NOSB Petition for Organic Processing and Handling

Sodium Dodecylbenzene Sulfonate (SDBS) as an active ingredient in an antimicrobial formulation for use in treating fruits and vegetables in the premises of organic food retail establishments.

Submitted by Ecolab, Inc.

October 9, 2015

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ECOLAB®

Dan Dahlman, CP-FS, RS
MANAGER
NORTH AMERICA FOOD, DRUGS, & COSMETICS
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October 9, 2015

USDA/AMS/TM/NOP – Manager
Room 2648-So.; Ag Stop 0268
1400 Independence Ave., SW.
Washington, DC 20250
Phone: (202) 720-3252
Fax: (202) 205-7808

RE: Petition for evaluation of Sodium Dodecylbenzene Sulfonate for inclusion on the National Organic List as a processing aid.

To Whom It May Concern:

Ecolab Inc. hereby requests an evaluation of Sodium Dodecylbenzene Sulfonate (SDBS) for inclusion on the National List of allowable synthetic substances in organic processing and handling (7 CFR 205.605(b)). More specifically, this will be used as an active ingredient in an antimicrobial formulation for use in treating fruits and vegetables in the premises of organic food retail establishments.

Pursuant to the guidelines posted in the Federal Registrar – "Notice of Guidelines on Procedures for Submitting National List Petitions" (Docket No. AMS-TM-06-0223; TM-06-12), the following petition addresses the items outlined in that document.

If you have any questions regarding the content of this petition, please contact me either at dan.dahlman@ecolab.com or at the telephone number listed above.

Best Regards,

Dan Dahlman

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1. SUBSTANCE INDENTIFICATION

Chemical Name:
Sodium Dodecylbenzene Sulfonate (SDBS)

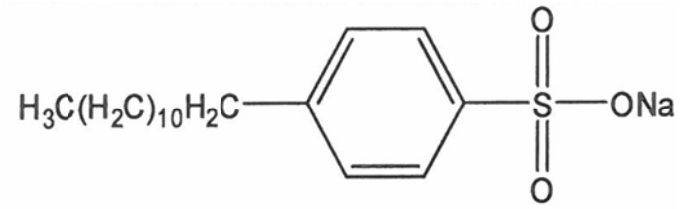
CAS Number:
25155-30-0

Synonyms:
Linear Alkylbenzene Sulfonate
Dodecylbenzenesulfonic acid, Sodium Salt
Sodium Branched Alkyl Benzene Sulfonate

Trade Name:
Nacconol 90G
Calimulse® EM-96F
Ufaryl DL 90C

Molecular Formula:
C_{18}-H_{29}-O_3-S.Na
C_{18}-H_{30}-O_3-S.Na

Chemical Structure:



Properties of the Substance:

Color/Form:	Off-white, powder
Flash Point:	>201°F (>93.9°C)
Specific Gravity:	4.41 lb/gal (0.53 g/ml)
Melting Point:	>572°F (>300°C)
Vapor Density:	Not Applicable, powder
Solubility:	Soluble
RVOC:	0%
pH Value:	7 @ 1% Aqueous
Molecular Weight:	348.49

Other: Sodium Dodecylbenzene Sulfonate is stable under normal conditions, but is incompatible with strong oxidizing agents. Upon decomposition, this product may yield sulfur dioxide and other oxides of sulfur.

2. MANUFACTURERS

Sodium Dodecylbenzene Sulfonate is manufactured by:

Pilot Chemical Company
11756 Burke Street
Santa Fe Springs, CA 90670
(562) 945-1867

Stepan Company
22 West Frontage Road
Northfield, IL 60093
(847) 446-7500

Unger Fabrikker A.S.
P.O. 254 N-1601
Fredrikstad, Norway
+47 69 70 82 00

3. INTENDED USE

Major Uses:

Sodium Dodecylbenzene Sulfonate (SDBS) is currently used in: “industrial, institutional, and chemical detergents and cleaners such as heavy duty laundry products; car, truck, and bus cleaners; metal cleaning products; specialty cleaners and sanitation products; emulsifiers, suspension or wetting agents, absorbents in pesticide and other agricultural chemicals; foaming and wetting agent in pulp and paper products; latex, textile, rubber, and polymer processing” (Toxnet 2014)[1].

Examples of Current Uses:

Attached is a list of current uses for SDBS, provided by the U.S. Department of Health and Human Services Household Product Database:

[1] TOXNET – Toxicology Data Network. 2014. Manufacturing/Use Information. Accessed July 7, 2014. Available at: http://toxnet.nlm.nih.gov/cgi-bin/sis/search2/r?dbs+hsdb:@term+@DOCNO+740

Chemical Information

Chemical Name: **Sodium dodecylbenzenesulfonate**

CAS Registry Number: 025155-30-0

Synonyms: Sodium dodecylbenzenesulfonate; Benzenesulfonic acid, dodecyl-, sodium salt; Dodecylbenzenesulfonic acid, sodium salt; Sodium dodecylphenylsulfonate; Sodium laurylbenzenesulfonate; Sodium Dodecylbenzene Sulfonate; Sodium Dodecyl Benzene Sulfonate

Information from other National Library of Medicine databases

Health Studies: Human Health Effects from Hazardous Substances Data Bank (HSDB)

Toxicity Information: Search TOXNET

Chemical Information: Search ChemIDplus

Biomedical References: Search PubMed

Products that contain this ingredient

Brand	Category	Form	Percent
Armor All OxiMagic Carpet & Upholstery Cleaner-06/01/2011	Auto Products	liquid	
Mothers Chrome Polish	Auto Products	liquid	
Black Magic All Wheel Cleaner-Old Product	Auto Products	liquid	<10
Smart Soap (Car Wash Plus)-discontinued	Auto Products	liquid	<10
Westleys Bleche Wite (Ready to Use)-Old Product	Auto Products	pump spray	
Westleys Megaconcentrate Car wash-discontinued	Auto Products	liquid	20-30
Westleys Wash n Wax-Old Product	Auto Products	liquid	
Turtle Wax Zip Wax Car Wash	Auto Products	liquid	
Armor All Carpet & Upholstery Cleaner-06/01/2011	Auto Products	liquid	1.0-5.0
Armor All Car Wash Wipes-Discontinued Product	Auto Products	wipes	0-20
Espree Wire Wheel Cleaner	Auto Products	liquid	
Sundance Car Wash	Auto Products	liquid	<25
Westleys Bleche-Wite All Wheel Cleaner	Auto Products	liquid	
Westleys Concentrated Car wash-discontinued	Auto Products	liquid	
Westleys Tire Dressing Remover-discontinued	Auto Products	liquid	
Red Devil Garage and Driveway Cleaner	Home maintenance	powder	2
UGL Mex All-Purpose Cleaner	Home maintenance	powder	<5
Fuller Brush Tile Clean, Tile & Grout Cleaner, Aerosol	Home maintenance	aerosol	
Sparkle Metal Polisher	Inside the Home	paste	
Soft Scrub Lavender-02/26/2009	Inside the Home	liquid	
Lysol Brand Cling Clip-OnToilet Bowl Deodorizer and Cleaner, Orange Grove-03/22/2007	Inside the Home	liquid	15-25
Vanish Drop-Ins, Blue, Continuous Toilet Bowl Cleaner-08/04/2008	Inside the Home	solid	30-60
Arm & Hammer with OxiClean Powder Laundry Detergent	Inside the Home	powder	1.0-2.0
Saaf Ultra Clean Fabric Detergent	Inside the Home	powder	
Arm & Hammer Concentrated Detergent-Old Product	Inside the Home	liquid	1.0-10.0

Vanish Hang Ins Automatic Toilet Bowl Cleaner-Old Product	Inside the Home	tablet	40-60
Mr Muscle Pot & Pan Detergent	Inside the Home	liquid	15-40
Windex Multi-Surface Glade Magic Meadow, Pump Spray	Inside the Home	pump spray	
Scrubbing Bubbles Extend-A-Clean Active Scrub Cream Cleanser, Citrus Scent	Inside the Home	liquid	1.0-5.0
Shout Free	Inside the Home	pump spray	
Ajax Fresh Multi-Purpose Cleaner, Pump Spray	Inside the Home	pump spray	
Palmolive Ultra Dish Liquid, Antibacterial, Orange	Inside the Home	liquid	
Heron Blue Barthan Cleaner	Inside the Home	powder	1.0-5.0
Soft Scrub Total Bath & Bowl Cleaner, Fresh Scent	Inside the Home	pump spray	1.0-5.0
Lysol Power & Free Toilet & Bathroom Wipes, Cool Spring Breeze	Inside the Home	wipes	
Lysol No Mess Automatic Toilet Bowl Cleaner, Complete Clean, Lavender	Inside the Home	solid	
Lysol Power Toilet Bowl Max Coverage Complete Clean with Bleach	Inside the Home	liquid	
Windex Multi-Surface Antibacterial-11/01/2012	Inside the Home	pump spray	
Windex Antibacterial Kitchen Touch-Up Cleaner, Glistering Citrus	Inside the Home	liquid	
OdoBan Professional Series BioLaundry Advanced Enzyme Detergent	Inside the Home	liquid	<10
Arm & Hammer Liquid Detergent, Sensitive Skin Formula-Old Product	Inside the Home	liquid	1.0-10.0
Arm & Hammer Liquid Detergent with Color Safe Bleach Alternate-Old Product	Inside the Home	liquid	1.0-10.0
Woolite Original Fabric Wash-Old Product	Inside the Home	liquid	1.0-10.0
Woolite Gentle Cycle Fabric Wash, Liquid, All Scents-Old Product	Inside the Home	liquid	5.0-10.0
Westleys Concentrated Bleche-Wite-Old Product	Inside the Home	liquid	2.0-10.0
Giant Auto Dish Detergent 75 OZ BOX-discontinued	Inside the Home	granules	10.0-25.0
Palmolive Dishwashing Liquid, Traditional-10/25/2006	Inside the Home	liquid	
Dermassage Hand Dishwashing Liquid, Regular-08/31/2006	Inside the Home	liquid	
Zep Tile & Grout Cleaner	Inside the Home	liquid	<5
Lysol Cling 2 in 1 Clip-On, In Toilet Bowl Cleaner with Bleach, Lime Scent	Inside the Home	gel	65-70
Vanish Drop-Ins, Blue-Old Product	Inside the Home	solid	30-45
Ajax Scouring Cleanser	Inside the Home	powder	1.7
Vanish Hang Ins Automatic Toilet Bowl Cleaner-10/14/2005	Inside the Home	tablet	40-60
Dynamo 2X Ultra Concentrated Laundry Detergent, Waterfall	Inside the Home	liquid	
Ajax 2X Ultra Liquid Detergent with Bleach Alternative	Inside the Home	liquid	
Formula 409 Carpet Cleaner Aerosol Spray-10/01/2000	Inside the Home	aerosol	1.0-5.0
Soft Scrub Cleanser with Lemon-02/26/2009	Inside the Home	liquid	
Toilet Duck Thick Liquid Toilet Bowl Cleaner-08/25/2008	Inside the Home	liquid	
Kaboom Ultra Scrub-06/17/2006	Inside the Home	liquid	<6
Dynamo Ultra Power-discontinued	Inside the Home	liquid	8
Masterpiece Neutral Cleaner Concentrate	Inside the Home	liquid	

Multi-Surface with Glade Clear Springs, Pump Spray	Inside the Home	pump spray	
Pledge 4 in 1 Tile & Vinyl Floor Cleaner	Inside the Home	liquid	
Scrubbing Bubbles Vanish Continuous Clean Drop-Ins	Inside the Home	solid	30.0-60.0
Ajax Triple Action Multi-Purpose Cleaner, Pump Spray-02/18/2011	Inside the Home	pump spray	
Ajax with Bleach Powder Cleanser-04/16/2012	Inside the Home	powder	1.0-5.0
Palmolive Ultra Pure + Clear Dish Liquid, Concentrated	Inside the Home	liquid	10.0-20.0
Dermassage Dishwashing Liquid-11/19/2012	Inside the Home	liquid	
Lysol Power & Free Multi-Purpose Cleaning Wipes, Oxygen Splash	Inside the Home	wipes	
Lysol No Mess Automatic Toilet Bowl Cleaner, Complete Clean, Citrus	Inside the Home	solid	
Lysol No Mess Automatic Toilet Bowl Cleaner, Complete Clean, Spring Waterfall	Inside the Home	solid	
Scrubbing Bubbles 5-in-1 Cream Cleanser Active Scrub with Fantastik	Inside the Home	liquid	1.0-5.0
Windex Antibacterial Bathroom Touch-Up Cleaner	Inside the Home	liquid	
OdoBan Professional Series BioGrease Kitchen Floor & Wall Degreaser	Inside the Home	liquid	<5
Fuller Brush Fulsol All-Purpose Degreaser	Inside the Home	liquid	
Arm & Hammer Ultra Liquid Detergent	Inside the Home	liquid	1.0-10.0
Palmolive Original Hand Dishwashing Liquid	Inside the Home	liquid	5.3
Ty D Bol Fresh Tabs 2 In 1, Blue	Inside the Home	tablet	24-33
Zep Tile and Terrazzo Cleaner-04/08/2002	Inside the Home	liquid	1.0-10.0
Woolite Gentle Cycle Original Powder	Inside the Home	powder	20-25
Lime-A-Way Automatic Toilet Bowl Cleaner-Old Product	Inside the Home	solid	8.0-12.0
Giant Pure Power Auto Dish Detergent Lemon 45 OZ BOX-discontinued	Inside the Home	granules	10.0-25.0
Palmolive Ultra Antibacterial Hand Soap-08/26/2004	Inside the Home	liquid	
Ajax Cleanser with Bleach-06/06/2007	Inside the Home	powder	
Dynamo Ultra Heavy Duty Detergent, Powder-11/11/2005-discontinued	Inside the Home	powder	
Lime-A-Way Automatic Toilet Bowl Cleaner (Solid)-08/04/2004	Inside the Home	liquid	8.0-12.0
Cling with Bleach Clip-On Toilet Bowl Deodorizer and Cleaner	Inside the Home	liquid	15-25
Vanish Bowl Cleaner Plus Deodorizer, Refreshing Rain	Inside the Home	solid	40-60
Toilet Duck Automatic with Bleach-04/18/2007	Inside the Home	tablet	30-45
Fab 2X Spring Magic Liquid Detergent	Inside the Home	liquid	
Dynamo 2X Ultra Concentrated Laundry Detergent, Sunrise Fresh	Inside the Home	liquid	
Toilet Duck Automatic with Bleach-Old Product	Inside the Home	tablet	45-60
Zep Commercial Patio Furniture Cleaner-05/24/1999-Old Product	Landscape/Yard	liquid	<3
Zep Commercial Patio Furniture Cleaner-Old Product	Landscape/Yard	liquid	<3
Fuller Brush Grill Clean, Foaming BBQ Grill Cleaner, Aerosol	Landscaping/Yard	aerosol	
Caress Moisturizing Body Bar with Bath Oil-discontinued	Personal care	solid	
Dove Soap Bar with 1/4 Moisturizing Lotion	Personal care	solid	

Caress Moisturizing Deodorant Body Bar-Shower Fresh-discontinued	Personal care	solid

Home | **Brands** | **Manufacturers** | **Ingredients** | **Health Effects**

Use and Technical Effect:

Sodium Dodecylbenzene Sulfonate is used as one of the active ingredients in a formulated product used as an antimicrobial processing aid in produce wash waters. The intended function of the product itself is to reduce the number of microorganisms in fruit and vegetable process water and on the surface of the fruit or vegetable. The primary application area for this product will be in food establishments such as restaurants, cafeterias, food service operations, commissaries, kitchens, grocery stores, and food processing facilities. The proposed use is on raw and processed fruits and vegetables and involves a minimum ninety (90) second immersion in the antimicrobial wash water, followed by a draining process prior to further processing and/or serving.

Produce Washing Procedures:

Produce washing procedures for the formulated product are provided as follows:

Use and Technical Effect

Minimum Contact Time	Ounces of Concentrate Per Gallon of Water	Dilution Ratio (Parts Concentrate : Parts Water)	Active ingredients	
			ppm SDBS*	ppm Lactic Acid
90 seconds	0.75 – 1.00	1:170 – 1:128	76 – 111	1061 – 1391

*Directions are consistent with the proposed EPA label.

The intended technical effect of the produce wash is to reduce the number of microorganisms in fruit and vegetable process water and on the surface of the commodity. The antimicrobial effect of the produce wash is provided by two active components, sodium dodecylbenzene sulfonate and lactic acid. Additional inert components aid in maintaining the product's compositional integrity as well as the surface wetting and cleaning properties. The primary application area for this product will be in food establishments such as restaurants, cafeterias, food service operations, commissaries, kitchens, grocery stores, and food processing facilities where produce will be received and processed by users for ultimate consumption by customers/consumers. The proposed use is on raw and processed fruits and vegetables and involves a minimum ninety (90) second immersion in the antimicrobial wash water followed by a draining process prior to further processing and/or serving.

Produce Washing Procedure
(Raw Agricultural Commodity RAC)

1

Fill sink to line with Produce Wash use-solution

2

Submerge produce in use-solution.

3

Slightly agitate produce. Soak for minimum 90 seconds.

4

Remove produce from sink.

5

Place produce in a colander.

6

Drain, process and store as desired.

Cut Produce Washing Procedure (Further processed)

1

Fill sink to line with Produce Wash use-solution

2

Place cut produce in a colander.

3

Submerge cut produce in use-solution.

4

Slightly agitate produce. Soak for minimum of 90 seconds.

5

Remove cut produce.

6

Drain and store as desired.

4. HANDLING ACTIVITIES

Handling Activities:

Sodium Dodecylbenzene Sulfonate (SDBS) is an active ingredient in an antimicrobial formulation for use in fruit and vegetable wash waters according to FDA and EPA limitations. The primary application area for this product will be in food establishments such as restaurants, cafeterias, food service operations, commissaries, kitchens, grocery stores, and food processing facilities where produce will be received and processed by users for ultimate consumption by customers/consumers. The proposed use is on raw and processed fruits and vegetables and involves a minimum ninety (90) second immersion in the antimicrobial wash water followed by a draining process prior to further processing and/or serving.

Please refer to Section 3 for illustrations on product use.

Mode of Action:

The activity of SDBS (CAS # 25155-30-0) is commonly hypothesized to be one of the three following mechanisms[1]:

1. Protein denaturing
2. Essential enzyme inactivation
3. Membrane disruption and alteration of cell permeability

[1] Cords, B.R., Burnett, S.L., Hilgren, J., Finley, M., and Magnuson, J., "Sanitizers: Halogens, Surface-Active Agents, and Peroxides," in *Antimicrobials in Food*, 3rd ed. Boca Raton, FL: CRC Press, 2005, ch.16, pp. 533-6.

5. MANUFACTURING PROCESS

Manufacturing Process:

Ecolab does not manufacture the substance Sodium Dodecylbenzene Sulfonate (SDBS), but purchases that and all other ingredients from suppliers and formulates it into a final product. There are no chemical reactions in the manufacture of the product which contains the active ingredient SDBS. Safety Data Sheets for the product SDBS and the final product in which SDBS is the active ingredient, SDBS, are attached in Section 10.

EPA Confidential Statements of Formula (CSF's) for the product are as follows:

Mix Instructions for the final product have been omitted from this section. Ecolab considers this to be Confidential Business Information (CBI), but can provide it upon request.

"CBI DELETED"

Confidential Business Information: Does Not Contain National Security Information (E. O. 12065)

Form Approved OMB No. 2070-0060. Approval expires 11/30/93

EPA

United States Environmental Protection Agency
Office of Pesticide Programs (TS-767)
Washington, DC 20460

Confidential Statement of Formula

A. X Basic Formulation ☐ Alternate Formulation

B. Page 1 of 2

See Instructions on Back

1. Name and Address of Applicant/Registrant *(Include Zip Code)*
Ecolab, Inc.
370 Wabasha Street North
St. Paul, MN 55102

2. Name and Address of Producer *(Include Zip Code)*
Same

2. Product Name Antimicrobial Fruit & Vegetable Treatment

4. Registration No./File Symbol **1677-234**

5. EPA Product Mgr/Team No. Mitchell / PM 32

6. Country Where Formulated USA

6. Pounds/Gal or Bulk Density 9.2 lb/gal

8. pH 0.740

9. Flash Point/Flame Extension >200F

EPA USE ONLY	10. Components in Formulation *(List as actually introduced into the formulation. Give commonly accepted chemical name, trade name, and CAS number.)*	11. Supplier Name and Address	12. EPA Reg. No.	13. Each Component in Formulation A. Amount B. % by Weight	14. Certified Limits % by Weight A. Upper Limit B. Lower Limit	15. Purpose in Formulation
	Dodecylbenzensulfonic acid, sodium salt, 90% CAS# 25155-30-0	See addendum		[redacted]		Active
	Lactic acid , 88% CAS# 50-21-5 or 79-33-4	See addendum				Active
	Tween 80 CAS# 9005-65-6	See addendum				Surfactant
	Xanthan Gum CAS# 11138-66-2	See addendum				Thickener
	Propylene Glycol CAS# 57-55-6	See addendum				Coupler
	Silicon Emulsion Antifoam CAS# 63148-62-9	See addendum				Antifoam
	Sodium Acid Sulfate CAS# 7681-38-1	See addendum				Acidulant
	Ethylene glycol-propylene glycol polymer CAS# 9003-11-6	See addendum				Surfactant
	FD &C Green #3 CAS # 2353-45-9	See addendum				Dye
	FD &C Yellow #5 CAS# 1934-21-0	See addendum				Dye
	Water	See addendum				Diluent

16. Typed Name of Approving Official: Rhonda Schulz

17. Total Weight 1000 lbs — 100%

18. Signature of Approving Official: Rhonda Schulz

19. Title: Director, Product Registration & Compliance

20. Phone No. *(Include Area Code)*: 651-293-4026

21. Date: 7/17/2012

A Form 8570-4 (Rev. 12-90) Previous editions are obsolete

Supplier Addresses for Antimicrobial Fruit Vegetable Treatment
EPA Reg No 1677-234

RM #	RM Name	CAS	EPA Reg No	Supplier	Supplier Address
171150	Linear alkylbenzene sulfonate	25155-30-0		Stepan Company	22 West Frontage Road, Northfield, IL 60093
171150	Linear alkylbenzene sulfonate	25155-30-0		AkzoNobel	15200 Almeda Road, Houston, TX 77053
171150	Linear alkylbenzene sulfonate	25155-30-0		Pilot Chemical Company	11756 Burke Street, Santa Fe Springs, CA 90670
171150	Linear alkylbenzene sulfonate	25155-30-0		Unger Fabrikker A. S.	P.O. 254 N-1601 Fredrikstad, Norway
132025	Sodium acid sulfate	7681-38-1		Jones-Hamilton Co.	8400 Enterprise Drive, Newark, CA 94560
132025	Sodium acid sulfate	7681-38-1		SAFC- Sigma Aldrich Fine Chemicals	3050 Spruce Street, St. Louis, MO 63103
132025	Sodium acid sulfate	7681-38-1		American Elements	1093 Broxton Avenue, Suite 2000, Los Angeles, CA 90024
132025	Sodium acid sulfate	7681-38-1		Jost Chemical Co.	8150 Lakeland Road, St. Louis, MO 63114
170787	Ethylene glycol-propylene glycol polymer	9003-11-6		BASF Corporation	100 Campus Drive, Florham Park, NJ 07932
271158	Food Green 3	2353-45-9		Pylam Prducts Company Inc.	2175 East Cedar Street, Tempe AZ 85281
271158	Food Green 3	2353-45-9		Noveon Hilton-Davis, Inc.	2235 Langdon Farm Road, Cincinnati, OH 45237
830414	Acid Yellow 23	1934-21-0		Pylam Prducts Company Inc.	2175 East Cedar Street, Tempe AZ 85281
830414	FD&C Yellow #5	1934-21-0		Noveon Hilton-Davis, Inc.	2235 Langdon Farm Road, Cincinnati, OH 45237
830414	Acid Yellow 23	1934-21-0		BASF Corporation	100 Campus Drive, Florham Park, NJ 07932
830792	Lactic acid	50-21-5 or 79-33-4		Archer Daniels Midland Co	P.O. Box 1470, Decatur, IL 62525
830792	Lactic acid	50-21-5 or 79-33-4		PURAC America, Inc	111 Barclay Blvd, Lincolnshire, IL 60089
830792	Lactic acid	50-21-5 or 79-33-4		Ashland Specialty Chemical Co.	P.O Box 2219, Columbus, OH 43216
830792	Lactic acid	50-21-5 or 79-33-4		Sterling Chemicas, Inc.	333 Clay Street, Suite 3600, Houston, TX 77002
830792	Lactic acid	50-21-5 or 79-33-4		BASF Corporation	100 Campus Drive, Florham Park, NJ 07932
170654	Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Uniquema	1000 Uniquema Blvd., New Castle, DE 19720
170654	Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Croda	300A Columbus Circle, Edison, NJ 08837
170654	Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Ivanhoe Industries Inc.	3333 20th Street, Zion, IL 60099
170654	Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Colonial Chemical Company	78 Carranza Road, Tabernacle, NJ 08088
290721	Polydimenthylsiloxane emulsion (20%)	63148-62-9		Dow Corning Corporation	South Saginaw Road Midland, Michigan 48686
830043	Propylene Glycol	57-55-6		Lyondell Chemical Company	One Houston Center, Suite 1600, 1221 McKinney St. P.O.Box 2583, Houston, TX 77252
830043	Propylene Glycol	57-55-6		The Dow Chemical Company	2030 Willard H. Dow Center, Midland, MI 48674
830043	Propylene Glycol	57-55-6		Arch Chemicals, Inc.	1405 Foulk Road, Wilmington, DE 19803
830043	Propylene Glycol	57-55-6		Equistar	One Houston Center, Suite 1600, 1221 McKinney St. P.O.Box 2583, Houston, TX 77252
830043	Propylene Glycol	57-55-6		Huntsman	P.O. Box 27707, Houson, TX 77227
230192	xanthan gum	11138-66-2		CP Kelco	A Huber Company, 8355 Aero Drive, San Diego, CA 92123
230192	xanthan gum	11138-66-2		Jungbunzlauer Inc.	7 Wells Ave, Newton Centre, MA 02459
230192	xanthan gum	11138-66-2		American Internatinal Corp.	135 Newbury Street, Framington, MA 01701
230192	xanthan gum	11138-66-2		Wego Chemical and Mineral Corp.	239 Great Neck Road, Great Neck, NY 11021
100016	Deionized Water	7732-18-5		Ecolab Inc	Ecolab facility water supply

Rhonda Schulz

Rhonda Schulz, Director, Product Registration Compliance

"CBI DELETED"

Confidential Business Information: Does Not Contain National Security Information (E. O. 12065)

Form Approved OMB No. 2070-0060. Approval expires 11/30/93

EPA

United States Environmental Protection Agency
Office of Pesticide Programs (TS-767)
Washington, DC 20460

Confidential Statement of Formula

A. ☐ Basic Formulation X Alternate Formulation

B. Page 1 of 2

See Instructions on Back

1. Name and Address of Applicant/Registrant *(Include Zip Code)*
Ecolab, Inc.
370 Wabasha Street North
St. Paul, MN 55102

2. Name and Address of Producer *(Include Zip Code)*
Same

2. Product Name DLSB-99

4. Registration No./File Symbol
1677-[pending]

5. EPA Product Mgr/Team No.
Mitchell / PM 32

6. Country Where Formulated
USA

6. Pounds/Gal or Bulk Density
9.2 lb/gal

8. pH
0.740

9. Flash Point/Flame Extension
>200F

EPA USE ONLY	10. Components in Formulation *(List as actually introduced into the formulation. Give commonly accepted chemical name, trade name, and CAS number.)*	11. Supplier Name and Address	12. EPA Reg. No.	13. Each Component in Formulation A. Amount B. % by Weight	14. Certified Limits % by Weight A. Upper Limit B. Lower Limit	15. Purpose in Formulation
	Dodecylbenzensulfonic acid, sodium salt, 90% CAS# 25155-30-0	See addendum		[redacted]		Active
	Lactic acid , 88% CAS# 50-21-5 or 79-33-4	See addendum				Active
	Tween 80 CAS# 9005-65-6	See addendum				Surfactant
	Xanthan Gum CAS# 11138-66-2	See addendum				Thickener
	Propylene Glycol CAS# 57-55-6	See addendum				Coupler
	Silicon Emulsion Antifoam CAS# 63148-62-9	See addendum				Antifoam
	Sodium Acid Sulfate CAS# 7681-38-1	See addendum				Acidulant
	Ethylene glycol-propylene glycol polymer CAS# 9003-11-6	See addendum				Surfactant
	FD &C Green #3 CAS # 2353-45-9	See addendum				Dye
	FD &C Yellow #5 CAS# 1934-21-0	See addendum				Dye
	Water	See addendum				Diluent
				17. Total Weight 1000 lbs	100%	

16. Typed Name of Approving Official
Theodore D. Head

18. Signature of Approving Official
Theodore D. Head

19. Title
Product Registration Manager

20. Phone No. *(Include Area Code)*
651-293-2848

21. Date
5-2-11

A Form 8570-4 (Rev. 12-90) Previous editions are obsolete

Supplier Addresses for DLSB-99
EPA Reg No 1677-[pending]

RM #	RM Name	CAS	EPA Reg No	Supplier	Supplier Address
171150	Linear alkylbenzene sulfonate	25155-30-0		Stepan Company	22 West Frontage Road, Northfield, IL 60093
171150	Linear alkylbenzene sulfonate	25155-30-0		AkzoNobel	15200 Almeda Road, Houston, TX 77053
171150	Linear alkylbenzene sulfonate	25155-30-0		Pilot Chemical Company	11756 Burke Street, Santa Fe Springs, CA 90670
171150	Linear alkylbenzene sulfonate	25155-30-0		Unger Fabrikker A. S.	P.O. 254 N-1601 Fredrikstad, Norway
132025	Sodium acid sulfate	7681-38-1		Jones-Hamilton Co.	8400 Enterprise Drive, Newark, CA 94560
132025	Sodium acid sulfate	7681-38-1		SAFC- Sigma Aldrich Fine Chemicals	3050 Spruce Street, St. Louis, MO 63103
132025	Sodium acid sulfate	7681-38-1		American Elements	1093 Broxton Avenue, Suite 2000, Los Angeles, CA 90024
132025	Sodium acid sulfate	7681-38-1		Jost Chemical Co.	8150 Lakeland Road, St. Louis, MO 63114
170787	Ethylene glycol-propylene glycol polymer	9003-11-6		BASF Corporation	100 Campus Drive, Florham Park, NJ 07932
271158	Food Green 3	2353-45-9		Pylam Prducts Company Inc.	2175 East Cedar Street, Tempe AZ 85281
271158	Food Green 3	2353-45-9		Noveon Hilton-Davis, Inc.	2235 Langdon Farm Road, Cincinnati, OH 45237
830414	Acid Yellow 23	1934-21-0		Pylam Prducts Company Inc.	2175 East Cedar Street, Tempe AZ 85281
830414	FD&C Yellow #5	1934-21-0		Noveon Hilton-Davis, Inc.	2235 Langdon Farm Road, Cincinnati, OH 45237
830414	Acid Yellow 23	1934-21-0		BASF Corporation	100 Campus Drive, Florham Park, NJ 07932
830792	Lactic acid	50-21-5 or 79-33-4		Archer Daniels Midland Co	P.O. Box 1470, Decatur, IL 62525
830792	Lactic acid	50-21-5 or 79-33-4		PURAC America, Inc	111 Barclay Blvd, Lincolnshire, IL 60089
830792	Lactic acid	50-21-5 or 79-33-4		Ashland Specialty Chemical Co.	P.O Box 2219, Columbus, OH 43216
830792	Lactic acid	50-21-5 or 79-33-4		Sterling Chemicas, Inc.	333 Clay Street, Suite 3600, Houston, TX 77002
830792	Lactic acid	50-21-5 or 79-33-4		BASF Corporation	100 Campus Drive, Florham Park, NJ 07932
170654	Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Uniquema	1000 Uniquema Blvd., New Castle, DE 19720
170654	Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Croda	300A Columbus Circle, Edison, NJ 08837
170654	Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Ivanhoe Industries Inc.	3333 20th Street, Zion, IL 60099
170654	Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Colonial Chemical Company	78 Carranza Road, Tabernacle, NJ 08088
290721	Polydimenthylsiloxane emulsion (10%)	63148-62-9		Dow Corning Corporation	South Saginaw Road Midland, Michigan 48686
830043	Propylene Glycol	57-55-6		Lyondell Chemical Company	One Houston Center, Suite 1600, 1221 McKinney St. P.O.Box 2583, Houston, TX 77252
830043	Propylene Glycol	57-55-6		The Dow Chemical Company	2030 Willard H. Dow Center, Midland, MI 48674
830043	Propylene Glycol	57-55-6		Arch Chemicals, Inc.	1405 Foulk Road, Wilmington, DE 19803
830043	Propylene Glycol	57-55-6		Equistar	One Houston Center, Suite 1600, 1221 McKinney St. P.O.Box 2583, Houston, TX 77252
830043	Propylene Glycol	57-55-6		Huntsman	P.O. Box 27707, Houson, TX 77227
230192	xanthan gum	11138-66-2		CP Kelco	A Huber Company, 8355 Aero Drive, San Diego, CA 92123
230192	xanthan gum	11138-66-2		Jungbunzlauer Inc.	7 Wells Ave, Newton Centre, MA 02459
230192	xanthan gum	11138-66-2		American Internatinal Corp.	135 Newbury Street, Framington, MA 01701
230192	xanthan gum	11138-66-2		Wego Chemical and Mineral Corp.	239 Great Neck Road, Great Neck, NY 11021
100016	Deionized Water	7732-18-5		Ecolab Inc	Ecolab facility water supply

"CBI DELETED"

Confidential Business Information: Does Not Contain National Security Information (E. O. 12065)

Form Approved OMB No. 2070-0060. Approval expires 11/30/93

EPA

United States Environmental Protection Agency
Office of Pesticide Programs (TS-767)
Washington, DC 20460

Confidential Statement of Formula

A. ☐ Basic Formulation X Alternate Formulation #2

B. Page 1 of 2

See Instructions on Back

1. Name and Address of Applicant/Registrant *(Include Zip Code)*
Ecolab, Inc.
370 Wabasha Street North
St. Paul, MN 55102

2. Name and Address of Producer *(Include Zip Code)*
Same

2. Product Name
Antimicrobial Fruit and Vegetable Treatment

4. Registration No./File Symbol
1677-234

5. EPA Product Mgr/Team No.
Jacqueline Campbell-McFarlane / PM 32

6. Country Where Formulated
USA

6. Pounds/Gal or Bulk Density
9.2 lb/gal

8. pH
0.740

9. Flash Point/Flame Extension
>200 F

EPA USE ONLY	10. Components in Formulation *(List as actually introduced into the formulation. Give commonly accepted chemical name, trade name, and CAS number.)*	11. Supplier Name and Address	12. EPA Reg. No.	13. Each Component in Formulation A. Amount B. % by Weight	14. Certified Limits % by Weight A. Upper Limit B. Lower Limit	15. Purpose in Formulation
	Dodecylbenzensulfonic acid, sodium salt, 90% CAS# 25155-30-0	See addendum		[redacted]		active
	Lactic acid , 88% CAS# 50-21-5 or 79-33-4	See addendum				active
	Polyoxyethylene (20) sorbitan monooleate CAS# 9005-65-6	See addendum				surfactant
	Xanthan gum CAS# 11138-66-2	See addendum				thickener
	Polydimethylsiloxane emulsion, 20% CAS# 63148-62-9	See addendum				antifoam
	Sodium acid sulfate CAS# 7681-38-1	See addendum				acidulant
	Ethylene glycol-propylene glycol polymer CAS# 9003-11-6	See addendum				surfactant
	FD &C green #3 CAS # 2353-45-9	See addendum				dye
	FD &C yellow #5 CAS# 1934-21-0	See addendum				dye
	Water CAS# 7732-18-5	See addendum				diluent
				17. Total Weight 1000 lbs	100%	

16. Typed Name of Approving Official
Ron Derbyshire

18. Signature of Approving Official
Ron Derbyshire

19. Title
Senior Manager, NA Biocides

20. Phone No. *(Include Area Code)*
651-293-2848

21. Date
1/24/14

A Form 8570-4 (Rev. 12-90) Previous editions are obsolete

Supplier Addresses for ANTIMICROBIAL FRUIT AND VEGETABLE TREATMENT
EPA Reg No 1677-234

RM Name	CAS	EPA Reg No	Supplier	Supplier Address
Linear alkylbenzene sulfonate	25155-30-0		Pilot Chemical Company	11756 Burke Street, Santa Fe Springs, CA 90670
Linear alkylbenzene sulfonate	25155-30-0		Stepan Company	22 West Frontage Road, Northfield,IL 60093
Linear alkylbenzene sulfonate	25155-30-0		Unger Fabrikker A. S.	P.O. 254 N-1601, Fredrikstad, Norway
Sodium acid sulfate	7681-38-1		American Elements	1093 Broxton Avenue, Suite 2000, Los Angeles, CA 90024
Sodium acid sulfate	7681-38-1		Jones-Hamilton Co.	8400 Enterprise Drive, Newark, CA 94560
Sodium acid sulfate	7681-38-1		Jost ChemicalCo.	8150 Lakeland Road, St. Louis, MO 63114
Sodium acid sulfate	7681-38-1		SAFC- Sigma Aldrich Fine Chemicals	3050 Spruce Street, St. Louis, MO 63103
Ethylene glycol-propylene glycol polymer	9003-11-6		BASF Corporation	100 Campus Drive, Florham Park, NJ 07932
FD&C green #3	2353-45-9		Noveon Hilton-Davis,Inc.	2235 Langdon Farm Road, Cincinnati, OH 45237
FD&C green #3	2353-45-9		Pylam Prducts Company Inc.	2175 East Cedar Street, Tempe, AZ 85281
FD&C yellow #5	1934-21-0		BASF Corporation	100 Campus Dnve, Florham Park,NJ 07932
FD&C yellow #5	1934-21-0		Noveon Hilton-Davis. Inc.	2235 Langdon Farm Road, Cincinnati,OH 45237
FD&C yellow #5	1934-21-0		Pylam Prducts Company Inc.	2175 East Cedar Street, Tempe, AZ 85281
Lactic acid	50-21-5 or 79-33-4		Archer Daniels Midland Co	P.O. Box 1470, Decatur, IL 62525
Lactic acid	50-21-5 or 79-33-4		Ashland Specialty Chemical Co.	P.O. Box 2219, Columbus, OH 43216
Lactic acid	50-21-5 or 79-33-4		BASF Corporation	100 Campus Drive, Florham Park, NJ 07932
Lactic acid	50-21-5 or 79-33-4		PURAC America, Inc	111 Barclay Blvd, Lincolnshire, IL 60089
Lactic acid	50-21-5 or 79-33-4		Sterling Chemicas, Inc.	333 Clay Street, Suite 3600, Houston, TX 77002
Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Colonial Chemical Company	78 Carranza Road, Tabernacle, NJ 08088
Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Croda	300A Columbus Circle, Edison, NJ 08837
Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Ivanhoe Industries Inc.	3333 20th Street, Zion, IL 60099
Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Uniquema	1000 Uniquema Blvd., New Castle, DE 19720
Polydimenthylsiloxane emulsion (20%)	63148-62-9		The Dow Chemical Company	South Saginaw Road, Midland, MI 48686
Xanthan gum	11138-66-2		American Internatinal Corp.	135 Newbury Street, Framington, MA 01701
Xanthan gum	11138-66-2		CP Kelco	A Huber Company, 8355 Aero Drive, San Diego, CA 92123
Xanthan gum	11138-66-2		Jungbunzlauer Inc.	7 Wells Ave, Newton Centre, MA 02459
Xanthan gum	11138-66-2		Wego Chemical and Mineral Corp.	239 Great Neck Road, Great Neck, NY 11021
Deionized Water	7732-18-5		Ecolab Inc	Ecolab facility water supply
Signature of Approving Official	651-293-2848	Date 1/30/14	Senior Manager, NA Biocides; Ron Derbyshire	

"CBI DELETED"

Confidential Business Information: Does Not Contain National Security Information (E. O. 12065)

Form Approved OMB No. 2070-0060. Approval expires 11/30/93

EPA

United States Environmental Protection Agency
Office of Pesticide Programs (TS-767)
Washington, DC 20460

Confidential Statement of Formula

A. ☐ Basic Formulation
X Alternate Formulation #3

B. Page 1 of 2

See Instructions on Back

1. Name and Address of Applicant/Registrant *(Include Zip Code)*
Ecolab, Inc.
370 Wabasha Street North
St. Paul, MN 55102

2. Name and Address of Producer *(Include Zip Code)*
Same

2. Product Name
Antimicrobial Fruit and Vegetable Treatment

4. Registration No./File Symbol
1677-234

5. EPA Product Mgr/Team No.
Jacqueline Hardy / PM 34

6. Country Where Formulated
USA

6. Pounds/Gal or Bulk Density
9.2 lb/gal

8. pH
0.740

9. Flash Point/Flame Extension
999

EPA USE ONLY	10. Components in Formulation *(List as actually introduced into the formulation. Give commonly accepted chemical name, trade name, and CAS number.)*	11. Supplier Name and Address	12. EPA Reg. No.	13. Each Component in Formulation A. Amount B. % by Weight	14. Certified Limits % by Weight A. Upper Limit B. Lower Limit	15. Purpose in Formulation
	Dodecylbenzensulfonic acid, sodium salt, 90% CAS# 25155-30-0	See addendum		[redacted]		active
	Lactic acid, 88% CAS# 50-21-5 or 79-33-4	See addendum				active
	Polyoxyethylene (20) sorbitan monooleate CAS# 9005-65-6	See addendum				surfactant
	Xanthan gum CAS# 11138-66-2	See addendum				thickener
	Polydimenthylsiloxane emulsion, 10% CAS# 63148-62-9	See addendum				antifoam
	Sodium acid sulfate CAS# 7681-38-1	See addendum				acidulant
	Ethylene glycol-propylene glycol polymer CAS# 9003-11-6	See addendum				surfactant
	FD &C green #3 CAS # 2353-45-9	See addendum				dye
	FD &C yellow #5 CAS# 1934-21-0	See addendum				dye
	Water CAS# 7732-18-5	See addendum				diluent
				17. Total Weight 1000 lbs	100%	

16. Typed Name of Approving Official
Nicole Listner

18. Signature of Approving Official
Nicole Listner

19. Title
Associate Regulatory Specialist I

20. Phone No. *(Include Area Code)*
651-250-3079

21. Date
03/30/2015

A Form 8570-4 (Rev. 12-90) Previous editions are obsolete

Supplier Addresses for ANTIMICROBIAL FRUIT AND VEGETABLE TREATMENT
EPA Reg No 1677-234

RM Name	CAS	EPA Reg No	Supplier	Supplier Address
Linear alkylbenzene sulfonate	25155-30-0		Pilot Chemical Company	11756 Burke Street, Santa Fe Springs, CA 90670
Linear alkylbenzene sulfonate	25155-30-0		Stepan Company	22 West Frontage Road, Northfield,IL 60093
Linear alkylbenzene sulfonate	25155-30-0		Unger Fabrikker A. S.	P.O. 254 N-1601, Fredrikstad, Norway
Sodium acid sulfate	7681-38-1		American Elements	1093 Broxton Avenue, Suite 2000, Los Angeles, CA 90024
Sodium acid sulfate	7681-38-1		Jones-Hamilton Co.	8400 Enterprise Drive, Newark, CA 94560
Sodium acid sulfate	7681-38-1		Jost ChemicalCo.	8150 Lakeland Road, St. Louis, MO 63114
Sodium acid sulfate	7681-38-1		SAFC- Sigma Aldrich Fine Chemicals	3050 Spruce Street, St. Louis, MO 63103
Ethylene glycol-propylene glycol polymer	9003-11-6		BASF Corporation	100 Campus Drive, Florham Park, NJ 07932
FD&C green #3	2353-45-9		Noveon Hilton-Davis,Inc.	2235 Langdon Farm Road, Cincinnati, OH 45237
FD&C green #3	2353-45-9		Pylam Prducts Company Inc.	2175 East Cedar Street, Tempe, AZ 85281
FD&C yellow #5	1934-21-0		BASF Corporation	100 Campus Drve, Florham Park,NJ 07932
FD&C yellow #5	1934-21-0		Emerald Performance Materials, LLC	2020 Front Street, Suite 100, Cuyahoga Falls, OH 44221
FD&C yellow #5	1934-21-0		Noveon Hilton-Davis. Inc.	2235 Langdon Farm Road, Cincinnati,OH 45237
FD&C yellow #5	1934-21-0		Pylam Prducts Company Inc.	2175 East Cedar Street, Tempe, AZ 85281
Lactic acid	50-21-5 or 79-33-4		Archer Daniels Midland Co	P.O. Box 1470, Decatur, IL 62525
Lactic acid	50-21-5 or 79-33-4		Ashland Specialty Chemical Co.	P.O. Box 2219, Columbus, OH 43216
Lactic acid	50-21-5 or 79-33-4		BASF Corporation	100 Campus Drive, Florham Park, NJ 07932
Lactic acid	50-21-5 or 79-33-4		PURAC America, Inc	111 Barclay Blvd, Lincolnshire, IL 60089
Lactic acid	50-21-5 or 79-33-4		Sterling Chemicas, Inc.	333 Clay Street, Suite 3600, Houston, TX 77002
Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Colonial Chemical Company	78 Carranza Road, Tabernacle, NJ 08088
Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Croda	300A Columbus Circle, Edison, NJ 08837
Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Ivanhoe Industries Inc.	3333 20th Street, Zion, IL 60099
Polyoxyethylene (20) sorbitan monooleate	9005-65-6		Uniquema	1000 Uniquema Blvd., New Castle, DE 19720
Polydimenthylsiloxane emulsion (10%)	63148-62-9		The Dow Chemical Company	South Saginaw Road, Midland, MI 48686
Polydimenthylsiloxane emulsion (10%)	63148-62-9		Momentive	180 East Broad Street, Columbus, OH 43215
Xanthan gum	11138-66-2		American Internatinal Corp.	135 Newbury Street, Framington, MA 01701
Xanthan gum	11138-66-2		CP Kelco	A Huber Company, 8355 Aero Drive, San Diego, CA 92123
Xanthan gum	11138-66-2		Great Earth Chemical	7007 SW Cardinal Lane, STE 135, Portland, OR 97224
Xanthan gum	11138-66-2		Jungbunzlauer Inc.	7 Wells Ave, Newton Centre, MA 02459
Xanthan gum	11138-66-2		Wego Chemical and Mineral Corp.	239 Great Neck Road, Great Neck, NY 11021
Deionized Water	7732-18-5		Ecolab Inc	Ecolab facility water supply

Nicole Listner, Associate Regulatory Specialist I
Ecolab Inc.
03/30/2015

6. CERTIFICATION REVIEWS

Certification Reviews:

To our knowledge, the Ecolab product Antimicrobial Fruit & Vegetable Treatment, or the active ingredient Sodium Dodecylbenzene Sulfonate have not been reviewed by any state or private certification agency regarding its use in fruit and vegetable wash waters. However, the product does possess both FDA and EPA clearances.

Please refer to Section 7 for FDA and EPA clearances regarding this product.

7. FDA, EPA REGISTRATIONS

FDA Registrations:

Sodium Dodecylbenzene Sulfonate is cleared for use as an antimicrobial agent in produce wash water under 21 CFR 173.405 as shown:

§173.405 Sodium Dodecylbenzene Sulfonate.

Sodium Dodecylbenzene Sulfonate (CAS No. 25155-30-0) may be safely used in accordance with the following prescribed conditions:

(a) The additive is an antimicrobial agent used in wash water for fruits and vegetables. The additive may be used at a level not to exceed 111 milligrams per kilogram in the wash water. Fruits and vegetables treated by the additive do not require a potable water rinse.

(b) The additive is limited to use in commissaries, cafeterias, restaurants, retail food establishments, nonprofit food establishments, and other food service operations in which food is prepared for or served directly to the consumer.

(c) To assure safe use of the additive, the label or labeling of the additive container shall bear, in addition to the other information required by the Federal Food, Drug, and Cosmetic Act, adequate directions to assure use in compliance with the provisions of this section.

[77 FR 71697, Dec. 4, 2012]

Other 21 CFR Clearances – 173.315, 176.210, 178.1010

EPA Registrations:

Ecolab's Antimicrobial Fruit & Vegetable Treatment product is currently registered with the United States Environmental Protection Agency per Registration No. 1677-234, and is also registered in all 50 states.

A copy of the Ecolab production label, EPA registered master label, and various literature for the Antimicrobial Fruit and Vegetable Treatment product are provided in Section 8.

8. CAS#'s, LABELS

CAS#'s:

Sodium Dodecylbenzene Sulfonate: 25155-30-0

Label:

Included is a copy of the Ecolab production label, EPA registered master label, and various literature for the Antimicrobial Fruit and Vegetable Treatment product in which SDBS will be the active ingredient:

PELIGRO: SI USTED NO PUEDE LEER EN INGLES, PIDA AYUDA Y PREGUNTE SOBRE EL CONTENIDO Y LAS INSTRUCCIONES DE USO ANTES DE USAR ESTE PRODUCTO.

PRECAUTIONARY STATEMENTS

HAZARDS TO HUMANS AND DOMESTIC ANIMALS

WARNING: Causes substantial but temporary eye injury. Harmful if absorbed through skin. Do not get in eyes, on skin or on clothing. Wear goggles, face shield, or safety glasses. Wash thoroughly with soap and water after handling and before eating, drinking, chewing gum, using tobacco or using the toilet. Remove and wash contaminated clothing before reuse. After the product is diluted, safety goggles are not required. Prolonged or frequently repeated skin contact with the concentrate may cause allergic reactions in some individuals.

FIRST AID

If in Eyes: Hold eye open and rinse slowly and gently with water for 15-20 minutes. Remove contact lenses, if present, after the first 5 minutes, then continue rinsing eyes. Call a Poison Control Center or doctor for treatment advice.
If on Skin or Clothing: Take off contaminated clothing. Rinse skin immediately with plenty of water for 15-20 minutes. Call a Poison Control Center or doctor for treatment advice.

FOR EMERGENCY MEDICAL INFORMATION CALL TOLL-FREE: 1-800-328-0026

STORAGE AND DISPOSAL

DO NOT CONTAMINATE WATER, FOOD OR FEED BY STORAGE OR DISPOSAL

PESTICIDE STORAGE: Store in a cool, dark, dry place in the original container. Always replace covers.

PESTICIDE DISPOSAL: Pesticide wastes are acutely hazardous. Improper disposal of excess pesticide, spray mixture, or rinsate is a violation of Federal Law. If these wastes cannot be disposed of by use according to label instructions, contact your State Pesticide or Environmental Control Agency, or the Hazardous Waste representative at the nearest EPA Regional Office for guidance. Waste resulting from the use of this product must be disposed of on site or at an approved waste disposal facility.

CONTAINER DISPOSAL: Non-refillable container. Do not reuse this container to hold materials other than pesticides or diluted pesticide rinsate. Offer for recycling if available or puncture and dispose in a sanitary landfill, or by other procedures approved by state and local authorities.

RESIDUE REMOVAL INSTRUCTIONS: Triple rinse container (or equivalent) promptly after emptying. Triple rinse as follows: Fill container 1/4 full with water and recap. Shake 10 seconds. Follow Pesticide Disposal instructions for rinsate disposal. Drain for 10 seconds after the flow begins to drip. Repeat procedure two more times.

For service or additional information, call 1-800-35-CLEAN (352-5326).

Antimicrobial Fruit & Vegetable Treatment

Water Additive for Pathogen Reduction in Fruit and Vegetable Wash or Process Waters

Controls the Growth of Spoilage and Decay-Causing, Non-Public Health Microorganisms in Wash or Process Waters

Reduces Bacterial Pathogens on Processed* Fruit and Vegetable Surfaces (This use not approved in the state of California)

ACTIVE INGREDIENTS:

Dodecylbenzenesulfonic acid, sodium salt	1.23%
Lactic Acid	17.29%
Other Ingredients:	81.48%
Total:	100.00%

FOR COMMERCIAL USE
KEEP OUT OF REACH OF CHILDREN

WARNING

See side panel for Precautionary Statements and First Aid.

Net Contents: 2.5 US gal (9.46L)

Areas of use: Food retail establishments such as restaurants, cafeterias, food service operations, commissaries, and kitchens.

DIRECTIONS FOR USE:
It is a violation of Federal law to use this product in a manner inconsistent with its labeling.

When used as directed under EPA regulations, Antimicrobial Fruit & Vegetable Treatment will:
1. Reduce 99.9% of the pathogens *Escherichia coli* 0157:H7 (ATCC 43895, 35150, 43890), *Listeria monocytogenes* (ATCC 49594, 19114, 19116) and *Salmonella enterica* (ATCC 10721,6962, 13311) in wash or process water for fruit and vegetable raw agricultural commodities (RACs).
2. Controls spoilage and decay-causing, non-public health microorganisms present in the wash or process water for fruit and vegetable raw agricultural commodities (RACs).

***To treat the surface of *processed* fruits and vegetables subject to FDA regulations:**
(This use not approved in the state of California) This product may be used in wash waters to reduce the pathogens *Escherichia coli* 0157:H7, *Listeria monocytogenes* and *Salmonella enterica* on the surface of processed fruits and vegetables introduced during handling or processing. This use must comply with all applicable FDA regulations, including but not limited to 21 CFR 173.405(a)(b), 21 CFR § 184.1061 and 21 CFR 170.3(o)(2).

Add **Antimicrobial Fruit & Vegetable Treatment** into the fruit and vegetable washing/processing vessel according to the table below, submerge and agitate fruits and vegetables for a minimum of 90 seconds. Drain thoroughly and allow to air dry. No rinse required.

Minimum Contact Time	Ounces of concentrate per gallon of water	Dilution ratio (parts concentrate : parts water)	Active Ingredients	
			ppm SDBS*	ppm Lactic Acid
90 seconds	0.75 – 1.00	1:170 – 1:128	76-111	1061-1391

* Sodium dodecylbenzenesulfonate

Ecolab Inc.
370 Wabasha Street N.
St. Paul, MN 55102-1390 USA
Made in USA

732768-02 · KUSA 732768/8002/0415

Antimicrobial Fruit & Vegetable Treatment can be applied to the following types of fresh fruits and vegetables, post harvest.

Vegetables
- Root and tuber vegetables such as carrot, potato, radish, rutabaga, sweet potato, yam and sugar beets.
- Leaves of root and tuber vegetables such as turnip greens and sugar beet
- Bulb vegetables such as onions, leeks, garlic and shallots.
- Leafy vegetables such as lettuce (head and leaf), celery, fennel, endive, escarole, parsley, radicchio, rhubarb, spinach
- Brassica leafy vegetables such as broccoli, brussel sprouts, cabbage, cauliflower, collards, kale, kohlrabi, mustard greens, mustard spinach and turnips.
- Legumes (succulent) such as beans, peas and alfalfa.
- Fruiting vegetables such as pepper (bell, pimento, hot, sweet), tomato, tomatillo and eggplant.
- Cucurbits such as cucumber, melon (crenshaw, honeydew, honey ball, mango, pineapple, watermelon), summer squash, pumpkins and winter squash.

Fruits
- Citrus fruits such as sweet orange, sour orange, lemon, lime, tangelo, tangerine, mandarin, citrus citron, kumquats and grapefruit.
- Pome fruits such as apples and pears
- Stone fruits such as sour and sweet cherry, peach, nectarine and plum.
- Small fruits and berries such as blackberries, blueberries, boysenberries, red and black raspberries and strawberries.

Herbs and spices such as basil, chives, dill, oregano, rosemary, sage, savory and thyme.
Miscellaneous such as apricots, artichoke, cranberry, dates, figs, grapes, guava, kiwi, mango, mushrooms, okra, olives, persimmons, pomegranate and watercress.

EPA Reg. No. 1677-234
EPA Est.: 1677-MN-1 (P), 60156-IL-1 (SI), 1677- CA-2 (R), 1677-TX-1 (D),1677-IL-2 (J), 1677-GA-1 (M), 1677-WV-1 (V), 5389-NC-1 (G), 6574-KY-1 (CA)
Superscript refers to first letter of date code

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, DC 20460

OFFICE OF CHEMICAL SAFETY
AND POLLUTION PREVENTION

April 21, 2015

Nicole Listner
Associate Regulatory Specialist I
Ecolab Inc.
370 N. Wabasha Street
St. Paul, MN 55102

Subject: Label Notification per PRN 98-10 – Updating Master label, adding additional marketing language; (adding a statement showing some claims not approved in CA); adding packaging size (64 oz.); and minor changes to the Secondary Container label in accordance with the PRN 98-10.
Product Name: Antimicrobial Fruit & Vegetable Treatment
EPA Registration Number: 1677-234
Application Date: 3/30/2015
Decision Number: 503102

Dear Ms. Listner:

The Agency is in receipt of your Application for Pesticide Notification under Pesticide Registration Notice (PRN) 98-10 for the above referenced product. The Antimicrobials Division has conducted a review of this request for its applicability under PRN 98-10 and finds that the action requested falls within the scope of PRN 98-10.

The label submitted with the application has been stamped "Notification" and will be placed in our records.

If you have any questions, you may contact Lorena Rivas at (703) 305-5027 or via email at rivas.lorena@epa.gov.

Sincerely,

for

Jacqueline Hardy, Product Manager 34
Regulatory Management Branch II
Antimicrobials Division (7510P)
Office of Pesticide Programs

Antimicrobial Fruit & Vegetable Treatment

Water Additive for Pathogen Reduction in Fruit and Vegetable Wash or Process Waters

Controls Spoilage and Decay Causing Bacteria in Fruit and Vegetable Wash or Process Waters

Reduces Bacterial Pathogens on *Processed* Fruit and Vegetable Surfaces†
†This(These) antimicrobial claim(s) not approved in the state of California

Antimicrobial Fruit and Vegetable Wash

Active Ingredients:	
Dodecylbenzenesulfonic acid, sodium salt	1.23%
Lactic Acid.....	17.29%
Other Ingredients:.....	81.48%
Total:.....	100.00%

NOTIFICATION
1677-234
The applicant has certified that no changes, other than those reported to the Agency have been made to the labeling. The Agency acknowledges this notification by letter dated:
4/21/2015

KEEP OUT OF REACH OF CHILDREN

WARNING

(See [back], [side], [other] label for [complete] [additional] [directions for use] [precautionary statements] [and] [first aid])

PRECAUTIONARY STATEMENTS

HAZARDS TO HUMANS AND DOMESTIC ANIMALS

WARNING: Causes substantial but temporary eye injury. Harmful if absorbed through skin. Do not get in eyes, on skin or on clothing. Wear goggles, face shield, or safety glasses. Wash thoroughly with soap and water after handling and before eating, drinking, chewing gum, using tobacco or using the toilet. Remove and wash contaminated clothing before reuse. After the product is diluted, safety goggles are not required. Prolonged or frequently repeated skin contact with the concentrate may cause allergic reactions in some individuals.

FIRST AID

If in Eyes:

- Hold eye open and rinse slowly and gently with water for 15-20 minutes. Remove contact lenses, if present, after the first 5 minutes, then continue rinsing eyes.
- Call a Poison Control Center or doctor for treatment advice.

If on Skin or Clothing:

- Take off contaminated clothing.
- Rinse skin immediately with plenty of water for 15-20 minutes.
- Call a Poison Control Center or doctor for treatment advice.

FOR EMERGENCY MEDICAL INFORMATION CALL TOLL-FREE:
1-800-328-0026
Areas of use: Food retail establishments such as restaurants, cafeterias, food service operations, commissaries, and kitchens.

[NOTE TO REVIEWER: language in parenthesis is interchangeable]

[Optional Marketing Language]

- See side/back panel for first aid
- See (outer container) (package insert) for (first aid) (precautionary statements) (additional directions for use)
- Mix one 4 oz. (packet) or (bottle) or (reservoir) with 4 – 5.3 gallons of water
- Use one filled 4 oz. reservoir to mix with 4 - 5.3 gallons of water
- Use 4 oz. of product with 4 – 5.3 gallons of water

DIRECTIONS FOR USE:
It is a violation of Federal law to use this product in a manner inconsistent with its labeling.

When used as directed, Antimicrobial Fruit & Vegetable Treatment will:

1. Reduce (Kill) 99.9% of the pathogens *Escherichia coli* O157:H7 (ATCC 43895, 35150, 43890), *Listeria monocytogenes (ATCC 49594, 19114, 19116)* and *Salmonella enterica* (ATCC 10721, 6962, 13311) in wash or process water for fruit and vegetable raw agricultural commodities (RACs).

2. Controls (Kill) spoilage and decay causing non-public health microorganisms present in the wash or process water for fruit and vegetable raw agricultural commodities (RACs).

To treat the surface of *processed* fruits and vegetables subject to FDA regulations[‡]:

This product may be used in wash waters to reduce the pathogens *Escherichia coli O157:H7, Listeria monocytogenes* and *Salmonella enterica* on the surface of *processed* fruits and vegetables introduced during handling or processing. This antimicrobial claim not approved in the state of California.

This use must comply with all applicable FDA regulations, including, but not limited to 21 CFR §173.405(a)(b), 21 CFR §184.1061 and 21 CFR §170.3(o)(2).

[†]This(These) antimicrobial claim(s) not approved in the state of California.

Cleans (removes) waxes and residue from produce (introduced during handling or processing)

Add Antimicrobial Fruit & Vegetable Treatment into the fruit and vegetable washing/processing vessel (sink) according to the table below, submerge and agitate fruits and vegetables for a minimum of 90 seconds. Drain fruit and vegetables thoroughly and allow to air dry. No rinse required.
If desired just before immediate use, rinse treated produce thoroughly with potable water. Place produce on a pre-cleaned and sanitized surface or in a pre-cleaned and sanitized container.

Minimum Contact Time	Ounces of concentrate per gallon of water	Dilution ratio (parts concentrate : parts water)	Active ingredients	
			ppm SDBS*	ppm Lactic Acid
90 seconds	0.75 – 1.00	1:170 – 1:128	76 –111	1061 – 1391

* Sodium dodecylbenzenesulfonate

Refer to the Antimicrobial Fruit & Vegetable Treatment package insert for the recommended list of fruits and vegetables.

STORAGE AND DISPOSAL:
DO NOT CONTAMINATE WATER, FOOD OR FEED BY STORAGE OR DISPOSAL

PESTICIDE STORAGE: Store in a cool, dark, dry place in the original container. Always replace covers.

PESTICIDE DISPOSAL: Pesticide wastes are acutely hazardous. Improper disposal of excess pesticide, spray mixture, or rinsate is a violation of Federal Law. If these wastes cannot be disposed of by use according to label instructions, contact your State Pesticide or Environmental Control Agency, or the Hazardous Waste representative at the nearest EPA Regional Office for guidance. Waste resulting from the use of this product must be disposed of on site or at an approved waste disposal facility.

CONTAINER DISPOSAL:
(Packet) Non-refillable container. Do not reuse packet. Wrap and put in trash.

Non-refillable container. Do not reuse this container to hold materials other than pesticides or diluted pesticide rinsate. Offer for recycling if available or puncture and dispose in a sanitary landfill, or by other procedures approved by state and local authorities.

RESIDUE REMOVAL INSTRUCTIONS: For containers less than 5 gallons. Triple rinse container (or equivalent) promptly after emptying. Triple rinse as follows: Fill container ¼ full with water and recap. Shake 10 seconds. Follow Pesticide Disposal instructions for rinsate disposal. Drain for 10 seconds after the flow begins to drip. Repeat procedure two more times.

RESIDUAL REMOVAL INSTRUCTIONS: For containers greater than 5 gallons. Triple rinse container (or equivalent) promptly after emptying. Triple rinse as follows: Fill container ¼ full with water. Tip container on its side and roll back and forth, ensuring at least one complete revolution for 30 seconds. Stand the container on its end and tip back and forth several times. Turn the container over its other end and tip back and forth several times. Follow Pesticide Disposal instructions for rinsate disposal. Repeat procedure two more times.

FOR COMMERCIAL USE

Net Contents:
4 oz.
64 oz.
96 oz.
1 U.S. Gal. (3.78 L)
2.5 U.S. Gal. (9.46 L)
4 U.S. Gal. (15.14 L)

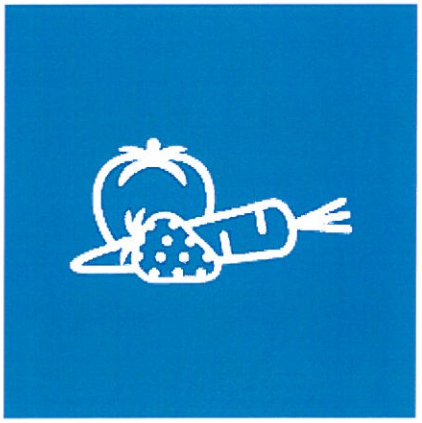
Manufactured by:
Ecolab Inc.
370 Wabasha Street N.
St. Paul, MN 55102

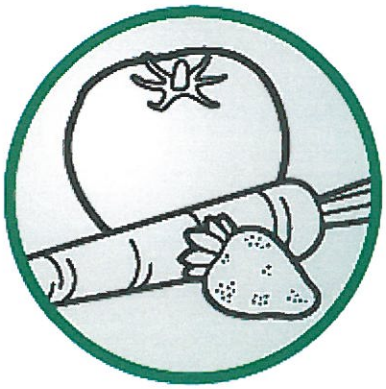
EPA Reg. No. 1677-234

EPA Est. No.: 1677-MN-1 (P), 60156-IL-1 (SI), 1677- CA-2 (R), 1677-TX-1 (D), 1677-IL-2 (J), 1677-GA-1 (M), 1677-WV-1 (V), 89566-IL-1 (C), 6574-KY-1 (CA)
Superscript refers to first letter of date code

(Made in USA) (Made in United States of America)

[Optional Marketing Graphics]





[NOTE TO REVIEWER: language in parenthesis is interchangeable]

PACKAGE INSERT

Water Additive for Pathogen Reduction in Fruit and Vegetable Wash or Process Waters

Controls Spoilage and Decay Causing Bacteria in Fruit and Vegetable Wash or Process Waters

Reduces Bacterial Pathogens on *Processed* Fruit and Vegetable Surfaces†
†This(These) antimicrobial claim(s) not approved in the state of California

When used as directed for the treatment of raw agricultural commodities and process water, Antimicrobial Fruit & Vegetable Treatment will:

1. Reduce (Kills) 99.9% of the pathogens *Escherichia coli* O157:H7 (ATCC 43895, 35150, 43890), *Listeria monocytogenes (ATCC 49594, 19114, 19116)* and *Salmonella enterica* (ATCC 10721, 6962, 13311) in wash or process water for fruit and vegetable raw agricultural commodities (RACs).

2. Control (Kills) spoilage and decay causing non-public health microorganisms present in the wash or process water for fruit and vegetable raw agricultural commodities (RACs).

Antimicrobial Fruit & Vegetable Treatment can be applied to the following types of fresh fruit, post harvest.

Vegetables

- Root and tuber vegetables such as carrot, potato, radish, rutabaga, sweet potato, yam and sugar beets.
- Leaves of root and tuber vegetables such as turnip greens and sugar beet
- Bulb vegetables such as onions, leeks, garlic and shallots.
- Leafy vegetables such as lettuce (head and leaf), celery, fennel, endive, escarole, parsley, radicchio, rhubarb, spinach
- B*rassica* leafy vegetables such as broccoli, brussel sprouts, cabbage, cauliflower, collards, kale, kohlrabi, mustard greens, mustard spinach and turnips.
- Legumes (succulent) such as beans, peas and alfalfa.
- Fruiting vegetables such as pepper (bell, pimento, hot, sweet), tomato, tomatillo and eggplant.
- Cucurbits such as cucumber, melon (crenshaw, honeydew, honey ball, mango, pineapple, watermelon, cantaloupe, muskmelon), summer squash, pumpkins and winter squash.

Fruits
- Citrus fruits such as sweet orange, sour orange, lemon, lime, tangelo, tangerine, mandarin, citrus citron, kumquats and grapefruit.
- Pome fruits such as apples and pears.
- Stone fruits such as sour and sweet cherry, peach, nectarine and plum.
- Small fruits and berries such as blackberries, blueberries, boysenberries, red and black raspberries and strawberries.

Herbs and Spices
- Basil, chives, dill, oregano, rosemary, sage, savory and thyme.

Other
- Apricots, artichoke, cranberry, dates, figs, grapes, guava, kiwi, mango, mushrooms, okra, olives, persimmons, pomegranate, watercress, coffee fruit (coffee cherry), and coffee bean.

When used as directed for the treatment of *processed* fruits and vegetables under FDA regulations, Antimicrobial Fruit and Vegetable Treatment will[†]:

Reduce the pathogens *Escherichia coli* O157:H7, *Listeria monocytogenes* and *Salmonella enterica* on the surface of *processed* fruits and vegetables introduced during handling or processing.

This use must comply with all applicable FDA regulations, including but not limited to 21 CFR §173.405(a)(b), 21 CFR §184.1061 and 21 CFR §170.3(o)(2).

[†]This(These) antimicrobial claim(s) not approved in the state of California.

Cleans (Removes) waxes and residue from produce (introduced during handling or processing).

SECONDARY/USE DILUTION CONTAINER LABEL

[Note to reviewer: This secondary/use dilution container label will be used when the product is diluted at 0.75 - 1 oz per gallon of water. Use dilution is to be prepared by end user. This secondary/use dilution label will only be used by the end user and will not be sold or distributed.]

Antimicrobial Fruit & Vegetable Treatment

Concentrate Ingredient Statement

Active Ingredients:	
Dodecylbenzenesulfonic acid, sodium salt	1.23%
Lactic Acid.....	17.29%
Other Ingredients:.....	81.48%
Total:.....	100.00%

Diluted product in this container is 0.75 - 1 oz per gallon water.
When diluted, the active ingredients are:

Active Ingredients:	
Dodecylbenzenesulfonic acid, sodium salt	76-111 ppm
Lactic Acid.....	1061-1391 ppm

KEEP OUT OF REACH OF CHILDREN
After product has been diluted according to label directions, goggles, face shield, or safety glasses are not required.

The product in this container is diluted as directed on the concentrate product label. Follow the directions for use on the pesticide label when applying this product.

Use solution prepared by end user.
NOT TO BE SOLD OR DISTRIBUTED.
[Do Not Drink]

EPA Reg. No. 1677-234

REDUCE PATHOGENS

Antimicrobial Fruit & Vegetable Treatment

- FDA clearance and EPA registered
- Effective on both whole and further processed produce
- Reduces harmful pathogens* on the surface of fresh cut produce and in wash water
- Cleans off waxes and residues
- Reduces spoilage organisms
- No rinse required

Reduces **99.9%** of the pathogens ***E. coli, Listeria*** and ***Salmonella**** in wash water**

**Pathogens: Escherichia coli O157:H7 , Listeria monocytogenes and Salmonella enterica*

***For fruit and vegetable raw agricultural commodities (RACs) when used according to the label instructions*

KILLS PATHOGENS

Antimicrobial Fruit & Vegetable Treatment reduces 99.9% of the pathogens ***E. coli, Listeria*** and ***Salmonella**** in produce wash or process water.** Water alone does not kill pathogens.

EPA Reg. No. 1677-234.

REQUIRES NO RINSING

Antimicrobial Fruit & Vegetable Treatment, at its registered use concentration, does not impart any off-flavor or odor. All components are Generally Regarded As Safe (GRAS) or have been cleared by the FDA for the intended use in a no-rinse application.

UNIQUE DISPENSING SYSTEM

Antimicrobial Fruit & Vegetable Treatment's unique dispensing design is easy to use, provides employees with visual verification that product is dispensed, and controls the delivery of antimicrobial concentrations for effectiveness and consistent results.

DIRECTIONS:

Dispense Antimicrobial Fruit & Vegetable Treatment into the sink according to the table below. Submerge and agitate fruits and vegetables for a minimum of 90 seconds. Drain thoroughly and allow to air dry. No rinse required.

Pictured Above:

Antimicrobial Fruit & Vegetable Treatment washes off waxes and residues from produce often making the produce look more appealing.

Pictured Right:

Kale washed with Antimicrobial Fruit & Vegetable Treatment. (Right kale leaf)

Kale washed with water only. (Left kale leaf)

MINIMUM CONTACT TIME	OUNCES OF CONCENTRATE PER GALLON OF WATER	DILUTION RATIO (PARTS CONCENTRATE: PARTS WATER)	ACTIVE INGREDIENTS	
			ppm SDBS*	ppm Lactic Acid
90 Seconds	0.75 - 1.00	1:170 - 1:128	76 - 111	1061 - 1391

* Sodium dodecylbenzenesulfonate

PRODUCT	PICK CODE	PACK SIZE
Antimicrobial Fruit & Vegetable Treatment	6100283	1-2.5 gal

370 Wabasha Street N St. Paul, MN 55102
www.ecolab.com 1 800 35 CLEAN

Antimicrobial Fruit & Vegetable Treatment

Food Safety. Made Easy.

Reduce 99.9% of *E. coli, Listeria* and *Salmonella* in produce wash water*

Water alone does not kill pathogens. Ecolab's Antimicrobial Fruit & Vegetable Treatment works in just 90 seconds with no rinse required. Cleared by both the EPA and FDA, it is effective on both whole and further processed produce, cleans off waxes and residues, and reduces spoilage organisms in wash water.

To learn more, visit: www.whycleanmatters.com/AFVT

OR CALL 1.800.942.3002 FOR MORE INFORMATION

** Pathogens: Escherichia coli O157:H7, Listeria monocytogenes and Salmonella enterica. For fruit and vegetable raw agricultural commodities (RACs) when used according to label instructions.*

WHAT'S THIS?
Use your smart-phone's QR code reader App and take a photo to go directly to the website.

ECOLAB®
Everywhere It Matters.™

JUST THE FACTS Foodborne Illness

Fruits and vegetables most associated with foodborne illness from 1996-2010

FDA, 2011


fresh herbs


berries


green onions


leafy greens


melons


sprouts


tomatoes

About 1 in 6 people gets sick each year from contaminated food

CDC, 2011

365M

Salmonella infection accounts for $365 million in direct medical costs each year

CDC, 2011

128K

Estimated number of annual hospitalizations resulting from foodborne illness

CDC, 2011

3,000

People die each year in the U.S. of foodborne diseases

CDC, 2011

9. PHYSICAL PROPERTIES, MODE OF ACTION

Physical Properties:

Linear Alkylbenzene Sulfonate (LAS) or Dodecylbenzenesulfonic acid, Sodium Salt (SDBS) is an anionic surfactant. It was introduced in 1964 as the readily biodegradable replacement for highly branched alkylbenzene sulfonates (ABS). LAS is a mixture of closely related isomers and homologues, each containing an aromatic ring sulfonated at the para position and attached to a linear alkyl chain. Alkylbenzene sulfonates are used largely as food-contact sanitizers in food processing plants and eating establishments. They are also used as disinfectants and sanitizers for agricultural, commercial, institutional, industrial, and public access uses.[5, 6] The linear alkyl carbon chain typically has 10 to 14 carbon atoms, with the approximate mole ratio varying somewhat regionally with weighted averages of 11.7-11.8. The alkyl chains are >95% linear.

Properties of the Substance:

Color/Form:	Off-white, powder
Flash Point:	> 93.9°C
Specific Gravity:	4.41 lb/gal (0.53 g/ml)
Melting Point:	> 300°C
Boiling Point	> 630°C
Vapor Pressure at 25°C:	5 x 10^{-13} Pa
Solubility in water:	250 g/liter
Octanol-water partition coefficient (log Kow)	3.32
pH Value:	7 @1% Aqueous
Molecular Weight:	348.49

Mode of Action:

Linear alkylbenzene sulfonates are used largely as food-contact sanitizers in food processing plants and eating establishments. They are also used as disinfectants and sanitizers for agricultural, commercial, institutional, industrial, and public access uses. Much of LAS consumption is in household detergency. Important application products are laundry powders, laundry liquids, dishwashing products and all-purpose cleaners. The remainder of the LAS (<20%) is used in Industrial and Institutional (I&I) cleaners, textile processing as wetting, dispersing and cleaning agents, industrial processes as emulsifiers, polymerization and in the formulation of crop protection agents.[5]

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[5] Human & Environmental Risk Assessment (HERA). 2013. LAS: linear alkyl benzene sulphonate. Revised HERA Report April 2013; accessed June 16, 2014. Available at:

http://www.heraproject.com/RiskAssessment.cfm

[6] Organization for Economic Cooperation and Development Screening Information Data Sets (OECD-SIDS). 2005. Linear Alkylbenzene Sulfonate (LAS) SIDS Initial Assessment Report, April 2005; accessed June 17, 2014. Available at: http://www.chem.unep.ch/irptc/sids/OECDSIDS/LAS.pdf

Toxicology Narrative – Human Health Assessment:

Introduction:

The following toxicological assessment of linear alkyl benzene sulfonate (LAS; which includes sodium dodecylbenzene sulfonate, CAS No. 25155-30-0) is excerpted from the 2006 Inert Ingredient Tolerance Reassessment by EPA and the toxicology chapter of the reregistration eligibility decision (RED) for alkyl benzene sulfonates.[7, 8]

Linear alkyl benzene Sulfonate (LAS) is an anionic surfactant which was introduced in 1964 as a more biodegradable replacement for highly branched Alkyl Benzene Sulfonates (ABS). LAS is a mixture of closely related isomers and homologues, each containing an aromatic ring sulfonated at the para position and attached to a linear alkyl chain. Their primary use is as a detergent for cleaning (residential, commercial, and on surfaces where food contact occurs). The presence of LAS in many commonly used household detergents gives rise to a variety of possible consumer contact scenarios such as: direct and indirect skin contact, inhalation, and oral ingestion derived either from residues deposited on dishes, from accidental product ingestion, or indirectly from drinking water. The EPA toxicology assessment drew heavily from two sources: WHO (1996)[9]; and HERA (2013).[10] The toxicology database consists almost entirely of published literature, was considered essentially complete and of acceptable quality by EPA to assess the potential hazard to humans.

Overview:

LAS are readily absorbed following oral ingestion, but not following dermal exposure. LAS are readily metabolized, excreted fairly rapidly, and do not accumulate in tissues. Available acute toxicity data show that LAS are not highly acutely toxic following oral exposure, but are moderately toxic via dermal and inhalation exposure, are irritating to the eye and skin, and they are not skin sensitizers. Sub-chronic and chronic exposures show that the liver, kidney and intestinal tract (following oral exposures) are the major target organs of toxicity. Both in vitro and in vivo genotoxicity data show that LAS are not toxic to the gene or the chromosome. LAS did not cause reproductive or developmental toxicity in acceptable studies. Early (pre-GLP) carcinogenicity studies indicate that LAS is not likely to be carcinogenic.

Absorption and excretion:

In animal tests (oral – monkeys, pigs, rats), LAS are readily absorbed from the gastrointestinal tract, are distributed throughout the body, and are extensively metabolized. Excretion is via both the urine and feces. Available dermal absorption data (rats and guinea pigs) indicate that LAS are poorly absorbed from the skin, although prolonged contact may lead to irritation and thus compromise the skin to permit more absorption.[9, 10]

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[7] U.S. Environmental Protection Agency (EPA); 2006c. Alkyl benzene sulfonates (ABS) toxicology chapter for the reregistration eligibility decision (RED) document. July 6, 2006; accessed July 22, 2010. EPA-HQ-OPP-2006-0156-0018. Available at: http://www.regulations.gov/#!docketDetail;D=EPA-HQ-OPP-2006-0156

[8] U.S. Environmental Protection Agency (EPA); 2006d. Environmental Fate Assessment of Alkylbenzene Sulfonates for the Registration Eligibility Document (RED). July 6, 2006; accessed June 16, 2014. EPA-HQ-OPP-2006-0156-0021. Available at: http://www.regulations.gov/#!docketDetail;D=EPA-HQ-OPP-2006-0156

[9] World Health Organization (WHO). 1996. Environmental health criteria document for linear alkyl benzene sulfonates and related compounds. EHC 169; accessed July 22, 2010. Available at:

http://www.inchem.org/documents/ehc/ehc/ehc169.htm.

[10] Human & Environmental Risk Assessment (HERA). 2013. LAS: linear alkyl benzene sulphonate. Revised HERA Report April 2013; accessed June 16, 2014. Available at:

http://www.heraproject.com/RiskAssessment.cfm

Acute toxicity including irritancy and sensitization:

LAS exhibit a wide range of acute toxicity via the oral route in rats (LD50 of 404 – 1980 mg/kg), with a narrower range in mice (LD50 of 1259-2300 mg/kg). This spans the acute oral toxicity categories of III-IV as assigned by the USEPA. LAS are classified as acute toxicity category II for the dermal and inhalation routes of exposure.

Repeated dose toxicity (sub-chronic and chronic):

There have been many oral repeated dose studies performed with LAS ranging from a 28-day study in monkeys to nine month studies conducted with rats and mice. There have also been repeated dose dermal (guinea pigs, rabbits, and rats) and inhalation studies (dogs and monkeys). Collectively, the animal data suggest that the liver, kidney and cecum (for oral studies) are the major target organs for toxicity. The liver and kidney effects were dose and duration related in that mild effects (organ weight changes and serum enzyme/clinical chemistry changes indicative of mild organ effects) were seen at lower doses, but increased in severity with both dose and time. For the purposes of this hazard assessment, several studies were considered collectively to determine a NOAEL of 50 mg/kg/day for the chronic dietary endpoint. The NOAELs in the three studies used to develop the chronic endpoint are 40, 50 and 85 mg/kg/day. The chronic endpoint is based on: increased cecum weight and slight kidney damage (at a LOAEL of 114 mg/kg/d in the six month rat study); reduced body weight in 21-day old pups (at a LOAEL of 250 mg/kg/day in a reproductive toxicity rat study); and significant decreases in renal biochemical parameters (at a LOAEL of 145 mg/kg/day in a nine month drinking water study in rats).

Developmental and reproductive toxicity:

A number of developmental studies via the oral and dermal routes have been performed with LAS in rats, mice and rabbits; there were also several subcutaneous injection developmental studies reported in mice.[11] There is a spectrum of quality in the 20+ studies in terms of dosing (some had only one or two doses), purity of LAS used (some used formulated products that ranged from 1-45% LAS content), and overt toxicity to the pregnant females in the dermal studies due to severe irritating effects. It is concluded that some developmental effects (including some terata) were observed at high doses at which maternal toxicity was observed and the available information does not suggest any qualitative or quantitative susceptibility differences between pups and pregnant animals. LAS were tested in several multigenerational studies in rats. There were no effects on reproductive parameters in any of these tests at doses up to 250 mg/kg/day.

Carcinogenicity:

The available long-term studies that assessed carcinogenicity were older studies (pre-1970) that would not be acceptable under current standards (due to low number of animals used, insufficient number of doses and extent of dosing, and limited histopathological examinations. However, the limited studies provide no evidence of carcinogenicity in animals given LAS orally.

Genotoxicity:

The toxicological data show that LAS was not genotoxic in vitro or in vivo.

Neurotoxicity:

There is no evidence in the literature to indicate any neurotoxic effects of LAS in humans or laboratory animals.

[11] World Health Organization (WHO). 1996. Environmental health criteria document for linear alkyl benzene sulfonates and related compounds. EHC 169; accessed July 22, 2010. Available at: http://www.inchem.org/documents/ehc/ehc/ehc169.htm.

Environmental Assessment:

Overview

The summary of the environmental risk assessment is extracted from the U.S. Environmental Protection Agency Reregistration Eligibility Decision (RED) for Alkylbenzene Sulfonate and Alkylbenzene Sulfonates (ABS) Risk Assessment for the Reregistration Eligibility Decision (RED) Document.[12, 13] The following risk characterization is intended to describe the magnitude of the estimated environmental risks for alkylbenzene sulfonates use sites and any associated uncertainties. For detailed discussions of all aspects of the environmental risk assessment, see the Environmental Fate Assessment of Alkylbenzene Sulfonates for the Reregistration Eligibility Decision.[14]

Environmental Hazard and Risk

The alkylbenzene sulfonates are slightly toxic to the Northern bobwhite quail, and moderately toxic to freshwater fish and freshwater invertebrates following acute exposure. The available data indicate that the alkylbenzene sulfonates are slightly toxic to green algae.

Available literature for linear alkylbenzene sulfonate (LAS) detergent use indicates that the alkylbenzene sulfonates are not expected to bioaccumulate in the environment or aquatic organisms (i.e. fish) and are expected to be soluble in water such that they will exhibit mobility through the soil. The model-calculated linear and non-linear biodegradation probabilities suggest that these chemicals will most likely biodegrade rapidly. The short half-life indicates that if these chemicals are present in the soil, they are not likely to be volatile and are expected to degrade rapidly in the environment.

Minimal or no environmental exposure is expected to occur from the majority of alkylbenzene sulfonate antimicrobial pesticide uses because a very small number of pounds of this chemical are sold for antimicrobial use per data provided by the manufacturers.

Ecological Toxicity Data

Acute toxicity to terrestrial organisms: As shown in the acute toxicity summary Table 8, alkylbenzene sulfonates are slightly toxic to the Northern bobwhite quail on an acute oral basis. The avian acute oral LD50 is > 500 ppm, therefore, an avian environmental hazard statement for birds is not required on manufacturing use product labels. No evidence of endocrine disrupting effects was observed in mammalian toxicity studies. No data are available or required for terrestrial plants.

Acute toxicity to aquatic organisms: As shown in Table 8, supplemental acute studies indicate that alkylbenzene sulfonates are moderately toxic to freshwater fish and freshwater aquatic invertebrates. In addition, 11 acute freshwater fish studies using commercially relevant LAS and LAB formulations indicate the LC50 values range from 1.67 to 7.7 mg/L [LAS SIDS Initial Assessment Report, (SIAR)]. Data using LAB sulfonic acids in the LAS SIAR report range in toxicity from 3.0 to 10.0 mg/L. In aquatic invertebrates, LAS toxicity is variable, depending on the length of the carbon chain. LAS/SIAR (page 37) summarizes 11 Daphnia magna studies on commercially relevant LAS that range in EC50 values from

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[12] U.S. Environmental Protection Agency (EPA); 2006a. Reregistration Eligibility Decision (RED) for Alkyl benzene sulfonates. July 27, 2006; accessed June 13, 2014. EPA-HQ-OPP-2006-0156-0016. Available at: http://www.regulations.gov/#!docketDetail;D=EPA-HQ-OPP-2006-0156

[13] U.S. Environmental Protection Agency (EPA); 2006b. Alkylbenzene Sulfonates (ABS) Risk Assessment for the Reregistration Eligibility Decision (RED) Document. PC Codes: 079010, 190116 and 098002.(active); 790102, 790116, 790101 (inert) Case No. 4006. July 19, 2006; accessed June 16, 2014. EPA-HQ-OPP-2006-0156-0017. Available at: http://www.regulations.gov/#!docketDetail;D=EPA-HQ-OPP-2006-0156

[14] U.S. Environmental Protection Agency (EPA); 2006d. Environmental Fate Assessment of Alkylbenzene Sulfonates for the Registration Eligibility Document (RED). July 6, 2006; accessed June 16, 2014. EPA-HQ-OPP-2006-0156-0021. Available at: http://www.regulations.gov/#!docketDetail;D=EPA-HQ-OPP-2006-0156

1.62 to 9.3 mg/L. Data on the LAB sulfonic acids give EC50 values for Daphnia magna ranging from 2.9 to 12 mg/L. Formulations tested included the C10-C16 benzene sulfonic acid and the dodecylbenzene sulfonic acid.

Chronic toxicity to aquatic organisms: A 28 day chronic freshwater fish toxicity test determined the NOAEC was 0.7 mg/L for a carbon chain C11.7. Scientists studying alkylbenzene sulfonates have concluded that a laboratory derived NOAEC of 0.4 mg/L alkylbenzene sulfonates is protective of ecosystem structure and function in experimental streams. Alkylbenzene sulfonates literature indicates slight toxicity to green algae (see Table 8).

Environmental Fate and Exposure Assessment.

There were no environmental fate studies for alkylbenzene sulfonates available in US EPA's files. Thus, the Agency relied on scientific literature and the Agency's EPI Suite model to obtain different environmental properties for the alkylbenzene sulfonates. The EPI Suite model predicts that alkylbenzene sulfonates are not likely to persist in water or microbial soils and sediments. Extensive literature are available that describe the fate and significance of alkylbenzene sulfonates in the environment from a long history of detergent use.[15]

Significant environmental exposure is not expected for the following reasons: total alkylbenzene sulfonate usage for these industrial applications is very minor - a very small percentage of the total pounds used in antimicrobials; commercial only use precludes broad environmental exposures that might occur with residential use; applications are mostly sprayed on and allowed to air dry; alkylbenzene sulfonate breakdown and degrade rapidly in the environment; alkylbenzene sulfonates are significantly reduced by sewage treatment; and industrial water treatment requires a NPDES permit in order to discharge effluents.

Ecological Risk Characterization.

Sodium dodecylbenzene sulfonate and is unlikely to bioaccumulate in the environment or aquatic animals. It is expected to be soluble in water such that it will exhibit mobility through the soil. Available modeling and literature suggest that this chemical will most likely biodegrade rapidly in soil due to microbial degradation. Minimal or no environmental exposure to terrestrial or aquatic organisms is expected to occur from the use of SDBS.

Linear alkyl benzene sulfonates (LAS) have been the principal ingredient in laundry detergent for 30+ years. Monitoring indicates that concentrations of 0.230 mg/L (continuous criterion concentration) and 0.625 mg/L (criterion maximum concentration) are rarely exceeded in aquatic systems protected by activated sludge treatment systems. Ecotoxicity studies indicate that a laboratory derived NOAEC value of 0.40 mg/L for LAS is protective of structure and function of experimental streams.[16]

Conclusion

No environmental exposure is expected to occur from the majority of linear alkylbenzene sulfonate uses and it is unlikely that any appreciable exposure to terrestrial or aquatic organisms would occur from limited commercial down-the-drain use because of the very small number of pounds sold for these uses plus rapid degradation in the environment.

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[15] U.S. Environmental Protection Agency (EPA); 2006c. Alkyl benzene sulfonates (ABS) toxicology chapter for the reregistration eligibility decision (RED) document. July 6, 2006; accessed July 22, 2010. EPA-HQ-OPP-2006-0156-0018. Available at: http://www.regulations.gov/#!docketDetail;D=EPA-HQ-OPP-2006-0156

[16] U.S. Environmental Protection Agency (EPA); 2006d. Environmental Fate Assessment of Alkylbenzene Sulfonates for the Registration Eligibility Document (RED). July 6, 2006; accessed June 16, 2014. EPA-HQ-OPP-2006-0156-0021. Available at: http://www.regulations.gov/#!docketDetail;D=EPA-HQ-OPP-2006-0156

EPA SUMMARY TABLES OF AVAILABLE TOXICITY STUDIES AND RELATED INFORMATION[17]

Table 1. Acute Toxicity Data on Linear Alkylbenzene Sulfonate (LAS):

Guideline No./ Study Type	MRID No.	Results	Toxicity Category
870.1100 Acute oral toxicity	Multiple	LD_{50} = range from 404 to over 5000 mg/kg	III-IV
870.1200 Acute dermal toxicity	94032006	LD_{50} = 1200 mg/kg	II
870.1300 Acute inhalation toxicity	Open Literature (HERA 2013)	LC_{50} = 310 mg/m3	II
870.2400 Acute eye irritation	0033443*	Corneal opacity not reversed at 72 hours.	I
870.2500 Acute dermal irritation	003444*	Severe irritation at 72 hours	II
870.2600 Skin sensitization	Open Literature	Non-sensitizer	

[17] Tables 1&2 extracted from the RED for Alkylbenzene sulfonates (EPA 2006a). Tables 3 through 8 extracted from Alkylbenzene Sulfonates (ABS) Risk Assessment for the Reregistration Eligibility Decision (RED) Document (EPA 2006b).

Table 2. Subchronic, Chronic and Other Toxicity Tables:

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
Subchronic Toxicity			
870.3100 Oral Subchronic (rodent)	Bornmann et al (1963) Study of a Detergent Based on Dodecylbenzene Sulfonate. Fette Seifen Anstrichm, 65 (10): 818-824. (EHC 169) **Open Literature**	0.01% of a preparation containing 51% LAS was administered in the drinking water for 100 weeks Rats (60/sex) Purity: Not Reported	No detrimental effects on body weight and no pathological effects, including tumors, were reported
870.3100 Oral Subchronic (rodent)	Ikawa et al., (1980)/ Ann. Rep. Tokyo Metrop. Res. Lab. Public Health. 29(2): 51-54(Z). 1978 (in Japanese, see WHO, 1996 and HERA, 2013). **Open Literature**	LAS was administered for 2, 4, or 12 weeks at a single dose of 1.5% in the diet (750 mg/kg/d). Male rats (five/group) Purity not reported.	LAS suppressed body weight gain and the relative liver weight was increased after two weeks. Serum biochemical alterations included: significant increases in ALP, GTP (at 2, 4, 12 weeks); significant decreases in cholesterol and protein (4 weeks); decreases in liver enzymes G6Pase and G6PDH and increases in isocitrate DH (all at 2, 4, 12 weeks). The following enzymes associated with kidney function were also altered: decreases in G6Pase, 5'nucleotidase (at 2, 4, 12 weeks) and Na,K-ATPase (12 wks); increase in LDH (12 wks) and IDH (2,4 wks).
870.3100 Oral Subchronic (rodent)	Ito, et al. (1978) Acute, Subacute, and Chronic Toxicity of Magnesium LAS (LAS-Mg). J. Med. Soc. Toho Univ. 25: 850-875. **Open Literature**	Administration by oral gavage at doses of 0, 155, 310, or 620 mg/kg/day (LAS-Mg) and 125, 250, and 500 mg/kg/day (LAS-Na) for one month Sprague-Dawley Rats (12/sex/group) Purity: 99.5%	LAS-Na: Body weight increase was suppressed; feed-efficacy was decreased, and liver weight increased at 500 mg/kg/day. NOAEL: 125 mg/kg bw/d.
870.3100 Oral Subchronic (rodent)	**MRID No. 43498412** Kay et al. (1965) Subacute Oral Toxicity of a Biodegradable, Linear Alkylbenzene Sulfonate. Toxicol Appl. Pharmacol. 7: 812-818 (HERA) **Acceptable** Guideline	SDDBS administered in the diet at dietary levels of 0, 200, 1000, and 5000 ppm for 90 days Weanling Sprague-Dawley Rat (10/sex/dose) Purity: 87.9% a.i.	NOEL: 5000 ppm (HDT) Two low dose males died early in the study from respiratory illness There was no compound-related effects in body weight, food consumption, hematology, urine analysis, organ weight, and histopathology.
870.3100 Oral Subchronic (rodent)	MRID No. 43511401 Mathur et al. (1986) Toxicological Evaluation of a Synthetic Detergent after Repeated Oral Ingestion in Rats. Industrial Toxicology Research Centre, Mahatma Ganghi Marg, Lucknow Study No. DDBSA JV-RP-013. Acceptable	LAS was administered as a commercial synthetic detergent solution at doses of 0, 50, 100, or 250 mg/kg/day in the feed for 10 weeks F Albino Rat (9/group) Purity: Not Reported	NOEL: < 50 mg/kg/d LOEL: 50 mg/kg/d based on alterations of several enzymes indicative of liver and kidney damage

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
870.3100 Oral Subchronic (rodent)	MRID No. 43498402 Oser et al. (1965) Toxicologic Studies with Branched and Linear Alkyl Benzene Sulfonates in the Rat. Toxicol. Appl. Pharmacol. 7: 819-825. (HERA) Acceptable Guideline	LAS and ABS were administered at dietary levels of 0, 50, or 250 mg/kg/day, adjusted for bw and fc, for 90 days FDRL Strain (Wistar-derived) Rat (15/sex/dose) Purity: Not Reported	NOEL: 50 mg/kg/d LEL: 250 mg/kg/d for increased absolute and relative liver weight in both sexes (21%) and increased relative cecal weight (21%) in males
870.3100 Oral Subchronic (rodent)	Watari et al. (1977) Ultrastructural Observations of the Protective Effect of Glycyrrhizin for Mouse Liver Injury Caused by Oral Administration of Detergent Ingredients (LAS), J. Clin. Electron. Microscopy (Nihon Rinsho Denshikenbikyo Kaishi) 10 (1-2): 121-139. **Open Literature**	Benzenesulfonic acid, C10-13- alkyl derivatives, sodium salt was administered in the drinking water for 6 months at 0 and 100 ppm with 2 months recovery (M: 0 and 17 mg/kg bw, F: 0 and 20 mg/kg bw) M/F ddy Mouse Purity: Not Reported	Liver effects were observed at the only dose tested (17-20 mg/kg/d), but they disappeared following the 2-month recovery period.
870.3100 Oral Subchronic (rodent)	Yoneyama & Hiraga (1977) Effect of Linear Alkylbenzene Sulfonate on Serum Lipid in Rats, J Ann Rep Tokyo Metrop Res Lab, Public Health 28(2): 109-111. (HERA) **Open Literature**	LAS was administered in the diet at concentrations of 180, 360, or 540 mg/kg bw/d for two and four weeks M Wistar Rat (5/group) Purity: 60% a.i.	Body weight gain was suppressed in the group receiving 540 mg/kg bw/d at four weeks, and the relative liver weight was increased at two weeks and thereafter in the groups receiving 360 mg/kg bw/d and 540 mg/kg bw/d. The levels of triglyceride and total lipids in the serum had decreased markedly at two weeks in all the experimental groups, and the levels of phospholipids and cholesterol in the serum had decreased significantly at two weeks in the groups given 360 and 540 mg/kg bw/d. These changes were less apparent at four weeks, but triglyceride, phospholipid, and cholesterol levels in serum were significantly decreased in the group given 540 mg/kg bw. Significant increases in triglyceride levels were seen in the liver after two weeks in the groups receiving 180 and 540 mg/kg bw/d, and in cholesterol levels in the group given 180 mg/kg bw.
870.3100 Oral Subchronic (rodent)	Yoneyama et al. (1978) Effects of LAS on Incorporation of Acetate-1-14C in Liver Lipids in Rats. J Ann Rep Tokyo Metrop Res Lab Public Health, 29 (2): 55-57. **Open Literature**	LAS was administered at a concentration of 200 mg/kg bw/d in the diet or in drinking water (560 mg/kg bw/d) for two weeks to determine the effect on the synthesis of lipids in the liver M Wistar Rat (5/group) Purity: Not Reported	Uptake of acetate-1-14C by lipids in the liver was increased in both groups; uptake of phospholipids and triglycerides tended to increase, and that of phospholipids increased significantly in rats given LAS in the diet.

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
870.3100 Oral Subchronic (rodent)	MRID No. 43498413 Heywood et al. (1978) Toxicology Studies of Linear Alkyl Sulfonate (LAS) in Rhesus Monkeys I. Simultaneous Oral and Subcutaneous Administration for 28 Days. Toxicol. Appl. Pharmacol. 11: 245-250. (HERA) Acceptable Guideline	LAS was given to four groups of three males and three females at doses of 30, 150, 300 mg/kg bw/day per gavage (po) and simultaneously with 0.1, 0.5, or 1.0 mg/kg bw/day subcutaneously (sc). Control groups were used. Rhesus Monkey (3/sex/dose), 18-36 months old Purity: Not Reported	At 300 (po) and 1.0 (sc) mg/kg bw/day, the monkeys vomited frequently and usually within 3 hours of administration. An increased frequency of loose or liquid faeces was recorded for animals receiving 150 (po) and 0.5 (sc) mg/kg bw/day. These effects are probably related to the inherent irritative effects of LAS rather than to its systemic toxicity. Fibrosis of the injection sites was found among the entire test group, the incidence and severity being dose related. Ophthalmoscopy, laboratory examination of blood and urine, organ weight analysis and histopathological investigation did not detect any further treatment-related responses. The LOAEL is 150 mg/kg bw/day (po) + 0.5 mg/kg bw/day (sc) based on an increase in liquid feces and the NOAEL is 30 mg/kg/d
870.3200 21-Day Dermal	Mathur et al. (1992) Effect of Dermal Exposure to LAS Detergent and HCH Pesticide in Guinea Pigs: Biochemical and Histopathologic Changes in Liver and Kidney. J Toxicol Cutan Ocular Toxicol, 11(1): 3-13. (WHO 1996) **Open Literature**	A solution of LAS in distilled water equivalent to 60 mg/kg bw was applied to a 4-cm2 area of clipped dorsal skin daily for 30 days 12 Guinea Pigs Purity: Not Reported	The activities of B-glucuronidase, gamma- glutamyl transpeptidase, 5-nucleotidase, and sorbitol dehydrogenase were increased in liver and kidney. Lipid peroxidation was increased in the kidney but not in liver, and the glutathione content was unchanged in both organs. Extensive fatty changes were found in hepatic lobules, with dilation of sinusoids; tubular lesions were found in the kidney, predominantly in the proximal and distal portions.
870.3200 21-Day Dermal	Tox Record No. 003441 Subchronic (28-day) Percutaneous Toxicity (Rabbit) of Compound: B0002.01, (Bio/dynamics Inc., Project No. 4717-77, March 17, 1978, submitted by Procter and Gambel Company, May 10, 1978). **Unacceptable** Core-Minimum Data	SDDBS (end use product Comet Cleanser) was applied to the skin of rabbits for 28 days at 200 mg/kg/d. The hair of each rabbit was clipped from its trunk, so as to expose approximately 25% of the total body surface area and the skin was abraded daily just prior to treatment. 20 M/F Albino New Zealand White Rabbits (5/sex/group) Purity: 10%	NOEL: > 200 mg/kg/d
870.3465 90-Day Inhalation	MRID No. 43498403 Coate et al. (1978) Respiratory Toxicity of Enzyme Detergent Dust. Toxicol. Appl. Pharmacol., 45: 477-496. Acceptable Non-Guideline	SDDBS was administered a SDDBS mixture at levels of 0, 100(detergent), and [.001, .01, 0.1 and 1 (enzyme)] together with [+0, 1, 10, and 100 (detergent)] mg/m3 for 6 hours daily, 5 days a week, for 6 months 12 groups of 5 M/4 F Cynomolgus Monkeys Purity: 13%	NOEL: 1 mg/m3 detergent dust combined with up to 0.1 mg/m3 enzyme dust. The detergent dust alone at 100 mg/m^3 caused gross signs of respiratory distress, pulmonary histopathological effects, and pulmonary function impairment indicative of constricted bronchioles. Exposure to 10 or 100 mg/m^3 together with 0.01 and 0.1 mg/m^3 enzyme dust produced the same effects along with weight loss and decreased weight gain.

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
Developmental Toxicity			
870.3700a Developmental Toxicity (rodent)	Daly et al. (1980) A Teratology Study of Topically Applied LAS in Rats, Fd. Cosmet. Toxicol. 18: 55-58. (HERA) **Open Literature**	LAS was applied to the skin on days 0 through 21 of gestation at doses of 20, 100, and 400 mg/kg bw/d Rat Purity: Not Reported	NOAEL (maternal): 20 mg/kg bw/d NOAEL (fetuses): 400 mg/kg bw/d Maternal toxicity: the dams treated with 400 mg/kg bw/day and 100 mg/kg bw/day showed inhibition of body weight gain and local skin effects that compromised the integrity of the skin and caused overt toxicity, like inhibition of the body weight gain. Teratogenicity: there were no findings indicative of effects of LAS on the foetal parameters evaluated. There were no indications of teratogenic or embryotoxic effects.
870.3700a Developmental Toxicity (rodent)	Endo et al. (1980) Studies of the Chronic Toxicity and Teratogenicity of Synthetic Surfactants, Ann. Rep. Tokyo Metrop. Res. Inst. Environ. Prot. (Tokyo Kogai Kenkyujo Nempo), 236-246. (HERA) **Open Literature**	LAS was administered in the drinking water at 0.1%, corresponding to 383 mg/kg bw/d for rats and up to 3030 mg/kg bw/d for rabits from day 6 to 15 (rats) and day 6 to 18 (rabbits) of pregnancy. F Rat and Rabbit Purity: Not Reported	NOAEL (maternal): 383 mg/kg bw/d (rat) LOAEL (maternal): 3030 mg/kg bw/d (rabbit) NOAEL (fetuses): 383 mg/kg bw/d (rat) LOAEL (fetuses): 3030 mg/kg bw/d (rabbit) The effect on the dams was a slight inhibition of body weight gain in the rabbits. The litter parameters of both species did not show any significant differences from those of the controls. Delayed ossification was observed in rabbits, but there was no increase in malformations in either the rabbits or the rats.
870.3700a Developmental Toxicity (rodent)	Imahori et al. (1976) Effects of LAS Applied Dermally to Pregnant Mice on the Pregnant Mice and their Fetuses, J. Jpn. J. Public Health (Nihon Koshueisei Zasshi) 23(2): 68-72. (HERA) **Open Literature**	LAS was applied daily at dermal doses of 15, 150, and 1500 mg/kg bw/d on days 6 through day 15 of pregnancy F Mouse Purity: Not Reported	NOAEL (maternal): 150 mg/kg bw/d NOAEL (fetuses): 1500 mg/kg bw/d The 1500 mg/kg bw/day group showed a clear decrease in the pregnancy rate (67.9%) when compared with a rate of 96.3% in the controls. However, there were no decreases in the litter size, and no changes in the litter parameters with the exception of a slight decrease in foetal body weight. There were no significant increases in the incidence of malformations in the foetuses.
870.3700a Developmental Toxicity (rodent)	**MRID No. 43498423** Masuda et al. (1974) Effects of LAS Applied Dermally to Pregnant Mice on the Development of their Fetuses. 15: 349-355. **Acceptable** Guideline	LAS was applied dermally at a level of 0.5 ml. The ICR-JCL strain received doses of 0, 0.85, 1.7, 2.55, and 3.4% solutions daily from days 1 to 13 of gestation and the ddY strain received doses of 0, 0.017, 0.17, and 1.7% solutions daily from days 2 to 14 of gestation. Mouse (ICR-JCL strain and ddY strain) Purity: Not Reported	NOEL (maternal and developmental toxicity - ddY): 1.7% (HDT) NOEL (maternal toxicity - ICR-JCL): 2.55% NOEL (developmental toxicity - ICR-JCL): 1.7% At 3.4% LAS, maternal body weight and the absolute weight of liver, kidney, spleen were significantly increased over control.. Pregnancy rates were significantly less (33.35) compared to controls (69%). The number of implantations, live fetuses, sex ratio, dead or resorbed fetuses, placenta weight and external malformations were comparable with control. Fetal body weights of 2.55% and 3.4% LAS-treated groups were significantly less than controls.

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
870.3700a Developmental Toxicity (rodent)	**MRID 43498424 and 43498425** Nomura, T et al. (1980) The Synthetic Surfactants AS and LAS Interrupt Pregnancy in Mice. Life Sciences, 26: 49-54. (HERA) Nomura, T. et al. (1987) Killing of Preimplantation Mouse Embryos by AS and LAS. Mutation Research 190: 25-29. (HERA) **Acceptable** Guideline	LAS (0.1 ml) was applied at a concentration of 20% to the dorsal skin of pregnant mice during the pre-implantation period twice a day from day 0 to day 3 of pregnancy Female ICR/Jcl Mouse, 9-10 weeks old Purity: 20%	Development was retarded and cleavage of eggs was interrupted. Significantly higher numbers of embryos were found to be deformed in the LAS group in comparison to controls, and most of these embryos were in the morula stage, whereas they were mostly in the last blastocyst stage in controls. Some dead, deformed, and growth-retarded embryos were observed in the treated group. Although the authors stated that these effects were not due to maternal toxicity since no maternal organs were affected, this statement is probably not correct in view of the high concentration of LAS and its irritation effects. A secondary effect due to maternal toxicity appears much more likely.
870.3700a Developmental Toxicity (rodent)	**MRID 43498426** Palmer et al. (1975) Assessment of the Teratogenic Potential of Surfactants, (Part I), Toxicology 3: 91-106. **Acceptable** Guideline	LAS was administered by gavage on days 6-15 of pregnancy in rats and mice and days 6-18 of pregnancy in rabbits at doses of 0.2, 2, 300, and 600 mg/kg bw/d 20 CD Rats, 20 CD-1 Mice, and 13 New Zealand White Rabbits Purity: 17%	NOAEL (rat - maternal): 300 mg/kg bw/d NOAEL (mouse - maternal): 2.0 mg/kg bw/d (However, there is a large difference between this dose and the next highest dose of 300 mg/kg bw/d, this study does not allow determination of a reliable maternal NOAEL for mice) NOAEL (rabbit - maternal): 2.0 mg/kg b/d (However, the study does not allow determination of reliable NOAELs, given the large difference between the maternal no-effects doses of 2 mg/kg bw/d and the maternal LOAEL dose (300 mg/kg bw/d) that is also the dose for which effects on litters could not be determined due to the high mortality rate in parent animals) NOAEL (rat - developmental): 300 mg/kg bw/d NOAEL (mouse - developmental): 2.0 mg/kg bw/d NOAEL (rabbit - developmental): 2.0 mg/kg bw/d NOAEL (rat - fetal): 600 mg/kg bw/d NOAEL (mouse - fetal): 300 mg/kg bw/d (Due to a high mortality rate of parent animals, no assessment was possible at 600 mg/kg bw/d) NOAEL (rabbit - fetal): could not be determined

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
870.3700a Developmental Toxicity (rodent)	**MRID 43511403** Palmer, et al. (1975) Assessment of the Teratogenic Potential of Surfactants, (Part III) - Dermal Application of LAS and Soap. Huntingdon Research Centre, Huntingdon, Great Britain. Study No. DDBSA JV-RP4-029. Toxicology 4: 171-181. **Acceptable** Guideline	LAS was administered percutaneously to shaved skin at solutions of 0.03%, 0.3%, and 3% during pregnancy on days 2-13 in mice, 2-15 in rats, and 1-16 in rabbits. Dosages employed were 0.5 ml/rat or mouse/day and 10 ml/rabbit/day CD-1 Mice (20/group), CD Rats (20/group), N2W Rabbits (13/group) Purity: 0.03%, 0.3%, and 3%	LOEL (maternal toxicity, mice): 0.3% (50 mg/kg/d) LOEL (maternal toxicity, rats): 3.0% (60 mg/kg/d) LOEL (maternal toxicity, rabbits): 0.3% (9.0 mg/kg/d) NOEL (maternal toxicity, mice): 0.03% (5.0 mg/kg/d) NOEL (maternal toxicity, rats): 0.3% (6.0 mg/kg/d) NOEL (maternal toxicity, rabbits): 0.03% ((0.9 mg/kg/d) LOEL (developmental toxicity): 0.3% (50 mg/kg/d) LOEL (developmental toxicity): 3.0% (60 mg/kg/d) LOEL (developmental toxicity): 3.0% (90 mg/kg/d) NOEL (developmental toxicity): 0.03% (5.0 mg/kg/d) NOEL (developmental toxicity): 0.3% (6.0 mg/kg/d) NOEL (developmental toxicity): 0.3% (9.0 mg/kg/d) Marked local skin reaction, irritability, weight loss and failure to maintain or establish pregnancy was evident in mice treated with LAS 3% soap, 3 or 30%: marked local reaction and weight loss also occurred in rabbits receiving LAS 3%. Moderate maternal toxicity was observed among mice treated with LAS, 0.3% and mild maternal toxicity in rats receiving LAS 3% or soap 30% and rabbits receiving LAS 0.3%. Effects on litter parameters were dose-dependent, causing marked maternal toxicity in mice, the principal higher fetal loss, reduction in viable litter size. LAS at 3% showed marked maternal toxicity in the rabbit The moderate maternal toxicity of LAS, 0.3% in the mouse correlated with a higher incidence of embryonic deaths and lower litter size but only the former differed significantly from the corresponding control value.
870.3700a Developmental Toxicity (rodent)	Sato et al. (1972) Studies on the Toxicity of Synthetic Detergents: (III), Examination of Teratogenic Effects of Alkylbenzene Sulfonates Spread on the Skin of Mice. Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 24: 441-448. (HERA) **Open Literature**	LAS was applied to the skin of female mice daily on days 0 through 13 of pregnancy with a single LAS dose of 110 mg/kg bw/d. Control group not specified. F Mouse Purity: Not Reported	NOAEL (maternal): 110 mg/kg bw/d No abnormalities were seen in the dam or foetuses.
870.3700a Developmental Toxicity (rodent)	Shiobara S., Imahori A. (1976) Effects of LAS Orally Administered to Pregnant Mice on the Pregnant Mice and their Fetuses. J.Food Hyg. Soc. Jpn. (Shokuhin Eiseigaku Zasshi) 17(4): 295-301. **Open Literature**	LAS was administered by gavage at doses of 10, 100, and 300 mg/kg bw/d at day 6 through 15 of gestation ICR-SLC Mouse (25-33/dose) Purity: Not Reported	LOAEL (maternal): 10 mg/kg bw/d NOAEL (fetuses): 300 mg/kg bw/d 1. Marked maternal and embryonic toxicities, such as maternal death, premature delivery, total litter loss and high fetal death rate, were observed at 300 mg/kg group. 2. Slight suppression of maternal body weight gain and slight body weight suppression of live fetuses were observed in each treated group. 3. External malformations such as cleft palate and exencephaly were observed sporadically both in the control and the treated groups. However, the incidence of these malformations was not significant, and considered to be within the spontaneous incidence of ICR mice.

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
870.3700a Developmental Toxicity (rodent)	Takahashi et al. (1975) Teratogenicity of Some Synthetic Detergent and LAS. Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 26(2): 67-78. (HERA) **Open Literature**	LAS doses of 40, and 400 mg/kg bw/d were administered daily from day 0 to day 6 of pregnancy or from day 7 to 13 of pregnancy by gavage Mouse (13-14/group) Purity: not reported	NOAEL (maternal): 40 mg/kg bw/d NOAEL (fetuses): 400 mg/kg bw/d At 400 mg/kg bw/day, the pregnancy rate was 46.2% compared to 92.9% in the controls. There was no increase in malformations. Although no information on maternal toxicity is available, it appears likely that maternal toxicity was present at the high dose group.
870.3700a Developmental Toxicity (rodent)	Tiba et al. (1976) Effects of LAS on Dam, Fetus, and Newborn Rat. J. Food Hyg. Soc. Jpn. (Shokuhin Eiseigaku Zassh) 17(1): 66-71. (HERA) **Open Literature**	LAS was administered in the diet at doses of 80 and 780 mg/kg bw/d from day 0 to 20 of gestation F Rat (16/dose) Purity: Not Reported	NOAEL (maternal): 780 mg/kg bw/d NOAEL (fetuses): 780 mg/kg bw/d At 780 mg/kg bw/day there were no abnormalities in the body weight gains of the dams, or in the occurrence and maintenance of pregnancy. The values of the litter parameters did not differ from those of the controls and there was no evidence of teratogenicity. The number of offsprings was rather low in the highest dose group, and the weaning rate of 78.3% was lower than the 100% rate observed in the controls. However, there were no abnormalities in body weight gain, organ weights or functions in the offsprings.
Reproduction Toxicity			
870.3800 Reproduction	**MRID 43498416** Buehler, E., Newmann, E., and King, W. (1971) Two Year Feeding and Reproduction Study in Rats with Linear Alkylbenzene Sulfonate (LAS). Tox. Appl. Pharm. 18: 83-91. (HERA) **Acceptable** Guideline	LAS was administered in the diet at doses of 0, 0.02, 0.1, and 0.5% , equivalent to (0, 10, 50, 250 mg/kg bw/day) for 84 days. Weanling Charles River CD Rat (20/sex/dose) Purity: 98.1%	NOAEL Parental: 250 mg/kg bw/day NOAEL Offspring: 50 mg/kg/d. The LOAEL of 250 mg/kg/day in the offspring is due to slight (non-significant) changes in hematology and histopathology and slight decrease in day 21 body weights.
870.3800 Reproduction	Endo et al. (1980) Studies of the Chronic Toxicity and Teratogenicity of Synthetic Surfactants, Ann. Rep. Tokyo Metrop. Res. Inst. Environ. Prot. (Tokyo Kogai Kenkyujo Nempo), 236-246. (HERA) **Open Literature**	LAS was administered at 70 mg/kg bw/day in the drinking water in a four generation rat study. M/F Wistar Rat Purity: Not Reported	NOAEL: > 70 mg/kg (only dose tested) No effects of LAS administration were observed
870.3800 Reproduction	Palmer et al. (1974) Effect of CLD Reproductive Function of Multiple Generations in the Rat, Report LFO10/731029, Unpublished results. (HERA) **Open Literature**	A commercial light duty liquid detergent of LAS (17%) and alkyl ethoxylate sulphate (7%) was continuously administered in the diet for three generations 60 days prior to mating at concentrations of 0, 40, 200, and 1000 mg/kg bw/d. The corresonding administration of LAS was of 0, 6.8, 34, and 170 mg/kg bw/d. Rat Purity: 17%	NOAEL: 170 mg/kg bw/d Among parental animals over the three generations there were no signs of adverse effects of treatment. Food consumption and bodyweight changes showed no consistent relationship to dosage. Necroscopy revealed no changes due to treatment. The mating performance, the pregnancy rate and the duration of gestation were unaffected. Among litter parameters, organ weight analysis, histopathology and skeletal staining of representative young from the F3b generation revealed no changes that could be conclusively related to treatment.

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
Chronic Toxicity			
870.4100a Chronic Toxicity (rodent)	Taniguchi et al. (1978) Results of Studies on Synthetic Detergents. Tokyo, Science and Technology Agency, Research and Coordination Bureau, pp. 18-54. (WHO 1996) **Open Literature**	LAS were applied to the dorsal skin of rats three times per week at doses of 1, 5, or 25 mg/rat for 24 months. Each application was washed from the skin with warm water after 24 hours. SLC-Wistar Rats Purity: 19.7% a.i.	Treatment had no effect on organ weights or histopathological appearance, and there was no evidence of toxicity or carcinogenicity.
870.3100 Chronic Toxicity (rodent)	Yoneyama et al. (1976) Subacute Toxicity of LAS, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health27(2): 105-112, See: IPCS, 1996. (HERA) **Open Literature**	LAS was administered in the diet at concentrations of 500 and 1000 mg/kg bw/d and in drinking water at concentrations of 100, 250, 600 mg/kg bw/d for males and 100, 250, 900 mg/kg bw/d for females for 9 months Mouse (8 or 9/sex/dose) Purity: Not Reported	LOAEL: 500 mg/kg bw/d (in diet) NOAEL: 250 mg/kg bw/d (in water) LAS in diet: in the mice given 500 mg/kg bw/day, body weight gain was not suppressed, but the weight of the liver increased in male and female mice. Enzymatic examinations revealed significant decreases in LDH of the liver and in acid phosphatase of the kidneys in the male mice. LAS in drinking water: body weight was depressed at the highest dose for male and females, increase in liver weight in females, significant decreases in renal Na,K-ATPase.
870.3100 Chronic Toxicity (rodent)	Yoneyama et al. (1976) Subacute Toxicity of LAS, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health27(2): 105-112, See: IPCS, 1996. (HERA) **Open Literature**	LAS was administered for 9 months in the drinking water at doses of 85, 145, 430 mg/kg bw/day M/F Wistar Rat Purity: Not Reported	NOAEL: 85 mg/kg bw/d LOAEL: 145 mg/kg bw/d Haematological examination revealed no significant changes in any experimental group and no organ weight changes were observed. Body weight gain was suppressed in the males of the highest dose group and also serum-biochemical and enzymatic parameters of the liver and kidney were affected. A significant decrease in renal Na,K-ATPase was seen in the group given 145 mg/kg bw/day of LAS.
870.4100a Chronic Toxicity (rodent)	Yoneyama et al. (1972) Studies on the Toxicity of Synthetic Detergents. (II) Subacute Toxicity of Linear and Branched Alkyl Benzene Sulfonates in Rats. Ann Rep Tokyo Metrop Res Lab Public Health, 24: 409-440. **Open Literature**	Technical-grade LAS was administered in the feed for 6 months at a concentration of 0, 0.07, 0.2, 0.6, or 1.8% Wistar SLC Strain Rat (10/sex/dose) Purity: Not Reported	NOAEL: 0.07% (40 mg/kg bw/day) At 1.8%, diarrhea, decrease in body weight gain and tissue damage in caecum liver and kidney were observed. The damage to the kidney was especially remarkable. At 0.6% of the LAS or ABS, the adverse effects observed were a slight decrease of body weight, increase of ceacum weight, increased activity of alkaline phosphatase, decrease of total protein in blood, and the tissue damage in the kidney. At 0.2% of the LAS or ABS, an increase of caecum weight and a slight damage to the kidney were observed.
Carcinogenicity			
870.4200a Oncogenicity (Rat)	**MRID 43498416** Buehler, E., Newmann, E., and King, W. (1971) Two Year Feeding and Reproduction Study in Rats with Linear Alkylbenzene Sulfonate (LAS). Tox. Appl. Pharm. 18: 83-91. (HERA) **Acceptable** Guideline	LAS was administered in the diet at doses of 10, 50, and 250 mg/kg/day for 2 years Weanling Charles River CD Rats (50/sex/group) Purity: Not Reported	Negative at 250 mg/kg/day (HDT)

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
870.4200a Oncogenicity (Rat)	Endo et al. (1980) Studies of the Chronic Toxicity and Teratogenicity of Synthetic Surfactants, Ann. Rep. Tokyo Metrop. Res. Inst. Environ. Prot. (Tokyo Kogai Kenkyujo Nempo), 236-246. (HERA) **Open Literature**	LAS was administered in the drinking water at the dose of 200 mg/kg bw/d 62 M/F Wistar Rat Purity: 38.74% a.i.	The administration of LAS had no effect on the intake of water, mortality, body weight gain, or general condition. In pathological examinations, looseness, atrophy, and fatty change of the hepatic cells in the liver were found in the experimental control group at 6 months, together with significant increases in GOT, GTP and bilirubin. In hematological examinations no effects due to LAS were observed.
870.4200a Oncogenicity (Rat)	Fujii et al. (1977) Pathological Examination of Rats Fed with LAS for their Lifespan, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 28(2): 85-108. (HERA) Yoneyama et al. (1977) Toxicity of LAS by Dietary Administration for Life-Span to Rats, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 28(2): 73-84. (HERA) **Open Literature**	LAS was administered in the feed at a concentration of 0.04, 0.16, and 0.60% for 24 months or lifespan Wistar Weanling Rat (15/sex/dose) Purity: Not Reported	Histopathological examination revealed that there was no evidence of a treatment-related effect on any tissue examined. Whereas a variety of tumors were observed in both linear alkylbenzene sulfonate treated and control rats, none was attributed for the exposure to linear alkylbenzene sulfonate. There was no relationship among the dosage groups, sex, type of tumor, or the site of occurrence.
870.4200a Oncogenicity (Rat)	**MRID 43498420** Takahasi et al. (1969) Effect of Alkylbenzenesulfonate as a Vehicle for 4-Nitroquinoline-1-Oxide on Gastric Carcinogenesis in Rats. GANN: 8, 241-261. **Acceptable** Guideline	For 560 days; Group I (79 rats): 1 mg 4-NQO and 80 mg SDDBS 2-3x per week for 18 weeks; Group I' (17 rats): same as Group 1, but fasted for 12 hours prior to dosing,; Group II (37 rats): 1 mg 4-NQO only; Group III (28 rats): 80 mg SDDBS only 97 M Wistar Rats Purity: Not Reported	In Groups I and I', the presence of SDDBS shifts the incidence of benign papillomas to malignant papillomas of the forestomach and the incidence of adenocarcinoma and sarcoma of the stomach were increased in comparison to Group II with only 4-NQO. The administration of SDDBS by itself has no effect on gastric tumors (Group III). The study authors concluded that the increased carcinogenicity produced by SDDBS was due to the better uptake of 4-NQO via LAS's surfactive/detersive effects on the protective mucous barrier which is normally found in the glandular stomach and other gastric compartments of the rat. The effect of SDDBS was physical rather than chemical in promoting the increased tumorigenicity.
870.4200a Oncogenicity (Rat)	**MRID 43498419** Takahasi et al. (1970) Effect of 4-Nitroquinoline-1-Oxide with Alkylbenzenesulfonate on Gastric Carcinogenesis in Rats. GANN: 61, 27-33. **Acceptable** Guideline	Rats were divided into three groups and gavaged with the following regimen for 560 days: Group I (37 rats) - 1 mg 4-NQO + 80 mg SDDBS + 20 mg ethanol in a 1 ml gavage for 18 weeks; Group II (13 rats) - 4-NQO and ethanol for 18 weeks; Group III (13 rats) - SDDBS + ethanol for 18 weeks 64 M Motoyama Strain Rat Purity: Not Reported	Survival: Mortality was 59% in Group I, 31% in Group II, and 23% in Group III Tumors: Group III - no gastric tumors; Group II - 9 benign papillomas of forestomach; Group I - 8 benign papillomas of forestomach, 2 malignant papillomas of forestomach, 1 hemangiosarcoma of forestomach. In glandular stomach, 2 adenocarcinomas, 1 hemangiosarcoma, 1 hemangioma, 5 squamous cell carcinomas, and 2 rats exhibited atrophic gastritis. The increased toxicity in Group I produced increased mortality and increased numbers of malignant tumors. The role of SDDBS in the tumorigenesis of 4-NQO was to promote increased absorption of 4-NQO through the forestomach and glandular stomach.

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
870.4200a Oncogenicity (Rat)	**MRID 43498421, -22** Takahasi et al. (1973) Carcinogenic Effect of N-Methyl-N'-Nitro-N-Nitrosoguanidine with Various Kinds of Surfactant in the Glandular Stomach of Rats. **Acceptable** Guideline	SDDBS was administered to 5 groups of rats: (I) 13 rats received 0.1g of MNNG + 4000 mg Tween 60 per L of drinking water for 36 weeks; (II) 16 rats received 0.1 g MNNG + 2000 mg nonipol per L of drinking water for 36 weeks; (III) 15 rats received 0.1 g of MNNG + 1000 mg branched ("hard") SDDBS per L of drinking water for 63 weeks; (IV) 10 rats received 0.1 g MNNG + 1000 mg of linear ("soft") SDDBS per L of drinking water for 63 weeks; (V) 14 rats received o.1 g MNNG per L of drinking water for 63 weeks M Wistar Rats Purity: Not Reported	Survivial was 100% in Groups I, III, and IV, and 93% and 94% in Groups V and II, respectively. The Group I and II rats had more tumors than the controls (Group V), whereas, the rats in Group III, ("hard" SDDBS, and particularly, Group IV (linear "soft" SDDBS) had the fewest tumors in comparison to controls.
870.4200a Oncogenicity (Rat)	Tiba S (1972) Studies on the Acute and Chronic Toxicity of LAS, J. Food Hyg. Soc. Jpn. (Shokuhin Eiseigaku Zasshi) 13(6): 509-516. (HERA) **Open Literature**	LAS was administered in drinking water for 2 years at doses of 20, 100, and 200 mg/kg bw/d M Wistar Rat (20/group) Purity: Not Reported	There were no changes due to the administration of LAS in regard to growth, mortality, the weight of major organs, or histopathological findings
Mutagenicity			
870.5100 Bacterial reverse mutation test	Huls, Report No. AM-93/12, Unpublished data, 1993. (As cited in HERA-2013) **Open Literature**	LAS was tested at 8-5000 ug/plate with and without metabolic activation. The cytotoxicity concentration was >5000 ug/plate. Salmonella typhimurium, strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538 Purity: Not Reported	Negative results
870.5100 Bacterial reverse mutation test	**MRID 43498429** Inoue et al. (1980) Studies of In Vitro Cell Transformation and Mutagenicity by Surfactants and other Compounds, Food. Cosmet. Toxicol 18: 289-296. (HERA) **Acceptable** Guideline	SDDBS was tested at cytotoxic levels or limit concentrations of 2,000-30,000 ug/plate for 2 days (Salmonella) or 8 days (SHE) Strain: Salmonella typhimurium - TA 98 and TA 100 cells and Embryonic Syrian Golden Hamster cells (SHE) Purity: Not Reported	Negative (both with and without S-9 metabolic activation)

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
870.5100 Bacterial reverse mutation test	Sunakawa et al. (1981) Studies on the Mutagenicity of Surfactants Following Activation with Various Liver Homogenates (S-9) and Mutagenicity in the Presence of Norharman, Hyg. Chem. (Eisei Kagaku) 27(4): 204-211, See: WHO, 1996. **Open Literature**	LAS was tested at up to 500 ug/plate Salmonella typhimurium Purity: Not Reported	Negative Results
870.5300 In Vitro mammalian cell gene mutation test	Inoue, K. et al. (1977) Osaka-furitsu Koshu Eisei Kenkyusho Kenkyu Hokoku, Shokuhin Eisei Hen 8: 25-8. (HERA) **Open Literature**	Sodium alkylbenzenesulfonate was added to culture at 62.5 ug/ml and 125 ug/l Hamster Lung Cell Purity: Not Reported	At 62.5 ug/ml: induced cell mutation, no effect on sister chromatid exchange At 125 ug/ml: destroyed the cells completely
870.5300 In Vitro cell transformation	**MRID No. 43498427** K. Inoue et al (1980) Food Cosmetic Toxicol. 18:289-296 **Acceptable** **Open Literature,**	Duplicate primary cultures of embryonic SHE and Salmonella typhimurium strain TA 98 and TA 100 cells were exposed to SDDBS and positive and negative controls for 8 days.	SDDBS was negative for transformation up to cytotoxic levels and did not induce mutation in either strains of Salmonalla when allplied up to cytotoxic levels or limit concentration of 2000-3000 ug/plate. SDDBS was tested negative at cytotoxic levels or limit concentrations (both with and without S-9 metabolic activation) of 2,000-30,000 ug/plate for 2 days (Salmonella) or 8 days (SHE)
870.5385 Mammalian bone marrow chomosomal aberration test	Inoue K, et al. (1979) In vivo Cytogenetic Tests of Some Synthetic Detergents in Mice, Ann. Rep. Osaka Perfect. Inst. Public Health 8: 17-24 (in Japanese), See: IPCS, 1996. (HERA) **Open Literature**	LAS was administered at doses of 200, 400, and 800 mg/kg bw/d by gavage for 1 and 5 days M Mouse Purity: Not Reported	There was no significant difference in the incidence of chromosomal aberrations between any of the groups
870.5385 Mammalian bone marrow chomosomal aberration test	Inoue, K. et al. (1977) In Vivo Cytogenetic Tests of Some Synthetic Detergents in Mice. Ann Rep Osaka Prefect Inst Public Health, 8: 17-24. (HERA) **Open Literature**	LAS was administered at a dose of 200, 400, and 800 mg/kg bw/d by gavage for 5 days. One commercial preparation containing 19.0% LAS was also given, at a dose of 800, 1600, or 3200 mg/kg bw, and another containing 17.1% LAS at a dose of 1000, 2000, or 4000 mg/kg bw once only by gavage. M ICR:JCL Mouse Purity: Not Reported	There was no significant difference between any of the groups given LAS and the negative control group in the incidence of chromosomal aberrations

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
870.5385 Mammalian bone marrow chomosomal aberration test	**MRID 43498428** J. Hope (1977) Absence of Chromosome Damage in the Bone Marrow of Rats Fed Detergent Actives for 90 Days. Mutation Research, 56: 47-50. **Acceptable** Guideline	SDDBS was administered in the diet for 90 days at 0, 280, and 565 mg/kg bw/d Colworth/Wistar Weanling Rat (6/sex/dose) Purity: Not Reported	All test preparations were negative for increased chromosomal damage over controls.
870.5385 Mammalian bone marrow chomosomal aberration test	Masabuchi et al. (1976) Cytogenetic Studies and Dominant Lethal Tests with Long Term Administration of Butylated Hydroxytoluene (BHT) and LAS in Mice and Rats, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 27(2): 100-104. (HERA) **Open Literature**	LAS was administered in the diet for 9 months at a dose of 0.9% in rats (450 mg/kg bw/d) and in mice (1170 mg/kg bw/d) Male Rat and Male Mouse Purity: Not Reported	There were no significant differences in the incidences of chromosomal aberrations between the experimental and control groups
870.5395 Mammalian erthrocyte micronucleus test	Kishi et al. (1984) Effects of Surfactants on Bone Marrow Cells, Bull. Kanagawa Public Health Lab. 14: 57-58. (HERA) **Open Literature**	LAS was administered as a single intraperitoneal injection at a dose of 100 mg/kg bw 3 M ddY Mice Purity: Not Reported	There were no differences in the incidences of polychromatic erythrocytes with micronuclei in the bone marrow cells between the treated group and the control group
870.5395 Mammalian erthrocyte micronucleus test	Koizumi et al. (1985) Implantation Disturbance Studies with LAS in Mice, Arch. Environ. Contam. Toxicol. 14: 73-81. (HERA) **Open Literature**	LAS were administered as a single oral dose of 2 mg to pregnant mice on day 3 of gestation. On day 17 of gestation, each animal received a subcutaneous dose of 1, 2, or 10 mg and were killed 24 h later. Pregnant ICR Mice Purity: Not Reported	There was no difference among treated groups in the incidence of polychromatic erythrocytes with micronuclei in maternal bone marrow or fetal liver or blood. No mutagenetic effect was found in any of the groups.
870.5450 Rodent dominant lethal assay	Masubuchi MA et al. (1976) Cytogenetic Studies and Dominant Lethal Tests with Long Term Administration of Butylated Hydroxytoluene (BHT) and Linear Alkylbenzene Sulfonate (LAS) in Mice and Rats. Ann Rep Tokyo Metrop Res Lab Public Heath, 27(2): 100-104. (HERA) **Open Literature**	A diet containing 0.6% LAS at 300 mg/kg bw/d was administered to mice for 9 months. Each of the male mice was then mated with two female mice that had not been given LAS, and 11 of the 14 females became pregnant. The pregnant mice were laparotomized on day 13 of gestation 7 M ICR:JCL Mice Purity: Not Reported	There were no significant differences in fertility, mortality of ova and embryos, the number of surviving fetuses, or the index of dominant lethal induction (Roehrborn) between the experimental and control groups.

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
Metabolism			
870.7485 General Metabolism	**MRID 43498410** Creswell et al. (1978) Toxicology Studies of Linear Alkylbenzene Sulfonate (LAS) in Rhesus Monkeys II. The Disposition of C14-LAS After Oral or Subcutaneous Administration. Toxicology, 11: 5-17. **Acceptable** Guideline	Single oral doses of C14-LAS (SDDBS; 25 ucuries) were administered to each animal, following 2-3 weeks between dose levels, at levels of 30, 150, and 300 mg/kg. Following 2-3 weeks after the last single oral dose, each monkey received 7 consecutive daily oral doses of 30 mg/kg/d of C14-LAS. 2 M/2 F Rhesus Monkeys Purity: Not Reported	After single 30 mg/kg doses the radioactivity was rapidly excreted, mostly during the first 24 hours. Feces and urine contained 23.1% and 71.2%, respectively, in the first 5 days after oral dosing. Plasma concentrations were comparable after the oral doses and averaged 34, 41, and 36 u/ml, respectively. Peak plasma concentrations increased proportional to the dose and were 0.16, 0.72, 1.13 u/ml, respectively. In urine samples analyzed for metabolites, there was no unchanged SDDBS and the 5 metabolites detected were polar, but were not sulphate or glucuronide conjugates.
870.7485 General Metabolism	Lay JP, et al. (1983) Toxicol. Letters 17 (1-2): 187-192 **Open Literature**	(14)C-labeled sodium dodecylbenzenesulfonate was administered daily in the diet at a concentration of 1.4 mg/kg for 5 weeks M Rat Purity: not reported	From a total uptake of 1.213 + or - 0.08 mg/animal of DBS, 81.8% was excreted during the dosing period: 52.4% in feces and 29.4% in urine. Low levels of (14)C-DBS-derived residues were detected in all tissues analyzed on day 35 of the study. Following 1 week on a normal diet, only 7.8% of the nominally stored amount of (14)C was found in the excreta.
870.7485 General Metabolism	Sunakawa et al. (1979) Yakuzaigaku 39 (2): 59-68 **Open Literature**	Sodium-para-dodecylbenzenesulfonate Rat Purity: Not Reported	Blood levels were max at 2 hr, negligible at 48 hr Excretion rate of radioactive label was 99.4% after 48 hr
870.7485 General Metabolism	The Royal Society of Chemistry. (1981) Foreign Compound Metabolism in Mammals. Volume 6: A Review of the Literature Published during 1978 and 1979. London: The Royal Society of Chemistry, p.354. **Open Literature**	(35)S-labeled sodium dodecylbenzenesulfonate was administered as a single oral dose Rat Purity: Not Reported	Rats excreted 64% and 24% of the dose in urine and feces, respectively
870.7485 General Metabolism	The Royal Society of Chemistry. (1981) Foreign Compound Metabolism in Mammals. Volume 6: A Review of the Literature Published during 1978 and 1979. London: The Royal Society of Chemistry, p.354.	Repeated doses of (14)C-labeled alkylbenzenesulfonate were orally administered Rhesus Monkey Purity: Not Reported	Radioactivity did not accumulate in the tissues
870.7485 General Metabolism	**MRID 43498431** W. Michael (1968) Metabolism of Linear Alkylate Sulfonate and Alkyl Benzene Sulfonate. Toxicol. Appl. Pharmacol. 12: 473-485. **Acceptable** Guideline	LAS-S35 was administered orally to fasted rats at doses of 0.6, 1.2, 8, and 40 mg Charles River CD M Rat Purity: Not Reported	The rate and distribution of the excreted dose was independent of concentration. Similar levels of radioactivity were found in urine and feces and within 3 days, 85.2% - 96.6% of the label was recovered. In the high dose rats, no detectable radioactivity was found in the carcasses after 3 days. Following methylation, one urinary metabolite was identified as 4-(4'-methylsulfophenyl) pentanoate. LAS-S35 in the feces remained unmetabolized.

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
Special Studies			
870.3700a Developmental Toxicity (rodent)	Koizumi et al. (1985) Implantation Disturbance Studies with LAS in Mice, Arch. Environ. Contam. Toxicol. 14: 73-81. (HERA) **Open Literature**	LAS was administered as a single oral dose of 350 mg/kg bw on day 3 of gestation Pregnant ICR Mice Purity: Not Reported	LAS was not detected in the uterus
Other	Inoue K, T Sunakawa. (1979) Mutagenicity Tests of Surfactants, Jpn. Fragr. J. 38: 67-75, (in Japanese), See: IPCS, 1996. (HERA) **Open Literature**	LAS tested in a recombination assay at concentrations up to 50 ug/plate Bacillus subtilis Purity: 99.5%	Negative results with and without metabolic activation
Other	Fujise, H. and Aoyama, M. (1984) Nagoya Med J, 28 (3-4): 211-5 **Open Literature**	The proliferation rate of the connective tissue was examined by measuring the activity of proline hydroxylase. The dorsal neck skin of rats was coated with sodium laurylbenzenesulfonate for 4 days, and on the 5th day, the enzyme activity in the skin was measured. Rat Purity: Not Reported	The proline hydroxylase in the part of the skin coated with the irritants showed clearly higher activity than normal skin, although it was still lower than the injured skin region prepared as a positive control.
Other	**MRID 43498430 and 43498408** Kimura et al. (1982) Mechanisms of Toxicities of Some Detergents Added to a Diet and the Ameliorating Effects of Dietary Fiber in the Rat. J. Nutrit. Science and Vitaminology, 28: 483-489. Kimura et al. (1982) Toxicity for Detergent Feeding and Effect of the Concurrent Feeding of Dietary Fiber in the Rat. Nutrition Reports International, 26(2): 271-279. **Acceptable** Guideline	Ringer's bicarbonate (containing sodium lauryl benzene sulfonate) at 0.5 ml/min was used to perfuse a 10 cm length of jejunal segment for 150 minutes; equilibrated for 30 minutes and then the perfusates were collected in 30 minute aliqouts for 120 minutes M Wistar Rat Purity: 0.5%	Alkaline phosphatase was released by an increase of 15-fold in comparison to Ringer's alone (controls without added sodium lauryl benzene sulfonate) and 3-7 times greater than other surfactants tested in Ringer's. The authors conclude that SDDBS has an exfoliative effect on the intestinal brush border
Other	Oba et al. (1968) Biochemical Studies of n-alpha-olefin sulfonates: (II) Acute Toxicity, Skin and Eye Irritation, and Some Other Physiological Properties. J Jpn Oil Chem Soc, 17 (11): 628-634. (EHC 169) **Open Literature**	Solutions of various concentrations of LAS were mixed with red blood cells from rabbits at room temperature for 3 hours Rabbit Red Blood Cell Purity: Not Reported	The 50% haemolytic concentration of LAS was 9 mg/litre

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
Other	Samejima Y (1991) Effects of Synthetic Surfactants and Natural Soap on the Development of Mouse Embryos In Vitro and the Fertilizing Capacity of Mouse and Human Sperm. J Osaka Univ Med Sch, 3 (12): 675-682. (EHC 169) **Open Literature**	Eggs were fertilized in vitro and incubated in culture medium containing LAS at concentrations between 0.015 and 0.03%. F B6C3F1 Mouse Egg Purity: Not Reported	Concentrations of LAS less than 0.025%: Eggs exposed for 1 hr, washed, and then cultured for 5 days developed normally to the blastocyst stage Concentrations of LAS higher than 0.03%: The eggs did not develop beyond the one-cell stage With continuous exposure to LAS for five days, a concentration of 0.01% slightly impaired development to the blastocyst stage, and 0.025% prevented development to the one-cell stage
Other	Takahashi et al. (1974) Inhibition of Thrombin by Linear Alkylbenzene Sulfonate (LAS). Ann Rep Tokyo Metrop Res Lab Public Health, 25: 637-645. (HERA) **Open Literature**	Purified LAS at various concentrations were added to 10 ul of plasma from rats and prothrombin time was determined M Rat Purity: Not Reported	Prothrombin time was prolonged; the 50% inhibitory concentration was about 0.6 mmol/litre. When LAS at various concentrations were added to a mixture of 1% fibrinogen and thrombin, the time of formation of a mass of fibrin was prolonged by inhibition of thrombin activity. The 50% inhibitory concentration was about 0.05 mmol/litre.
Other	Yanagisawa et al. (1964) Biochemical Studies of Dodecylbenzene Sulfonates; Differences Between Soft and Hard Detergents. Jpn. J Public Health, 11(13): 859-864. (EHC 169) **Open Literature**	The haemolytic action of LAS was investigated by mixing red blood cells from rabbits with solutions of LAS at concentrations of 1-1000 mg/litre at 38 C for 30 min Rabbit Red Blood Cell Purity: Not Reported	Haemolysis occurred at concentrations >= 5 mg/litre.

Table 3. Summary of Toxicological Dose and Endpoints for Alkylbenzene Sulfonates:

Exposure Scenario	Dose Used in Risk Assessment, UF	Special FQPA SF*, endpoint and Level of Concern for Risk Assessment	Study and Toxicological Effects
Acute Dietary (All populations)	No endpoint was selected. No effects are attributable to a single dose.		
Chronic Dietary (All populations)	Systemic/ Reproductive NOAEL= 50 mg/kg/day UF = 100 **Chronic RfD** = 0.5 mg/kg/day	FQPA SF = 1X **cPAD** = chronic RfD FQPA SF = 0.5 mg/kg/day	Systemic/Reproductive NOAEL= 50 mg/kg/day; LOAEL = 250 mg/kg/day based on decreased Day 21 female pup body weight (Buehler, E. et al. 1971. Tox. Appl. Pharmacol. 18:83-91) **plus** NOAEL = 85 mg/kg/day; LOAEL= 145 mg/kg/day from 9 month drinking water rat study based on decreased body weight gain, and serum/ biochemical and enzymatic changes in the liver and kidney (Yoneyama et al. 1976 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 27(2):105-112) **plus** NOAEL= 40 mg/kg/day (0.07%) LOAEL= 114 mg/kg/day (0.2%) based on increased caecum weight and slight kidney damage in a 6 month rat dietary study (Yoneyama et al 1972 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 24:409-440)
Short-Term Incidental Oral (1-30 days)	Oral NOAEL = 50 mg/kg/day	**Residential** LOC for MOE < 100	Systemic/Reproductive NOAEL= 50 mg/kg/day; LOAEL = 250 mg/kg/day based on decreased Day 21 female pup body weight (Buehler, E. et al. 1971. Tox. Appl. Pharmacol. 18:83-91) **plus** NOAEL = 85 mg/kg/day; LOAEL= 145 mg/kg/day from 9 month drinking water rat study based on decreased body weight gain, and serum/ biochemical and enzymatic changes in the liver and kidney (Yoneyama et al. 1976 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 27(2):105-112) **plus** NOAEL= 40 mg/kg/day (0.07%); LOAEL= 114 mg/kg/day (0.2%) based on increased caecum weight and slight kidney damage in a 6 month rat dietary study (Yoneyama et al 1972 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 24:409-440)

Table 3. Summary of Toxicological Dose and Endpoints for Alkylbenzene Sulfonates:

Exposure Scenario	Dose Used in Risk Assessment, UF	Special FQPA SF*, endpoint and Level of Concern for Risk Assessment	Study and Toxicological Effects
Short-, intermediate- and Long-Term Inhalation (1 to 30 days, 1-6 months, >6 months)	Inhalation study NOAEL= 1mg/m^3 detergent dust combined with up to 0.1 mg/m^3 enzyme dust Equivalent to approximately 0.14 mg/kg/day (a) (inhalation absorption rate = 100%) purity= 13% active ingredient	**Residential** LOC for MOE < 100 **Occupational** LOC for MOE < 100	Subchronic Inhalation Monkey Study LOAEL = 10 mg/m^3 detergent combined with 0.1 mg/m^3 enzyme dust based on weight loss and decreased weight gain (W. Coates, et al 1978. Tox. Appl. Pharmacol. 45: 477-496) This air concentration is equivalent to approximately 1.4 mg/kg/day (a)
Dermal Endpoint	Quantification of dermal risk is not required since: 1) the alkylbenzene sulfonates are surfactants that are dermal irritants at concentrations generally greater than 20% solution (WHO 1996). Thus, dermal exposure would be self-limiting to preclude dermal irritation. Most pesticide formulations have less than 5% alkylbenzene sulfonates as an inert ingredient, with the vast majority of household products containing approximately 2%. Additionally, the requirement of the dermal toxicity studies with the end-use product will determine whether personal protective clothing would be necessary to protect against irritation during product use; 2) no systemic toxicity was seen following repeated dermal applications to rabbits at 200 mg/kg/day (with an end use product); 3) no developmental toxicity concerns were seen following repeated dermal applications to pregnant mice, rats or rabbits (developmental effects were seen either in the presence of maternal toxicity or at doses higher than those that caused maternal toxicity); and 4) there is no residential exposure to alkylbenzene sulfonates as an active ingredient, however, residential exposure from its use as an inert ingredient in pesticide formulations is expected to be of an intermittent nature (i.e, no continuous, constant contact, multi-day exposure) from household products.		
Cancer (oral, dermal, inhalation)	No evidence of carcinogenicity in reported studies in rats done before 1980 GLPs		

UF = uncertainty factor, FQPA SF = Special FQPA safety factor, NOAEL = no observed adverse effect level, LOAEL = lowest observed adverse effect level, PAD = population adjusted dose (a = acute, c = chronic) RfD = reference dose, MOE = margin of exposure, LOC = level of concern, NA = Not Applicable

(a) Equation used to convert inhalation air concentration to a dose= mg/L* absorption*respiratory volume (L/hr)*duration (hrs) * activity factor / body weight. Thus, 0.001 mg/L * 1*67.94 L/hr (based on default respiratory volumes for a New Zealand Rabbit which is used as a surrogate for a cynomolgus monkey) * 6 hrs * 1 / 2.98 kg (body weight for New Zealand Rabbit used as a surrogate for cynomolgus monkey, study reports monkey body weight ranges from 1.6 to 3.7 kg).

Table 4. Tolerance Exemptions for Food Contact Sanitizer Uses (Active Uses):

Tolerance Exemption Expression/ Chemical Name	CAS No.	PC Code	40 CFR Part 180.	Use Pattern (Pesticidal)
Benzenesulfonic acid, dodecyl-	27176-87-0	098002	940 (b)	food contact sanitizing solutions for dairy processing equipment, and food processing equipment and utensils; end use concentration not to exceed 5.5 ppm
			940 (c)	food contact sanitizing solutions for food processing equipment and utensils; end use concentration not to exceed 400 ppm
Benzenesulfonic acid dodecyl-, sodium salt	25155-30-0	079010	940 (c)	food contact sanitizing solutions for food processing equipment and utensils; end use concentration not to exceed 430 ppm

Table 5. Summary of Dietary Exposure and Risk for Alkylbenzene Sulfonates Pesticidal Active Uses:

Use	Population Subgroup	Chronic Dietary	
		Dietary Exposure (mg/kg/day)[a]	% cPAD[b]
Food Service Industry (treated surfaces, utensils, glassware, etc.)	adult male	0.023	4.6
	females (13-50 years)	0.027	5.4
	infants/children	0.053	10.6
Food Processing Industry (Food Processing Equipment)	adult male	0.00043	0.086
	females (13-50 years)	0.0005	0.1
	infants/children	0.001	0.2
Total Food Contact Surface Sanitizing Uses	adult male	0.023	4.6
	females (13-50 years)	0.027	5.4
	infants/children	0.054	10.8
Fruit and Vegetable Wash	U.S population	0.0979	19.6
	children 1-2 yrs	0.3558	71.2
	children 3-5 yrs	0.2573	51.5

NA=not applicable
[a] chronic exposure analysis based on body weights of 70 kg, 60 kg, and 15 kg for adult males, females and children, respectively.
[b] %PAD = dietary exposure (mg/kg/day) / cPAD, where cPAD=0.5 mg/kg/day for all populations.

Table 6. Tolerance Exemptions for Inert Use:		
Tolerance Exemption Expression	**40 CFR □ 180. (a)**	**Use Pattern**
Alkyl (C8-C24) benzenesulfonic acid and its ammonium, calcium, magnesium, potassium , sodium and zinc salts	910	Surfactants, related adjuvants of surfactants
	930	Surfactants, emulsifier, related adjuvants of surfactants
(a) Residues listed in 40 CFR §180.910 are exempted from the requirement of a tolerance when used as inert ingredients in pesticide formulations when applied to growing crops or to raw agricultural commodities after harvest (i.e., pre- and post-harvest). Residues listed in 40 CFR §180.930 are exempted from the requirement of a tolerance when used as inert ingredients in pesticide formulations when applied to animals only.		

Table 7. Summary of Dietary Exposure and Risk for Alkylbenzene Sulfonates as Inert Ingredients:		
Population Subgroup	**Chronic Dietary**	
	Dietary Exposure (mg/kg/day)	**% cPAD [a]**
U.S. population	0.120	24
females (13-50 years)	0.087	17
children 1-2 yrs	0.422	84
children 3-5 yrs	0.310	62
[a] %PAD = dietary exposure (mg/kg/day) ÷ cPAD, where cPAD=0.5 mg/kg/day for all populations.		

EPA SUMMARY TABLES OF AVAILABLE ENVIRONMENTAL TOXICITY STUDIES AND RELATED INFORMATION[18]

Table 8. Acute Toxicity of Alkylbenzene Sulfonates:

Species	Chemical, % active ingredient (ai)	Endpoint	Toxicity Category (TGAI)	Satisfies Guidelines/Comments	Reference (MRID)
Birds					
Northern bobwhite *(Colinus virginianus)*	87.6%Carbon chain not identified. (Nacconal 90G used)	LD_{50} > 1382 mg/kg NOEL = 279 mg/kg	Slightly toxic	Yes. Acceptable. 14 day test	41143901
Freshwater Fish					
Fathead Minnow (*Pimephales promelas*)	14.0% (Carbon chain not identified.)	96hr LC50 = 3.4 mg/L	Moderately toxic	Yes. Supplemental study.	44260002
Rainbow trout *Oncorhynchus mykiss*)	65.0% C11, C12	96 hr LC50 = 1.68 mg/L	Moderately toxic	Yes. Supplemental study.	44260009
Freshwater Invertebrates					
Waterflea *(Daphnia magna)*	Not reported.	48-hr. EC_{50} = LAS-C10 = 29.5 mg/L, LAS-C12 = 6.84 mg/L, LAS-C14 = 0.80 mg/L, LAS-C16 = 0.20 mg/L.	C-12 = Moderately toxic	Yes. Supplemental study.	47025025
Green Algae					
Selenastrum capricornutum	Not Reported. (Carbon chain not identified.)	96 hr. EC50 = 70.27 ppm	Slightly toxic	No. Supplemental.	42439803

[18] Tables 1&2 extracted from the RED for Alkylbenzene sulfonates (EPA 2006a). Tables 3 through 8 extracted from Alkylbenzene Sulfonates (ABS) Risk Assessment for the Reregistration Eligibility Decision (RED) Document (EPA 2006b).

10. SDS, SAFETY INFORMATION

SDS, Safety Information:

Safety Data Sheets for Antimicrobial Fruit & Vegetable Treatment and SDBS are as follows.

SAFETY DATA SHEET

ANTIMICROBIAL FRUIT & VEGETABLE TREATMENT

SECTION 1. PRODUCT AND COMPANY IDENTIFICATION

Product name	:	ANTIMICROBIAL FRUIT & VEGETABLE TREATMENT
Other means of identification	:	not applicable
Recommended use	:	Sanitizer
Restrictions on use	:	Reserved for industrial and professional use.
Product dilution information	:	0.58 % - 0.78 %
Company	:	Ecolab Inc. 370 N. Wabasha Street St. Paul, Minnesota USA 55102 1-800-352-5326
Emergency telephone	:	1-800-328-0026 (US/Canada), 1-651-222-5352 (outside US)
Issuing date	:	06/04/2014

SECTION 2. HAZARDS IDENTIFICATION

GHS Classification

Product AS SOLD

Acute toxicity (Dermal)	:	Category 4
Eye irritation	:	Category 2A
Skin sensitization	:	Category 1

Product AT USE DILUTION
Not a hazardous substance or mixture.

GHS Label element

Product AS SOLD
Hazard pictograms :

Signal Word : Warning

Hazard Statements : Harmful in contact with skin.
May cause an allergic skin reaction.
Causes serious eye irritation.

Precautionary Statements : **Prevention:**
Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray. Wash skin thoroughly after handling. Contaminated work clothing should not be allowed out of the workplace. Wear eye protection/ face protection. Warning! Do not use together with other products. May release dangerous gases (chlorine).
Response:
IF ON SKIN: Wash with plenty of soap and water. IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Call a POISON CENTER or doctor/ physician if you feel unwell. If skin irritation or rash occurs: Get

medical advice/ attention. If eye irritation persists: Get medical advice/ attention. Wash contaminated clothing before reuse.
Disposal:
Dispose of contents/ container to an approved waste disposal plant.

Product AT USE DILUTION
Precautionary Statements : **Prevention:**
Wash hands thoroughly after handling.
Response:
Get medical advice/ attention if you feel unwell.
Storage:
Store in accordance with local regulations.

Other hazards : None known.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Product AS SOLD
Pure substance/mixture : Mixture

Chemical Name	CAS-No.	Concentration (%)
Dodecylbenzenesulfonic acid, sodium salt	25155-30-0	1.23
Lactic acid	79-33-4	17.29
Sodium hydrogensulfate	7681-38-1	5 - 10
oxirane, methyl-, polymer with oxirane	9003-11-6	0.1 - 1

Product AT USE DILUTION

No hazardous ingredients

SECTION 4. FIRST AID MEASURES

Product AS SOLD
In case of eye contact : Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical attention.

In case of skin contact : Wash off immediately with plenty of water for at least 15 minutes. Use a mild soap if available. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

If swallowed : Rinse mouth. Get medical attention if symptoms occur.

If inhaled : Get medical attention if symptoms occur.

Protection of first-aiders : If potential for exposure exists refer to Section 8 for specific personal protective equipment.

Notes to physician : Treat symptomatically.

Product AT USE DILUTION
In case of eye contact : Rinse with plenty of water.

In case of skin contact : Rinse with plenty of water.

If swallowed : Rinse mouth. Get medical attention if symptoms occur.

If inhaled : Get medical attention if symptoms occur.

See toxicological information (Section 11)

SECTION 5. FIRE-FIGHTING MEASURES

Product AS SOLD

Suitable extinguishing media	:	Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.
Unsuitable extinguishing media	:	None known.
Specific hazards during fire fighting	:	Not flammable or combustible.
Hazardous combustion products	:	Decomposition products may include the following materials: Carbon oxides nitrogen oxides (NOx) Sulfur oxides Oxides of phosphorus
Special protective equipment for fire-fighters	:	Use personal protective equipment.
Specific extinguishing methods	:	Fire residues and contaminated fire extinguishing water must be disposed of in accordance with local regulations. In the event of fire and/or explosion do not breathe fumes.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Product AS SOLD

Personal precautions, protective equipment and emergency procedures	:	Ensure clean-up is conducted by trained personnel only. Refer to protective measures listed in sections 7 and 8.
Environmental precautions	:	Do not allow contact with soil, surface or ground water.
Methods and materials for containment and cleaning up	:	Stop leak if safe to do so. Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Flush away traces with water. For large spills, dike spilled material or otherwise contain material to ensure runoff does not reach a waterway.

Product AT USE DILUTION

Personal precautions, protective equipment and emergency procedures	:	Refer to protective measures listed in sections 7 and 8.
Environmental precautions	:	No special environmental precautions required.
Methods and materials for containment and cleaning up	:	Stop leak if safe to do so. Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Flush away traces with water. For large spills, dike spilled material or otherwise contain material to ensure runoff does not reach a waterway.

SECTION 7. HANDLING AND STORAGE

Product AS SOLD

Advice on safe handling	:	Do not get in eyes, on skin, or on clothing. Wash hands thoroughly after handling. Warning! Do not use together with other products. May release dangerous gases (chlorine).
Conditions for safe storage	:	Keep away from strong bases. Keep out of reach of children. Store in suitable labeled containers.
Storage temperature	:	0 °C to 50 °C

Product AT USE DILUTION

Advice on safe handling	:	Wash hands after handling. For personal protection see section 8.
Conditions for safe storage	:	Keep out of reach of children. Store in suitable labeled containers.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Product AS SOLD
Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures	:	Effective exhaust ventilation system. Maintain air concentrations below occupational exposure standards.

Personal protective equipment

Eye protection	:	Safety goggles Safety glasses with side-shields Face-shield
Hand protection	:	No special protective equipment required.
Skin protection	:	No special protective equipment required.
Respiratory protection	:	No personal respiratory protective equipment normally required.
Hygiene measures	:	Handle in accordance with good industrial hygiene and safety practice. Wash face, hands and any exposed skin thoroughly after handling.

Product AT USE DILUTION

Engineering measures	:	Good general ventilation should be sufficient to control worker exposure to airborne contaminants.

Personal protective equipment

Eye protection	:	No special protective equipment required.
Hand protection	:	No special protective equipment required.
Skin protection	:	No special protective equipment required.
Respiratory protection	:	No personal respiratory protective equipment normally required.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

		Product AS SOLD	Product AT USE DILUTION
Appearance	:	liquid	liquid
Color	:	cloudy, dark green	light green
Odor	:	odorless	odorless
pH	:	0.5 - 1.0, 100 %	2.1 - 3.2
Flash point	:	not applicable	
Odor Threshold	:	no data available	
Melting point/freezing point	:	no data available	
Initial boiling point and boiling range	:	> 100 °C	
Evaporation rate	:	no data available	
Flammability (solid, gas)	:	no data available	
Upper explosion limit	:	no data available	
Lower explosion limit	:	no data available	
Vapor pressure	:	no data available	
Relative vapor density	:	no data available	
Relative density	:	1.069 - 1.135	
Water solubility	:	soluble	
Solubility in other solvents	:	no data available	
Partition coefficient: n-octanol/water	:	no data available	
Autoignition temperature	:	no data available	
Thermal decomposition	:	no data available	
Viscosity, kinematic	:	907.757 mm2/s (40 °C)	
Explosive properties	:	no data available	
Oxidizing properties	:	The substance or mixture is not classified as oxidizing.	
Molecular weight	:	no data available	
VOC	:	no data available	

SECTION 10. STABILITY AND REACTIVITY

Product AS SOLD

Chemical stability	:	Stable under normal conditions.
Possibility of hazardous reactions	:	Warning! Do not use together with other products. May release dangerous gases (chlorine).
Conditions to avoid	:	None known.
Incompatible materials	:	Bases Metals
Hazardous decomposition products	:	Decomposition products may include the following materials: Carbon oxides nitrogen oxides (NOx)

Sulfur oxides
Oxides of phosphorus

SECTION 11. TOXICOLOGICAL INFORMATION

Information on likely routes of exposure	:	Inhalation, Eye contact, Skin contact

Potential Health Effects

Product AS SOLD

Eyes	:	Causes serious eye irritation.
Skin	:	Harmful in contact with skin. May cause allergic skin reaction.
Ingestion	:	Health injuries are not known or expected under normal use.
Inhalation	:	Health injuries are not known or expected under normal use.
Chronic Exposure	:	Health injuries are not known or expected under normal use.

Product AT USE DILUTION

Eyes	:	Health injuries are not known or expected under normal use.
Skin	:	Health injuries are not known or expected under normal use.
Ingestion	:	Health injuries are not known or expected under normal use.
Inhalation	:	Health injuries are not known or expected under normal use.
Chronic Exposure	:	Health injuries are not known or expected under normal use.

Experience with human exposure

Product AS SOLD

Eye contact	:	Redness, Pain, Irritation
Skin contact	:	Redness, Irritation, Allergic reactions
Ingestion	:	No symptoms known or expected.
Inhalation	:	No symptoms known or expected.

Product AT USE DILUTION

Eye contact	:	No symptoms known or expected.
Skin contact	:	No symptoms known or expected.
Ingestion	:	No symptoms known or expected.
Inhalation	:	No symptoms known or expected.

Toxicity

Product AS SOLD

Acute oral toxicity	:	Acute toxicity estimate : > 5,000 mg/kg
Acute inhalation toxicity	:	no data available
Acute dermal toxicity	:	no data available

Skin corrosion/irritation	:	no data available
Serious eye damage/eye irritation	:	no data available
Carcinogenicity	:	no data available
Reproductive effects	:	no data available
Germ cell mutagenicity	:	no data available
Teratogenicity	:	no data available
STOT-single exposure	:	no data available
STOT-repeated exposure	:	no data available
Aspiration toxicity	:	no data available

Ingredients

Acute inhalation toxicity	:	Lactic acid 4 h LC50 rat: > 7.94 mg/l Sodium hydrogensulfate 4 h LC50 rat: > 2.4 mg/l oxirane, methyl-, polymer with oxirane 4 h LC50 rat: 0.147 mg/l

Ingredients

Acute dermal toxicity	:	Lactic acid LD50 rabbit: > 2,000 mg/kg

SECTION 12. ECOLOGICAL INFORMATION

Product AS SOLD
Ecotoxicity

Environmental Effects	:	This product has no known ecotoxicological effects.

Product

Toxicity to fish	:	no data available
Toxicity to daphnia and other aquatic invertebrates	:	no data available
Toxicity to algae	:	no data available

Ingredients

Toxicity to fish	:	Dodecylbenzenesulfonic acid, sodium salt 96 h LC50: 3.2 mg/l Lactic acid 96 h LC50 Fish: 130 mg/l Sodium hydrogensulfate 96 h LC50 Fish: 7,960 mg/l oxirane, methyl-, polymer with oxirane 96 h LC50 Fish: > 100 mg/l

Persistence and degradability

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

Other adverse effects

no data available

SECTION 13. DISPOSAL CONSIDERATIONS

Product AS SOLD

Disposal methods	:	Where possible recycling is preferred to disposal or incineration. If recycling is not practicable, dispose of in compliance with local regulations. Dispose of wastes in an approved waste disposal facility.
Disposal considerations	:	Dispose of as unused product. Empty containers should be taken to an approved waste handling site for recycling or disposal. Do not re-use empty containers.
RCRA - Resource Conservation and Recovery Authorization Act Hazardous waste	:	D002 (Corrosive)

Product AT USE DILUTION

Disposal methods	:	Where possible recycling is preferred to disposal or incineration. If recycling is not practicable, dispose of in compliance with local regulations. Dispose of wastes in an approved waste disposal facility.
Disposal considerations	:	Dispose of as unused product. Empty containers should be taken to an approved waste handling site for recycling or disposal. Do not re-use empty containers.

SECTION 14. TRANSPORT INFORMATION

Product AS SOLD

The shipper/consignor/sender is responsible to ensure that the packaging, labeling, and markings are in compliance with the selected mode of transport.

Land transport (DOT)

UN number	:	3265
Description of the goods	:	Corrosive liquid, acidic, organic, n.o.s. (Lactic acid)
Class	:	8
Packing group	:	III
Environmentally hazardous	:	no

Sea transport (IMDG/IMO)

UN number	:	3265
Description of the goods	:	CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (Lactic acid)
Class	:	8

Packing group : III
Marine pollutant : no

Product AT USE DILUTION
Not intended for transport.

SECTION 15. REGULATORY INFORMATION

Product AS SOLD

EPA Registration number : 1677-234

EPCRA - Emergency Planning and Community Right-to-Know

CERCLA Reportable Quantity

Ingredients	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Dodecylbenzenesulfonic acid, sodium salt	25155-30-0	1000	76834

SARA 304 Extremely Hazardous Substances Reportable Quantity
This material does not contain any components with a section 304 EHS RQ.

SARA 311/312 Hazards : Acute Health Hazard

SARA 302 : SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 : SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

California Prop 65
This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

The ingredients of this product are reported in the following inventories:

1907/2006 (EU) :
not determined

Switzerland. New notified substances and declared preparations :
not determined

United States TSCA Inventory :
On TSCA Inventory

Canadian Domestic Substances List (DSL) :
All components of this product are on the Canadian DSL.

Australia Inventory of Chemical Substances (AICS) :
On the inventory, or in compliance with the inventory

New Zealand. Inventory of Chemical Substances :
On the inventory, or in compliance with the inventory

Japan. ENCS - Existing and New Chemical Substances Inventory :
not determined

Japan. ISHL - Inventory of Chemical Substances (METI) :
not determined

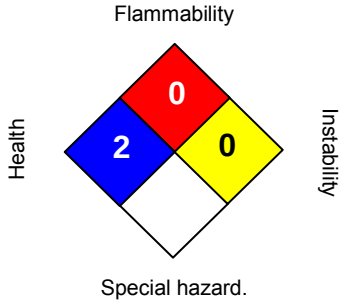
Korea. Korean Existing Chemicals Inventory (KECI) :
On the inventory, or in compliance with the inventory

Philippines Inventory of Chemicals and Chemical Substances (PICCS) :
On the inventory, or in compliance with the inventory

China. Inventory of Existing Chemical Substances in China (IECSC) :
On the inventory, or in compliance with the inventory

SECTION 16. OTHER INFORMATION

Product AS SOLD
NFPA:

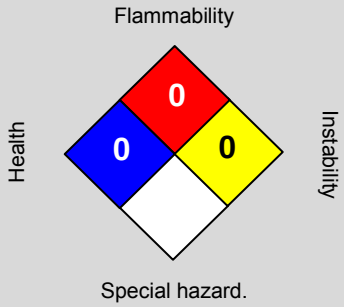


HMIS III:

HEALTH	2
FLAMMABILITY	0
PHYSICAL HAZARD	0

0 = not significant, 1 =Slight,
2 = Moderate, 3 = High
4 = Extreme, * = Chronic

Product AT USE DILUTION
NFPA:



HMIS III:

HEALTH	0
FLAMMABILITY	0
PHYSICAL HAZARD	0

0 = not significant, 1 =Slight,
2 = Moderate, 3 = High
4 = Extreme, * = Chronic

Issuing date	:	06/04/2014
Version	:	1.1
Prepared by	:	Regulatory Affairs

REVISED INFORMATION: Significant changes to regulatory or health information for this revision is indicated by a bar in the left-hand margin of the SDS.

The information provided in this Material Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text.

MATERIAL SAFETY DATA SHEET

1. Product and Company Identification

Material name NACCONOL 90G
Version # 22
Revision date 12-20-2013
Product code 0533
Chemical class Linear alkylbenzene sulfonate
Manufacturer Stepan Company
22 West Frontage Road
Northfield, IL 60093
Emergency Medical 1-800-228-5635
Chemtrec 1-800-424-9300
Chemtrec Int'l +1 703-527-3887
General information General 1-847-446-7500

2. Hazards Identification

Emergency overview WARNING
Product may form explosive dust/air mixtures if high concentration of product dust is suspended in air.
Moderately irritating to the eyes. Contact with this product may cause severe eye damage. Contact with skin may cause irritation. May cause irritation of respiratory tract.

Potential health effects

Eyes Contact can cause moderate to severe irritation and possible injury to the eyes.
Skin This product may cause irritation to the skin.
Inhalation Inhalation of dusts may produce respiratory irritation and may cause allergic respiratory sensitization reactions.
Ingestion Ingestion of large amounts may produce gastrointestinal disturbances including irritation, nausea, and diarrhea.

3. Composition / Information on Ingredients

Components	CAS #	Percent
_Sodium dodecylbenzenesulfonate	25155-30-0	90 - 93
Sodium sulfate	7757-82-6	5
Water	7732-18-5	1.5
Sodium chloride	7647-14-5	1

4. First Aid Measures

First aid procedures

Eye contact Immediately flush eyes with plenty of water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical attention immediately.
Skin contact Immediately flush skin with plenty of water. Immediately take off all contaminated clothing. If irritation persists get medical attention. Wash clothing separately before reuse.
Inhalation If symptoms are experienced, remove source of contamination or move victim to fresh air. If symptoms persist, get medical attention. If the affected person is not breathing, apply artificial respiration. If breathing is difficult, give oxygen. Get medical attention immediately.
Ingestion IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell. Rinse mouth. Do not induce vomiting without advice from poison control center.

General advice Ensure that medical personnel are aware of the material(s) involved, and take precautions to protect themselves.

5. Fire Fighting Measures

Flammable properties Dust accumulation from this product may present an explosion hazard in the presence of an ignition source. Fire hazard. Class II Dust for National Electric Code (NFPA 70)

Extinguishing media

Suitable extinguishing media	Water. Water fog. Foam. Dry chemical powder. Carbon dioxide (CO2).

Protection of firefighters

Protective equipment and precautions for firefighters	As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Move containers from fire area if you can do so without risk. In the event of fire, cool tanks with water spray.
Specific methods	Cool containers exposed to flames with water until well after the fire is out.

6. Accidental Release Measures

Personal precautions	Ventilate closed spaces before entering them. Isolate area.
Environmental precautions	Prevent further leakage or spillage if safe to do so. Do not contaminate water.
Methods for containment	ELIMINATE all ignition sources (no smoking, flares, sparks or flames in immediate area). Stop the flow of material, if this is without risk. Dike the spilled material, where this is possible.
Methods for cleaning up	Should not be released into the environment. Avoid dust formation. Avoid the generation of dusts during clean-up. Do not create a powder cloud by using a brush or compressed air. Wear appropriate protective equipment and clothing during clean-up. Cover powder spill with plastic sheet or tarp to minimize spreading. Use clean non-sparking tools to collect absorbed material. Shovel into suitable container for disposal.

7. Handling and Storage

Handling	DO NOT handle, store or open near an open flame, sources of heat or sources of ignition. Protect material from direct sunlight. Avoid contact with skin and eyes. Wash hands thoroughly after handling. Avoid release to the environment. Avoid breathing dusts from this material.
Storage	Keep away from heat, sparks and open flame. Store in cool place. Store in a well-ventilated place. Keep container tightly closed. Keep out of the reach of children. Guard against dust accumulation of this material. Prevent electrostatic charge build-up by using common bonding and grounding techniques.

8. Exposure Controls / Personal Protection

Engineering controls	Use explosion-proof equipment if high dust/air concentrations are possible. Keep formation of airborne dusts to a minimum. Use general ventilation. Local exhaust is suggested for use, where possible, in enclosed or confined spaces.

Personal protective equipment

General	Eye wash fountain and emergency showers are recommended.
Eye / face protection	Wear dust goggles.
Skin protection	Wear protective gloves. Wear suitable protective clothing.
Respiratory protection	If ventilation is not sufficient to effectively prevent buildup of aerosols or vapors, appropriate NIOSH/MSHA respiratory protection must be provided.
General hygiene considerations	Wash hands after handling and before eating. Keep away from food and drink. Handle in accordance with good industrial hygiene and safety practice.

9. Physical & Chemical Properties

Color	Off-white.
Physical state	Solid.
Form	Powder. Class II Dust for National Electric Code (NFPA 70) Pmax = 6.4bar Kst = 56 bar m/s Minimum Ignition Energy (MIE) = > 1000 mJ Minimum Explosible Concentration (MEC) = 74 g/m3 Minimum Autoignition Temperature (MAIT Cloud) = 460 C Limiting Oxygen Concentration (LOC) = 15 vol. % Mean particle size = 218 (11% < 75) micrometer
pH	6.0000 - 7.5000 @1% Aqueous
Melting point	> 572 °F (> 300 °C)
Flash point	> 201 °F (> 93.9 °C)
Flammability limits in air, upper, % by volume	NOT DETERMINED.
Vapor density	Not applicable, powder.
Specific gravity	0.5300

Solubility (water)	Soluble.
RVOC	0 %

10. Stability & Reactivity

Chemical stability	Material is stable under normal conditions.
Conditions to avoid	Dust may form explosive mixture in air.
Incompatible materials	Strong oxidizing agents.
Hazardous decomposition products	Upon decomposition, this product may yield sulfur dioxide and oxides of sulfur.
Possibility of hazardous reactions	Will not occur.

11. Toxicological Information

Toxicological data

Product	Test Results
NACCONOL 90G	Acute Dermal LD50 Rabbit: > 2000 mg/kg
	Acute Oral LD50 Rat: > 1000 mg/kg

Sensitization	Not a skin sensitizer.
Carcinogenicity	This product is not considered to be a carcinogen by IARC, ACGIH, NTP, or OSHA.
Mutagenicity	No data available to indicate product or any components present at greater than 0.1% are mutagenic or genotoxic.
Reproductive effects	Contains no ingredient listed as toxic to reproduction

12. Ecological Information

Ecotoxicological data

Product	Test Results
NACCONOL 90G	EC50 Algae: 29 mg/l 96 hours
	EC50 Daphnia: 2.4 mg/l 48 hours
	LC50 Fish: 1.67 mg/l 96 hours
Components	**Test Results**
_Sodium dodecylbenzenesulfonate (25155-30-0)	EC50 Water flea (Ceriodaphnia dubia): 3.26 - 14.51 mg/l Not reported 48 hours
	LC50 Rainbow trout,donaldson trout (Oncorhynchus mykiss): 3.2 - 5.6 mg/l Renewal 96 hours
Sodium chloride (7647-14-5)	EC50 Water flea (Daphnia magna): 340.7 - 469.2 mg/l Static 48 hours
	LC50 Fathead minnow (Pimephales promelas): 6020 - 7070 mg/l Static 96 hours
Sodium sulfate (7757-82-6)	EC50 Water flea (Ceriodaphnia dubia): 2807 - 3535 mg/l Not reported 48 hours
	LC50 Striped bass (Morone saxatilis): 790 mg/l Static 96 hours

Ecotoxicity	Readily biodegradable.

13. Disposal Considerations

Disposal instructions	Dispose of contents/container in accordance with local/regional/national/international regulations. Dispose in accordance with all applicable regulations. Regulations vary.

14. Transport Information

General	The following transportation classifications are for bulk shipments only: DOT: UN3077, RQ, Environmentally Hazardous Substance, Solid, N.O.S., (Sodium Dodecylbenzene Sulfonate), 9, III, Marine Pollutant (Linear Alkylbenzene Suflonate) IATA CLASSIFICATION: IATA prohibits air cargo transport. IMDG CLASSIFICATION: UN3077, RQ, Environmentally Hazardous Substance, Solid, N.O.S., (Sodium Dodecylbenzene Sulfonate), 9, III, Marine Pollutant (Linear Alkylbenzene Suflonate)

15. Regulatory Information

US federal regulations All components are on the U.S. EPA TSCA Inventory List.

US CERCLA Hazardous Substances: Reportable quantity

_Sodium dodecylbenzenesulfonate (CAS 25155-30-0) 1000 lbs

Reportable Quantity Reportable Quantity (RQ) of this product is 1085 pounds based upon _Sodium dodecylbenzenesulfonate(25155-30-0) which yielded the lowest resultant RQ according to the following formula: CERCLA ingredient RQ / % of that ingredient in the product.

CERCLA (Superfund) reportable quantity

_Sodium dodecylbenzenesulfonate: 1000

Superfund Amendments and Reauthorization Act of 1986 (SARA)

Section 302 extremely hazardous substance No

Section 311 hazardous chemical Yes

Clean Water Act (CWA) Hazardous substance

Inventory status

Country(s) or region	Inventory name	On inventory (yes/no)*
Australia	Australian Inventory of Chemical Substances (AICS)	Yes
Canada	Domestic Substances List (DSL)	Yes
Canada	Non-Domestic Substances List (NDSL)	No
China	Inventory of Existing Chemical Substances in China (IECSC)	Yes
Europe	European Inventory of Existing Commercial Chemical Substances (EINECS)	Yes
Europe	European List of Notified Chemical Substances (ELINCS)	No
Japan	Inventory of Existing and New Chemical Substances (ENCS)	Yes
Korea	Existing Chemicals List (ECL)	Yes
New Zealand	New Zealand Inventory	Yes
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	Yes
United States & Puerto Rico	Toxic Substances Control Act (TSCA) Inventory	Yes

*A "Yes" indicates that all components of this product comply with the inventory requirements administered by the governing country(s)
A "No" indicates that one or more components of the product are not listed or exempt from listing on the inventory administered by the governing country(s).

State regulations

US - New Jersey RTK - Substances: Listed substance

_Sodium dodecylbenzenesulfonate (CAS 25155-30-0) Substance no. 1698

US - Pennsylvania RTK - Hazardous Substances: Listed substance

_Sodium dodecylbenzenesulfonate (CAS 25155-30-0) Listed.
Sodium sulfate (CAS 7757-82-6) Listed.

16. Other Information

Further information Refer to NFPA 654, Standard for the Prevention of Fire and Dust Explosions from the Manufacturing, Processing, and Handling of Combustible Particulate Solids, for safe handling.

HMIS® is a registered trade and service mark of the NPCA.

HMIS® ratings
Health: 2
Flammability: 1
Physical hazard: 0
Personal protection: X

NFPA ratings
Health: 2
Flammability: 1
Instability: 0

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Issue date	12-20-2013
This data sheet contains changes from the previous version in section(s):	Physical & Chemical Properties: Multiple Properties Transport Information: Material Transportation Information Transport Information: General Transport Information: Notes

11. RESEARCH INFORMATION

Results of Recent Literature Search:

Results of a recent literature search for Sodium Dodecylbenzene Sulfonate (SDBS) are listed immediately following this page:

Reviews of Safety and Environmental Information:

Reviews on safety and environmental information for SDBS are provided after the results of the literature search, and are obtained via the sources listed below. Reviews are ordered as follows:

1. Human & Environmental Risk Assessment (HERA). 2013. LAS: linear alkyl benzene sulphonate. Revised HERA Report April 2013; accessed June 16, 2014. Available at:
http://www.heraproject.com/RiskAssessment.cfm

2. Organization for Economic Cooperation and Development Screening Information Data Sets (OECD-SIDS). 2005. Linear Alkylbenzene Sulfonate (LAS) SIDS Initial Assessment Report, April 2005; accessed June 17, 2014. Available at: http://www.chem.unep.ch/irptc/sids/OECDSIDS/LAS.pdf

3. U.S. Environmental Protection Agency (EPA); 2006a. Reregistration Eligibility Decision (RED) for Alkyl benzene sulfonates. July 27, 2006; accessed June 13, 2014. EPA-HQ-OPP-2006-0156-0016. Available at: http://www.regulations.gov/#!docketDetail;D=EPA-HQ-OPP-2006-0156

4. U.S. Environmental Protection Agency (EPA); 2006b. Alkylbenzene Sulfonates (ABS) Risk Assessment for the Reregistration Eligibility Decision (RED) Document. PC Codes: 079010, 190116 and 098002.(active); 790102, 790116, 790101 (inert) Case No. 4006. July 19, 2006; accessed June 16, 2014. EPA-HQ-OPP-2006-0156-0017. Available at: http://www.regulations.gov/#!docketDetail;D=EPA-HQ-OPP-2006-0156

5. U.S. Environmental Protection Agency (EPA); 2006c. Alkyl benzene sulfonates (ABS) toxicology chapter for the reregistration eligibility decision (RED) document. July 6, 2006; accessed July 22, 2010. EPA-HQ-OPP-2006-0156-0018. Available at: http://www.regulations.gov/#!docketDetail;D=EPA-HQ-OPP-2006-0156

6. U.S. Environmental Protection Agency (EPA); 2006d. Environmental Fate Assessment of Alkylbenzene Sulfonates for the Registration Eligibility Document (RED). July 6, 2006; accessed June 16, 2014. EPA-HQ-OPP-2006-0156-0021. Available at: http://www.regulations.gov/#!docketDetail;D=EPA-HQ-OPP-2006-0156

7. U.S. Environmental Protection Agency (EPA); 2006e. Ecological Hazard and Environmental Risk Assessment of alkylbenzene sulfonates for the Registration Eligibility Document (RED). July 12, 2006; accessed June 16, 2014. EPA-HQ-OPP-2006-0156-0023. Available at:
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8. World Health Organization (WHO). 1996. Environmental health criteria document for linear alkyl benzene sulfonates and related compounds. EHC 169; accessed July 22, 2010. Available at: http://www.inchem.org/documents/ehc/ehc/ehc169.htm.

[redacted]

This message contains search results from the National Center for Biotechnology Information (NCBI) at the U.S. National Library of Medicine (NLM). Do not reply directly to this message

Sent on: Fri Jun 13 15:24:06 2014

Search: ("dodecylbenzenesulfonic acid"[NM]) AND ("2011/01/01"[Date - Publication] : "3000"[Date - Publication])

PubMed Results

Items 1 - 59 of 59 (Display the 59 citations in PubMed)

1. Sodium dodecyl sulfate and sodium dodecyl benzenesulfonate are ligands for peroxisome proliferator-activated receptor γ.

   Iida K, Yonezawa T, Choi SS, Nagai K, Woo JT.

   J Toxicol Sci. 2013;38(5):697-702.

   PMID: 24025786 [PubMed - indexed for MEDLINE] **Free Article**

   Related citations

2. Size-controlled preparation of α-calcium sulphate hemihydrate starting from calcium sulphate dihydrate in the presence of modifiers and the dissolution rate in simulated body fluid.

   Chen J, Gao J, Yin H, Liu F, Wang A, Zhu Y, Wu Z, Jiang T, Qin D, Chen B, Ji Y, Sun M.

   Mater Sci Eng C Mater Biol Appl. 2013 Aug 1;33(6):3256-62. doi: 10.1016/j.msec.2013.04.007. Epub 2013 Apr 10.

   PMID: 23706208 [PubMed - indexed for MEDLINE]

   Related citations

3. Continuous bioproduction of short-chain fatty acids from sludge enhanced by the combined use of surfactant and alkaline pH.

   Chen Y, Liu K, Su Y, Zheng X, Wang Q.

   Bioresour Technol. 2013 Jul;140:97-102. doi: 10.1016/j.biortech.2013.04.075. Epub 2013 Apr 28.

   PMID: 23685363 [PubMed - indexed for MEDLINE]

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4. The impact of alkyl sulfate surfactant geometry and electrolyte on the co-adsorption of anionic surfactants with model perfumes at the air-solution interface.

   Bradbury R, Penfold J, Thomas RK, Tucker IM, Petkov JT, Jones C.

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5. Dynamics in anionic micelles: effect of phenyl ring.
   Sharma VK, Mitra S, Johnson M, Mukhopadhyay R.
   J Phys Chem B. 2013 May 23;117(20):6250-5. doi: 10.1021/jp401831y. Epub 2013 May 6.
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6. Sodium dodecyl benzene sulfonate functionalized graphene for confined electrochemical growth of metal/oxide nanocomposites for sensing application.
   Zhou S, Wei D, Shi H, Feng X, Xue K, Zhang F, Song W.
   Talanta. 2013 Mar 30;107:349-55. doi: 10.1016/j.talanta.2013.01.041. Epub 2013 Feb 4.
   PMID: 23598233 [PubMed - indexed for MEDLINE]
   Related citations

7. Fate of (14)C-organic pollutant residues in composted sludge after application to soil.
   Haudin CS, Zhang Y, Dumény V, Lashermes G, Bergheaud V, Barriuso E, Houot S.
   Chemosphere. 2013 Aug;92(10):1280-5. doi: 10.1016/j.chemosphere.2013.02.041. Epub 2013 Mar 29.
   PMID: 23545187 [PubMed - indexed for MEDLINE]
   Related citations

8. Adsorption mechanism of sodium dodecyl benzene sulfonate on carbon blacks by adsorption isotherm and zeta potential determinations.
   Zhao Y, Lu P, Li C, Fan X, Wen Q, Zhan Q, Shu X, Xu T, Zeng G.
   Environ Technol. 2013 Jan-Feb;34(1-4):201-7.
   PMID: 23530331 [PubMed - indexed for MEDLINE]
   Related citations

9. Layered double hydroxides intercalated with anionic surfactants/benzophenone as potential materials for sunscreens.
   Cursino AC, Lisboa Fda S, Pyrrho Ados S, de Sousa VP, Wypych F.
   J Colloid Interface Sci. 2013 May 1;397:88-95. doi: 10.1016/j.jcis.2013.01.059. Epub 2013 Feb 12.
   PMID: 23481517 [PubMed - indexed for MEDLINE]
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10. Influence of calcium ions on rhamnolipid and rhamnolipid/anionic surfactant adsorption and self-assembly.
    Chen M, Dong C, Penfold J, Thomas RK, Smyth TJ, Perfumo A, Marchant R, Banat IM, Stevenson P, Parry A, Tucker I, Grillo I.
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11. Investigation on the co-luminescence effect of europium (III)-lanthanum(III)-dopamine-sodium dodecylbenzene sulfonate system and its application.
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12. Conductive polyaniline helixes self-assembled in the absence of chiral dopant.
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PMID: 23282864 [PubMed - indexed for MEDLINE]
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13. Microstructure transformation of PDMS-E grafted gelatin polymers induced by SDS and SDBS.
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18. Toxicity evaluation of two typical surfactants to Dunaliella bardawil, an environmentally tolerant alga.
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22. Simultaneous determination of ofloxacin and gatifloxacin on cysteic acid modified electrode in the presence of sodium dodecyl benzene sulfonate.
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23. Implications of surfactant-induced flow for miscible-displacement estimation of air-water interfacial areas in unsaturated porous media.
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Human and Environmental Risk Assessment
on ingredients of Household Cleaning Products

LAS

Linear Alkylbenzene Sulphonate

(CAS No. 68411-30-3)

Revised HERA Report

April 2013

1. Contents

2. Executive Summary

Linear alkylbenzene sulphonate (LAS) is an anionic surfactant. It was introduced in 1964 as the readily biodegradable replacement for highly branched alkylbenzene sulphonates (ABS). LAS is a mixture of closely related isomers and homologues, each containing an aromatic ring sulphonated at the *para* position and attached to a linear alkyl chain.

The European consumption of LAS in detergents applications covered by HERA was about 350 kt in 2005. This represents more than 80% of the total European consumption of LAS, which was estimated to be about 430 kt in the year 2005. LAS is one of the major anionic surfactants used on the market. Important application products are household detergents, such as laundry powders, laundry liquids, dishwashing products and all-purpose cleaners. The minor other final uses of LAS, namely in the field of textile and fibres, chemicals, and agriculture, are outside HERA's scope.

Environmental assessment

- The present environmental risk assessment of LAS is based on the HERA methodology document, which in its turn is based on the EU Technical Guidance Document (TGD, 2003). It makes use of the EUSES programme following the HERA detergent scenario (EUSES, 2008). LAS concentrations (PEC values) measured or modelled in the various environmental compartments were compared with extrapolations of the many available eco-toxicity data leading to PNEC values protective of each compartment.

- In raw sewage, the LAS concentration was in the range of 1-15 mg/l. When the sewage was properly treated in activated sludge STPs (Sewage Treatment Plant). LAS was highly removed leading to an effluent concentration in the 0.008-0.27 mg/l range.

- LAS concentration was further decreased by dilution in the receiving waters where it could be found in the <0.002-0.047 mg/l concentration range. LAS degrades rapidly aerobically (half-life in rivers about 3 hours), whereas it does not degrade under anaerobic conditions, except under particular conditions.

- Typical LAS concentrations in aerobic sludge are <0.5 $g/kg_{dw\ sludge}$ (dry weight). In STP anaerobic sludge, the calculated median LAS concentration was 5.6 $g/kg_{dw\ sludge}$ (dry weight) (15.1 $g/kg_{dw\ sludge}$ at 95th percentile). During sludge transportation to the farmland, sludge storage, and application on agricultural soil, aerobic conditions are restored and rapid degradation of LAS resumes.

- In sludge-amended soils, LAS had a maximum half-life of one week (primary biodegradation) and monitored concentrations were around 1 $mg/kg_{dw\ soil}$ (maximum 1.4 $mg/kg_{dw\ soil}$) at harvesting time. No accumulation in soil and no bioaccumulation in plants could be detected experimentally.

- In freshwater sediments, measured LAS concentrations typically ranged from <1 $mg/kg_{dw\ sed.}$ to a maximum value of 5.3 $mg/kg_{dw\ sed.}$.

- Ecotoxicity data are abundant and well documented. The aquatic PNEC value (0.27 mg/l) was calculated from: i) a statistical extrapolation including a set of high quality single species chronic data and ii) the no-observed effect concentration of a stream community experimentally exposed to LAS.

- The terrestrial PNEC value (35 $mg/kg_{dw\ soil}$) was calculated from: i) the equilibrium partitioning method , ii) statistical extrapolation of a set of high quality chronic data on plants and soil fauna , iii) an expert judgement on the toxicity of several microbial processes and functions, and 4) field toxicity studies.

- The sludge PNEC value (49 $g/kg_{dw\ sludge}$) was back-calculated from the soil PNEC on the basis of the EU TGD scenario (TGD, 2003).

- The sediment PNEC value (23.8 $mg/kg_{dw\ sed.}$) was calculated from i) the lowest available chronic effect value and an application factor, and ii) the equilibrium partitioning method, the PNEC was normalized for organic carbon content.

- The STP PNEC (5.5 mg/l) was calculated from acute and chronic microbial inhibition data and the use of the relevant application factor (TGD, 2003).

- The risk characterisation as expressed by the PEC/PNEC ratio was below 1 for all environmental compartments. It was concluded that the ecotoxicological parameters of LAS have been adequately and sufficiently characterized and that the ecological risk of LAS is judged to be low.

Human health assessment

- The presence of LAS in many commonly used household detergents gives rise to a variety of possible consumer contact scenarios including direct and indirect skin contact, inhalation, and oral ingestion derived either from residues deposited on dishes, from accidental product ingestion, or indirectly from drinking water.

- The consumer aggregate exposure from direct and indirect skin contact as well as from inhalation and from oral route in drinking water and dishware results in an estimated total body burden of 34.6 mg/kg bw/day. This body burden is substantially higher than the body burden of 0.4 µg/kg bw/day reported in the previous version of this HERA document. The higher estimated body burden is a result of using information from the RIVM report Cleaning Products Fact Sheet (RIVM,2006) to assess the risk to consumers in additional to the AISE overview concerning habits and practices on uses of detergents and surface cleaners in Western Europe (THPCPWE,2002). Furthermore, some additional use scenarios have been identified.

- The toxicological data show that LAS was not genotoxic *in vitro* or *in vivo,* did not induce tumours in rodents after two years daily dosing, and failed to induce either reproductive toxicity or developmental or teratogenic effects. The critical adverse effect identified after repeated long term high dosing of LAS to animals was a change in renal biochemical parameters. A systemic NOAEL of 68 mg/kg bw/day was established.

- Comparison of the aggregate consumer exposure to LAS with the systemic NOAEL results in an estimated Margin of Exposure (MOE) of 1.97. The estimated Margin of Exposure is based on conservative estimations of both exposure and NOAEL (which is a systemic NOAEL given the existence of oral toxicokinetic data). This MOE is substantially less than the MOE of 17000

reported in the previous version of of this HERA document. The lower MOE is a direct result of the higher estimated body burden (see above).

- Neat LAS is an irritant to skin and eyes. The irritation potential of aqueous solutions of LAS depends on concentration. Local effects of hand wash solutions containing LAS do not cause concern given that LAS is not a contact sensitizer and that the concentrations of LAS in such solutions are well below 1% and therefore not expected to be irritating to eye or skin. Laundry pre-treatment tasks, which may translate into brief hand skin contact with higher concentrations of LAS, may occasionally result in mild irritation easily avoided by prompt rinsing of the hands in water. Potential irritation of the respiratory tract is not a concern given the very low levels of airborne LAS generated as a consequence of cleaning sprays aerosols or laundry powder detergent dust.

- In view of the extensive database on toxic effects, the low exposure values calculated and the resulting Margin of Exposure described above, it can be concluded that use of LAS in household laundry and cleaning products raises no safety concerns for the consumers.

3. Substance Characterisation

Linear alkylbenzene sulphonate (LAS) is an anionic surfactant. It was introduced in 1964 as the readily biodegradable replacement for highly branched alkylbenzene sulphonates (ABS). LAS is a mixture of closely related isomers and homologues, each containing an aromatic ring sulphonated at the *para* position and attached to a linear alkyl chain.

3.1 CAS No. and grouping information

LAS, used on the European market and covered in this focused risk assessment, is represented by the list in Table 1.

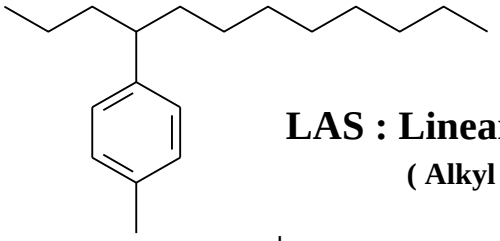
Table 1: CAS and EINECS numbers of LAS in the European market

CAS No.	EINECS No.	NAME
68411-30-3	270-115-0	Benzenesulphonic acid, C_{10-13} alkyl derivs., sodium salts
1322-98-1	215-347-5	Sodium decylbenzenesulphonate
25155-30-0	246-680-4	Benzenedodecylsulfonic acid, sodium salt
90194-45-9	290-656-6	Benzenesulphonic acid, mono-C_{10-13} alkyl derivs., sodium salt
85117-50-6	285-600-2	Benzenesulphonic acid, mono-C_{10-14} alkyl derivs., sodium salt

The present assessment focuses on LAS levels in consumer products used on the European market and found in the various environmental compartments. LAS represented by the CAS No. 68411-30-3 and EINECS No. 270-115-0 is by far the most used on the European market (>98%).

3.2 Chemical Structure and Composition

LAS on the European market is a specific and rather constant mixture of closely related isomers and homologues generated in the manufacture of the raw material Linear Alkyl Benzene (LAB), the LAS precursor, each containing an aromatic ring sulphonated at the “para” position and attached to a linear alkyl chain at any position except the terminal carbons (Schönkaes, 1998; Cavalli et al., 1999b; Valtorta et al., 2000), as shown in the figure below:



LAS : Linear Alkyl Benzene Sulfonate

(Alkyl Chain : C_{10} - C_{13})

The linear alkyl chain has typically 10 to 13 carbon units, approximately in the following mole ratio C_{10}:C_{11}:C_{12}:C_{13}=13:30:33:24, an average carbon number near 11.6 and a content of the most hydrophobic 2-phenyl isomers in the 18-29% range (Feijtel et al., 1995b; Feijtel et al., 1999; Cavalli et al., 1999b; Valtorta et al., 2000). This commercial LAS consists of more than 20 individual components. The ratio of the various homologues and isomers, representing different alkyl chain lengths and aromatic ring positions along the linear alkyl chains, is relatively constant across the various household applications. This LAS constant ratio is unique and does not apply to the other major surfactants. Therefore, the present assessment adopted a category approach, i.e., considered the fate and effects of the LAS mixture as described above rather than of each isomer and homologue separately. However, fingerprints in the different environmental compartments are reported.

The linearity of the alkyl chain is between 93% and 98% depending on the different manufacturing processes of LAB, the LAS precursor (Cavalli et al., 1999b). The mono-methyl substituted alkylbenzene sulphonate (iso-LAS) (Nielsen et al., 1997) represent on average 2 to 7% of the raw material. The kind of substitutions of iso-LAS was shown not to limit their biodegradation, which under realistic environmental conditions was comparable to the one of LAS (Nielsen et al., 1997; Dunphy et al., 2000). Non-linear components such as DiAlkylTetralin Sulphonates (DATS) can be present at levels of 3-10% in the LAS derived from $AlCl_3$ catalysed LAB process (see par. 3.3). This process, however, was less than 5% in 2005 (ECOSOL, 2005).

The data presented in Table 2 are fully described in IUCLID, 1994 and SIDS, 2005 and refer to the commercial $C_{11.6}$ LAS or the pure C_{12} homologue.

Table 2: Physical chemical data of the commercial $C_{11.6}$ LAS (IUCLID, 1994; SIDS, 2005)

LAS	Protocol	Results
Molecular description	Solid organic acid sodium salt	-
Molecular weight (g/M)	$(C_{11.6}H_{24.2})C_6H_4SO_3Na$	342.4
Vapour pressure at 25°C (Pa)	Calculated as C_{12}	$(3\text{-}17) \cdot 10^{-13}$
Boiling point (°C)	Calculated as C_{12}	637
Melting point (°C)	Calculated as C_{12}	277
Octanol-water partition coefficient ($\log K_{ow}$)	Calculated as $C_{11.6}$	3.32
Organic carbon-water partition coefficient K_{oc} (l/kg)	Calculated as $C_{11.6}$	2500
Critical micelle concentration (g/l)	Experimental	0.65
Water solubility (g/l)	Experimental	250

Sorption coefficient between soil/sediment and water, K_d (l/kg)	Experimental	2-300
Density (kg/l)	Experimental	1.06 (relative) 0.55 (bulk)
pH (5% LAS water solutions)	Experimental	7-9
Henry's constant (Pa · m^3/mole)	Calculated as C_{12}	$6.35 \cdot 10^{-3}$

Molecular weight was calculated according to the structure of the sodium salt of the benzenesulphonic acid with an average $C_{11.6}$ linear alkyl chain.

Vapour pressure ($3 \cdot 10^{-13}$ Pa) was estimated for C_{12}LAS (Lyman, 1985) and calculated ($17 \cdot 10^{-13}$ Pa) using EPI database by a Syracuse Research Corporation (SRC) software (SIDS, 2005).

Melting and boiling points were calculated using Estimation Program Interface (EPI) database by SRC software (SIDS, 1999).

The octanol-water partition coefficient, log K_{ow}, cannot be experimentally measured for surfactants because of their surface–active properties, but only approximately calculated (Roberts, 2000). A log K_{ow} of 3.32, for the $C_{11.6}$LAS structure was calculated with a method (Leo et al., 1979) modified to take into account the various aromatic ring positions along the linear alkyl chain (Roberts, 1991). This value was used in the aquatic risk assessment carried out in the Netherlands (Feijtel, 1995b). Organic carbon-water partition coefficient (K_{oc}) values of 110 and 278 were calculated for C_{12}benzenesulphonate using regression equations from water solubility and log K_{ow} data (Lyman, 1990).

A better indication of this association can, however, be represented by the sludge partition coefficient, K_p (l/kg), assessed by QSAR analyses (Feijtel et al., 1999; Garcìa et al., 2002)). For pure compounds, log K_p of 3.0 and 3.5 for C_{11}LAS and C_{12}LAS respectively were derived and used in full-scale studies of activated sludge plants (Feijtel, 1995a; Feijtel, 1995b). Laboratory experiments (Temmink et al., 2004) with LAS showed that sorption of the C_{12}LAS homologue over sludge is a fast and reversible process that can be described by a K_p value (K_p = 3210 l/kg) in agreement with the above QSAR calculations. Applying the same QSAR for the commercial $C_{11.6}$LAS mixture, a log K_p value of 3.4 (K_p = 2500 l/kg) can thus be derived and confidently assumed as a measure of the partition of the surfactant between organic matter and water and assimilated to K_{oc}. An average log K_{oc} value of 4.83 was also reported for C_{12}LAS as a measure of its association with dissolved organic compounds, basically represented by humic acids (Traina et al., 1996).

A critical micelle concentration (CMC) of 0.65 g/l for the commercial $C_{10\text{-}13}$LAS was reported (Smulders, 2002); the value is in line with that of other anionic surfactants. CMCs were also measured for the different LAS homologues in deionized and hard waters (Garcìa et al., 2002).
The reported water solubility and density values were experimentally derived (IUCLID, 1994). pH values in water solutions depend on the free caustic soda content in LAS after neutralisation of the sulphonic acid; in general, 5% water solutions of commercial LAS have pH values in the 7-9 range. Soil/sediment and water sorption coefficients, K_d (l/kg), were experimentally measured; they ranged from 2 to 300 l/kg, depending on the organic content, and fit the Freundlich equation (Painter, 1992). K_d sediment values were higher than K_d soil ones, as a consequence of the higher organic content in sediment than in soil (Marchesi et al., 1991; TGD, 2003).

Using a structure estimation method (Meylan et al., 1991) the Henry's constant for C_{12} benzenesulphonate was calculated to be $6.35 \cdot 10^{-3}$ ($Pa \cdot m^3$/mole).

3.3 Manufacturing route and production/volume statistics

LAS is produced by sulphonation of LAB with a variety of sulphonating agents. In the past, oleum (fuming sulphuric acid), as well as sulphuric acid were the predominant agents used either in batch reactors or in the so-called "cascade" systems. The sulphonation technology, however, has been considerably improved since the mid 60s and nowadays, although oleum is still used, modern falling film reactors (FFR) (mono-tube or multi-tube) and SO_3 gas are the state of art of the technology in most of the sulphonation facilities in Europe. In these modern plants both the sulphonation of LAB and the sulphation of fatty alcohols are normally practised.

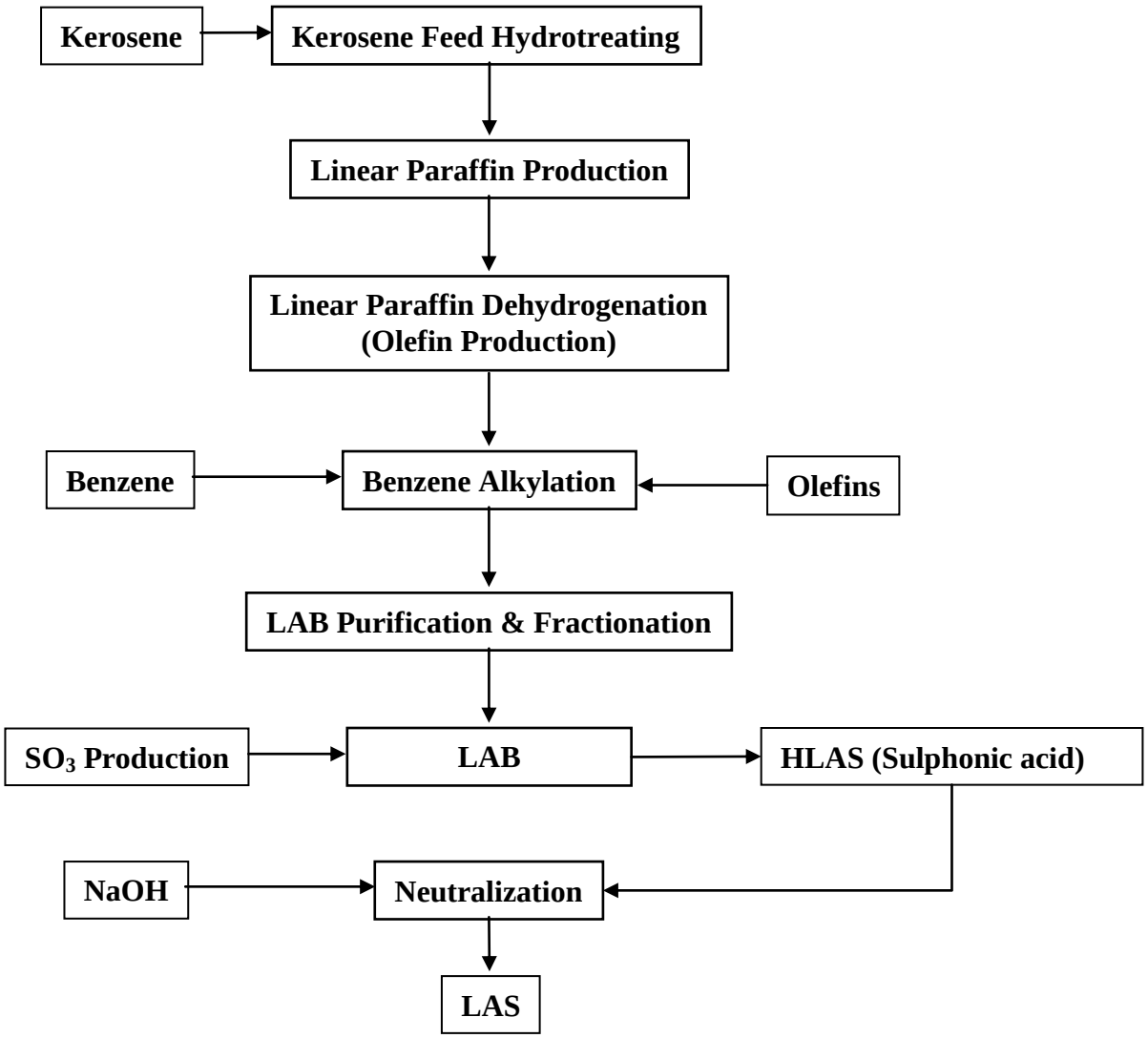
LAB, the precursor of LAS, is manufactured in large scale industrial processes by alkylating benzene with linear mono-olefins or alkyl halides such as chloro-paraffins by using HF or $AlCl_3$ as the alkylation catalyst (Cavalli et al., 1999b), and recently also over heterogeneous solid super-acids in a fixed-bed reactor (Erickson et al., 1996). LAB production quality, as measured by its bromine and colour indexes as well as by impurities and alkyl chain linearity, has been enhanced over time following significant technological improvements (Marr et al., 2000). Alkylation with $AlCl_3$ was the first commercial process used in the mid 60s when branched dodecylbenzene (DDB) was replaced by LAB. At the end of the 60s the HF technology was applied for the first time and immediately it became the preferred technology to be installed in the world to produce LAB.

In the mid 90s a new alkylation technology based on heterogeneous catalyst in a fixed-bed reactor, Detal®, appeared on the market (Berna et al., 1994) and was rapidly adopted, as testified by several new units recently installed with this technology. The new technology offers considerable advantages over the old ones, namely: process simplification, elimination of acids handling and disposal (HF, HCl) as well as an overall production yield improvement and improved LAB quality.
Production of commercial LAS involves a series of processes as shown schematically in the below scheme.

Total LAB world production capacity in the year 2005 is estimated to be more than 3 million tons, with a split by technology as follows: 75 % HF, 5% $AlCl_3$, and 20 % fixed-bed. In Europe, in the year 2005, the estimated installed LAB capacity was around 600 kt/y with a corresponding demand of 325 kt/y (ECOSOL, 2005; CESIO, 2005).

The result of sulphonating LAB is the formation of alkylbenzene sulphonic acid, which has the consistency of a liquid with a high active content, >97% by titration with hyamine (ISO 2271; EN 14480), containing about 1% of unsulphonated matter and 1-2% of H_2SO_4 (IUCLID, 1994; Schönkaes, 1998). It represents commercially the most important supply form. The acid is then neutralised with a base to give the final LAS surfactant salt. Sodium neutralised LAS is by far the predominant grade. As salt, it can also be supplied in various forms and active contents, for example as paste (50-75%) and powder (80-90%) (Schönkaes, 1998).

Processing Steps in LAB-LAS Production



3.4. Consumption scenario in Europe

The most recent and realistic market survey was completed by the Ecosol companies (ECOSOL, 2005), which estimated a total consumption tonnage of about 430 kt for the year 2005, with a breakdown by household applications of about 350 k, corresponding to more than 80% of the total according to an independent survey of AISE companies.

Table 3: Tonnage consumption estimates of LAS in Europe in 2005

Survey	Total kt	Household Kt
ECOSOL	430	350 (>80% vs. total)

The present focused risk assessment models the use of the highest realistic LAS figure available for the household products, namely 350 kt/y. In addition, the reported monitoring data, related to total

tonnage consumption and degradation in the environment, have been used in the final higher tier risk assessment.

3.5 Use application summary

Most of LAS European consumption is in household detergency (>80%). Important application products are laundry powders, laundry liquids, dishwashing products and all purpose cleaners. The remainder of the LAS (<20%) is used in Industrial and Institutional (I&I) cleaners, textile processing as wetting, dispersing and cleaning agents, industrial processes as emulsifiers, polymerisation and in the formulation of crop protection agents.

4. Environmental risk assessment

The extensive body of research studies on the environmental properties of LAS present in the literature is reported below.

4.1 Environmental exposure assessment

4.1.1 Biotic and abiotic degradability

Aerobic biodegradation in aqueous medium

LAS primary biodegradation is the transformation induced by microorganisms with formation of sulpho phenyl carboxylates (SPCs) as biodegradation intermediates (Swisher, 1987). This biodegradation stage corresponds to the disappearance of the parent molecule and to the loss of interfacial activity and toxicity towards organisms present in the environment (Kimerle et al., 1977; Kimerle, 1989). The change of the interfacial activity of the surfactant during biodegradation has much more importance on the aquatic toxicity than the biodegradation as measured, for example, by the biological oxygen demand (BOD); that was shown by a recent detailed study on the relation between interfacial activity and aquatic toxicity during primary LAS biodegradation (Oya et al., 2010).

Biodegradation proceeds further with i) the cleavage of the aromatic ring and the complete conversion of LAS and SPCs into inorganic substances (H_2O, CO_2, Na_2SO_4) and ii) the incorporation of its constituents into the biomass of micro-organisms (ultimate biodegradation) (Karsa et al., 1995).

One of the first evidences that the alkyl and ring portions of LAS can extensively biodegrade and convert to CO_2 in the environment was shown in a STP simulating laboratory equipment using a ^{14}C ring-labelled commercial product and some pure unlabelled homologues (Nielsen and Huddleston, 1981). The primary biodegradation of LAS, measured by MBAS (Methylene Blue Active Substance) or by specific analytical methods such as HPLC (High Performance Liquid Chromatography), in any OECD tests (OECD, 1993), is >99% (EU Commission, 1997). The ultimate biodegradation measured by DOC (Dissolved Organic Carbon) is in a range going from 80% to >95% for CAS (Continuous Activated Sludge) simulation tests (OECD 303 A), and in the 95-98% range for inherent tests (OECD 302) (EU Commission, 1997).

CAS simulation tests (OECD 303 A) were run for the commercial LAS product in the 9-25°C temperature range (Prats et al., 2003). The acclimation lag phase was significantly different at the various temperatures, being longer at lower temperatures. The percent LAS removal measured by MBAS and HPLC, however, was always similar and high (>95%) in all cases, indicating that the

microorganism community can also reach a proper acclimation and that kinetics are also adequate at low temperatures (Prats et al., 2006; Leòn et al., 2006). These results are in agreement with some stream mesocosm studies which concluded that the mineralization of surfactants under realistic environmental conditions, where various algal species are acclimated following natural temperature fluctuations, was at least maintained and often increased during significant seasonal decreases in temperature (Lee et al., 1997).

The commercial LAS product is readily biodegradable (EU Commission, 1997). The 10-day window is not deemed necessary for assessing ready ultimate biodegradability of surfactants in detergents (CSTEE, 1999). However, in the literature LAS is reported to pass the 10-day window rule as shown by: i) a comparative CO_2 evolution study (Ruffo et al., 1999; Anon, 2002), ii) OECD 301 F tests following the biodegradation by O_2-consumption and specific C_{12}LAS analysis (Temmink et al., 2004) and iii) recent tests run according to the GLP principles, namely, CO_2 evolution test following OECD 301B (LAUSa, 2005), DOC die-away test following OECD 301A (LAUSb, 2005) and mineralization under ISO 14593/1999 test in compliance with the Detergent Regulation 648/2004 (Lòpez et al., 2005). The formation of persistent biodegradation intermediates can be excluded as demonstrated by high tier tests (Gerike et al., 1986; Moreno et al., 1991; Cavalli et al., 1996b). Biodegradation intermediates, i.e. the sulpho phenyl carboxylates (SPCs), are not persistent and their toxicities are several orders of magnitude lower than that of the parent molecule (Kimerle et al., 1977).

Considering the absence of persistent metabolites and the relatively low toxicity of the transient degradation products, the rate of primary biodegradation, rather than that of the ultimate biodegradation is the relevant parameter for risk assessment purposes. Specific analytical methodologies based on High Performance Liquid Chromatography (HPLC), Gas Chromatography/Mass Spectrometry (GC/MS) and Liquid Chromatography/Mass Spectrometry (LC/MS) have been developed for LAS, which provided kinetic data relevant for exposure assessments (Matthijs et al., 1987; Trey et al., 1996; Di Corcia et al., 1999). Relevant kinetics of LAS biodegradation were obtained in a die-away laboratory test applying innovative testing procedures to radio-labelled materials, measuring $^{14}CO_2$ evolution by Liquid Scintillation Counting (LSC) and following the biodegradation by Radio Thin-layer Chromatography (RAD-TLC) (Federle et al., 1997). In these studies, using river water as test medium, the primary biodegradation rate was approximately $k = 0.06\ h^{-1}$ ($t_{0.5}$ = ca.12 h) (Itrich et al., 1995) and about 10-15 times lower than that found using activated sludge as test medium (Federle et al., 1997).

Field studies (further described in Section 4.1.3), carried out in some rivers under realistic environmental conditions specifically to measure in-stream removal kinetics of LAS, showed $t_{0.5}$ in the 1-3 h range indicating that kinetics are faster than those displayed in laboratory studies (Takada et al., 1992; Schröder, 1995; Fox et al., 2000),. This is due to the more favourable biodegradation conditions in the real environment vs. those reproduced in laboratory.
Considering the above available field data, **a protective primary biodegradation half-life of 3 hours in aqueous medium was considered in the present risk assessment.**

Biodegradation under anaerobic conditions
Results with Standard Tests that Model Anaerobic Sludge Digesters
In the existing laboratory screening and simulation tests (ECETOC, 1994; OECD TG 307, 2002; OECD TG 308, 2002; OECD TG 311, 2006; ISO 11734: 1995; ISO 13641-1,-2: 2003), which are extensively reviewed in literature (ERASM, 2007; Berna et al., 2007; Berna et al., 2008), ultimate biodegradation was measured by determining the final gas production (CO_2 and CH_4) after about two months of incubation. In these studies LAS did not show any significant biodegradation (Steber et al., 1989; Steber, 1991; Federle et al., 1992;; Gejlsbjerg et al., 2004; Garcìa et al., 2005).

Another approach has been recently proposed to assess the anaerobic biodegradation of substances as they relate to sewage treatment. This approach is based on OECD guideline (OECD TG 314, 2008). This standard describes an analytical procedure made by a set of five separate but complementary simulation tests, which assess the primary and ultimate biodegradation of chemicals in the sewer wastewater, in the secondary treatment of the activated sludge system, in the anaerobic sludge digester, in the treated effluent and surface water mixing zone, and in the untreated wastewater directly discharged to surface water. The third test (test C) evaluates biodegradation during anaerobic sludge digestion, in particular aims to demonstrate whether chemicals have the potential for anaerobic biodegradation or not. LAS has been tested with this method: results confirm the absence of anaerobic biodegradation (Procter & Gamble, 2008).
Conclusion: LAS does not pass standard tests for anaerobic biodegradation. These tests model anaerobic sludge digesters. The lack of LAS biodegradation in these tests is consistent with the lack of LAS biodegradation noted in anaerobic sludge digesters. Nonetheless, some studies suggest that LAS can biodegrade under anaerobic conditions, but low bioavailability prevents any substantial biodegradation in wastewater treatment plant reactors (Angelidaki et al., 2000a; Mogensen et al., 2003). LAS anaerobic biodegradation has been demonstrated under laboratory and field conditions using other test methods (see below).

Risk Perspective
The preferred method for disposal of sewage sludge is use as a soil fertilizer. The following information is relevant when considering the fate of LAS in sludge-amended soil:

1) Biodegradation under strict anaerobic conditions was shown to have little direct ecological relevance (Heinze et al., 1994; ERASM 2007) and are not formally considered in the EUSES modelling program (see 4.1.4).
2) In oxygen-limited conditions, which occur in the real world, LAS biodegradation can initiate and then continue in anaerobic conditions (Larson et al., 1993; Leon et al., 2001).
3) Field testing takes precedence over simulation test data. There is a very significant amount of field monitoring data available for LAS in agricultural soils (Jensen et al., 2007; Schowanek et al., 2007)

In addition, the opinion of the Scientific Committee on Health and Environment Risks (SCHER), a committee of experts who serve an advisory role within the European Commission (EC), on the environmental risk posed by detergent surfactants that are poorly biodegradable under anaerobic conditions, such as LAS, is as follows:…"A poor biodegradability under anaerobic conditions is not expected to produce substantial modifications in the risk for freshwater ecosystems as the surfactant removal in the STPs seems to be regulated by its aerobic biodegradability" (SCHER, 2005). This statement was again confirmed by SCHER in its opinion of 2008: "The LAS-HERA report of 2004 contained no recent publications which affected the conclusion of SCHER in its opinion of 2005. Similarly recent publication, later than 2004 (Garcia et al., 2005; Garcia et al. 2006a and b; references cited in LAS-HERA report of 2007), did not give grounds for any change of that opinion" (SCHER, 2008).
As a consequence, the requirement of ultimate biodegradability under anaerobic conditions cannot be considered an effective measure for environmental protection.

A specific risk assessment in anaerobic environments would include effects on anaerobic bacteria in anaerobic digesters. It has been shown that LAS at concentrations up to 30 g/kg_{dw} sludge does not affect the microbial processes in these digesters (Berna et al., 1989). The LAS effect on the anaerobic sludge digestion process was investigated showing that toxicity on the anaerobic microorganisms depended on the concentration of the bioavailable LAS homologues in the liquid phase of the STP anaerobic digesters; an EC_{50} of 14 mg/l was calculated (Garcìa et al., 2006b). Poor

primary LAS degradation in anaerobic discontinuous systems was confirmed showing also that the inhibition extent of the biogas production was significantly related to the sludge used as inoculum (Garcìa et al., 2006a).

Results with Other Test Methods, Other Anaerobic Digesters and Tests that Model Other Environmental Compartments

Consideration of the LAS structure suggests that it should be anaerobically biodegradable. First, the LAS structure consists of a sulfonate group attached to the aromatic ring. Certain bacteria are capable of biodegrading such compounds and using them as a sole sulphate source. This has been demonstrated for LAS (Denger et al., 1999).

In addition, LAS has a long alkyl chain (C_{10}-C_{13}). Long alkyl chains are known to be anaerobically biodegradable by sulphate-reducing, denitrifying and methanogenic bacterial communities (review in Wentzel et al., 2007). LAS anaerobic biodegradation has been reported in the following studies:

1) In a modified standard test for anaerobic biodegradation, loss of parent LAS is observed after several months of incubation (Prats et al., 2000a).
2) In continuous stirred tank (CST) reactors, 14-25% biodegradation is observed (Angelidaki et al., 2000b; Haggensen et al., 2002)
3) In upflow anaerobic sludge blanket (UASB) reactors, 5-44% biodegradation is observed (Sanz et al., 1999; Mogensen et al., 2003).

The most complete set of experiments demonstrating LAS anaerobic biodegradation is on sulphate-reducing marine sediments (Lara-Martin et al., 2007; Lara-Martin et al., 2008; Lara-Martin et al, 2010). Laboratory experiments, performed on anoxy marine sediments spiked with 10-50 ppm of LAS, showed that degradation is feasible, reaching a value of 79% in 165 days, with a half-life time of ca. 90 days. The anaerobic process was also observed in the field with several marine sediment samplings at anoxy depths in the sedimentary column. LAS concentrations in pore waters decreased sharply and the biodegradation intermediates (SPC) reached the maxima. These observations provide the first real evidence of partial degradation of LAS under anaerobic conditions (Lara-Martin et al., 2007; Lara-Martin et al., 2008). A more recent paper claimed to provide for the first time an anaerobic biodegradation bathway for LAS (Lara-Martin et al., 2010).

Biodegradation in soil

Several measurements of LAS in sludge-amended soil from both laboratory and field studies have been carried out and are reviewed in the literature (De Wolf et al., 1998; Jensen, 1999; Cavalli et al., 1999a). These investigations were performed, after application of sludge containing LAS to soil usually at rates higher than that recommended in agriculture, maximum 5 t DS (Dry Solids)/ha/y (TGD, 2003). For example, the annual sludge spreading averaged 6 t/ha in the UK (Holt et al., 1989; Waters et al., 1989), 32 t/ha in Spain (Berna et al., 1989; Prats et al., 1993), 13.5 t/ha in Switzerland (Marcomini et al., 1988) and 6 t/ha in Germany (Matthijs et al., 1987). In all these studies the calculated LAS removal corresponded to half lives in the range of $t_{0.5}$= 3-33 days.

The most reliable results in the laboratory were obtained by investigating mixtures of sludge and LAS-spiked soils using ^{14}C materials, measuring ultimate biodegradation. LAS mineralization rates corresponding to $t_{0.5}$ = 13-26 days (Figge and Schöberl, 1989) and $t_{0.5}$ = 7.0-8.5 days (Gejlsbjerg et al., 2001) were estimated. Mineralization with $t_{0.5}$ = 2.1-2.6 days was obtained after a lag time of 1.9-2.5 days at 10 mg/kg_{dw} LAS concentration in soil, which is the highest expected environmental concentration of the surfactant in an agricultural land (Gejlsbjerg et al., 2003).

Laboratory sludge-soil mixtures with ^{14}C-labelled LAS at concentrations in the $\mu g/kg_{dw\ soil}$ range, corresponding to predicted steady concentrations (at least after a waiting period of 30 days from sludge application) of the surfactant in sludge-amended soil, were also investigated (Gejlsbjerg et

al., 2004). After relative long lag times (ca. 2 weeks), LAS was mineralized rapidly and extensively showing two phase kinetics: a first rapid mineralization ($t_{0.5}$ = ca. 2 days) followed by a slow mineralization phase ($t_{0.5}$ = 7.9 days), the latter likely governed by sorption and desorption processes in the soil. Even subsurface soils, sampled below a septic system drain field and investigated in laboratory sorption and biodegradation studies using groundwater and radiolabeled materials, showed to have the potential to mineralize LAS (ultimate $t_{0.5}$ from 0.32 to 8.7 d) (Doi et al., 2002). Other LAS leaching properties in soils and groundwater were investigated to develop a mathematical model for septic systems to predict the fate and transport of consumer product ingredients (McAvoy et al., 2002).

However, most laboratory studies and all field monitoring studies in sludge-amended soil measure the disappearance of LAS, estimating, thus, the primary biodegradation.

In the laboratory tests it was shown that for soil spiked with aqueous LAS and LAS-spiked sewage sludge, the disappearance (primary biodegradation) of the surfactant was more than 73% after 2 weeks (Elsgaard et al., 2001b). A soil mesocosm study showed that the primary degradation of LAS was rapid with $t_{0.5}$ of 1-4 days (Elsgaard et al., 2003). A field study, at sludge application rates close to those recommended in agriculture (equal or below 5 t_{dw}/ha/y), estimated $t_{0.5}$ values in the range of 3-7 days (Küchler et al., 1997).

Accurate data for degradation of LAS in sludge-amended soil under realistic field conditions were reported by Mortensen et al., 2001. Its degradation in soil increased by the presence of crop plants with soil concentrations decreasing from 27 mg/kg_{dw} to 0.7-1.4 mg/$kg_{dw\ soil}$ at harvesting time after 30 days ($t_{0.5}$ <4d).
Considering the above available field data**, a conservative protective primary biodegradation half-life of 7 days in agricultural soils was considered in the present risk assessment.**

Hydrolysis and photolysis degradation
Reactions of hydrolysis (Cross, 1977) and photolysis (Matsuura et al., 1970; Venhuls et al., 2005) of LAS are described in literature (Table 4) in conditions not relevant to the environment. The corresponding results are, thus, not considered in the present assessment.

The set of data on LAS biodegradation properties relevant to this risk assessment are summarized in Table 4.

Table 4: Biodegradation properties

LAS	Protocol	Results	References
Screening, confirmatory	OECD 301 D OECD 303 A	>99 (% primary biod.)*	EU Commission, 1997
Ready test	OECD 301 A, B, D, E, F ISO 1493/1999	Readily biodegradable >70 (% DOC removal) >60 (% CO_2 evolution) >60 (% O_2 uptake)	EU Commission, 1997 Ruffo et al., 1999 Temmink et al., 2004 LAUS, 2005a-b Lòpez et al.,2005
Inherent test	OECD 302 A, B	95-98 (% DOC removal)	EU Commission, 1997
Simulation test	OECD 303 A	80->95 (% DOC removal)	EU Commission, 1997

Biodegradation rate in activated sludge	Die-away	$t_{0.5}$ = 0.6-0.7 h (prim. biod.) $t_{0.5}$ = 1.3-1.4 h (ultim. biod.)	Federle et al., 1997
Biodegradation rate in river water	Die-away Die-away River monitoring	$t_{0.5}$ = 12 h (prim. biod.) $t_{0.5}$ = 18 h (ultim. biod.) $t_{0.5}$ = 1-3 h (prim. biod.)	Itrich et al., 1995 Itrich et al., 1995 Fox et al., 2000
Anaerobic biodegradation	ECETOC Research study	ca.0 (% ultim. biod.) 5-44 (% prim. biod. in UASB reactors)	AISE/CESIO, 1994 Mogensen et al., 2003
Biodegradation rate in soil	Field study Laboratory study	$t_{0.5}$ = 1-7 d (prim. biod.) $t_{0.5}$ = 2-26 d (ultim. biod.)	Küchler et al., 1997 Elsgaard et al., 2003 Figge et al., 1989 Gejlsbjerg et al., 2001, 2003, 2004
Hydrolysis	Research study	Decomposition: 60-70% in presence of inorganic acids at 150-200°C	Cross, 1977
Photolysis	Research study	Degradation: 80-95% under mercury lamp (200-450 nm)	Matsuura et al., 1970 Venhuls et al., 2005

(*) measured by MBAS and by additional HPLC analysis

4.1.2 Removal

Sewers
LAS removal rates in sewers, due to a combination of biodegradation, adsorption and precipitation, were measured during field studies in different countries up to a degree of 68% (Moreno et al., 1990; Matthijs et al., 1999). Laboratory studies have demonstrated that the concentration of all surfactants can be significantly reduced in sewers, depending on the length of the sewer, travel time and the degree of microbial activity present in the sewer (Matthijs et al., 1995).

Laboratory CAS systems
Accurate confirmatory CAS data, using MBAS and specific analytical methods (such as HPLC) or ^{14}C measurements to determine the LAS removal rate, are available (Schöberl et al., 1988; Cavalli et al., 1996a; Leon et al., 2006). In these tests the removal rate of the parent surfactant was always >99%.

Sewage Treatment Plants
LAS removal in Activated Sludge Sewage Treatment Plants, (as-STPs), has been documented in several studies and found to be mostly in the 98-99.9% range (Berna et al., 1989; Painter et al., 1989; Waters et al., 1995; Cavalli et al., 1993; Matthijs et al., 1999). This elimination efficiency can be further increased when membrane biological reactors (MBR) will become economically available (Terzic et al., 2005). The LAS removal in as-STPs, measured in five European countries, averaged 99.2% (6 records in the range 98.5-99.9%) (Waters et al., 1995) and 99.4% (4 records in the range 98.9-99.9%) (Holt et al., 2003).

Total LAS removal in Trickling Filter Sewage Treatment Plants (tf-STPs), are lower and more variable and were found in the 89.1-99.1% range (24 records) in Europe with an average value of 95.9% (Holt et al., 2003). These values are higher than those reported for tf-STPs in USA where average removals of 83% (Trehy et al., 1996) and 77% (McAvoy et al., 1993) were recorded.
The following proportions are based on as-STP mass balance studies: 80-90% degraded, 10-20% adsorbed onto sludge and about 1% released to surface waters (Berna et al., 1989; Painter et al., 1989; Cavalli et al., 1993; Di Corcia et al., 1994).
For EUSES modelling assessment, Predicted Exposure Concentrations (PECs) were calculated assuming 79% degradation, 20% to sludge and 1% release to water (see 4.1.6).

The dataset of removal rates relevant to this risk assessment are summarised in Table 5.

Table 5: Removal data

LAS	Results	References
Removal in CAS test (%)	>99	Schöberl et al., 1988 Cavalli et al., 1996
Total STP removal (%)	as-STP: 98-99.9 (range) as-STP: 99.2 (arithmetic mean)	Matthijs et al., 1999 Waters et al., 1995
as-STP: degraded (%)	80-90	Berna et al., 1989 Painter et al., 1989 Cavalli et al., 1993 Di Corcia et al., 1994
as-STP: released to water (%)	ca. 1	
as-STP: adsorption into sludge in (%)	10-20	

4.1.3 Monitoring studies
Several monitoring studies on LAS in the different environmental compartments are available in Europe. Here below monitoring data for surface waters, ground waters, sludge, soils and sediments are summarized.

Surface waters
The present aquatic risk assessment refers specifically to the European monitoring project carried out in five different countries (UK, Germany, Netherlands, Spain, Italy), using a common and agreed protocol in the context of the Dutch risk assessment of surfactants (Feijtel et al., 1995b). The results of this multi-years EU monitoring project were consistent with previous monitoring studies (Berna et al., 1989; Painter et al., 1989; Cavalli et al., 1993) and with other recent monitoring programmes in Europe (Holt et al., 2003). The results illustrate well the actual European LAS content in the as-STP effluents and sludge as well as in the corresponding receiving rivers (Schöberl et al., 1994; Di Corcia et al., 1994; Sànchez Leal et al., 1994; Feijtel et al., 1995a; Holt et al., 1995; Waters et al., 1995; Matthijs et al., 1999).

In the EU monitoring study project LAS levels in raw sewage ranged from 1 to 15 mg/l (Feijtel et al., 1995b; Matthijs et al., 1999). In the same EU project LAS effluent concentrations under normal as-STP operating conditions were altogether in the 8-220 µg/l range with an arithmetic mean of 42.8 µg/l (46 records), considering all the available results.

In the receiving waters downstream the above as-STP effluents, just after the mixing zone, the LAS concentration was in the <2-47 µg/l range with an arithmetic mean of 14.2 µg/l (23 records) (Feijtel et al., 1995b; Matthijs et al., 1999). The highest LAS concentration (47 µg/l) would decrease to <2 µg/l in one day, considering a conservative in-stream biodegradation half-life of 3 hours (see par. 4.1.1).

LAS environmental fingerprints in effluent and surface waters differ from the composition of the commercial material. The relative ratio of the various homologues detected in the aquatic environmental samples is as follows: C_{10}:C_{11}:C_{12}:C_{13} = 45:30:23:2 with an average carbon number of 10.8 (Prats et al., 1993; Cavalli et al., 1993; Di Corcia et al., 1994; Tabor et al., 1996). That is a consequence of two processes: i) biodegradation in the water phase which is faster for the higher homologues and ii) adsorption into sediments and suspended solids which is more pronounced for higher homologues.

In another comprehensive European monitoring programme, carried out in the context of the GREAT-ER project (Geography-Referenced Exposure Assessment Tool for European Rivers), thousands of effluent samples from different STPs and samples of river waters were measured in UK for their LAS content over a 2-year period (Holt et al., 2003). All effluents from as-STPs were in the 7-273 µg/l range; those with an additional tertiary treatment were found below 50 µg/l.

In US monitoring studies LAS concentrations in river waters below STP mixing zones were also generally found below 50 µg/l (McAvoy et al., 1993; Trehy et al., 1996; Tabor et al., 1996).
A US study conducted to assess a weight of evidence (WoE) risk of alkyl sulfates (AS), alkyl ethoxy sulfates (AES) and LAS was based on accurate monitoring of STP streams located in 3 different sites (Sanderson et al., 2006). The total LAS concentrations were in the range 2.75-3.96 mg/l in influents, 1.3-2.9 µg/l in effluents and 0.26-3.8 µg/l in the receiving river waters.

A study to evaluate the validity of as-STP fate models was carried out, monitoring the C_{12}LAS concentrations under controlled and well-established conditions in a pilot-scale municipal as-STP. C_{12}LAS concentrations were 2-12 mg/l in influents, 5-10 µg/l in effluents and 37-69 mg/kg_{dw} in the waste aerobic sludge. The removal of the LAS homologue (>99%) was totally ascribed to biodegradation (Temmink et al., 2004).

The tf-STP effluents, on the contrary, have usually higher and more variable LAS concentrations because these plants are not so efficient as the (as)-STPs. BOD_5 removals are in the 85-95% range for tf-STPs (Holt et al., 2000), whereas they are always >95% for as-STPs. tf-STP effluent LAS concentrations, in flow proportional composite samples, were in the 40-430 µg/l range with an average value of 240 µg/l in Europe (Holt et al., 2000; Holt et al., 2003) and up to 1.5 mg/l in the US (Rapaport et al., 1990; McAvoy et al., 1998).

In river waters receiving effluents either from tf-STPs (Fox et al., 2000) or from undersized as-STPs (Gandolfi et al., 2000), LAS was shown to be removed rapidly. Downstream the mixing zones of tf-STP, the LAS concentrations were 0.42-0.77 mg/l and decreased to 72 and 33 µg/l at 4.8 and 3.3 km respectively from the tf-STP outfall (Fox et al., 2000). From an undersized as-STP, LAS concentrations in 24-h composite samples were on average 120 µg/l at the mixing zones and 27 µg/l

at 26 km (Gandolfi et al., 2000). These results indicate that in-stream removal is an efficient process and were used to validate a dynamic quality model to assess the fate of xenobiotics in the river water compartment and benthic sediment (Deksissa et al., 2004).

Other types of discharges, including direct discharges, exist in Europe. Downstream these discharges, higher concentrations of BOD, NH_3, LAS and other contaminants can be monitored. According to some studies (McAvoy et al., 2003; Dyer et al., 2003), the relative in-stream removal of LAS is higher than the removal of BOD and therefore the impact of untreated discharges on the receiving ecosystem is not caused by LAS but rather by low dissolved O_2 and high unionised ammonia.

As recommended by the TGD (TGD, 2003), only monitoring data of river waters receiving effluents from as-STPs, as well as the highest concentrations found in the European monitoring studies, were considered relevant to the present risk assessment.
Conclusion: PEC effluent (PEC_{STP}) = 0.27 mg/l; PEC river waters = 0.047 mg/l.

Ground waters
No LAS monitoring data in ground waters are available for Europe. In samples collected in the USA, LAS concentrations were below the detection limit in several monitored wells drilled in an area near a pond system exposed to high concentrations of detergent chemicals for more than 25 years (Larson, 1989). LAS concentrations in ground waters, 500 m downstream a sewage infiltration, were below the analytical detection limit (<10 µg/l). In one well, using an improved analytical methodology, a maximum LAS concentration of 3 µg/l was recorded (Field, 1992).

Sludge
Measured LAS concentrations in sewage sludge have been reviewed (De Wolf et al., 1998; Jensen et al. 1999; Cavalli et al. 1999; Fraunhofer, 2003; Leschber, 2004 Jensen and Jepsen, 2005; Schowanek et al., 2007). Typical LAS concentrations in aerobic sludge are <0.5 $g/kg_{dw\ sludge,}$ higher LAS concentrations are noted in anaerobic sludge (<1 $g/kg_{dw\ sludge}$ up to 30 $g/kg_{dw\ sludge}$). The highest LAS concentrations in anaerobic sludge (ca. 30 $g/kg_{dw\ sludge}$) were found in one specific Spanish region in the presence of a very high water hardness (>500 mg/l as $CaCO_3$) (Berna et al., 1989). Water hardness data collected by AISE companies are available for Europe and indicate that on average 13% of the European population use water with hardness <70 mg/l, 33% with medium hardness (70-212 mg/l) and 53% with hardness >212 mg/l (Jensen et al., 2006). This high LAS value in Spanish sludge is clearly an outlier.

Although these reports cover LAS concentrations in sludge for a number of wastewater treatment plants in different European countries, they do not represent the situation in one specific country. A comprehensive survey of LAS measurements in aerobic and anaerobic sludge was reported (Jensen and Jepsen, 2005) from the ongoing monitoring program of pollutants in sludge in Denmark. LAS concentrations are annually measured and reported to the Danish EPA for approximately 1,400 waste water treatment plants in Denmark. This survey allowed to derive the Danish LAS distribution in sludge: a mean concentration of 0.24 $g/kg_{dw\ sludge}$ (0.5 to 1.5 $g/kg_{dw\ sludge}$; 5^{th} to 95^{th} percentile) (Jensen et al., 2006).

At the European level, approximate sludge distributions were also calculated based on literature data over the time period 1988-2006 (Schowanek et al., 2007). The result of the distribution of the anaerobic sludges (ca. 155 records) was a mean of 5.56 $g/kg_{dw\ sludge}$ (0.49 to 15.07 $g/kg_{dw\ sludge}$; 5^{th} to 95^{th} percentile), where the highest point in the data set was the already mentioned Spanish value of ca. 30 $g/kg_{dw\ sludge}$, a clear outlier.

The LAS homologue distribution in sludge is approximately in the mole ratio C_{10}:C_{11}:C_{12}:C_{13} = 7:24:39:30 with an average carbon number of 11.9, as a consequence of a preferential adsorption of higher homologues (Berna et al., 1989; Cavalli et al., 1993; Di Corcia et al., 1994).
It is worth taking into account possible differences of LAS concentration in wet sludge, freshly produced at STP, from that in dry sludge, aged and dried before its use in agriculture (several months after). It was found that the LAS concentration in the bulk of dry sludge could drop by 74% compared to that of wet sludge (Carlsen et al., 2002). Removal of LAS from sludge can also effectively be performed by composting systems. This methodology for handling sludge in general was extensively discussed in a workshop in Denmark (SPT/EPA, 1999) and was recognised as a useful method to reduce the level of some xenobiotics. Several composting studies have demonstrated that LAS can be removed (>98%) with half-life of 7-9 days (Petersen, 1999; Prats et al., 2000b; Sanz et al., 2006).
Conclusion: PEC in anaerobic sludge = 5.56 g/kg$_{dw\ sludge}$ (mean 50th percentile) and 15.07 g/kg$_{dw\ sludge}$ (95th percentile).

Soil
Results from several monitoring studies of LAS concentrations in soil are available for various soil types, sludge application rates, and averaging times. For example, concentrations of up to 3.0 mg LAS/kg$_{dw}$ were measured in sludge-amended soil at a sludge application rate of 6 t DS/ha/y for extended periods in the UK and Germany (Matthijs et al., 1987; Holt et al., 1989). LAS concentrations in sludge-amended soils were reviewed concluding that they were generally below 20 mg/kg soil, depending on the application rate or sampling time after sludge application (Solbè, 1999). At sludge application rates less than 5 t/ha/y, 30 days after its application, LAS concentrations in soil are expected to be in the low mg/kg range. With sludge application rates higher than those used in the normal agricultural practice (6-10 t/ha/y), LAS concentration in an experimental field of soil-pots with rapes dropped from an initial measured value of 27 mg/kg$_{dw\ soil}$ to 0.7-1.4 mg/kg$_{dw\ soil}$ in soil at harvest time after 30 days (Mortensen et al., 2001).

A series of soils having a known history of sludge amendment and selected to be typical for Denmark were monitored (Carlsen et al., 2002). In regions where the sludge application was carried out according to the prevailing agricultural rules, the concentration of LAS in all soils was found to be <1 mg/kg$_{dw\ soil}$, well below the soil quality criterion for LAS of 5 mg/kg$_{dw\ soil}$ proposed in Denmark (Jensen et al., 1995). The LAS concentration that can be found in soil at any time after sludge applications, in any case, is always too low to contribute significantly to the mobilization of hydrophobic organic compounds in sludge-amended soil (Haigh, 1996).
Conclusion: PEC in soil = 1.4 mg/kg$_{dw\ soil}$.

Sediments
Available measured LAS data in fresh water sediments were reviewed (Cavalli et al., 2000). Typical LAS values in sediments below sewage outfalls were found in the 0.5-5.3 mg/kg$_{dw\ sed.}$ range with an arithmetic mean of 2.9 mg/kg$_{dw\ sed.}$ (12 records).
Homologue distributions were also measured for some river sediment samples and the corresponding fingerprint was found similar to that of sludge and soils (Cavalli et al., 2000).
Conclusion: PEC in sediment = 5.3 mg/kg$_{dw\ sed.}$.

The set of monitoring data relevant to this risk assessment are summarised in Table 6. The effluent and river data refer to representative EU monitoring studies and to samples collected downstream of (as)-STPs. Most of the data were used in the aquatic risk assessment carried out in the Netherlands (Feijtel et al., 1995b). Sludge and soil data refer to studies developed in the context of the terrestrial risk assessment in Europe (Jensen et al., 2007; Schowanek et al., 2007).

Table 6: Monitoring data

LAS	Results	References
Effluent (µg/l)	as-STP: 8-220 (range) as-STP: 2-273 (range) as-STP: 42.8 (arithmetic mean) as-STP: 1.3-2.9	Feijtel et al., 1995b Holt et al., 2003 Matthijs et al., 1999 Sanderson et al., 2006
River water (µg/l)	down as-STP: <2-47 (range) down as-STP: 14.2 (arithmetic mean) down as-STP: 0.3-3.8	Feijtel et al., 1995b Matthijs et al., 1999 Sanderson et al., 2006
Ground water (µg/l)	0-3	Field et al., 1992
Anaerobic sludge ($g/kg_{dw\ sludge}$)	5.56 (median 50th percentile) 0.49-15.07 (5th to 95th percentile)	Schowanek et al., 2007
River sediment ($mg/kg_{dw\ sed.}$)	<1-5.3 (typical range) 2.9 (arithmetic mean)	Cavalli et al., 2000
Soil ($mg/kg_{dw\ soil}$)	0.7-1.4, measured at harvest time (30 d) <1, typical agricultural value	Mortensen et al., 2001 Carlsen et al., 2002

4.1.4 Exposure modelling: scenario description

The HERA environmental risk assessment of LAS is based on the Technical Guidance Document for new and existing substances (TGD, 2003). At screening level it makes use of the EUSES programme (EUSES, 2008) to calculate the local and regional exposure to LAS. The total estimated LAS tonnage of 330 kt/y was assumed to follow the down-the-drain pathway to the environment.

The production and formulation releases at local level were not considered because they fall outside the scope of HERA. For the calculation, the HERA exposure scenario was adopted; this scenario assigns 7% of the EU tonnage to the standard EU region, instead of the TGD default 10%, and a factor of 1.5, instead of the TGD default factor of 4, to increase the emissions at local level. These changes introduced by HERA more realistically represent the regional emissions and the local input of substances used in household detergents, as experimentally demonstrated (Fox, 2001). More details and justification of this modification can be found in chapter 2.6 of the HERA methodology document (www.heraproject.com).

Table 7: HERA exposure scenario

LAS	HERA scenario
Total yearly LAS use in household (HERA scope), kt	350
LAS continental usage going to standard EU region, %	7
Increase factor for local usage	1.5

4.1.5 Substance data used for the exposure calculations

The essential input data used for exposure calculations following the TGD and EUSES are derived from Table 2, 3, 4, and 5, and are summarized in Table 8.

The biodegradation rate in STP is the default value as assumed by TGD for readily biodegradable substances. It should be noted that this rate is not used in the assessment, as the Simple Treat output is overridden by experimental removal data. K_{ow} is also not considered in the calculations, which are rather based on K_{oc}.
The biodegradation rates in water and soil are experimentally measured values as reported in Table 4, whereas the biodegradation rates in aerated sediments and in bulk sediments are the default values as suggested in TGD (TGD, 2003).

The (as)-STP data, as measured by mass balance results and reported in Table 5, are the most protective ones for all environmental compartments. For the fraction to sludge, the extreme high value of the range, namely 0.20, was employed (see 4.1.2).

Table 8: Data for exposure calculations

General name	Linear Alkylbenzene Sulphonate (LAS)	References
Description	$(C_{11.6}H_{24.2})C_6H_4SO_3Na$	-
CAS No.	68411-30-3	-
EINECS No.	270-115-0	-
Average molecular weight (g/mole)	342.4	-
Melting point (°C)	277	SIDS, 2005
Boiling point (°C)	637	SIDS, 2005
Vapour pressure at 25 C° (Pa)	$3 \cdot 10^{-13}$	Lyman, 1985
Water solubility (g/l)	250	IUCLID, 1994
Henry's constant ($Pa \cdot m^3$/mole)	$6.35 \cdot 10^{-3}$	Meylan et al., 1991
Octanol-water partition coefficient, log K_{ow}	3.32	Feijtel et al., 1995b
Organic carbon-water partition coefficient, K_{oc} (l/kg)	2500	Feijtel et al., 1999
Biodegradation rate in STP	$k = 1\ h^{-1}$ ($t_{0.5} = 0.693$ h)	EU Commission, 1997
Biodegradation rate in river water (primary)	$k = 0.23\ h^{-1}$ ($t_{0.5} = 3$ h)	Fox et al., 2000
Biodegradation rate in soil (primary)	$k = 0.1\ d^{-1}$ ($t_{0.5} = 7$ d)	Küchler et al., 1997
Biodegradation rate in oxic sediments	$k = 0.1\ d^{-1}$ ($t_{0.5} = 7$ d)	TGD, 2003
Biodegradation rate in bulk sediments	$k = 0.01\ d^{-1}$ ($t_{0.5} = 70$ d)	TGD, 2003
STP removal (%)	99	Waters et al., 1995 Berna et al., 1989 Painter et al., 1989 Cavalli et al., 1993 Di Corcia et al., 1994
Fraction to air by STP	0	
Fraction to water by STP	0.01	
Fraction to sludge by STP	0.20	
Fraction degraded in STP	0.79	

4.1.6 PEC calculations

Column A of Table 9 reports values calculated by EUSES v2.1 (EUSES, 2008) on the basis of data in Table 7 and 8, according to the HERA scenario, considering the tonnage used in household applications (350 kt/y). In-sewer removal (50%) was not taken into account in this calculation.

Column B of Table 9 was not obtained by modelling but by using monitoring data. The values given are the high concentrations of the (as)-STP related monitoring findings in each environmental

compartment, as presented in Table 6. The concentrations listed in column B can, thus, be considered the worst-case PEC of a realistic exposure scenario, excluding, as already said in 4.1.3, data related to (tf)-STPs and other discharges where LAS concentrations are only a marker of poor organic matter removal (McAvoy et al., 2003; Dyer et al., 2003). Data in the aquatic compartment are based on the monitoring results of the European project (Matthijs et al.,1999) and supported by the high tier modelling exercise of the GREAT-ER project (Fox et al., 2000; Holt et al., 2003).

The results of scenario A (modelling) and B (monitoring) are within a factor of 2 for all the environmental compartments except for soil. LAS, however, biodegrades during sludge storage, transport and the waiting period (several months) before its application to soil (Carlsen et al., 2002). A conservative degradation rate of 50% for the pre-application period would lead to a calculated soil concentration of 2.8 mg/$kg_{dw\ soil}$, closer to the highest measured ones (1.4 mg/$kg_{dw\ soil}$).

Table 9: Calculated environmental LAS concentrations

	A Modelling of household LAS usages	B LAS monitoring data
Local conc., influent, mg/l	23.7	**15**
Local conc., effluent, (PEC in STP), mg/l	0.237	**0.27**
Local conc., sludge, g/$kg_{dw\ sludge}$	12.1	**5.56** (50^{th} percentile) **15.07** (95^{th} percentile)
Local PEC in water, mg/l	0.027	**0.047**
Local PEC in soil (30 d), mg/$kg_{dw\ soil}$	10.9	**1.4**
Local PEC in sediment, mg/$kg_{dw\ sed.}$	1.51	**5.3**
Regional PEC in water, mg/l	0.004	-

The monitoring data presented in column B were used in the risk assessment.

4.1.7 Bioaccumulation potential

The purpose of the estimation of bioconcentration is to assess whether there is any potential for the chemical to accumulate in organisms to a high degree and hence, for further transfer up the food chain.

In the absence of measured data, the bioconcentration potential for fish, based on the lipid solubility characteristics of chemicals can be estimated based on QSARs (Quantitative Structure Activity Relationships). Due to the relationship between the bioconcentration of a chemical and its lipophilicity it is possible to predict the BCF for a particular organic compound from its octanol/water partition coefficient (K_{ow}). However, bioconcentration predictions based on K_{ow} are restricted to chemicals with a log K_{ow} <3 and >7. Such predictions are not applicable to surfactants because of their surface active properties. It must be also born in mind that bioconcentration is not a solely hydrophobicity/diffusion-driven process, and as such organismal (ADME) processes, i.e. Absorption, Distribution, Metabolism, Excretion, should as well be considered. Chemicals with a high molecular weight (MW >700) and certain molecular sizes (length, cross sectional diameters) are not likely to cross the biological membranes and therefore their bioconcentration in fish will be limited. Similarly, chemicals which can be metabolized (biotransformed) by an organism will not bioconcentrate to the extent that would be expected if diffusion was the only process involved. Reliable alternative methods already exist and are being further developed to estimate in vitro the absorption and biotransforrmation potential of chemicals in fish. These methods will finally limit the cost of in vivo bioconcentration tests on thousands of chemicals.

Early experimental studies on bioconcentration of LAS were not appropriate because of the analytical methods based on radio-analysis, which consistently overestimated the parent concentration present in the aquatic organism and consequently the true bioconcentration (reviewed by Tolls et al., 1994).

An in depth research project on bioconcentration of surfactants was completed and concluded that LAS is not bioaccumulative, likely due to biotransformation (metabolic) processes taking place in the fish, and therefore doesn't transfer through the aquatic food chain (Tolls, 1998).

LAS was studied employing a flow-through test system, in line with the OECD guidelines, using *Pimephales promelas* as test fish. Single homologue and isomer representatives of the commercial LAS were synthesised and then tested, determining their uptake and elimination rates in fish. Specific HPLC analysis in the water phase and in the fish body showed that LAS reaches a steady state concentration in the fish body in about 3 days. Biotransformation contributes to more than 40% of the elimination as shown for the C_{12}-2-LAS homologue (Tolls et al., 2000). BCF data for the tested LAS standards ranged between 2 l/kg (6-phenyl C_{10}LAS) to 990 l/kg (2-phenyl C_{13}LAS), allowing calculating the potential BCF of any LAS mixture (Tolls et al., 1997). BCFs were also calculated for the commercial LAS ($C_{11.6}$ alkyl chain length) and a representative sample found in river water ($C_{10.8}$ alkyl chain length, see 4.1.3). The respective BCFs were 87 l/kg and 22 l/kg, indicating that the bioconcentration potential of LAS is low and is decreased by environmental processes such as biodegradation and absorption (Tolls, 1998).

This has been confirmed recently by Dyer et al. (2008) and ERASM reports (www.erasm.org/study.html) evaluating the feasibility of *in vitro* assays with surfactants, including C_{12}LAS as prediction tools for their biotransformation and, hence, bioconcentration potential. All fish liver *in vitro* systems investigated are capable of transforming rapidly C_{12}LAS. The immortalised hepatocytes are less effective as immortalised cells and tend to loose much of their specific activity. It can be concluded that biotransformation (metabolic) processes in the fish are contributing to the lower than predicted bioconcentration potential of LAS in fish.

Pimephales promelas and three invertebrates species were caged in streams during a C_{12}LAS model ecosystem experimental study (Versteeg et al., 2003). Total C_{12}LAS BCFs for the investigated species ranged from 9 to 116 l/kg. In general, bioconcentration was affected by isomer position, exposure concentration, and species. BCF values tended to decrease as isomer position moved from external (e.g., 2-phenyl) to internal (e.g., 5,6-phenyl). BCFs also decreased as exposure concentration increased. BCFs for *Lumbriculus variegatus* exposed to freshwater sediments spiked with the C_{12}-2-LAS homologue were measured and found in the range 0.5-4.7 l/kg depending on the sediment organic content (Mäenpää and Kukkonen, 2006).
Bioconcentration potential estimation: i) ca. 87 l/kg for commercial LAS mixture ($C_{11.6}$ alkyl chain length); ii) ca. 22 l/kg for LAS in river water ($C_{10.8}$ alkyl chain length).

4.2 Environmental effects assessment

4.2.1 Ecotoxicity

The toxicity database of the present LAS risk assessment basically refers to that used in the risk assessments carried out for the aquatic compartment in the Netherlands (AISE/CESIO, 1995; Van de Plassche et al., 1999a) and to that used in a revisited risk assessment for the terrestrial environment (Jensen et al., 2007).

Robust summaries and validity ratings based on Klimisch scores have been validated for all studies during the compilation of this risk assessment and are available (www.lasinfo.org).

4.2.1.1 Aquatic ecotoxicity

The toxicity database for LAS (Kimerle, 1989; SDA, 1991; Painter, 1992; IPCS, 1996) is very rich and well documented. A comprehensive review of environmental information for the aquatic compartment that includes all data of the above mentioned literature is the BKH report (BKH, 1993). This report collects 749 records of toxicity data for LAS, specifically collated for an aquatic environmental risk assessment in the Netherlands (AISE/CESIO, 1995; Feijtel et al., 1995b; Van de Plassche et al., 1999a). The database covers several taxonomic groups; intra- and inter-species variability is large, particularly in case of algae. The reason is due to the fact that data refer to different individual compounds and mixtures of LAS and also to differences in test design as well as to the large range of species sensitivity.

In the aquatic environment, different homologues and isomers are present. Each of these components has a different degree of ecotoxicity, with the shorter chain lengths being less toxic than the longer ones. This trend is illustrated in Table 10, where geometric means of experimental aquatic toxicities of LAS homologues as extracted from the BKH review (BKH, 1993: list 12) are compared for two organisms, an invertebrate (*Daphnia magna*) and a fish (*Pimephales promelas*).

Table 10: Average measured aquatic toxicity (mg/l) of LAS homologues (BKH, 1993)

Alkyl chain	Invertebrate (*Daphnia magna*)		Fish (*Pimephales promelas*)	
	EC_{50}	NOEC	LC_{50}	NOEC
C_{10}	16.7 (7)	9.8 (2)	39.6 (4)	14 (1)
C_{11}	9.2 (17)	-	19.8 (4)	6.4 (3)
C_{12}	4.8 (37)	0.58 (7)	3.2 (9)	0.67 (3)
C_{13}	2.35 (20)	0.57 (1)	1.04 (10)	0.1 (1)
C_{14}	1.5 (13)	0.1 (2)	0.5 (3)	0.05 (1)

No. of records in parenthesis

The average chain length of the environmental fingerprint in water of LAS is $C_{10.8}$ (see 4.1.3). However, the actual ecotoxicity of the environmental fingerprint is probably not the same as the ecotoxicity associated with this average structure, because toxicity is not linearly related with chain length. Instead, ecotoxicity increases exponentially with the carbon chain length (see Table 10). Because of that, the contribution to the overall ecotoxicity of the longer (more toxic) homologues is probably more than proportional to their percentage in the fingerprint. Hence, the average structure is expected to be more ecotoxic than the real fingerprint. To take this into account, a toxicity-weighted average structure was calculated as shown in Table 11. To avoid influences of experimental variability, calculated toxicity values, instead of those reported in Table 10, were used for this exercise, obtained by means of QSAR calculations (Könemann, 1981). This resulted in a toxicity weighted average corresponding to a structure of LAS $C_{11.6}$, instead of the original LAS fingerprint average $C_{10.8}$.

Table 11: Toxicity-weighted average structure, LAS $C_{11.6}$

Chain length CL	Homologue % in fingerprint	Calculated LC_{50} (mg/l)	Weight % · $1/LC_{50}$	Weight · CL
10	45	12.48	3.6	36
11	30	4.89	6.1	67.1

12	23	1.91	12.0	144.0
13	2	0.75	2.7	35.1
SUM ⇒			24.4	282.2
Toxicity weighted average structure = SUM (weight · CL) / SUM (weight) ⇒				11.6

The ecotoxicity associated with the $C_{11.6}$ alkyl chain is, thus, expected to be representative of the overall LAS aquatic fingerprint. Below, all reported aquatic ecotoxicity data are related to, or normalised (Könemann, 1981), to this weighted average structure.

Aquatic acute ecotoxicity

Acute toxicity data, selected from the BKH report (BKH, 1993) for the commercial LAS (average carbon numbers near $C_{11.6}$) are summarized in Table 12. *Daphnia magna* and *Pimephales promelas* and *Lepomis macrochirus* were chosen as representative organisms of the toxicity of invertebrates and fish. Data for algae refer to various species. The toxicity values are the geometric means of several records as indicated in parenthesis. However, they were not used directly in the risk assessment, as higher tier data are available.

Table 12: Aquatic acute test results for commercial LAS

Taxon	$IC_{50,}$; EC_{50}; LC_{50} (mg/l) Geometric mean
Algae, IC_{50}	9.1 (n = 12, SD = ±3.9)
Invertebrate (*D. magna*), EC_{50}	4.1 (n = 17, SD = ±2.0)
Fish *(L. macrochirus*), LC_{50}	4.1 (n = 12, SD = ±1.7)
Fish (*P. promelas*), LC_{50}	3.2 (n = 4, SD = ±1.6)

No. of records in parenthesis with Standard Deviations (SD)

Aquatic chronic ecotoxicity

Chronic toxicity data from the BKH report are summarised in Table 13 (BKH, 1993). These long term toxicity data are geometric mean NOEC values obtained over fifteen freshwater species and normalised to the average structure of $LASC_{11.6}$ (Van de Plassche et al., 1999a).

Test durations for algae were 72 to 120 hours, whereas exposure periods of NOECs for crustacean and fish were at least 21 days. The lowest NOEC is that for the fish *Tilapia mossambica* (0.25 mg/l). All known literature data were incorporated and the use of a geometric mean allows deriving sound NOECs, as used in the Dutch risk assessment (Feijtel et al., 1995b). A validity rating of 1 to 2 (Klimisch et al., 1997) can be assigned to all these toxicity data points.

Table 13: Aquatic chronic NOEC data for commercial LAS (BKH, 1993; Van de Plassche et al., 1999a)

Species	End point	NOEC (mg/l) Geometric mean	Range (mg/l)
Chlamydomonas reinhardtii, alga	growth	12 (1)	-
Chlorella kessleri, alga	growth	3.5 (1)	-
Microcystis sp., alga	population density	0.80 (4)	0.05-6.1
Plectonema boryanum, alga	growth	15 (1)	-
Desmodesmus subspicatus, alga	growth	7.7 (4)	0.8-105
Selenastrum sp., alga	population density	3.8 (9)	0.58-17
Ceriodaphnia sp., crustacean	reproduction	3.2 (1)	-
Daphnia magna, crustacean	mobility	1.4 (12)	0.3-6.6
Chironomus riparius, insectum	emergence	2.8 (1)	-

Paratanytarsus parthenogenica, insectum	growth	3.4 (1)	-
Danio rerio, fish	mortality	2.3 (1)	-
Pimephales promelas, fish	mortality and others	0.87 (14)	0.5-4.8
Poecilia reticulata, fish	reproduction	3.2 (1)	-
Oncorhynchus mykiss, fish	-	0.34 (7)	0.23-0.89
Tilapia mossambica, fish	reproduction	0.25 (1)	-

No. of records in parenthesis

Since the outcome of the BKH report in 1993, several new chronic studies have become available. These studies all have Klimish validity ratings of 1 or 2 and NOEC values within the range of values reported in Table 13. The additional studies are summarised below.

Chronic (32 days) toxicity tests of C_{12}LAS to single species (one fish and three new invertebrates), caged in model ecosystem streams, were also obtained (Versteeg et al., 2003). The chronic values, associated to body burden concentrations were: 1 mg/l for the fish *Pimephales promelas*, 0.27, 0.95, and >2.9 mg/l for the invertebrates *Corbicula fluminea, Hyalella azteca* and *Elimia* sp. respectively.

Two aquatic plant (other than algae) studies were conducted. In the first study (Maki, 1981), the chornic toxicity of $C_{11.6}$ LAS to the aquatic macrophyte (*Elodea canadensis*) was determined in a 28 day model ecosystem test. The nominal test concentrations were 0.5, 1.0, 2.0, and 4.0 mg/l and were confirmed by analytical measurements. Growth inhibition was not observed even at highest tested concentration (4 mg/l). Growth throughout the exposure period approximately doubled the initial biomass of the vegetative shoots used at the start of the exposure. Hence, the NOEC was found to be $\geq$4 mg/l. The data are for $C_{11.6}$LAS and no normalization is required.

In the second study (Bishop and Perry, 1981; Bishop, 1980; Van de Plassche et al, 1999a), the duckweed, *Lemna minor*, was exposed to $C_{11.8}$LAS. Endpoints included frond count, dry weight, growth rate and root length after a 7 day exposure period in a flow through study. The measured test concentrations were 0, 2.1, 3.8, 8, 17 and 34 mg/l. The resultant EC_{10} value, based on frond number, was 0.21 mg/l. The EC_{50} value, also based on frond number, was 2.30 mg/l $C_{11.8}$ LAS. Normalizing the EC_{10} of 0.21 mg/l to $C_{11.6}$ LAS results in a final value of 0.30 mg/l.

In a more recent study (Unilever, 2010), fertilized eggs of rainbow trout (*Oncorhynchus mykiss*, formerly *Salmo gairdneri*) were exposed to mean measured concentrations of 0.03, 0.23, 0.35, 0.63, 0.95 and 1.9 mg/l, for 72 days. The responses recorded included the survival of eggs, time to eyed egg stage, time to hatch, survival and final weight of sac-fry (eleutheroembryos), and time and extent of swim-up (external feeding). The lowest NOEC value found was 0.23 mg/l based on survival of eggs exposed from eyed stage, survival of eggs exposed from fertilization, survival of sac fry, and overall survival from fertilization to swim-up. The data are for $C_{11.6}$ LAS and no normalization is required.

Furthermore, a chronic toxicity test (Maki, 1981) with juvenile bluegills (*Lepomis macrochirus*) was conducted on C_{12} LAS. Fish growth was determined after 28 days exposure in a flow-through model ecosystem to measured concentrations of 0, 0.5, 1.0, 2.0, and 4.0 mg/l. Results showed that the growth of juvenile bluegills was not affected at 0.5 and 1.0 mg LAS/l, but was reduced at 2.0 and 4.0 mg/l. At the end of the exposure period, fish at 1.0 mg/l LAS had a biomass of 44 g/m^2 compared to 10.5 g/m^2 for the 2.0 mg/l concentration. Based on these effects on growth rate, the NOEC was 1.0 mg/l.

Model ecosystem studies

A variety of model ecosystem and mesocosm studies have been conducted on LAS. Many of these studies have been evaluated and summarized in two papers (Van de Plassche et al., 1999a; Belanger et al, 2002). NOEC values for standing (lentic) and flowing (lotic) water model ecosystems varied from 0.12 to 3.5 mg/l. The lowest NOEC value (≥0.12 mg/l) was observed in an artificial stream study (Tattersfield et al., 1995, 1996).

In a specific stretch of the studied mesocosm (rifle zone) and after a prolonged exposure (56 days), some data appeared to show an exceptional sensitivity of the *Gammarus pulex* (NOEC = 0.03 mg/l), clearly an outlier in the sensitivity distribution. An ERASM study (ERASM, 2000) has tentatively tried to confirm this sensitivity in a 107 days single species laboratory exposure; the NOEC was significantly higher (0.1 mg/l), but the control mortality was particularly high (22-40%), which indicates that the study was not valid for risk assessment purposes (Klimish reliability score: 3).

The fate and effects of a C_{12}LAS homologue has been studied in an experimental stream facility (ESF) (Belanger et al., 2002). The C_{12}LAS test substance had a high content (35.7%) of its most hydrophobic and toxic 2-phenyl isomer. The 56-day ESF study included a representative community encompassing over 250 taxa. A NOEC of 0.27 mg/l, equivalent to 0.37 mg/l, if normalised to the commercial $C_{11.6}$LAS structure by QSAR calculations (Könemann, 1981), was found. A critical literature review of all mesocosm studies available for LAS (13 studies), including the Tattersfield et. al. studies, was conducted and concluded that a NOEC value of 0.27 mg/l was a reliable and robust value protecting aquatic ecosystems (Belanger et al., 2002). A validity rating of 1 can be applied to this toxicity value (Klimish et al., 1997). This value approximates the LTE (Long-Term Effect) of 0.30 mg/l for LAS present in the DID list (Detergent Ingredient Database) of the European eco-labelling of laundry detergents (EU Commission, 1999).

Table 14: Results of model ecosytem studies for commerical LAS (Van de Plassche et al., 1999a; Belanger et al., 2002)

	Lowest NOEC range (mg/l)
Mesocosm studies	0.12-0.50 (13)

No. of studies in parenthesis.

4.2.1.2 Terrestrial ecotoxicity

A large number of LAS toxicity data, both in laboratory and field, are available for the terrestrial environmental risk assessment. Data refer to the effects of LAS on soil organisms, namely toxicity to soil plants, soil fauna, soil micro-organisms and microbial soil processes (Kloepper-Sams et al., 1996; Jensen, 1999; Jensen et al., 2001; Holmstrup et al., 2001a; Elsgaard et al., 2001a).

Using new standard protocols, updated results were obtained to extend the existing toxicity data and to contribute to an improved terrestrial risk assessment (Krogh et al., 2007; Jensen et al., 2007). All available data were obtained with the commercial LAS (average alkyl chain length of $C_{11.6}$). The soil samples were collected in agricultural field. The soil was coarse with a total C content of about 1.5%, representative of cultivated area in Europe. Considering that the toxicities are mainly driven by the LAS pore water concentration, the same toxicity weighted average as that in water was used for the terrestrial and the sediment effects assessments (see par. 4.2.1.1).

The ecotoxicity of surfactants in the terrestrial environment were recently reviewed: eight groups of the most often used surfactants, representing the three largest classes (anionic, non-ionic and cationic), were selected and studied. Soil toxicity data in general are limited. Only for one group, represented by LAS, a full dataset of toxicity is available. The conclusion reported was: "The risk characterizations estimated for LAS are usually significantly lower than 1, what allows for the

conclusion that the ecological risk of this surfactant in the terrestrial environment is relatively low" (Liwarska-Bizukojc, 2009).

The range of the acute and chronic test results on LAS are summarised in Table 15 and Table 16 respectively. A first terrestrial risk assessment, using data available at the time, was presented and discussed at an international workshop (SPT/EPA, 1999) and at a world surfactant Congress (Lokke et al., 2000; Solbè et al., 2000). The figures presented in Table 15 are indicative of acute effects. They were not directly used in the present risk assessment, as higher tier data are available. The figures in Table 16 are a summary of chronic effects, refer to updated results and are used for a revisited terrestrial risk assessment, as described below (Jensen et al., 2007).

Table 15: Terrestrial acute test results for commercial LAS.

Taxon	Range ($mg/kg_{dry\ soil}$)
Plants, EC_{50}	167 – 316
Soil fauna, EC_{50}	41 - >1000
Micro-organisms, EC_{50}	17 - >1000

Table 16: Terrestrial chronic test results for commercial LAS (Jensen et al., 2007)

Taxon	Range ($mg/kg_{dry\ soil}$)
Plants, NOEC or EC_{10}	52 - 200 (12)
Soil fauna, NOEC or EC_{10}	27 - 320 (9)
Micro-organisms, EC_{10}	<8 - >793 (10)

No. of records in parenthesis.

Terrestrial chronic ecotoxicity

Twenty one laboratory chronic data points for plants and soil fauna are available (Jensen et al., 2007). The values and the most sensitive endpoints for each species are indicated in Table 17. Following multi-peer reviews, a validity rating of 1 (Klimisch, 1997) can be assigned to all these chronic toxicity data.

The twelve data for plants were separated for crop and non-crop species, considering that only the former ones would be exposed to LAS via sludge application. The toxicity data were critically analysed reconsidering and consulting the original works. Toxicity results were calculated using graphical estimations and extrapolations with improved software and methodologies (Jensen et al., 2007).

The nine data for soil fauna were separated according to three classes: Oligochaetes, Insects and Arachnids. These toxicity data are basically the ones reported in the previous terrestrial risk assessment (Jensen et al., 2001) with the exception of the updated results for *Aporrectodea caliginosa, Enchytraeus sp.* and *Folsomia candida* (Krogh et al., 2007). The dataset was combined to develop a final $HC_{5,50}$ of LAS in soil (see par. 4.2.2.2).

As a measure of chronic toxicity, when possible, EC_{10} (equivalent to a no-observed effect concentration) were preferred to NOEC (no-observed effect concentration). A full discussion on the relevance of EC_x in risk assessments has been reported (Bruce and Versteeg, 1992).

The mixture toxicity of LAS with a PAH, pyrene, towards the micro-arthropod *Folsomia sp.* was tested (Holmstrup et al., 1996). No synergistic effects were observed and pyrene bioavailability was not enhanced by LAS in the experiment conditions. According to the authors, LAS is not likely to affect the solubility of PAH in soil at levels below its critical micelle concentration and LAS concentration in soil pore waters are orders of magnitude lower.

Table 17: Plants and soil fauna. Terrestrial chronic toxicity data for commercial LAS (Krogh et al., 2007; Jensen et al., 2007)

Species	Most sensitive end point	Value ($mg/kg_{dw\ soil}$)	
		EC_{10}	Extrapolated NOEC
Plants, non crop species:			
Malvia pusilla	growth	110	-
Solanum nigrum	growth	120	-
Chenopodium album	growth	120	-
Amaranthus retroflexus	growth	110	-
Nigella arvensis	growth	-	52
Galinsoga parviflora	growth	55	-
Plants, crop species			
Brassica rapa	growth	86	-
Avena sativa	growth	80	-
Sinapis alba	growth	200	-
Sorghum bicolor	growth	68	-
Helianthus annuus	growth	116	-
Phaseolus aureus	growth	126	-
Invertebrates: class oligocheates			
Eisenia foetica	growth	277	-
Aporrectodea caliginosa	reproduction	46	-
Enchytraeus sp.	reproduction	27	-
Invertebrates: class insects			
Folsomia fimetaria	reproduction	108	-
Folsomia candida	reproduction	205	-
Isotoma viridis	growth	41	-
Hypogastrura assimilis	reproduction	100	-
Invertebrates: class arachnids			
Hypoaspis aculeifer	reproduction	82	-
Platynothrus peltifer	reproduction	-	320

Ten chronic soil microbial data points (Table 18) are also available (Jensen et al., 2001; Elsgaard et al., 2001a).

Table 18: Microbial parameters. Effect of commercial LAS on micro-organisms and microbial processes in soil (Jensen et al., 2001; Elsgaard et al., 2001a)

Endpoint	Incubation (d)	EC_{10} ($mg/kg_{dw\ soil}$)
Ethylene degradation	0.5	9
Ammonium oxidation	7	<8
Dehydrogenase activity	7	22

ß-Glucosidase activity	7	47
Iron reduction	7	<8
Cellulolytic bacteria	7	11
Cellulolytic fungi	7	<8
Cellulolytic actinomycetes	7	8
Basal soil respiration	1-9	>793
PLFA content	11	>488

Effects of both chemical- and bio-surfactants on soil biochemical processes are extensively reported by review papers in literature. Many beneficial applications in microbial, environmental and agricultural biotechnology, oil processing, enzyme technology and other bioprocessing operations are described (Cameotra et al., 2004; Van Hamme et al., 2006; Muller et al., 2007; Singh et al., 2007).

Some key soil physico-chemical and bio-chemical parameters show to be temporarily affected by sludge amendment of soil (Dunbabin et al., 2006). As to LAS, for example:

- the presence of LAS in agricultural soil stimulated the uptake of N, P and K with a surfactant dose of 15-30 g/m^2; Ca and Mg were reduced (Moreno-Caselles et al., 2006); the average LAS doses in agriculture, however, with anaerobic sludge are much lower (2.8 g/m^2) (Schowanek et al., 2007);
- laboratory studies on the growth of isolated soil bacteria cultures in presence of 50 µg/ml LAS concentration indicate that application of sewage sludge (also wastewater or pesticides formulations) containing LAS to an agricultural soil could be considered a potential risk for selected aerobic heterotrophic soil microbiota and their microbial activities (Sanchez-Peinado et al., 2008).

As LAS degrades rapidly and the sludge integrates in the soil, such effects disappear rapidly. In addition, it is difficult to distinguish whether any observed effect is due to the sludge organic matter itself, LAS (ca. 10%, the lowest sludge organic fraction) or other components (e.g. metals) and to understand whether the disturbance is adverse and permanent. In any case, field studies have never provided evidence of adverse and permanent impact of LAS in sludge on these parameters.

Specific effects of surfactants, present in municipal wastewaters, considering in particular the main soil regulatory factors, haven't been much considered (Muller et al., 2006). Regulatory requirements relevant to "pristine/natural" soil should not be used for agricultural soil that receives sewage sludge. Again, as already said before, it is also impossible to separate effects related to the organic carbon of sewage sludge solids itself, and perhaps to other persistent contaminants, from effects of biodegradable surfactants.

On the contrary, no significant effects to the microbial community were observed after prolonged exposure to heterogeneous LAS distributions in agricultural soil following sludge amendment. For example:

- no effects were observed in the soil even at LAS concentrations >31 $g/kg_{dw\ sludge}$ (Brandt et al., 2003);
- LAS at the concentration levels of 22 and 174 $mg/kg_{dw\ soil}$ in sandy agricultural soil (worst-case scenario in terms of high bioavailability and toxicity in the soil environment) was rapidly degraded (>93% in 4 weeks) and had little or no significant influence of the functional diversity of aerobic heterotrophic bacterial community (Winther et al., 2003);
- effects of LAS (at concentrations of 10 or 50 mg/l for periods of time up to 21 days) on the bacterial community of a microcosm system consisted of agricultural soil columns were evaluated, applying a molecular-based community-level analysis. The structures of

three bacteria communities (*Alphaproteo-, Actino- and Acido-bacteria*) were analysed. The conclusions were that the alphaproteobacterial population identified in the work was enriched in the LAS polluted soil, suggesting its relevant role and ability to biotransform and degrade LAS. LAS had no remarkable effects on the other two community bacteria, even when present at concentrations widely exceeding those reached in soil immediately after sludge application (Sànchez-Peinado et al., 2010).

Micro-organisms and overall soil processes were thus considered protected by the PNEC derived from the relative higher sensitivity of plants and invertebrates (Brandt et al., 2003; Petersen et al., 2003) and therefore not considered in the risk assessment.

Field observations are also available (Jensen, 1999; Jensen et al., 2001; Brandt et al., 2003) and are summarized in Table 19. The application of LAS-containing sludge generally stimulated the microbial activity and, hence, the abundance of soil fauna and growth of plants. Paddy growth was stimulated when LAS was <80 $mg/kg_{dw\ soil}$ (Liang-Qing et al., 2005). It was found that application of LAS-containing sludge on soil did not produce any short- and long-term adverse effects on microbial functions and processes or the abundance and diversity of soil invertebrates.

Table 19: Field studies for commercial LAS (Jensen et al. 2001; Figge and Schöberl, 1989)

Taxon	Range ($mg/kg_{dry\ soil}$)
Soil ecosystem, NOEC	>15
Biomass, NOEC	>16, >27

A laboratory agricultural ecosystems study used a "plant metabolism box" to measure the growth of grass, beans, radishes and potatoes for a period up to 106 days after application of sludge spiked with radiolabelled LAS material (Figge and Schöberl, 1989; Figge and Bieber, 1999). At LAS soil concentrations of 16 and 27 $mg/kg_{dw\ soil}$, no significant uptake and accumulation by plants and no adverse effects on the biomass were observed. Jensen et al. (2001) concluded that soil LAS concentrations of 5 to 15 $mg/kg_{dw\ soil}$ did not cause any harm to the soil ecosystem. Selected microbial populations in sandy soils (low organic matter content) surrounding sludge bands spiked with high levels of LAS were also studied (Brandt et al., 2003). In this study the observed disturbance of the soil microbial community lasted only two months and was confined to soil close to sludge, confirming that LAS doesn't pose any significant threat to the function of the microbial community in sludge-amended soils.

4.2.1.3 Sediment ecotoxicity

The organic carbon content of the sediment may influence the bioavailability and therefore the toxicity of the test substance. Therefore, for comparison of sediment tests, the organic carbon content of the test sediment should be within a certain range. The organic carbon content of a standard sediment is set to 5 % (TGD, 2003). It is recommended that the organic carbon content of the test sediments is between these two values. As some of the available data are tested with sediments that have an organic carbon content that fall outside the ranges, all results are converted to a standard sediment, which is defined as a sediment with an organic matter content of 5%.

Toxicity information is available for sediments and is summarized in Table 20. A NOEC of 319 $mg/kg_{dw\ sed.}$ (Klimish score of 1) was observed for the larvae of a benthic organism, *Chironomus riparius* (Pittinger, 1989; Kimerle, 1989). The organic carbon content of the tested sediment was 4.2%. The organic carbon normalized NOEC is 380 $mg/kg_{dw\ sed.}$ New toxicity experiments for the same organism, looking at larval growth and mortality, were performed using two different sediments spiked with both radiolabelled and unlabelled C_{12}-2-LAS homologue (Mäenpää and Kukkonen, 2006). After 10-days exposure, NOECs were 362 $mg/kg_{dw\ sed.}$ and 537 $mg/kg_{dw\ sed.}$

(Klimish score of 1). The organic carbon content of the sediments were 1.06% and 1.57%, respectively. The organic carbon normalized NOECs are 1,710 mg/$kg_{dw\ sed.}$ for both sediments. For one sediment the NOEC as body residue (measure of internal exposure) was 30 mg/kg larval wet weight.

A tubificid species, *Branchiura sowerbyi*, a benthic filter organism, was exposed for a long period (220 days) to a sediment with LAS concentrations varying from 26 to 7 mg/$kg_{dw\ sed.}$ (Klimish score of 1, absence of any observed effect) over the exposure period and no effects were observed in any of the test concentrations (Casellato et al., 1992). While the absence of reported toxicity is reassuring, it appears that the range of exposure concentrations was too low to derive a toxicity data directly useful in risk assessment. However, the results of this test do not invalidate the PNEC calculation. Two freshwater mollusc species, *Unio elongatulus* and *Anodonta cygnea*, were exposed to sediments with LAS concentration >200 mg/$kg_{dw\ sed.}$ (Klimish score of 2, due to lack on description of the experimental details) without noticing any adverse effects (Bressan et al., 1989).

Chronic studies were conducted with *Lumbriculus variegatus* and *Caenorhabditis elegans* (Comber et al., 2006). As to the first species, a 28 days NOEC of 81 mg/$kg_{dw\ sed.}$ was derived for survival, reproduction and growth, using sediment spiked with radio-labelled material, the organic carbon content of the sediment was 1.7%. The organic carbon normalized NOEC is 238 mg/$kg_{dw\ sed.}$.For the second species, a 3 day NOEC of 100 mg/$kg_{dw\ sed.}$ was obtained for egg production, the organic carbon normalized NOEC is 294 mg/$kg_{dw\ sed}$. Both experiments are well described (Klimish score of 1).

LAS sorbed to sediments was assessed for its level and potential perturbations on benthos; comparative sediment contamination analyses came to the conclusion that LAS risk for both aquatic and sediment compartment is low (Sanderson et al., 2006).

Table 20: Sediment chronic test results for commercial LAS

Species	Most sensitive end point	NOEC (mg/$kg_{dw\ sed.}$)	Organic carbon normalized NOEC (mg/$kg_{dw\ sed.}$)	Organic carbon content (%)	References
Chironomus riparius	reproduction, survival	319 362, 537	380 1,710	4.2 1.06, 1.57	Pittinger, 1989 Kimerle, 1989 Mäenpää and Kukkonen, 2006
Unio elongatulus *Anodonta cygnea*	survival survival	>200 >200	- -	- -	Bressan et al., 1989
Lumbriculus variegatus	survival, reproduction, growth	81	238	1.7	Comber et al., 2006
Caenorhabditis elegans	egg production	100	294	1.7	Comber et al., 2006

It is also worth mentioning LAS safety in the coastal marine environment.

LAS is highly biodegradable, not only under aerobic conditions in sea water (Leon et al, 2004), but also under anaerobic conditions in marine sediments (Lara-Martin et al., 2007; Lara-Martin et al.,

2008). Monitoring studies have shown that LAS is only present in coastal sediments close to points of municipal and industrial discharges (Petrovic et al., 2002).

Laboratory experiments, performed on anoxy marine sediments spiked with 10-50 ppm of LAS, showed that degradation is feasible reaching a value of 79% in 165 days, with a half-life time of ca. 90 days. The anaerobic process was also observed in the field with several marine sediment samplings: at anoxy depths in the sedimentary column, LAS concentrations in pore waters decreased sharply and the biodegradation intermediates (SPC) reached the maxima. These observations were claimed as the first real evidence of a partial degradation of LAS under anaerobic conditions (Lara-Martin et al., 2007; Lara-Martin et al., 2008). An anaerobic biodegradation pathway for LAS has recently been described (Lara-Martin et al., 2010).

Sortion and desorption experiments with two marine sediments were carried out using C_{12}-2-LAS molecule to study its toxicity on a marine mud shrimp, *Corophium volutator*, in water-only exposure as well as in spiked sediments (Rico-Rico A et al., 2009). Pore water LC_{50} values were calculated in the range 100-700 μg/l. These values are considerably higher than pore water concentrations for LAS (maximum 15 μg/l) found in marine sediments of coastal areas close to wastewater discharges (Lara-Martin et al., 2006).

The mud snail *Hydrobia ulvae* was exposed to marine LAS-spiked sediments: LC_{50} toxicity values were comprised between 203 mg/kg (48 h) and 94 mg/kg (9 d) (Hampel et al., 2009). The results confirm that *H. ulvae* is an appropriate candidate organism for routine marine sediment toxicity testing with surfactants.

4.2.1.4 Ecotoxicity to sewage microorganisms

The 3-h EC_{50} of LAS for microorganisms present in the aerobic activated sludge was experimentally measured at 550 mg/l (Verge et al., 1993; Verge et al., 1996). Assuming an average content of suspended matter in the activated sludge of 3 g/l, the EC_{50} value corresponds to about 18% LAS in sludge on dry basis (i.e., 183 g LAS/$kg_{dw\ sludge}$).

A consortium of two bacteria (*Pantoea agglomerans and Serratia odorifera*) was isolated from a STP sludge. They complement each other in the ability to degrade LAS. Optimizing their culture growth conditions, complete laboratory mineralization of 200 mg/l LAS was obtained within 48-72 h (Khleifat et al., 2006).

Laboratory toxicities of commercial surfactants were carried out using a specific type of micro organism isolated from a STP activated sludge (the phosphate-accumulating bacterium: *Acinetobacter junii*). The anionic surfactants were the most toxic, with LAS having a 50% growth inhibition of 0.15-1.8 mg/l (Ivankovic et al., 2009).

A NOEC value of 35 mg/l, normalised to the $C_{11.6}$LAS structure, was found for *Pseudomonas putida* after a growth inhibition test (Feijtel et al., 1995b).

The microbial population present in the STP activated sludge digesters was not found to be inhibited even by a high and atypical concentration (30 g/$kg_{dw\ sludge}$) of LAS in sludge (Berna et al., 1989).

4.2.1.5 Reassurance on absence of estrogenic effects

LAS was also investigated to check whether it could be an endocrine disruptor, using an estrogens-inducible yeast screen (Routledge et al., 1996; Navas et al., 1999) and the vitellogenin assay with

cultured trout hepatocytes (Navas et al., 1999). LAS as well as its biodegradation intermediates, Sulpho Phenyl Carboxylates (SPC), did not display any estrogenic effects.

4.2.2 PNEC calculations

4.2.2.1 Aquatic PNEC

In a previous environmental risk assessment of LAS for the aquatic compartment (Van de Plassche et al., 1999a), NOECs for fifteen freshwater species were considered (Table 13), a dataset that justified the application of a statistical extrapolation method (Aldenberg & Slob, 1993). They were normalised to the average structure $C_{11.6}$ LAS by the use of QSARs. A geometric mean NOEC for each species was calculated. $HC_{5,50}$, the median value of the 5^{th} percentile of the log-normal distribution including all available NOEC values, was derived and was 0.32 mg/l. This value is in good agreement with the lowest available freshwater NOEC, found for the fish *Tilapia mossambica* (0.25 mg/l).

Various mesocosm studies (Tattersfield et al., 1995; Tattersfield et al., 1996; Belanger et al., 2002) indicate that the lower limits of mesocosm studies can be considered between 0.12 to 0.5 mg/l. Following a critical review of all the mesocosm studies, however, it was also concluded that a NOEC = 0.27 mg/l for a C_{12}LAS homologue, corresponding to 0.37 mg/l when normalised to the $C_{11.6}$ LAS structure, is the most reliable, robust and defendable mesocosms value, to which an application factor of 1 has to be applied Belanger et al., 2002). The reasons for this are many, but include:

- presence of a large number of sensitive flora and fauna, accompanied by a high degree of overall biodiversity (a total of 149 alga species and 6 phylogenetic divisions; 117 benthic invertebrates including insects, molluscs, crustaceans, and aquatic worms; 77 macroinvertebrate taxa collected in drift; 110 adult insect species);
- 16 weeks of colonization and exposure, longer than single species chronic toxicity tests represented in the database;
- use of a large array of endpoints, including many that reveal subtle and indirect effects; endpoints combine relevant environmental aspects of fate (biodegradation, chemical metabolism, sorption, and exposure verification) with effects (invertebrate, autotrophic and heterotrophic periphyton);
- the experimental stream facility (ESF) has a long history of biological and chemical data that has been used to interpret and re-interpret past studies (Belanger et al., 1994, 1995, 2000); two pairs of studies have been conducted to assess repeatability and findings have been consistent in different years (Belanger, 1992; Belanger et al., 2000 and unpublished data);
- ESF streams have relatively low levels of variability and are sampled intensively (i.e., at relatively high levels of replication) (Lowe et al., 1996; Belanger et al., 2000);
- ESF stream population and community structure has been compared to local and regional flora and fauna to ensure that the ESF communities are representative of sensitive ecosystems (Belanger et al., 1995; Dyer and Belanger, 1999); ecological investigations of nutrient dynamics of ESF streams support their being representative of headwater streams at the relevant discharge levels (Peterson et al., 2001).

It seems reasonable and in agreement with the results on single species to assign a PNEC value of 0.27 mg/l to the PNEC of LAS in the water compartment.
Conclusion: PNEC in water = 0.27 mg/l.

4.2.2.2 Terrestrial PNEC

In a typical disposal scenario, LAS enters soil predominantly via addition of (anaerobic) sewage sludge to agricultural land.

Modelling approach: The terrestrial PNEC of LAS can be calculated by using the TGD equilibrium partitioning method (EqP - TGD, 2003, Part II: eq. 72, page 117). On the basis of a local PNEC in water of 0.27 mg/l and assuming a value of 2500 l/kg as partition coefficient between organic matter and water (see 3.2), a value of 11.9 mg/kgdw soil can be obtained. No additional safety factor is required for LAS because the substance has a log Kow <5. This value is in the same order of magnitude as the values derived below based on the all available experimental toxicity results for soil organisms.

Analysis of soil experimental data: In a previous environmental risk assessment carried out for LAS in the soil compartment (Jensen et al., 2001), the estimation of PNEC, performed for soil fauna and plants using a data set of twenty three records and applying a statistical extrapolation method (Wagner et al., 1991), was 4.6 mg/kgdw soil. This PNEC was calculated as the HC5,50, the median value of the 5th percentile of the log-normal distribution, and includes the microbial processes and functions that have been examined (Jensen et al., 2001).

Comparison with the EqP approach and with available more recent information suggest that this value can be considered as rather low/conservative. Following an extensive review and update of the plant and invertebrate ecotoxicological data, and a further interpretation of the relevance of the microbial endpoints for the functioning of the soil ecosystem, the terrestrial risk assessment of LAS has been revisited (Jensen et al., 2007). The new PNEC, using a data set of twenty one toxicity values (as reported in Table 17), was derived at 35 mg/kgdw soil.

The opinion of SCHER (2008) however disagrees with the argument that soil microbial functions (and with particular reference to iron reduction) are adequately covered by the proposed PNEC of 35 mg/kgdw soil, and considers that an evaluation of the relevance of LAS effects on microbial activity is essential for a proper PNECsoil derivation. Thus, SCHER considers that the information provided is not sufficient for justifying the newly proposed PNEC value of 35 mg/kg. In this respect, HERA experts remark that at present there is no consistent and universally accepted framework of how microbial species, and in particular single biochemical endpoints, should be included in a soil or sediment risk assessment for a given chemical. The EU TGD (2003) provides only very basic guidance in this respect, emphasizing the function of “primary producers” (plants), “consumers” (soil fauna) and “decomposers” (mainly microbes). Given the enormous diversity and metabolic/genetic flexibility of microbial communities, and the variability and diversity of potentially measurable microbial endpoints in soil, a careful interpretation is required. Each result should be evaluated for its true environmental relevance with respect to the size of the effect, duration, essential soil function impairment, etc., and not necessarily the lowest observed number should therefore be retained as a NOEC.

The salt speciation of LAS and the soil type were included in the evaluation and did not significantly modify the toxicity of LAS to soil organisms (Holmstrup et al., 2001b; Jensen et al., 2001). Dosage of LAS via sewage sludge, instead, generally reduced the effects for microbial parameters, showing also recovery potentials for most parameters as a result of prolonged incubation (Elsgaard et al., 2001b). Disturbance of soil microbial community were confined to soil close to sludge and disappeared after two months (Brandt et al., 2003). In addition, field observations (Table 19) after experimental sludge amendment at high application rates concluded that LAS, at an average soil concentration of > 15 mg/kgdw soil, does not seem to be detrimental to the soil ecosystem in the long term (Jensen et al., 2001). The HERA experts therefore judge that the impact of LAS on the soil community has been adequately assessed, in particular if one

combines the laboratory data with the holistic weight of evidence provided by available controlled field studies at high LAS levels. These show no impact on 'ecosystem service' parameters such as soil fertility and crop yield (see studies reported in Schowanek et al. 2007, where a probabilistic pan-European risk assessment for LAS in soil is also presented). With respect to the protection of the agro-ecosystem, reference is also made to discussion on setting protection levels on the basis of 'ecosystem services" in the EU Commission document (2012) "Addressing the new challenges for Risk Assessment" (http://ec.europa.eu/health/scientific_committees/consultations/public_consultations/scenihr_consultation_16_en.htm)

Conclusion: PNEC in soil = 35 mg/kg$_{dw\ soil}$.

4.2.2.3 Sludge PNEC

A sludge PNEC, also called sludge quality standard (SQS), of LAS can be back-calculated from the soil PNEC taking into account the TGD (TGD, 2003) scenario for exposure of sewage sludge on agricultural soil and the soil PNEC of 35 mg/kg$_{dw\ soil}$ (see par. 4.2.2.2). A PNEC of 49 g/kg$_{dw\ sludge}$ was calculated (for details of its calculation and interpretation we refer to Schowanek et al., 2007)(*).

Conclusion: PNEC in sludge = 49 g/kg$_{dw\ sludge}$.

4.2.2.4 Sediment PNEC

As for soil, sediment PNEC of LAS can be calculated using the TGD equilibrium partitioning method (TGD, 2003: Part II, eq. 70, page 113). The resulting PNEC is 14.9 mg/kg$_{dw\ sed}$.

Good quality chronic data on sediment toxicity for LAS are available for five species representing different living and feeding conditions. An application factor of 10 can be applied to the lowest available NOEC figure normalized for organic carbon, deriving a conservative PNEC for sediment of 23.8 mg/kg$_{dw\ sed}$.

The available sediment toxicity data, as reported in Table 20, in particular those relative to oligochaetes, well represent the different benthic taxa (Comber et al., 2006) and are recommended by the European TGD (TGD, 2003) in the sediment testing for the risk assessment of chemicals.

Conclusion: PNEC in sediment = 23.8 mg/kg$_{dw\ sed.}$.

4.2.2.5 STP PNEC

Although the lowest effect concentration is a NOEC value of 35 mg/l, normalised to the $C_{11.6}$LAS structure, for *Pseudomonas putida* after a growth inhibition test, this value will not be taken into account. Results of the cell multiplication inhibition test with *P. putida* should only be used for calculation of the STP PNEC in cases where no other test results employing mixed inocula are available. As a respiration inhibition test with activated sludge is available, results from this study will be used to derive the STP PNEC (TGD, 2003). Thus the most relevant reported effective concentration for STP organisms is the 3-h EC_{50} value of 550 mg/l for activated sludge. This value with an application factor of 100 gives a PNEC of 5.5 mg/l, as recommended by the TGD.

Conclusion: PNEC in STPs = 5.5 mg/l.

4.3 Environmental risk assessment

PEC and PNEC values with the corresponding PEC/PNEC ratios are summarized in Table 21.

(*) A LAS limit value in sludge of 1.3 g/kg$_{dw\ sludge}$ is actually in force in Denmark (Executive Order 823 DK).

Table 21: Risk characterization

LAS	PEC	PNEC	PEC/PNEC
Water, mg/l	0.047	0.27	**0.17**
Soil (30 d), mg/$kg_{dw\ soil}$	1.4	35	**0.04**
Sludge, g/$kg_{dw\ sludge}$	5.56 (50th percentile) 15.07 (95th percentile)	49	**0.11** **0.31**
Sediment, mg/$kg_{dw\ sed.}$	5.3	23.8	**0.22**
STP, mg/l	0.27	5.5	**0.05**

This assessment shows that the use of LAS in HERA applications results in risk characterisation ratios (PEC/PNEC) less than one. To demonstrate this, higher tier exposure and effects data were needed. PEC values were estimated based on monitoring data for each environmental compartment and PNEC values were based on chronic effects data. This conclusion can be generalized to all LAS usages in Europe including the non-HERA minor applications, since exposure has been based on the actual LAS concentrations measured in the various environmental compartments.

5. Human health assessment

5.1 Consumer exposure

5.1.1 Product types

LAS is one of the major anionic surfactants used in laundry and cleaning products. LAS is commonly used in many household detergents, including laundry powders, liquids, and tablets (at a typical concentration range from 3% to 22%), laundry bleach additives (at a typical concentration range from 3% to 11%), hand dishwashing liquids (at a typical concentration range from 2% to 30%), and all-purpose cleaning powders, liquids, sprays, and tablets (at a typical concentration range from 1% to 37%). LAS is also used in some industrial applications, such as in the fields of textile and fibers, chemicals, and agriculture and in cosmetics and glues. These other uses of LAS are minor relative to the laundry and cleaning applications (which represent about 80% of the total use of LAS in the market) and are outside the scope of HERA. They are not evaluated in this assessment.

5.1.2 Consumer Contact Scenarios

Based on the product types, the consumer contact scenarios that were identified and considered in this assessment include: direct and indirect skin contact, inhalation of aerosols from cleaning sprays, and oral ingestion derived either from residues deposited on dishes, from accidental product ingestion, or indirectly from drinking water.

5.1.3 Consumer exposure estimates

There is a consolidated overview concerning habits and practices of use of detergents and surface cleaners in Western Europe which was tabulated and issued by AISE (THPCPWE,2002). This table reports the consumer's use of detergents in g/cup, tasks/week, duration of task and other uses of products. All exposure estimates that follow were calculated using relevant data from this table. Information from the RIVM report Cleaning Products Fact Sheet - To assess the risks for the consumer has also been used (RIVM,2006)

(Editorial note: across this section and throughout the report the term "conservative" is used frequently to refer to the nature of an estimation of exposure. For clarification, the term "conservative" is always meant here as indicating the higher end of likely exposure).

5.1.3.1 Direct skin contact from hand washed laundry

During the hand-wash laundry, the diluted laundry liquid comes into direct contact with the skin of hands and forearms.

The following worst case should address this scenario:

- The exposed area is the skin surface area of forearms and hands, which is 1900 cm^2 (RIVM, 2006).
- It is assumed that not the total amount of diluted product is in contact with the skin but only a layer of 0.01 cm around the exposed skin (TGD,2003). The exposure area is 1900 cm^2, therefore the amount of diluted product is 19 cm^3, or 19 g (RIVM,2006).
- The concentration of laundry detergent for the hand-wash is 0.1% to 1%. Worst-case, the weight fraction of the diluted detergent is 1% of the used detergent powder/liquid (AISE,2002).
- Taking the above into account, the following local dermal exposure can be calculated:

0.01 (dilution factor) x 19 (g) / 1900 (cm^2) = 0.10 mg/cm^2/day
$Exp_{dermal,local}$ = 0.10 mg/cm^2/day

Assuming a frequency of 104 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

0.01 (dilution factor) x 19 (g) / 65 (kg) / 365/104 (frequency) = 0.83 mg/kg bw/day
$Exp_{dermal,sys}$ = 0.83 mg/kg bw/day

5.1.3.2 Direct skin contact from laundry tablets

Contact time is so low and area of contact with skin is so small that the amount absorbed percutaneously is considered insignificant.

5.1.3.3 Direct skin contact from pre-treatment of clothes

Direct skin contact with LAS is possible when clothing stains are being removed by spot-treatment with a 60 % (600 mg/ml) detergent paste powder (THPCPWE,2002) or neat liquid. As only a fraction of the skin surface area of the hands (840 cm^2) (TGD,2003) is exposed, it can be assumed that the amount of LAS systemically available via percutaneous absorption, if any, is quite low.

The following worst case should address this scenario:

- Highest concentration of LAS in powder laundry detergents amounts to 22% (internal AISE data). Therefore highest concentration of LAS in hand washing paste (600 mg/ml) is approximately 132 mg/ml. Highest concentration of LAS in liquid laundry detergents amounts to 14% (140 mg/ml) (internal AISE data). Because liquid detergents may be used neat for pre-treatment, the worst case value of 14% will be used in the calculation.

- Contact of hands into solution would expose a maximum of 840 cm² (TGD,2003). This value is very conservative because only a fraction of the two hands surface skin will be exposed.
- Assuming a film thickness of 100 µm (0.1 mm or 0.01 cm) (TGD,2003) on the hands and an assumed applied amount of 0.65 g (RIVM,2006), the following local dermal exposure can be calculated:

0.14 (dilution factor) x 0.65 (g) / 840 (cm^2) = 0.11 mg/cm^2/day
$Exp_{dermal,local}$ = 0.11 mg/cm^2/day

Assuming a frequency of 128 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

0.14 (dilution factor) x 0.65 (g) / 65 (kg) / 365/128 (frequency) = 0.49 mg/kg bw/day
$Exp_{dermal,sys}$ = 0.49 mg/kg bw/day

5.1.3.4 Direct skin contact and inhalation from hand dishwashing

Dermal
When doing the dishes, there is dermal exposure to the diluted dishwashing liquid.

The following worst case should address this scenario:
- Highest concentration of LAS in hand dishwashing solution is $6.54 \cdot 10^{-5}$% (RIVM,2006).
- Immersion of hands and forearms into solution would expose about 1900 cm² (RIVM,2006).
- Assuming a film thickness of 100 µm (0.1 mm or 0.01 cm) (TGD,2003) on the hands and an assumed applied amount of 15000 g, the following local dermal exposure can be calculated:

$6.54 \cdot 10^{-7}$ (dilution factor) x 15000 (g) / 1900 (cm^2) = $5.16 \cdot 10^{-3}$ mg/cm^2/day
$Exp_{dermal,local}$ = $5.16 \cdot 10^{-3}$ mg/cm^2/day

Assuming a frequency of 426 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

$6.54 \cdot 10^{-7}$ (dilution factor) x 15000 (g) / 65 (kg) / 365/426 (frequency) = 0.18 mg/kg bw/day
$Exp_{dermal,sys}$ = 0.18 mg/kg bw/day

Inhalation
When doing the dishes, there is inhalation exposure to the diluted dishwashing liquid.

The following worst case should address this scenario:
- Highest concentration of LAS in hand dishwashing solution is $6.54 \cdot 10^{-5}$% (RIVM,2006).

- The exposure duration is the time of being in the kitchen, which is estimated at 60 min. The application duration is set at 16 min. (RIVM,2006)
- The room volume is 15 m^3 (kitchen). The release area, based on the surface area of the sink, is set at 0.15 m^2. (RIVM,2006)
- Default values are used for ventilation rate (2.5 hr^{-1} = $6.9 \cdot 10^{-4}$ s^{-1}), applied amount (15000 g), molecular weight matrix (18 g/mol) and mass transfer rate (2100 m/min) (RIVM,2006).
- Based on the above, the inhalation exposure to LAS is estimated using the ConsExpo v4.1 evaporation model:

$Exp_{inhalation}$ = $3.90 \cdot 10^{-20}$ mg/m^3/day

This amount does not contribute significantly to the total exposure of LAS.

5.1.3.5 Indirect skin contact from wearing clothes

Residues of components of laundry detergents may remain on textiles after washing and could come in contact with the skin via transfer from textile to skin. The amount of LAS deposited on fabric remaining after 10 repeats of a typical washing process with typical laundry detergents was experimentally measured to be in the order of 2.5 mg of LAS per g of fabric (Rodriguez et al., 1994). However, this amount of compound deposited on the textile depends on the type of chemical and on the product itself. Therefore, extrapolating to the total amount of detergent residues is not feasible (RIVM,2006).

- It is assumed that clothers are worn every day, for 24 hours; resulting in a frequency of exposure of 365 $year^{-1}$.
- The leachable fraction is the relative amount of chemical which can leach from a product, i.e. the fraction of deposits of the detergent which can leach from textile. This fraction is determined to be 0.0023 (RIVM,2006).
- The average weight of the product that is worn on the body is estimated at 1000 g (RIVM, 2006).
- The exposed area is 17600 cm^2.
- Assuming a skin contact factor, the part of the product that is in contact with bare skin, of 0.8, the following local dermal exposure can be calculated:

1000 (g) x 0.8 x 0.0023 / 17600 (cm^2) = 0.105 mg/cm^2/day
$Exp_{dermal.local}$ = 0.11 mg/cm^2/day

Assuming a frequency of 365 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

1000 (g) x 0.8 x 0.0023 / 65 (kg) = 28.31 mg/kg bw/day
$Exp_{dermal,sys}$ = 28.31 mg/kg bw/day

5.1.3.6 Inhalation of detergent dust during washing processes

Charging the washing machine with laundry powder may lead to generation of dust particles and may lead to inhalation exposure.

- The powder laundry detergents contain up to 22% LAS.
- The exposure duration includes picking up the package, opening it, filling the machine and closing the package, and is set at 15 s (0.25 min.) (RIVM,2006).
- The room volume is 1 m^3; room volume is interpreted here as 'personal volume', a small area of 1 m^3 around the user.
- Default values are used for ventilation rate (2 hr^{-1} = $5.6 \cdot 10^{-4}$ s^{-1}), and applied amount ($2.7 \cdot 10^{-4}$ mg).
- In the worst case assumptions that all of the dust is inhaled during machine loading and that this task is done once daily, the inhalation exposure to LAS is estimated to be:

$$\mathbf{Exp_{inhalation}} = [(2.7 \cdot 10^{-4} \text{ (mg)} \times 0.22 \times e^{-5.6.10\text{-}4 \text{ (s-1)} \times 15 \text{ (s)}}) / 1 \text{ (m}^3\text{)}] \times 1.7 \cdot 10^{-4} \text{ (day)} = \mathbf{1.03 \cdot 10^{-8}\ mg/m^3/day}$$

This amount does not contribute significantly to the total exposure of LAS. Similarly, lint formation during drying of fabrics in tumble-dryers which vent indoors is considered not to contribute to inhalation exposure of LAS, since washed fabrics do not contain any relevant amount of LAS (see above).

5.1.3.7 Inhalation of and skin contact with aerosols from cleaning sprays

LAS is present in some surface cleaning spray products at a typical concentration range of 3% to 6% (internal AISE data).

Inhalation

When cleaning a surface using a spray cleaner, inhalation exposure to the aerosols from the cleaning spray can occur.

The following worst case should address this scenario:

- Highest concentration of LAS in spray cleaner is 6 % (internal AISE data).
- The exposure duration is the time of being in the room, which is estimated at 60 min. The application duration is set at 0.41 min. (RIVM,2006)
- The room volume is set at 15 m^3, the room height at 2.5 m (RIVM,2006).
- The mass generation rate is 0.78 g/s, and the weight fraction non-volatile is 0.06.
- Default values are used for ventilation rate (2.5 hr^{-1} = $6.9 \cdot 10^{-4}$ s^{-1}), inhalation cut-off diameter (15 µm), density non-volatile (1.8 g/cm^3) and airborn fraction (0.2) (RIVM,2006).
- Based on the above, the inhalation exposure to LAS is estimated using the ConsExpo v4.1 exposure to spray model:

$$\mathbf{Exp_{inhalation}} = \mathbf{1.31 \cdot 10^{-5}\ mg/m^3/day}$$

Dermal

When cleaning a surface using a spray cleaner, dermal exposure to the aerosols from the cleaning spray can occur.

The following worst case should address this scenario:

- Highest concentration of LAS in spray cleaner is 6 % (internal AISE data).
- Immersion of hands and forearms into solution would expose about 1900 cm² (RIVM,2006).
- Assuming a contact rate of 100 mg/min (1.67 mg/s) and a release duration 24.6 s, the following local dermal exposure can be calculated:

$$1.67 \text{ (mg/s)} \times 24.6 \text{ (s)} \times 0.06 / 1900 \text{ (cm}^2\text{)} = 1.29 \cdot 10^{-3} \text{ mg/cm}^2\text{/day}$$
$$\mathbf{Exp_{dermal,local} = 1.29 \cdot 10^{-3} \text{ mg/cm}^2\text{/day}}$$

Assuming a frequency of 365 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

$$1.67 \text{ (mg/s)} \times 24.6 \text{ (s)} \times 0.06 / 65 \text{ (kg)} / 365/365 \text{ (frequency)} = 3.78 \cdot 10^{-2} \text{ mg/kg bw/day}$$
$$\mathbf{Exp_{dermal,sys} = 3.78 \cdot 10^{-2} \text{ mg/kg bw/day}}$$

5.1.3.8 Oral exposures to LAS

Oral exposures can be assumed to originate from drinking water and food (fruits and vegetables) and from residues over eating utensils and dishes washed in hand dishwashing detergents (machine dishwashing products do not contain LAS).

- It is assumed that every day dinnerware is used for food and drinks, resulting in a frequency of 365 year^{-1}.
- The value for amount of water left on dishes is $5.5 \cdot 10^{-5}$ mL/cm² and the value for the area of dishes in daily contact with food is 5400 cm². The concentration of the dishwashing water is 1.4 g/L. Using these data, the ingested product amount is $5.5 \cdot 10^{-5}$ mL/cm² x 5400 cm² x 1.4 mg/mL = 0.42 mg (RIVM,2006).
- Assuming a weight fraction of 0.3 and a body weight of 65 kg, the oral exposure to LAS is estimated to be:

$$0.42 \text{ (mg)} \times 0.3 / 65 \text{ (kg)} = 1.94 \cdot 10^{-3} \text{ mg/kg bw/day}$$
$$\mathbf{Exp_{oral,sys} = 1.94 \cdot 10^{-3} \text{ mg/kg bw/day}}$$

5.1.3.9 Inhalation and skin contact from laundry pretreatment products: Spray spot removers

Inhalation

When pretreating laundry with spray spot remover, inhalation exposure to the aerosols from the spray spot remover.

The following worst case should address this scenario:

- Highest concentration of LAS in spray spot remover is 14 % (internal AISE data).

- The exposure duration is the time per task for the use of laundry-pre-treatment, which is estimated at 10 min (AISE data). The spray duration is set at 0.05 min (3 s) (RIVM,2006).
- The room volume is set at 10 m^3, the room height at 2.5 m (RIVM,2006).
- The mass generation rate is 1.5 g/s, and the weight fraction non-volatile is 0.14.
- Default values are used for ventilation rate (2 hr^{-1} = $5.6 \cdot 10^{-4}$ s^{-1}), inhalation cut-off diameter (15 µm), density non-volatile (1.8 g/cm^3) and airborn fraction (0.2) (RIVM,2006).
- Based on the above, the inhalation exposure to LAS is estimated using the ConsExpo v4.1 exposure to spray model:

$$\mathbf{Exp_{inhalation} = 3.51 \cdot 10^{-6}\ mg/m^3/day}$$

Dermal
When pretreating laundry with spray spot remover, dermal exposure to the aerosols from the spray spot remover can occur.

The following worst case should address this scenario:
- Highest concentration of LAS in spray spot remover is 14 % (internal AISE data).
- The exposed area would be two hands, 840 cm².
- Assuming a contact rate of 46 mg/min (0.77 mg/s) and a release duration of 3 s, the following local dermal exposure can be calculated:

$$0.77\ (mg/s) \times 3\ (s) \times 0.14 / 840\ (cm^2) = 3.83 \cdot 10^{-4}\ mg/cm^2/day$$
$$\mathbf{Exp_{dermal,local} = 3.83 \cdot 10^{-4}\ mg/cm^2/day}$$

Assuming a frequency of 128 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

$$0.77\ (mg/s) \times 3\ (s) \times 0.14 / 65\ (kg) / 365/128\ (frequency) = 1.74 \cdot 10^{-3}\ mg/kg\ bw/day$$
$$\mathbf{Exp_{dermal,sys} = 1.74 \cdot 10^{-3}\ mg/kg\ bw/day}$$

5.1.3.10 Skin contact from laundry pretreatment products: Liquid spot removers

When using a liquid spot remover to remove spots from laundry, dermal exposure to the spot remover can occur.

The following worst case should address this scenario:
- Highest concentration of LAS in spray spot remover is 14 % (internal AISE data).
- The exposed area would be two hands, 840 cm².
- Assuming an applied amount of 650 mg, the following local dermal exposure can be calculated:

$$650\ (mg) \times 0.14 / 840\ (cm^2) = 0.11\ mg/cm^2/day$$

$$\mathbf{Exp_{dermal,local} = 0.11\ mg/cm^2/day}$$

Assuming a frequency of 128 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

650 (mg) x 0.14 / 65 (kg) / 365/128 (frequency) = 0.49 mg/kg bw/day

$$\mathbf{Exp_{dermal,sys} = 0.49\ mg/kg\ bw/day}$$

5.1.3.11 Inhalation and skin contact from liquid cleaner products: Oven cleaner (spraying)

This scenario describes the cleaning of a cold oven once every fortnight with a trigger spray. The oven has a surface area of 0.9 m^2 (30 cm x 40 cm x 45 cm). After spraying the oven door is closed and the product has to soak.

Inhalation

The following worst case should address this scenario:

- Highest concentration of LAS in oven cleaner is 10 % (internal AISE data).
- The exposure duration is the time of being in the room, which is estimated at 60 min. The spray duration is set at 0. 5 min (30 s) (RIVM,2006).
- The room volume is set at 15 m^3, the room height at 2.5 m (RIVM,2006).
- The mass generation rate is 0.78 g/s, and the weight $6.9 \cdot 10^{-4}$ s^{-1}), inhalation cut-off diameter (15 µm), density non-volatile (1.8 g/cm^3) and airborn fraction (0.2) (RIVM,2006).
- Based on the above, the inhalation exposure to LAS is estimated using the ConsExpo v4.1 exposure to spray model:

$$\mathbf{Exp_{inhalation} = 1.90 \cdot 10^{-6}\ mg/m^3/day}$$

Dermal

The following worst case should address this scenario:

- Highest concentration of LAS in spray spot remover is 10 % (internal AISE data).
- The exposed area would be half of two hands, 430 cm^2.
- Assuming a contact rate of 46 mg/min (0.77 mg/s) and a release duration of 30 s, the following local dermal exposure can be calculated:

0.77 (mg/s) x 30 (s) x 0.1 / 430 (cm^2) = $5.35 \cdot 10^{-3}$ mg/cm^2/day

$$\mathbf{Exp_{dermal,local} = 5.35 \cdot 10^{-3}\ mg/cm^2/day}$$

Assuming a frequency of 26 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

0.77 (mg/s) x 30 (s) x 0.1 / 65 (kg) / 365/26 (frequency) = $2.52 \cdot 10^{-3}$ mg/kg bw/day

$Exp_{dermal,sys}$ = $2.52 \cdot 10^{-3}$ mg/kg bw/day

5.1.3.12 Skin contact from liquid cleaner products: Oven cleaner (cleaning)

After treatment with the cleaner, the oven is wiped clean with a wet cloth or sponge and one has to ringe frequently. It is assumed users will not wear gloves, therefore the dermal exposure has been determined.

The following worst case should address this scenario:

- Highest concentration of LAS in spray spot remover is 10 % (internal AISE data).
- The exposed area would be half of two hands, 430 cm².
- Assuming an applied amount of 200 mg, the following local dermal exposure can be calculated:

200 (mg) x 0.1 / 430 (cm^2) = $4.65 \cdot 10^{-2}$ mg/cm^2/day

$Exp_{dermal,local}$ = $4.65 \cdot 10^{-2}$ mg/cm^2/day

Assuming a frequency of 26 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

200 (mg) x 0.1 / 65 (kg) / 365/26 (frequency) = $2.19 \cdot 10^{-2}$ mg/kg bw/day

$Exp_{dermal,sys}$ = $2.19 \cdot 10^{-2}$ mg/kg bw/day

5.1.3.13 Inhalation and skin contact from liquid cleaner products: Bathroom cleaners (mixing & loading)

Bathroom cleaning liquids are periodically applied as descaling products. In this scenario the mixing and loading of bathroom cleaning liquid in a bucket of water is described.

Inhalation

The following worst case should address this scenario:

- Highest concentration of LAS in spray spot remover is 2.2 % (RIVM,2006).
- The exposure duration is the time per task for the use of bathroom cleaners, which is estimated at 0.75 min. The application duration is set at 0.3 min (18 s) (RIVM,2006).
- The room volume is set at 1 m^3; room volume is interpreted here as 'personal volume', a small area of 1 m^3 around the user (RIVM,2006). The release area is 20 cm^2.
- The mass transfer rate is $2.04 \cdot 10^3$, and the molecular weight matrix is 26 g/mol.
- Default value is used for ventilation rate (2 hr^{-1} = $5.6 \cdot 10^{-4}$ s^{-1}), and the amount used is 500 g.
- Based on the above, the inhalation exposure to LAS is estimated using the ConsExpo v4.1 evaporation model:

$$\mathbf{Exp_{inhalation} = 2.37 \cdot 10^{-19}\ mg/m^3/day}$$

This amount does not contribute significantly to the total exposure of LAS.

Dermal
The following worst case should address this scenario:

- Highest concentration of LAS in spray spot remover is 2.2 % (RIVM,2006).
- The exposed area would be one palm, 215 cm².
- Assuming an applied amount of 10 mg, the following local dermal exposure can be calculated:

$$10\ (mg) \times 0.022 / 215\ (cm^2) = 1.02 \cdot 10^{-3}\ mg/cm^2/day$$
$$\mathbf{Exp_{dermal,local} = 1.02 \cdot 10^{-3}\ mg/cm^2/day}$$

Assuming a frequency of 4 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

$$10\ (mg) \times 0.022 / 65\ (kg) / 365/4\ (frequency) = 3.71 \cdot 10^{-5}\ mg/kg\ bw/day$$
$$\mathbf{Exp_{dermal,sys} = 3.71 \cdot 10^{-5}\ mg/kg\ bw/day}$$

5.1.3.14 Inhalation and skin contact from liquid cleaner products: Bathroom cleaners (cleaning)

Bathroom cleaning liquids are periodically applied as descaling products. In this scenario the mixing and loading of bathroom cleaning liquid in a bucket of water is described.

Inhalation
The following worst case should address this scenario:

- Highest concentration of LAS in spray spot remover is 2.2 % (RIVM,2006).
- The exposure duration is the time per task for the use of bathroom cleaners, which is estimated at 25 min. The application duration is set at 20 min (1200 s) (RIVM,2006).
- The room volume is set at 10 m^3 (RIVM,2006). The release area is $6.4 \cdot 10^4$ cm^2.
- The mass transfer rate is $2.04 \cdot 10^3$, and the molecular weight matrix is 18 g/mol.
- Default value is used for ventilation rate (2 hr^{-1} = $5.6 \cdot 10^{-4}$ s^{-1}), and the amount used is 260 g.
- Based on the above, the inhalation exposure to LAS is estimated using the ConsExpo v4.1 evaporation model:

$$\mathbf{Exp_{inhalation} = 9.26 \cdot 10^{-18}\ mg/m^3/day}$$

This amount does not contribute significantly to the total exposure of LAS.

Dermal
The following worst case should address this scenario:

- Highest concentration of LAS in spray spot remover is 2.2 % (RIVM,2006).
- The exposed area would be the hands and forearms, 1900 cm².
- Assuming an applied amount of 19000 mg, the following local dermal exposure can be calculated:

19000 (mg) x 0.022 / 1900 (cm^2) = 0.22 $mg/cm^2/day$
$Exp_{dermal,local}$ = 0.22 $mg/cm^2/day$

Assuming a frequency of 4 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

19000 (mg) x 0.022 / 65 (kg) / 365/4 (frequency) = $7.04 \cdot 10^{-2}$ mg/kg bw/day
$Exp_{dermal,sys}$ = $7.04 \cdot 10^{-2}$ mg/kg bw/day

5.1.3.15 Inhalation and skin contact from liquid cleaner products: Floor cleaners (mixing)

Floor cleaners, which contain soap, are meant for daily or periodically removing all kinds of grease and dirt from different sorts of floors.

Inhalation
The following worst case should address this scenario:

- Highest concentration of LAS in spray spot remover is 5 % (RIVM,2006).
- The exposure duration is the time per task for the use of floor cleaners, which is estimated at 0.75 min. The application duration is set at 0.3 min (18 s) (RIVM,2006).
- The room volume is set at 1 m^3; room volume is interpreted here as 'personal volume', a small area of 1 m^3 around the user (RIVM,2006). The release area is 20 cm^2.
- The mass transfer rate is $2.04 \cdot 10^3$, and the molecular weight matrix is 22 g/mol.
- Default value is used for ventilation rate (0.5 hr^{-1} = $1.3 \cdot 10^{-4}$ s^{-1}), and the amount used is 500 g.
- Based on the above, the inhalation exposure to LAS is estimated using the ConsExpo v4.1 evaporation model:

$Exp_{inhalation}$ = $1.23 \cdot 10^{-17}$ $mg/m^3/day$

This amount does not contribute significantly to the total exposure of LAS.

Dermal
The following worst case should address this scenario:

- Highest concentration of LAS in spray spot remover is 5 % (RIVM,2006).
- The exposed area would be one palm, 215 cm².
- Assuming an applied amount of 10 mg, the following local dermal exposure can be calculated:

10 (mg) x 0.05 / 215 (cm^2) = $2.33 \cdot 10^{-3}$ mg/cm^2/day
$Exp_{dermal,local}$ = $2.33 \cdot 10^{-3}$ mg/cm^2/day

Assuming a frequency of 104 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

10 (mg) x 0.05 / 65 (kg) / 365/104 (frequency) = $2.19 \cdot 10^{-3}$ mg/kg bw/day
$Exp_{dermal,sys}$ = $2.19 \cdot 10^{-3}$ mg/kg bw/day

5.1.3.16 Inhalation and skin contact from liquid cleaner products: Floor cleaners (cleaning)

Floor cleaners, which contain soap, are meant for daily or periodically removing all kinds of grease and dirt from different sorts of floors.

Inhalation
The following worst case should address this scenario:

- Highest concentration of LAS in spray spot remover is 5 % (RIVM,2006).
- The exposure duration is the time per task for the use of floor cleaners, which is estimated at 240 min. The application duration is set at 30 min (1200 s) (RIVM,2006).
- The room volume is set at 58 m^3 (RIVM,2006). The release area is $2.2 \cdot 10^5$ cm^2.
- The mass transfer rate is $2.04 \cdot 10^3$, and the molecular weight matrix is 18 g/mol.
- Default value is used for ventilation rate (0.5 hr^{-1} = $1.3 \cdot 10^{-4}$ s^{-1}), and the amount used is 8800 g.
- Based on the above, the inhalation exposure to LAS is estimated using the ConsExpo v4.1 evaporation model:

$Exp_{inhalation}$ = $5.43 \cdot 10^{-15}$ mg/m^3/day

This amount does not contribute significantly to the total exposure of LAS.

Dermal
The following worst case should address this scenario:

- Highest concentration of LAS in spray spot remover is 5 % (RIVM,2006).
- The exposed area would be the hands and forearms, 1900 cm^2.
- Assuming an applied amount of 19000 mg, the following local dermal exposure can be calculated:

19000 (mg) x 0.05 / 1900 (cm^2) = 0.5 mg/cm^2/day
$Exp_{dermal,local}$ = 0.5 mg/cm^2/day

Assuming a frequency of 104 times per year, and a body weight of 65 kg, the resulting dermal systemic dose is:

19000 (mg) x 0.05 / 65 (kg) / 365/104 (frequency) = 4.16 mg/kg bw/day

$Exp_{dermal,sys}$ = 4.16 mg/kg bw/day

5.1.3.17 Accidental or intentional overexposure

Accidental or intentional overexposure to LAS may occur via household detergent products, which may contain up to 30% of LAS.
No fatal cases or serious injuries arising from accidental ingestion of LAS by humans are known to us. The accidental or intentional overexposure to LAS directly is not considered a likely occurrence for consumers, but it may occur via household detergent products. The German Federal Institute for Health Protection of Consumers and Veterinary Medicine (BgVV,1999) published recently a report on products involved in poisoning cases. No fatal case of poisoning with detergents was reported in this report. Detergent products were not mentioned as dangerous products with a high incidence of poisoning.

Equally, in the UK, the Department of Trade and Industry (DTI) produces an annual report of the home accident surveillance system (HASS). The data in this report summarizes the information recorded at accident and emergency (A&E) units at a sample of hospitals across the UK. It also includes death statistics produced by the Office for National Statistics for England and Wales. The figures for 1998 show that for the representative sample of hospitals surveyed, there were 33 reported accidents involving detergent washing powder (the national estimate being 644) with none of these resulting in fatalities (DTI,1998). In 1996 and 1997, despite their being 43 and 50 reported cases, respectively, no fatalities were reported either.

Accidental exposure of the eye to LAS will occur in consumers only via splashes or spills with a formulated product. Therefore, the eye irritation potential has to be considered in the context of accidental exposure.

5.2 Hazard assessment

5.2.1 Summary of the available toxicological data

5.2.1.1 Toxicokinetics

The absorption, distribution, metabolism and elimination of LAS (radio-labelled with ^{35}S; chain length: C_{10-14}) were studied in male Charles River rats (Michael,1968). LAS was administered as an aqueous solution. The compound was readily absorbed from the gastrointestinal tract (80-90% of the dose). Most of the absorbed ^{35}S was eliminated within 72 hours and 60-65% of the absorbed dose was eliminated in the urine, with sulfophenyl butanoic and sulfophenyl pentatonic acid as metabolites. These metabolites were not reabsorbed from the kidney tubules. 35% of the absorbed ^{35}S was excreted in the bile and then reabsorbed completely from the gastrointestinal tract.
Although the metabolites in the bile were not identified, it was shown that no unchanged LAS was eliminated via this pathway. The authors suggested that metabolism proceeded via omega oxidation with subsequent beta-oxidation. Retention of radioactivity was not observed in any organ.

LAS is well absorbed via the gastrointestinal tract of pigs treated with 3.3 mmol/animal ^{35}S-Na-dodecylbenzene sulphonate (Havermann et al.,1959). At 200 hours after oral administration, the radioactivity was relatively high in bristles and bones, while low in liver, kidney and spleen. After 10 weeks only traces of radioactivity were still in the body. 40 hours after the administration, 40% of the dose was excreted into the urine and 60% of the dose via the faeces.

Rhesus monkeys (*Macaca mulatta*) were dosed orally with ^{14}C-LAS at a dose level of 150 mg/kg (Cresswell et al.,1978). Plasma radioactivity concentrations reached a maximum of 41.2 µg/ml at 4 hr and then declined during the following 6-24 hours with a biological half-life of about 6.5 hrs. After 7 consecutive daily doses of 30 mg/kg, both plasma concentrations of radioactivity and the biological half-life were almost identical to those observed after single administration. Two hours after the last dose, the highest radioactivity was observed in the stomach. Radioactivity was also observed in the intestinal tract, kidneys, liver, lung, pancreas, adrenals and pituitary. At 24 hours, concentrations were highest in the intestinal tract, probably indicating biliary excretion. Since the concentrations in the tissues were in general lower than in plasma, no specific accumulation of LAS occurred. When ^{14}C-LAS was injected into the skin, most of the radioactivity remained at the site of injection. During the 120 hours after single oral (30 mg/kg) or subcutaneous (1 mg/kg) doses, average rates of excretion were between 63% and 74% in the urine and between 9% and 26% in the faeces. TLC of the urine extracts after oral or subcutaneous doses showed that only trace amounts of unchanged LAS were present. Five metabolites were excreted but they were not identified. Incubations with beta-glucuronidase/sulfatase did not affect the metabolites, indicating that the metabolites were probably not present as the corresponding conjugates.

Rats were dosed orally with ^{14}C-NaLAS and radioactivity was detected 0.25 hr after administration, reaching a maximum at 2 hrs (Sunakawa et al.,1979). The biologically half-lives were calculated to be 10.9 hrs. The distribution was high in the digestive tract and in the bladder at 4 hours after administration. Concentrations were also high in the liver, kidney, testis, spleen and lung. Sixty-eight hours after administration, the rates of excreted radioactivity were 47% in the urine and 50% in the faeces.

^{35}S-LAS ($15 \cdot 10^8$ cpm) was administered topically, once, onto the back skin of rats and guinea pigs (Chikara Debane,1978). Absorption and distribution in major organs and blood were studied. Urine was collected 24 hours after topical application of the test substance. In the guinea pig, the amount of ^{35}S excreted in the urine was about 0.1% of the total administered dose. Organ distribution in the rat was about 5 times greater than in the guinea pig and "relatively large amounts" of ^{35}S were noted in the liver and kidneys.
Conclusion: when 0.2-0.5% LAS is topically applied once, it is approximately absorbed by 0.1-0.6%; there was no accumulation in specific organs; the test chemical was quickly excreted in the urine after being metabolised.

Studies (Howes,1975) with isolated human skin preparations as well as in vivo investigations of percutaneous administration of LAS to rats have demonstrated that penetration through skin and subsequent systemic absorption of this surfactant does not occur to any significant extent at 24 to 48 hours. ^{14}C-LAS was applied on the clipped dorsal skin of the rats, which was washed after 15 min. No radioactivity was detected in urine or faeces.

LAS was not detected in the uterus of pregnant ICR mice administered with a single oral dose of 350 mg/kg bw on day 3 of gestation (Koizumi et al.,1985).

Conclusions
- LAS is readily absorbed by the gastro-intestinal tract (80-90% of the administered dose)
- The LAS absorption through intact skin is very poor (0.1-0.6% of the administered dose)
- LAS is distributed to most organs, except uterus, and the major part is metabolised in the liver to sulfophenyl carboxyl acids
- LAS metabolites are eliminated primarily via the urine and faeces

- Main urinary LAS metabolites are sulfophenyl butanoic and sulfophenyl pentanoic acids; most of them are normally excreted within 24 hours.
- Accumulation of LAS or of its main metabolites has not been observed after repeated oral administration
- The good absorption of LAS by the gut and its very poor adsorption by the skin is an interesting observation. To explain it, one could speculate that the gut microflora may be adapting with time and causing metabolism of LAS before it is absorbed.

5.2.1.2 Acute toxicity

5.2.1.2.1 Acute oral toxicity

Six acute toxicity tests are available, five with rats (Hüls-a,1984; Hüls-b,1984; Hüls-c,1984; Ito et al.,1978; Huntingdon,1984; Murmann,1984), and one with mice (Ito et al.,1978).

In a well documented and conducted study with rats (Huntingdon,1984), according to GLP and the OECD 401 method, clinical observations, at doses near the LD_{50} values (1980 mg/kg bw), were piloerection, hunched posture, abnormal gait (waddling), lethargy, decreased respiratory rate, ptosis, pallor of the extremities and diarrhoea. Recovery was apparently complete by day 4 for survivors. Deaths occurred within 24 hours after administration. Autopsy of rats that died revealed isolated cases of pallor of the kidneys or spleen. Terminal necropsy findings for survivors were normal.

The oral acute toxicity of the test substance in rats was also examined in another study (Murmann,1984). Groups of 5 male and 5 female rats were exposed orally via gavage to 0, 1075, 1220, 1360, or 1710 mg/kg bw of test substance (all doses reported were adjusted from the original for 86% activity). The animals were then monitored for 14 days for mortality and clinical signs. Body weights were measured on days 7 and 14, and necropsies were performed at the end of the study. No effects on body weight were observed, but all animals showed some signs of toxicity. Symptoms beginning about 30 minutes past application included diarrhea, squatting attitude, breathing difficulties, nose bleeding, ataxia, and lethargy. These symptoms had disappeared in surviving animals by 120 hours. In the animals that died before the end of the study, red mucous was seen in the stomach and intestine. In the surviving animals, hyperemia of the stomach was noted, along with abnormalities of the stomach, liver, spleen, kidneys, and the peritoneum. Mortality was seen at all dose levels, with 4 of 10 animals at the lowest dose level dying. All animals at the highest dose level died. The acute oral LD_{50}, when adjusted for active content was 1080 mg/kg bw.

Conclusion
The acute oral LD_{50} for rats was 1080 mg/kg bw. Mortality was seen at all dose levels. In addition, all animals showed some signs of toxicity, with symptoms including diarrhea, squatting attitude, breathing difficulties, nose bleeding, ataxia, and lethargy, though all of these symptoms had disappeared in surviving animals by 120 hours. In the surviving animals, hyperemia of the stomach was noted, along with abnormalities of the stomach, liver, spleen, kidneys, and the peritoneum.
According to the CLP-Regulation, the test substance is a Category IV toxicant (H302: Harmful if swallowed).

5.2.1.2.2 Acute inhalation toxicity

Acute inhalation data are available for LAS (Kinney,1985). Groups of six 8-week old rats underwent nose-only exposures to aerosol atmospheres containing 65, 120, 260 or 310 mg/m^3 particulate LAS (C_{12}, 98% activity) for 4 hours, followed by 14 days of observations for clinical signs. During exposures, rats in all groups had clear to red nasal discharge. During the recovery

period, rats exhibited dose dependent weight loss 1 day post exposure followed by normal weight gains. No mortality or adverse clinical signs occurred at concentrations up to 260 mg/m^3. At 310 mg/m^3, MMAD (Mass Median Diameter) = 2.5 microns, one rat died during the exposure and two rats died one day post exposure.

It is important to note that this laboratory exposure is not representative of the possible LAS exposure during actual production or use and, therefore, its relevance is limited. In the study, animals were given high exposures to respirable-sized particles, which were generated by special, difficult laboratory procedures. LAS particles of that size do not occur under normal conditions. Spray products containing LAS are designed to produce large particle sizes. These large particles are needed for efficient delivery of the spray to the surface being cleaned. This results in particle sizes that are much larger than the respirable particle sizes used in testing and, therefore, would not be able to reach far into the lungs where effects could occur. Given this lack of relevance to real-world exposure potential, the use of this study for risk assessment purposes is limited.

Conclusion
Given this lack of relevance to real-world exposure potential, the use of this acute inhalation study for risk assessment purposes is limited. Due to the irritant nature of LAS, it is expected that high LAS aerosol concentrations may be irritating to the upper respiratory tract.

5.2.1.2.3 Acute Dermal Toxicity

The acute dermal toxicity of LAS was investigated in three rabbit studies (Monsanto,1971; Monsanto-a,1972; Monsanto-b,1972). Toxicity effects were found at doses ranging from 251 mg/kg bw to 794 mg/kg bw. Control groups were not used. The number of animals was 1 per dose substance and not from the same sex. Clinical observations were reduced appetite, reduced activity, increased weakness and collapse. Necropsy findings consisted of haemorrhagic lungs, liver discoloration, enlarged gall bladder, and gastro-intestinal inflammation (only observed in the animals that died).

A limit test study was performed on rats, according to the OECD 402 Method and GLP (Huntingdon-a,1986). There were no deaths following a single dermal application of 2000 mg/kg bw of LAS at 47% of active matter. No signs of systemic reaction to treatment. Well-defined or slight erythema and slight oedema were observed at all test sites after removal of the occlusive dressings on day 2. These reactions were unresolved before progressive hardening of the skin that was first detected on day 4. All test sites were entirely covered by scab formation from day 7. Sloughing from the scabbed skin began at various times between day 7 and day 12 and was completed before termination. Low bodyweight gains or loss of bodyweight were recorded for one male and three female rats on day 8. The three female rats also showed low bodyweight gains between day 8 and 15. Terminal necropsy findings were normal in all animals.

The clipped skin on the backs (approximate 10% of the area) of five male and five female rats was exposed to a dose of 2000 mg/kg bw LAS and kept under an occlusive dressing for 24 hours, then observed for another 14 days after the dressing was removed and the skin washed in warm water. The treated areas were examined daily for signs of dermal irritation and assessed according to the standard scoring system for erythema, eschar and oedema. On day 15 all animals were sacrificed and given a macroscopic post-mortem examination of internal organs. No mortality was observed at exposures to 2000 mg/kg of the undiluted test material. There were no signs of systemic reaction. Well defined or slight erythema and slight oedema were observed at all test sites after removal of the occlusive dressings, and these reactions were unresolved before progressive hardening of the skin was first detected on day 4. All test sites were entirely covered by scab formation from day 7.

Sloughing from the scabbed skin began at various times between day 7 and day 12 and was completed before test termination. Therefore, results indicate slight erythema and slight oedema but no acute mortality. The dermal LD_{50} is > 2000 mg/kg bw.

Conclusion
The quality of the data of studies by Monsanto,1971; Monsanto-a,1972; Monsanto-b,1972 on rabbits has to be rated as non reliable, mainly due to the fact that the animals were not sufficient number (only 1 per dose) and were not of the same sex. No information was provided about the concentration of the tested substance.

Reliable results come from a well-performed and documented limit test on rats (Huntingdon-a,1986), with a LD_{50} >2000 mg/kg bw at the LAS concentration of 47% (LD_{50} >1000 mg/kg bw at 100%). In the study by Kynoch,1986 no mortality was seen at exposures to 2000 mg/kg of undiluted LAS and no other signs of systemic reactions were observed. However, well defined or slight erythema and slight oedema were observed at all test sites immediately after removal of the occlusive dressings, and these reactions were unresolved before progressive hardening of the skin was first detected on day 4. All test sites were entirely covered by scab formation from day 7, and complete sloughing from the scabbed skin was completed before test termination. Therefore, results indicate slight erythema and slight oedema but no acute mortality from dermal exposures, with a dermal LD_{50} of > 2000 mg/kg. Therefore the substance is not classified for acute dermal toxicity under CLP.

5.2.1.3 Skin Irritation

Several skin irritation studies on rabbits are available for LAS at the concentration of about 50%. (Huntingdon-b,1986; Hüls,1983; Kaestner-a,1987; Kaestner,1977; BIOLAB-a,1989). Findings of all the studies were consistent, showing similar irritation effects.

The most reliable study (Huntingdon-b,1986) was performed on three animals with a semi-occlusive application, according to the OECD Guideline 404 and GLP. LAS concentration as active matter was 47%. Three rabbits were exposed to 0.5 ml of the test substance dermally for 4 hours on clipped skin under a gauze pad held in place by an adhesive dressing. Examination of the treated skin was made approximately 30 minutes after removal of the patch and daily through 14 days. Grading and scoring of the dermal reactions was performed using the standard numerical scoring system. Irritation was noted in all animals at the first observation (maximum score of 2). Symptoms worsened, and desquamation, necrosis, and hyperkeratinization was noted by day 4. Symptoms resolved in one animal by day 12, but in the other two animals, symptoms were seen through the end of the observation period. The primary dermal irritation index was 2.17.

In other studies (BIOLAB,1988; BIOLAB-b,1989; BIOLAB,1983) LAS was tested at 1%, 2.5% and 5%, according to the modified Draize test. Six rabbits were used with a 24-hour application on intact and abraded skin. An occlusive dressing was applied in all experiments. For LAS at 1% and 2.5% no effects were found. The 5% dilution is considered a moderate irritant according to the Draize criteria.

Conclusion
LAS in aqueous solutions, after a 24 hour application on intact and abraded skin of rabbits under occlusive dressing, did not show any irritation effects at concentrations of 1% and 2.5%, while it was moderately irritating at the concentration of 5% (Draize criteria). At higher concentrations, 47-50%, LAS is irritating, on the base of the available tests on the intact skin of rabbits with a 4 hour application under occlusive or semi-occlusive dressing. Irritation symptoms worsened after

exposure, and desquamation, necrosis, and hyperkeratinization were noted by day 4 in all animals. These resolved in one animal by day 12, but in the other two animals symptoms continued through the end of the observation period. Therefore, LAS is considered a Category 2 skin irritant.

5.2.1.4 Eye irritation

Four eye irritation studies on rabbits are available for LAS at the concentration of about 50% (Kaestner-b,1987; Hüls-b,1983; Huntingdon-c,1986; BIOLAB-c,1989). Findings of all the studies were consistent and showed significant irritation effects.

The most reliable and documented study (Huntingdon-c,1986), performed according to GLP and OECD Guidelines, was conducted on three rabbits with LAS at 47%. Groups of three rabbits had 0.1 ml of test substance placed in each of their eyes. In one group, the eyes were not rinsed. In the second group, the eyes were rinsed after 4 seconds of exposure. In the third group, the eyes were rinsed after 30 seconds of exposure. Observations were made one hour and 1, 2, 3, 4, 7, 14, and 21 days after exposure. Severe irritation was noted in the animals whose eyes were not rinsed. This irritation was not resolved in one of these animals at the end of 21 days. Irritation was also seen in the animals rinsed after 30 seconds, although the irritation was not as severe, and the effects were fully reversible within 14 days. Mild irritation was seen in the animals rinsed after 4 seconds. These effects were fully reversible within 7 days. Since OECD guideline 405 for eye irritation studies calls for an exposure of at least 24 hrs, the results for unrinsed eyes were used for classification.

Another study (BIOLAB-c,1989), conducted with LAS at 50% on six rabbits, showed significant irritation effects on iris and conjunctivae. These effects were persistent at day 6.

LAS was tested at lower concentrations as well. In two Japanese studies (Iimori et al.,1972; Oba et al.,1968), no abnormalities were found for animals treated with a test solution at 0.01% LAS. Slight and considerable irritation of the conjunctivae at 0.05% LAS, considerable irritation at 0.1% LAS within 2 hours, which disappeared at 24 hours, and marked reactions at 0.5% LAS (severe irritation and oedema, increased secretion, turbidity of the cornea and disappearance of the corneal reflex) for 24 hours. The eye tended to recovery and the effects disappeared completely after 120 hours. Averaged irritation scores are not available and the effects at 24, 48 and 72 hours cannot be quantitatively evaluated.

In two other studies (BIOLAB,1984; BIOLAB,1988), LAS at concentrations of 1% and 5% was tested on six rabbits, according to the OECD guidelines. Findings were that LAS is not irritating to eye at 1%, while it is moderately irritating at 5%. However, it is not classifiable as an irritant according the EU criteria.

Conclusion
LAS is not irritating to eye at 1%. It is moderately irritating at 5% (not classifiable as an irritant according the EU criteria). It is irritating to eye at concentrations of 47-50%.

Severe irritation was noted in the animals whose eyes were not rinsed and was not resolved by day 21. Milder irritation was observed in animals that had the test substance rinsed from their eye after 4 or 30 seconds, and effects seen in these rinsed animals were reversible within 7 or 14 days. Based on the irreversible irritation observed in the unrinsed animals, LAS is considered a Category 1 eye irritant (H318: Causes serious eye damage).

5.2.1.5 Sensitisation

Tests on animals

There are several studies available and the most reliable ones were selected (Hüls,1988; Procter & Gamble,1985; RBM,1985).

In the first study (Hüls,1988), performed with the Guinea Pig Maximisation Test (OECD method), LAS was used at 50%. With applications of LAS solutions at 0.1% as intracutaneous and at 3% as epicutaneous, negative results were obtained for all tested animals.

In the second study (Procter & Gamble,1985), carried out under the Buehler test (OECD method) and GLP, 10 animals (5M/5F) remained untreated and were used as controls to be treated at a first challenge, 10 animals (5M/5F) remained untreated and were used as additional controls to be treated at a second challenge, and 20 animals (10M/10F) were treated with LAS. Induction concentration was 1.0% LAS in water; first and second challenge concentrations were 0.8% LAS in water. Zero of 20 animals responded in the treated group; 0/10 animals responded in the control group.

In the last study, the potential of the test substance to be sensitising to skin was investigated (RBM,1985). Ten male and ten female guinea pigs were given intradermal injections of 25% test solution. Control animals (5 male and 5 female) were given injections of vehicle only. One week later, a second induction was done by dermal exposure to 25% test solution for 24 hrs. Control animals were again exposed to vehicle only. On day 21, the challenge exposure was performed. All animals were exposed to 12.5% test solution dermally. Exposure was for 24 hrs, with observations made at 48 and 72 hrs after the start of exposure. No positive reactions were noted.

Tests on human volunteers
Two Human Repeat Insult Patch Tests are available.

In the first (Procter & Gamble,1997) 95 volunteers were treated with LAS at 0.10% (w/v) on the upper arms, under occlusive patch conditions. Test material was applied for 24 hours, 3 times a week, for 3 weeks during the induction period. After a 14- to 17-day rest, a 24-hour challenge patch was applied on the original and alternate arm sites. There was no evidence of skin sensitisation on the 95 subjects who completed the test.

In the second test 2294 volunteers were exposed to LAS as a raw material and 17,887 exposed to LAS in formulations (Nusair et al.,1988). No evidence of skin sensitisation was found.

An occlusive epicutaneous test was carried out on volunteers in Europe. LAS was applied once at 1%. The test duration was 6 days. The authors concluded that LAS was sufficiently compatible to the skin (Matthies,1989).

Conclusion
No sensitisation potential was found for LAS when tested either on animals or on human volunteers.

5.2.1.6 Repeated Dose Toxicity

5.2.1.6.1 Oral route
LAS was administered for 90 days in the diet to groups of 15 male and 15 female rats at doses of 50 and 250 mg/kg bw/day (Oser,1965). Control groups were used. No behavioural abnormalities were noted during the test period. Growth responses were equal in all groups. There were no differences in food intake or in efficiency of food utilisation. The clinical data showed no abnormal variations in any of the dose groups. The relative organ weights and the histopathological evaluation did not show significant differences among the dose groups except for a slight liver weight increase in females of the highest dose group.

The NOAEL is 50 mg/kg bw/day.

LAS was administered for 90 days in the diet to 10 male/females rats per dose groups. Doses were 0.02%, 0.1% and 0.5% (8.8, 44, 220 mg/kg bw/day) (Kay et al.,1965). No adverse effects were found upon the following parameters: growth, food efficiency, survival, haematologic values, urinary analytical values, absolute and relative organ weights, gross and histopathological changes.
The NOAEL is 220 mg/kg bw/day, the highest tested dose.

LAS was administered for six months at doses of 0.07%, 0.2%, 0.6%, 1.8% in the diet (40, 115, 340 and 1030 mg/kg bw/day) to 10 rats per each sex (Yoneyama et al.,1972). Control groups were used. The 1.8% group showed diarrhoea, markedly suppressed growth, increased weight of the cecum, and remarkable degeneration of the renal tubes. The 0.6% (340 mg/kg bw/day) group showed slightly suppressed growth, increased weight of the cecum, increased activity of serum ALP, a decrease in serum protein and degeneration of the renal tubes. The 0.2 % (115 mg/kg bw/day) group showed increased weight of the cecum and slight degeneration of the renal tubes. The 0.07% (40 mg/kg bw/day) group showed no adverse effects related to the administration of LAS.
A NOAEL of 40 mg/kg bw/day was estimated.

LAS was administered for 9 months at doses of 0.6% and 1.8% (260 and 780 mg/kg bw/day) in the diet to male/female rats (8 animals per groups). Control groups were included (Yoneyama et al., 1976). In the 1.8% dose group, the body weight gain was suppressed and haematological and serum-biochemical adverse effects were observed in both treatment groups of both sexes. The weight of the cecum of the male rats and the weight of the liver and cecum of the females in the high dose groups were significantly increased. Enzymatic examinations of the liver and kidneys revealed changes in enzyme activities in the 1.8% groups.
A NOAEL of 260 mg/kg bw/day was estimated.

LAS was administered for 2, 4 and 12 weeks, at the a single dose of 1.5% in the diet (750 mg/kg bw/day) to groups of 5 male rats, with control groups (Ikawa et al.,1978). LAS suppressed body weight gain, and the relative liver weight was increased after 2 weeks of LAS administration. Serum biochemical examinations revealed significant increases in ALP and GTP at each observation period and significant decreases in cholesterol and protein in 4 weeks. Enzymatic examinations of the liver revealed decreases in G6Pase and G6PDH and an increase in isocitrate dehydrogenase (IDH) at each observation period. Enzymatic examinations of the renal cortex revealed decreases in G6Pase and 5'-nucleotidase at each observation period, an increase in LDH at 12 weeks, and an increase in IDH at 2 and 4 weeks. Enzymatic examinations in the renal medulla revealed a decrease in Na,K-ATPase, an increase in LDH at 12 weeks, a decrease in IDH at 2 weeks, and an increase in IDH at 12 weeks.
Effects were found at the only dose tested, equivalent to 750 mg/kg bw/day.

LAS was administered to male/female rats for 9 months in drinking water, at doses of 0.07%, 0.2% and 0.6% (85, 145, 430 mg/kg bw/day) (Yoneyama et al.,1976). Control groups were used.
Haematological examination revealed no significant changes in any experimental group and no organ weight changes were observed. Body weight gain was suppressed in the males of the highest dose group and also serum-biochemical and enzymatic parameters of the liver and kidney were affected. A significant decrease in renal Na,K-ATPase was seen in the group given 145 mg/kg bw/day of LAS.
The NOAEL is 85 mg/kg bw/day and the LOAEL is 145 mg/kg bw/day.

LAS was administered by gavage to male/females rats (12 animals per dose group) for one month, at daily doses of 125, 250, 500 mg/kg bw/day (Ito et al.,1978). Control groups were used. Diarrhoea was observed in the 500 mg/kg group and soft stools were observed in the other 2 groups. Body weight gain was suppressed in all the male groups and in the female 500 mg/kg bw/day group.

Haematological examinations revealed no abnormalities. Serum-biochemical examinations revealed several differences among the mid and high dose group compared to the control group. The weight of the spleen and the heart significantly decreased in the male high dose group. In the female high dose group, the weight of the liver increased while the weight of the heart and thymus decreased.
Histological findings of the liver revealed no abnormalities.
The NOAEL was 125 mg/kg bw/day.

LAS was administered to mice for six months in drinking water, at the dose of 100 ppm, corresponding to 20 mg/kg bw/day (Watari et al.,1977). No data about sex and number of animals are available. Control groups were used. The animals were sacrificed at 1, 2, 3, and 6 months. Some animals were observed an additional 2 months without test substance administration. Liver slices were investigated using electron microscopy. Hepatic damage was observed at one and six months. In mice examined after the two-month recovery some hepatic damage was seen, while other cellular effects had reversed, indicating that the liver cells had recovered.
LOAEL = 20 mg/kg bw/day
.
Groups of 8 or 9 male/females mice were given diets containing LAS at concentrations of 0.6 and 1.8% (corresponding to 500 and 1000 mg/kg bw/day) or drinking water containing LAS at concentrations of 0.07%, 0.2% and 0.6% for 9 months (corresponding to 100, 250, 600 mg/kg bw/day for males and to 100, 250, 900 mg/kg bw/day for females) (Yoneyama et al.,1976). Control groups were used.
LAS in diet: in the mice given 500 mg/kg bw/day, body weight gain was not suppressed, but the weight of the liver increased in male and female mice. Enzymatic examinations revealed significant decreases in LDH of the liver and in acid phosphatase of the kidneys in the male mice.
LAS in drinking water: body weight was depressed at the highest dose for male and females, increase in liver weight in females, significant decreases in renal Na,K-ATPase.
LOAEL: 500 mg/kg bw/day (in diet)
NOAEL: 250 mg/kg bw/day (in water)

A 28-day study on male/female Rhesus monkeys (*Macaca mulatta*) was conducted (Heywood et al.,1978). LAS was given to four groups of three males and three females at doses of 30, 150, 300 mg/kg bw/day per gavage (po) and simultaneously with 0.1, 0.5, or 1.0 mg/kg bw/day subcutaneously (sc). Control groups were used. At 300 (po) and 1.0 (sc) mg/kg bw/day, the monkeys vomited frequently and usually within 3 hours of administration. An increased frequency of loose or liquid faeces was recorded for animals receiving 150 (po) and 0.5 (sc) mg/kg bw/day. These effects are probably related to the inherent irritative effects of LAS rather than to its systemic toxicity. Fibrosis of the injection sites was found among the entire test group, the incidence and severity being dose related. Ophthalmoscopy, laboratory examination of blood and urine, organ weight analysis and histopathological investigation did not detect any further treatment-related responses.
The demonstrated systemic NOAEL is 150 mg/kg bw/day (po) + 0.5 mg/kg bw/day (sc), since animals vomited at the higher dose level and may not have been truly exposed to LAS.

In a well-documented study of teratogenicity (Nolen et al.,1975) (see 5.2.1.9), a mixture of 55% of tallow alkyl ethoxylate sulphate and 45% of LAS was fed to two generations of rats either continuously to males and females during the 8-week growth period or only to females during the organogenesis period. Control groups were used. Seven groups of 25 male and 25 female rats received dietary levels of the mixture of 0.1%, 0.5% and 1% (50, 250 and 500 mg/kg bw/day). The corresponding doses of LAS were 22.5, 112.5 and 225 mg/kg bw/day. No significant effects were seen in weight gain, organ/body weight ratios, haematology values and histopathology during both the first generation 8-week period and the second-generation period.
The NOAEL for LAS is the highest dose tested of 225 mg/kg bw/day.

In a three-generation study with rats for reproductive toxicity (Palmer et al.,1974) (see 5.2.1.8), findings of the oral administration for 60 days of LAS in a commercial light duty liquid detergent (17% LAS and 7% alkyl ethoxylate sulphate) are available. This study is well documented and complies with guidelines recommended by the US-FDA and GLP. Dietary concentrations of 0, 0.08%, 0.4% and 2% (0, 40, 200 and 1000 mg/kg bw/day) of the formulation were continuously administered throughout three generations for 60 days prior to mating. The corresponding administration of LAS was of 0, 6.8, 34 and 170 mg/kg bw/day. The number of parental animals per group, control groups included, were 11 males and 22 females for the F0 generation and 10 males and 20 females for F1b and F2b. Among parental animals over the three generations there were no signs of adverse effects to treatment. Food consumption and bodyweight changes showed no consistent relationship to dosage. The terminal necroscopy revealed no changes attributable to treatment.
The NOAEL for LAS is the highest dose tested of 170 mg/kg bw/day.

5.2.1.6.2 Inhalation

Long-term studies on LAS inhalation are not available. Given the irritant nature of LAS, it is expected that repeated inhalation of LAS might be irritating to the respiratory tract.

5.2.1.6.3 Dermal route

LAS was applied for 15 days to the backs of male rats, at daily doses of 0.5 g of solutions at 20 and 30% (about 286 and 427 mg/kg bw/day) (Sadai et al.,1972). On the 16th day of the experiment, the animals were assessed. Body weight gain was suppressed in the 20% group (286 mg/kg bw/day) and the body weight was decreased in the 30% group (427 mg/kg bw/day). An infiltrating, yellowish-reddish brown crust was observed after 2-3 days in the lower dose group, and after 1-2 days in the high dose group. After 4-6 days the crust was abraded and erosion occurred at the abraded site. Histological examinations of the application site revealed severe necrosis of the region from the epidermis cuticle to the upper layer of the dermis, severe infiltration of leukocytes in the necrotic site, and diffuse inflammatory cell infiltration of all layers of the corium. The effects on body weight are to be considered related to the LAS irritation.
The LOAEL for these effects is 286 mg/kg bw/day, the lower dose tested.

The repeated dose toxicity tests are summarised in Table 23.

Table 23: Summary of the repeated dose toxicity tests

Animal	**Route**	**Duration**	**NOAEL** mg/kg bw/day	**LOAEL** mg/kg bw/day	**Doses** mg/kg bw/day	**Reference**
Monkey	Gavage+ subcutaneous injection	28 days	150 (po) + 0.5 (sc)		30,150,300 (po) + 0.1, 0.5, 1.0 (sc)	Heywood et al.,1978
Rat	Gavage	1 month	125	250	125, 250, 500	Ito et al.,1978
Rat	Oral feed	60 days	170		6.8, 34, 170	Palmer et al., 1974
Rat	Oral feed	2 months	225		22.5, 112.5, 225	Nolen et al.,1975
Rat	Oral feed	90 days	50	250	50, 250	Oser et al.,1965
Rat	Oral feed	90 days	750 (*)		750	Ikawa et al.,1978
Rat	Oral feed	90 days	220		8.8, 44, 220	Kay et al.,1965
Rat	Oral feed	6 months	40	115	40,115,340, 1030	Yoneyama et al.,1972
Mouse	Drinking	6 months		20 (**)	20	Watari et al.,1977

	water					
Rat	Oral feed	9 months	260	780	260, 780	Yoneyama et al.,1976
Rat	Drinking water	9 months	85	145	85, 145, 430	Yoneyama et al.,1976
Mouse	Oral feed	9 months	< 500	500	500, 1000	Yoneyama et al.,1976
Mouse	Drinking water	9 months	100	250	100, 250, 750	Yoneyama et al.,1976
Rat	Dermal	15 days	< 286	286	286, 427	Sadai et al.,1972

(*) the only dose tested
(**) effects disappeared during the course of the study

Conclusion

LAS was tested for toxicity in several repeated dose toxicity experiments by the oral and dermal routes in rodents (rats, mice) and non-rodents (monkeys).
In monkeys dosed for 28 days by gavage and subcutaneous injection, the observed effects were diarrhoea at 150 mg/kg bw/day (oral) +0.5 mg/kg bw/day and vomiting at 300 mg/kg bw/day (oral) +1 mg/kg bw/day (subcutaneous), but effects of systemic toxicity were not found (Heywood et al.,1978).

In some studies, with duration from 1 to 3 months, no effects were observed in rats at oral doses (by gavage or in diet) from 125 to 750 mg/kg bw/day, except for a slight liver increase in females administered with 250 mg/kg bw/day for 3 months.

Ultra-structural changes in liver cells were observed at the dose of 20 mg/kg bw/day in one 6-month study in mice which were dosed orally (drinking water), but effects were not seen at higher doses in other studies. These changes seem to be reversible as they disappeared in the course of the study (as did liver effects reported at higher doses in two 24-month carcinogenicity studies in rats (see 5.2.1.7), in which proliferation of hepatic cells and other effects were observed after one and six months and later disappeared). Since these alterations later disappeared, they are considered to represent adaptation to the administration of LAS.

Increased weight of the cecum and slight degeneration of the renal tubes were noted in a 6-month study at the dose of 115 mg/kg bw/day administered by oral feed (Yoneyama et al.,1972). The dose with no adverse effects was 40 mg/kg bw/day.

In a 9-month study in rats, a significant decrease in renal Na,K-ATPase was seen at the oral dose (drinking water) of 145 mg/kg bw/day, while no effects were seen at 85 mg/kg bw/day (Yoneyama et al.,1976).

In two other 9-month studies by the same authors, oral administration of higher doses (250 and 780 mg/kg bw/day), to mice in drinking water and to rats in diet, resulted in suppressed body weight gain, changes in weight of spleen, heart, thymus, cecum, liver, and degeneration of renal tubes. Also haematological, serum-biochemical and enzymatic alterations were seen in liver and kidneys. The NOAELs were 100 and 260 mg/kg bw/day respectively.

Repeated dermal application on rats of 280 mg/kg bw/day of LAS for 15 days, the only dose tested, caused local irritation effects and, most likely as a consequence, suppression of the body weight gain (Sadai,1972).

NOAEL
In view of the available information it is not possible to determine which single study among those summarized above is the most reliable or appropriate for the determination of a NOAEL. Because of that, based on the data from all the studies, a NOAEL of 85 mg/kg bw/day is proposed, which was derived from a 9 month oral study and corresponds to the NOAEL which is closest to the lowest available oral LOAEL of 115 mg/kg bw/day.

5.2.1.7 Genetic Toxicity

5.2.1.7.1 *In vitro*

Bacterial tests
A reliable and well documented test (Hüls,1993) was conducted according to OECD Guidelines and GLP on TA 98, TA 100, TA 1535, TA 1537, TA 1538 Salmonella typhimurium strains with and without metabolic activation. Concentrations tested were 8-5000 µg/plate and the cytotoxicity concentration was >5000 µg/plate, both with and without metabolic activation. The LAS concentration was 91.3%. Negative and positive controls were used.

Another bacterial mutagenicity study (Ames test) (Schoeberl,1993) using Salmonella typhimurium strains TA 1535, TA 1537, TA 98 and TA 100, as well as TA1538, at test concentrations of 8, 40, 200, 1000 and 5000 µg/plate is also available. All strains tested negative with and without S9 activation.

Two other Ames tests are available. Although conducted on limited Salmonella typhimurium strains compared those recommended by the OECD Guidelines and with no information about cytotoxicity and controls, they showed negative results (Inoue et al.,1980; Sunakawa et al.,1981). Concentrations tested were up to 200 µg/plate in the first assay and up to 500 µg/plate in the second one. The LAS concentration was 20%.

One recombination assay (Inoue-a et al.,1979) is available on *Bacillus subtilis*, with and without metabolic activation. Concentrations tested were up to 50 µg/plate. The LAS concentration was 99.5%. Results were negative.

An *Escherichia coli* reverse mutation assay, with and without metabolic activation, reported negative results (Inoue-a et al.,1979). No data on the concentration tested were given.

Non bacterial tests
A transformation test with Syrian hamster embryo (SHE) cells without metabolic activation was conducted with negative results (Inoue et al.,1980). Concentrations tested were up to 50 µg/plate. The LAS concentration was 22.2%.

In the second test (Anon.,1995), the potential of LAS to cause mutations in mammalian cells was examined. Chinese Hamster Ovary (CHO) cells were exposed to concentrations of 0, 0.6, 1, 1.8, 3, and 6 µg/ml without S9, and 0, 6, 10, 18, 30, and 60 µg/ml with S9. The cells were then examined for cytogenicity and mutation frequency. Ethyl methane sulfonate and 3-(20-)methylcholanthrene were used as positive control substances. Preliminary tests show the test substance was cytotoxic at concentrations of 50 µg/ml or greater with metabolic activation, and 100 µg/ml or above without metabolic activation. There was no biologically significant increase in mutation frequency in the treated groups. Therefore, results show that LAS was not mutagenic to CHO cells both in the presence and absence of S9.

The third study (Murie and Innes,1997) examined the potential of LAS to cause chromosomal

aberrations in mammalian cells. Chinese hamster ovary cells were exposed to concentrations of 2.5, 5, 10, 15, 20, 26, 33, and 39 µg/ml with S9, and 20, 39, 58, 78, 104, 130, and 156 µg/ml without S9. No biologically significant results were seen in treated cultures in the absence of metabolic activation. In the presence of metabolic activation the results were more equivocal. In the first of three tests, no cytotoxicity, and no increase in chromosome aberrations were observed at doses of 10 or 20 µg/ml and 100% cytotoxicity was observed at 39 µg/ml. In the second test, a steep cytotoxicity curve was observed between 10 and 20 µg/ml with a cell count of 68/90 % at the 10 µg/ml dose and no living cells remaining at the 20 µg/ml dose. An increased in aberration frequency could be observed at the 10 µg/ml dose. No increase in aberration frequency has been observed at lower doses which also did no show any cytotoxicity. To gain clarity on the positive result an additional test was conducted. Here, no cytotoxicity and no increase in chromosomal aberration frequency have been observed at the 10 µg/ml dose. At the 15 µg/ml dose the cell number was reduced to 25 % which is why this dose group cannot be evaluated due to excessive cytotoxicity. These results indicate that LAS is weakly clastogenic at cytotoxic concentrations but negative at concentrations below cytotoxic concentrations in this *in vitro* assay.

Conclusion
In bacterial test and in a test with mammalian cells the substance did not induce gene mutations. In a chrosomal aberration test LAS was weakly clastogenic at cytotoxic concentrations but negative at concentrations below cytotoxic concentrations.

5.2.1.7.2 *In vivo*

A cytogenetic assay (chromosomal aberrations) on male mice was carried out (Inoue-b et al.,1979). Doses of 200, 400, 800 mg/kg bw/day of LAS were administered by gavage for 1 and 5 days. The maximum dose was half the LD_{50}. Bone marrow was examined 6, 24, 48 hours after administration. There was no significant difference in the incidence of chromosomal aberrations between any of the groups given LAS and the negative control group. Mitomycin was used as a positive control and induced severe chromosomal aberrations.

Another cytogenetic assay was performed on male rats and male mouse (Masabuchi et al.,1976). LAS was administered by oral feed for 9 months, at a dose of 0.9% in rats (450 mg/kg bw/day) and in mice (1170 mg/kg bw/day). Chromosomes of the bone marrow cells were examined. There were no significant differences in the incidences of chromosomal aberrations between the experimental and control groups.

A dominant lethal assay is available (Masabuchi et al.,1976). LAS was administered as oral feed for 9 months to 7 male mice, at the dose of 0.6% (300 mg/kg bw/day). One of the male mice was mated with 2 female mice that were not given LAS. The pregnant mice were laparotomized on day 13 of gestation to determine the numbers of luteal bodies, implantations, surviving foetuses, and dead foetuses. There were no significant differences in fertility, the mortality of ova and embryos, the number of surviving foetuses, or the index of dominant lethal induction between the experimental groups and the control group. Details are not available about eventual signs of toxicity and the number of animals is very limited.

In one micronucleus assay on male mice (Kishi et al.,1984), a single intraperoneal application at the dose of 100 mg/kg bw was administered. There were no differences in the incidences of polychromatic erythrocytes with micronuclei in the bone marrow cells between the treated group and the control group.

An *in vivo* mammalian micronucleus study is available on the structurally related substance LAS Acid (CAS#85536-14-7, Benzenesulfonic acid, C10-13-sec alkyl derivatives). In this study (Fedtke,1991), 40 male and 40 female mice were given a single oral dose by gavage of 1122 mg/kg LAS Acid (read across) and evaluated for chromosome aberrations. Only a single dose has been evaluated which was in the range of the acute oral LD50 value for LAS Acid in rats (LD50 = 1470 mg/kg). Furthermore, slight cytotoxicity has been observed after 48 hours. No statistically significant or biologically relevant increases in the number of polychromatic erythrocytes with micronuclei were observed; therefore the test material is considered negative for cytogenicity.

Conclusion
LAS was tested in cytogenetic assays in rat and mouse, in a dominant lethal assay in rat, and in an micronucleus test in mice. None of these tests indicated any genetic toxicity of the test compound *in vivo*. An additional micronucleus study with mice conducted on the structural analogue LAS Acid further supports that LAS is not clastogenic *in vivo*.

The positive result in the *in vitro* chromosome aberration study using a rodent cell line (CHO cells) derived from cancer tissues that is lacking proper cell cycle control has to be seen in the context of the extensive *in vivo* data. *In vivo* studies do assess genotoxicity under more realistic conditions, including exposure. Therefore, LAS is not considered a genotoxic compound.

5.2.1.8 Carcinogenicity
Four studies are available.

A test was conducted on male/female rats (Buehler et al.,1971). Doses of LAS (98.1%) of 0.02%, 0.1% and 0.5% (10, 50, 250 mg/kg bw/day) were administered for 2 years in the diet. A control group was used. No information about the method used was given. Fifty animals per dose group and sex were tested. Adverse effects on growth or feed efficiency were not observed during the experiment. Five males and females from each of the groups at 8 and 15 months and all survivors at 24 months were necrospied, haematologic values were determined, and tissues were taken for histologic studies.

These examinations revealed no consistent dietary-induced changes, which could be considered a toxic response. In addition, animals, which showed significant loss of weight, development of tumours or other evidence of abnormalities, were sacrificed and tissues were preserved for study. The incidence of tumours and the common incidental diseases were similar in all dietary groups.

In a second study, Wistar rats were exposed for 2 years at doses of 0.01%, 0.05%, 0.1% LAS (34.55%) in drinking water, corresponding to 20, 100, 200 mg/kg bw/day. (Tiba et al.,1972). Control groups were used. There were no changes due to the administration of LAS in regard to growth, mortality, the weight of major organs, or histopathological findings. There is no description of tumours in the report.

In a third study, male/female Wistar rats were fed LAS at doses of 0.04, 0.16. 0.6% (20, 80 and 300 mg/kg bw/day) for 1, 3, 6, 24, or more months (Fujii. et al.,1977; Yoneyama et al.,1977). A control group was used. Groups of 5 rats of both sexes were fed for 1, 3, 6, and 12 months and groups of 15 rats of both sexes were fed for 24 months or more. During the experiment, the 0.6% group showed slight increases in weights of liver and cecum, and in GPT and ALP in serum. LAS administration had no adverse effects upon the intake of food, body weight gain, general condition, and mortality or mean survival period. On the basis of these results, it was concluded that the diet containing LAS at a concentration of 0.6% (300 mg/kg bw/day) did not have any adverse effects on rats.

Detailed histopathological examinations were made on the rats. At one month, proliferation of hepatic cells in the liver and slight swellings of the renal tubes and narrowing of the tubular lumen in the kidneys were found in the 0.16% and 0.6% groups. Since these findings disappeared later on, they were thought as being adaptation phenomena to the administration of LAS. There were no histopathological lesions attributable to LAS administration in any of the organs in the rats, which were fed for 24 months or more. Various types of tumours were observed in different organs, but findings suggestive of tumorigenicity of LAS were not present.

Male and female rats were exposed up to 26 months to LAS at the dose of 0.1% in drinking water (200 mg/kg bw/day) (Endo et al.,1980). A control group was used. A group of 62 rats of both sexes were treated with LAS and a control group of 37 rats of both sexes were given pure water. Five to 12 of the rats in the experimental group and 3 to 12 rats in the control group at 3, 6, 12, and 18 months, and all surviving rats between 24 and 26 months were sacrificed for pathological, biochemical, and haematological examinations. The administration of LAS had no effect on the intake of water, mortality, body weight gain, or general condition. In pathological examinations, looseness, atrophy, and fatty change of the hepatic cells in the liver were found in the experimental group at 6 months, together with significant increases in GOT, GTP and bilirubin. In haematological examinations no effects due to LAS were observed.

Conclusion
Even though the studies are conducted per-1980 and were not performed and/or evaluated according to GLP and current requirements (number of animals, doses, scope of investigations) the information that they provide is still useful. All the studies were well conducted according to common practice at the time and toxicity was observed at the higher dose tested in some of the studies. All of the studies consistently showed lack of evidence of carcinogenicity in all species tested (rats and mice). There is no reason to believe that LAS has carcinogenic potential.

5.2.1.9 Reproductive toxicity

A four-generation reproduction study is available on male/female Wistar rats (Endo et al.,1980). Animals were administered 0.1% LAS in drinking water (corresponding to 70 mg/kg bw/day). A control group was used. The administration of LAS had no adverse effects on fertility, parturition, gestation period, or lactation in any of the generations. Five to 10 rats of both control and experimental groups were sacrificed at 12 weeks for pathological examinations. No effects of LAS administration were observed.

A three-generation reproduction study was conducted on male/female rats. LAS was administered in the diet at doses of 0.02, 0.1, 0.5% (14, 70, 350 mg/kg bw/day) (Buehler et al.,1971). A control group was used. Animals were fed for 84 days to the 4 groups of weaning rats, each consisting of 50 animals of both sexes (FO-generation). Twenty females from each dose group were mated with 20 males from the same group. The first litters of each generation (F1a-generation) were sacrificed at 21 days of age. Ten days after the first litter was sacrificed, all females were re-mated with different males from the same group. The F2a-generation was sacrificed at the F1a-generation. From the resulting F1b-generation, 20 males and females of each group were selected at weaning to continue their respective diets for 80 to 85 days until they were mated to produce the F2b-generation. This generation was treated with LAS for a further 8 weeks and mated again. The first litter (F3a) was sacrificed; the F3b-generation was treated until the animals were weaned. General reproduction including fertility gestation, parturition, neonatal viability, lactation, and post-weaning growth was normal for all test groups and did not deviate from the controls in each generation. No gross abnormalities were noted. No definitive adverse effects due to the test material were noted in the haematology and pathology.
NOAEL Parental: 350 mg/kg bw/day
NOAEL F1 Offspring: 350 mg/kg bw/day

NOAEL F2 Offspring: 350 mg/kg bw/day
The NOAEL is the highest tested dose.

Another three-generation study on rats is available for a commercial light duty liquid detergent, containing 17% LAS and 7% alkyl ethoxylate sulphate (Palmer et al.,1974). This study is well documented and complies with guidelines recommended by the US-FDA and GLP. Dietary concentrations of 0, 0.08%, 0.4% and 2% (0, 40, 200 and 1000 mg/kg bw/day) of the formulation were continuously administered throughout three generations for 60 days prior to mating. The corresponding administration of LAS was of 0, 6.8, 34 and 170 mg/kg bw/day. The number of parental animals per group, control groups included, were 11 males and 22 females for the F0 generation and 10 males and 20 females for F1b and F2b. Among parental animals over the three generations there were no signs of adverse effects of treatment. Food consumption and bodyweight changes showed no consistent relationship to dosage. The terminal necroscopy revealed no changes attributable to treatment. The mating performance, the pregnancy rate and the duration of gestation were unaffected. Among litter parameters, statistically significant differences were occasionally recorded, but as these showed non-consistent dosage related trends, they were considered to be unrelated to treatment. The incidences of sporadic deaths and total litter losses were unrelated to dosage. The incidence of malformations was unaffected by treatment. Additional organ weight analysis, histopathology and skeletal staining of representative young from the F3b generation revealed no changes that could be conclusively related to treatment.
The NOAEL for LAS is 170 mg/kg bw/day, corresponding to the highest tested dose.

Conclusion
Results of two tests on three generations and one on four generations did not show any adverse effects on reproduction at any of the doses tested. Based on these studies, a NOAEL of 350 mg/kg bw/day, corresponding to the highest tested dose, is assessed.

5.2.1.10 Developmental Toxicity and Teratogenicity

5.2.1.10.1 Oral route

Female rats and rabbits were administered 0.1% LAS in drinking water, corresponding to 383 mg/kg bw/day for rats and to 3030 mg/kg bw/day for rabbits (Endo et al.,1980). Control groups were used. LAS was given to 40 rats (20 controls) and 22 rabbits (11 controls) from day 6 to 15 (rats) and day 6 to 18 of pregnancy (rabbits). The effect on the dams was a slight inhibition of body weight gain in the rabbits. The litter parameters of both species did not show any significant differences from those of the controls. Delayed ossification was observed in rabbits, but there was no increase in malformations in either the rabbits or the rats.
NOAEL Maternal: 383 mg/kg bw/day (rat)
LOAEL Maternal: 3030 mg/kg bw/day (rabbit)
NOAEL Foetuses: 383 mg/kg bw/day (rat)
LOAEL Foetuses: 3030 mg/kg bw/day (rabbit)

Palmer et al. conducted studies on female rats, mice and rabbits (Palmer-a et al.,1975). They were all conducted according to GLP and standard guidelines and their results are summarised below:
Rat study (Palmer-a et al.,1975)
Twenty animals per dose group were used. Animals were daily administered at day 6-15 of pregnancy by gavage with LAS at doses of 0.2, 2, 300, 600 mg/kg bw/day and sacrificed at day 20 of gestation. A control group was used. The body weight gain was retarded in the highest dose group from the start of dosing and showed partial recovery toward the end of the dosing period. One animal died in this group, but it could not be conclusively related to treatment. The toxic effects were associated with disturbance of the gastrointestinal tract. Pregnancy rates were comparable at all dosage.

No differences were observed among the dose groups and the control group with respect to: number of litters, viable young, litter weight, foetal weight, embryonic deaths, implantations, corpora lutea, pre- and post-implantation embryonic loss, major malformations, and minor visceral or skeletal anomalies or incidence of pups with extra ribs.
NOAEL Maternal: 300 mg/kg bw/day
NOAEL Foetuses: 600 mg/kg bw/day
Mice study (Palmer-a et al.,1975)
Animals were administered 0.2, 2, 300, 600 mg/kg bw/day LAS by gavage on days 6-15 of pregnancy, then sacrificed on day 17 of pregnancy (Palmer-a et al., 1975). A control group was used. Among parent animals, treatment at 300 and 600 mg/kg bw/day was associated with increased mortality (35% and 90% respectively). At 300 mg/kg bw/day weight gain was retarded only during the first four days. No assessment could be done at 600 mg/kg bw/day due to the high mortality rate. Necropsy revealed an almost invariable picture of tympanites, sometimes associated with gastritis. Pregnancy rates were essentially comparable for all groups. At doses with no maternal toxicity, no differences were observed among the dose group and the control group with respect to: number of litters, viable young, litter weight, foetal weight, embryonic deaths, implantations and post-implantation embryonic loss. At these doses the incidences of major malformations and minor abnormalities were not affected. At doses with maternal toxicity there was increased foetal loss and reduced litter size due almost entirely to total litter loss, which was considered to be a secondary effect due to the maternal toxicity. The incidences of major malformations and minor abnormalities were not significantly affected, apart from a higher, but not statistically significant, incidence of skeletal anomalies at 300 mg/kg bw/day (extra ribbed pups). Given the large difference between the maternal no-effects dose of 2 mg/kg bw/day and the LOAEL dose (300 mg/kg bw/day), this study, although well documented and conducted according to GLP, does not allow determination of a reliable maternal NOAEL.
Since no assessment was possible at 600 mg/kg bw/day, due to the high mortality rate of parent animals, the NOAEL for litters is 300 mg/kg bw/day.
Rabbits study (Palmer-a et al.,1975)
Animals were administered 0.2, 2, 300, 600 mg/kg bw LAS by gavage at days 6-18 of pregnancy, then sacrificed at day 29 of pregnancy (Palmer-a et al.,1975). A control group was used. At 300 and 600 mg/kg bw/day, parent animals showed anorexia, diarrhoea, weight loss and death; mortality rates were 85 and 100% and necropsy revealed changes in the gastrointestinal tract. At 0.2 and 2 mg/kg bw/day, treatment did not adversely affect bodyweight changes and pregnancy rates of parent animals. The influence of maternal toxicity at higher doses restricted assessment of the effects on litter parameters to animals treated with lower dosages, which showed no adverse effects on litter parameters.
This study, although well documented and conducted according to GLP, does not allow determination of reliable NOAELs, given the large difference between the maternal no-effects doses of 2 mg/kg bw/day and the maternal LOAEL dose (300 mg/kg bw/day) that is also the dose for which effects on litters could not be determined due to the high mortality rate in parent animals.

A test was conducted on female mice. Doses of 40, 400 mg/kg bw/day LAS was administered daily by gavage from day 0 to day 6 of pregnancy or from day 7 to 13 of pregnancy (Takahashi et al.,1975). Thirteen to fourteen mice were used in each dose and control groups. In mice given 400 mg/kg bw/day, the pregnancy rate was 46.2% compared to 92.9% in the controls. There was no increase in malformations. Although no information on maternal toxicity is available, it appears likely that maternal toxicity was present at the high dose group.
NOAEL Maternal: 40 mg/kg bw/day
NOAEL Foetuses: 400 mg/kg bw/day

Female mice were administered doses of 10, 100, 300 mg/kg bw/day LAS daily by gavage at day 6 through day 15 of pregnancy (Shiobara et al.,1976). There were 25 to 33 mice in each dose group and a control group was used. The dams showed inhibition of body weight gains in all groups, especially in the high dose group. In this group, two dams died, and there was one case of premature delivery and death of all foetuses. There were findings such as decreased body weight and delayed ossification among the living foetuses, but there was no increase in malformations.
LOAEL Maternal: 10 mg/kg bw/day
NOAEL Foetuses: 300 mg/kg bw/day

Pregnant female rats were fed doses of 0.1%, 1.0% LAS (16 rats/dose) in the diet (80 and 780 mg/kg bw/day) from day 0 to 20 of gestation (Tiba et al.,1976). Control groups were used, but information about the numbers of animals is not available. At the LAS dose of 780 mg/kg bw/day there were no abnormalities in the body weight gains of the dams, or in the occurrence and maintenance of pregnancy. The values of the litter parameters did not differ from those of the controls and there was no evidence of teratogenicity. The number of offsprings was rather low in the highest dose group, and the weaning rate of 78.3% was lower than the 100% rate observed in the controls. However, there were no abnormalities in body weight gain, organ weights or functions in the offsprings.
NOAEL Maternal: 780 mg/kg bw/day
NOAEL Foetuses: 780 mg/kg bw/day

In a well-documented study, a mixture of 55% of tallow alkyl ethoxylate sulphate and 45% of LAS was fed to rats and rabbits (Nolen et al.,1975).
Rats. Seven groups of 25 male and 25 female rats were kept at dietary levels of 0.1%, 0.5% and 1% of the surfactant mixture (50, 250 and 500 mg/kg bw/day). The corresponding doses of LAS were 22.5, 112.5 and 225 mg/kg bw/day. The surfactant mixture was fed to two generations either continuously to males and females during the 8-week growth period or to females during the organogenesis period (days 6-15) of six pregnancies. Control groups were used. No significant effects were seen in weight gain, organ/body weight ratios, haematology values and histopathology during both the first generation 8-week period and the second-generation period. No adverse effects were noted on conception, foetal viability or post-natal survival in either generation of rats. There were no statistical differences among the groups of rat foetuses examined for birth defects. Of 1210 rat foetuses, the overall incidence of abnormal young was 9%.
NOAEL Maternal: 225 mg/kg bw/day (rat)
NOAEL Foetuses: 225 mg/kg bw/day (rat)
Rabbits. Pregnant rabbits were given 50, 100, and 300 mg/kg bw/day of the surfactant mixture by intubation on days 2-16 of gestation during a single pregnancy (22.5, 45 and 135 mg/kg bw/day of LAS). No symptoms of maternal toxicity and no adverse effects in foetuses were noted. Of 855 rabbit foetuses, 5.7% were abnormal, but the incidences of defective foetuses in the test groups were not significantly different from those in controls.
NOAEL Maternal: 135 mg/kg bw/day (rabbit)
NOAEL Foetuses: 135 mg/kg bw/day (rabbit)

In the three generation study for reproductive toxicity with rats (Palmer et al.,1974), already mentioned in 5.2.1.8, there were no signs of adverse effects of treatment over the three generations at dietary concentrations of a formulation containing 0, 6.8, 34 and 170 mg/kg bw/day of LAS. Food consumption and bodyweight changes showed no consistent relationship to dosage. The terminal necroscopy revealed no changes attributable to treatment. The incidence of malformations was unaffected by treatment. Additional organ weight analysis, hystopatology and skeletal staining of representative young from the F3b generation revealed no changes that could be conclusively related to treatment.

NOAEL both for parental animals and foetuses is 170 mg/kg bw/day of LAS, corresponding to the highest tested dose.

5.2.1.10.2 Dermal route

Pregnant female rats were exposed daily at days 2 through 15 of gestation to LAS at doses of 0.03%, 0.3%, or 3% on the shaved skin as 0.5 ml aqueous solution (0.6, 6, 60 mg/kg bw/day) (Palmer-b et al.,1975). A control group was used.
Maternal toxicity: at the high dose, local irritation was observed, resulting in a slightly lower body weight gain and hypersensitivity. Teratogenicity: no differences were observed among the dose groups and the control group with respect to: number of litters, viable young, litter weight, foetal weight, embryonic deaths, implantations, corpora lutea, pre- and post implantation embryonic loss. The incidences of major malformations, minor visceral or skeletal anomalies, and skeletal variants were not different between controls and dose groups even at maternal toxic doses.
NOAEL Maternal: 6 mg/kg bw/day
NOAEL Foetuses: 60 mg/kg bw/day

Another dermal study was conducted on female rats (days 0 through 21 of gestation), with daily exposure at 1.0%, 5.0%, and 20% of LAS (20, 100, and 400 mg/kg bw/day). Controls groups were used (Daly et al.,1980).
Maternal toxicity: the dams treated with 400 mg/kg bw/day and 100 mg/kg bw/day showed inhibition of body weight gain and local skin effects that compromised the integrity of the skin and caused overt toxicity, like inhibition of the body weight gain.
Teratogenicity: there were no findings indicative of effects of LAS on the foetal parameters evaluated. There were no indications of teratogenic or embryotoxic effects.
NOAEL Maternal: 20 mg/kg bw/day
NOAEL Foetuses: 400 mg/kg bw/day

Doses of 0.03, 0.3, or 3% LAS (5, 50, and 500 mg/kg bw/day) in aqueous solution were applied daily onto the shaved skin of females mice (days 2 through 13 of gestation) (Palmer-b et al.,1975). The dosage volume was 0.5 ml, which was applied to an area of skin (2 x 3 cm). Controls groups were used. At the high dose, severe local irritation was observed resulting in body weight loss and hypersensitivity, which was also observed at the medium dose. Teratogenicity: at the lowest dose, the dose with no maternal toxicity, no differences were observed among the LAS group and the control group with respect to: number of litters, viable young, litter weight, foetal weight, embryonic deaths, implantations, corpora lutea, pre- and post-implantation embryonic loss. The incidences of major malformations minor visceral or skeletal anomalies, and skeletal variants were not different between controls and the tested group. Maternally toxic dosages were associated with a significantly increased foetal loss and consequent reduction of litter size. This was due almost entirely to total litter losses, as values for the one surviving litter at the highest dose were similar to the control litters. At the medium dose, the moderate degree of maternal toxicity correlated with a moderate effect on litter values in that, whilst the higher incidence of embryonic deaths differed significantly from control values, the consequent reduction in litter size was not statistically significant. With regard to major malformations and minor skeletal or visceral anomalies, the assessment of litters was not possible in the highest dose group due to the low survival. At the low doses, no treatment related increases of the incidences of major malformations or minor skeletal and visceral anomalies were observed.
The maternal NOAEL is 5 mg/kg bw/day.
Given the large difference between the no observed effects dose for litters of 50 mg/kg bw/day and the dose of 500 mg/kg bw/day, for which the assessment of litters was not possible due to the low survival, this study does not allow determination of a reliable foetal NOAEL.

Female mice were daily treated (day 0 through day 13 of pregnancy) with a single LAS dose of 2.2% (110 mg/kg bw/day) (Sato et al.,1972). An area of 4 x 4 cm on the backs of mice was depilated and LAS was applied at a dose of 0.5 ml/mouse/day. No information about control groups. No abnormalities were seen in the dam or foetuses.
NOAEL Maternal: 110 mg/kg bw/day

Female mice were treated daily from day 6 through day 15 of pregnancy at dermal doses of 0.03%, 0.3%, 3% (15, 150, and 1500 mg/kg bw/day) of LAS (Imahori et al.,1976). Control groups were used. The 1500 mg/kg bw/day group showed a clear decrease in the pregnancy rate (67.9%) when compared with a rate of 96.3% in the controls. However, there were no decreases in the litter size, and no changes in the litter parameters with the exception of a slight decrease in foetal body weight. There were no significant increases in the incidence of malformations in the foetuses.
NOAEL Maternal: 150 mg/kg bw/day
NOAEL Foetuses: 1500 mg/kg bw/day

LAS (99.5%) was administered daily via subcutaneous injection to female mice at doses of 0.35, 1% in water (20, 200 mg/kg bw/day) from day 0 to 3 or day 8 to 11 of pregnancy (Takahashi et al.,1975). There were 12-19 mice in each treatment group. Control groups were used. When dams were administered the 200 mg/kg bw/day solution from day 0 to 3 of pregnancy, there was an initial decrease in body weight and necrosis at the injection sites. The number of pregnancies decreased in the mice given the 1% solution compared to the controls (61.5% vs. 93.3%). There were no significant changes with respect to litter parameters, major malformations or minor abnormalities.
NOAEL Maternal: 20 mg/kg bw/day
NOAEL Foetuses: 200 mg/kg bw/day

Female rabbits were exposed (days 1 through 16 of gestation) to aqueous solutions of LAS at 0.03%, 0.3%, or 3% on shaved skin (0.9, 9.0, and 90 mg/kg bw/day) (Palmer-a et al.,1975). Control groups were present. The dosage volume was 10 ml, which was applied to an area of skin (12 x 20 cm) from which the fur was removed. At the highest dose, local irritation was observed in parental animals, resulting in body weight loss an hypersensitivity. The medium dose caused retarded body weight gain and hypersensitivity. At the medium and low dose, no differences were observed among the dose groups and the control group with respect to: number of litters, viable young, litter weight, foetal weight, embryonic deaths, implantations, corpora lutea, pre- and post-implantation embryonic loss. The high dose was associated with a slightly, but not significantly, higher foetal loss and lower litter size. The incidences of major malformations, minor visceral or skeletal anomalies, and skeletal variants were not different between controls and dose groups even at maternal toxic doses.
NOAEL Maternal: 0.9 mg/kg bw/day
NOAEL Foetuses: 90 mg/kg bw/day, corresponding to the highest dose tested

LAS was applied at the concentration of 20% to the dorsal skin of pregnant mice during the pre-implantation period. On day 3 of gestation the embryos were flushed from the uterus (Nomura et al.,1980). Some dead, deformed and growth-retarded embryos were observed in the treated group. Although the authors stated that these effects were not due to maternal toxicity since no maternal organs were affected, this statement is probably not correct in view of the high concentration of LAS and its irritation effects. A secondary effect due to maternal toxicity appears much more likely. This is also corroborated by a study in which LAS were not detected in the uterus of pregnant ICR mice administered a single oral dose of 350 mg/kg bw on day 3 of gestation (Koizumi et al.,1985) (see 5.2.1.10).

The developmental and teratogenicity tests are summarised in Table 24.

Table 24: Summary of the developmental and teratogenicity tests

Animal	**Route**	**Exposure in pregnancy**	**NOAEL maternal** mg/kg bw/day	**NOAEL Teratogenicity** mg/kg bw/day	**Dose** mg/kg bw/day	**Reference**
Rat	Drinking water	Day 6-15	383	383	383	Endo et al.,1980
Rat	Oral feed	Day 0-20	780	780	80, 780	Tiba et al.,1976
Rat	Oral feed	Day 6-15 + 60 days prior mating	225	225	22.5, 112.5, 225	Nolen et al.,1975
Rat	Gavage	Day 6-15	300	600	0.2, 2, 300, 600	Palmer-a et al.,1975
Mouse	Gavage	Day 7-13	40	400	4, 40, 400	Takahashi et al.,1975
Mouse	Gavage	Day 6-15	10	300	10, 100, 300	Shiobara et al.,1976
Mouse	Gavage	Day 6-15	(2)	300	0.2, 2, 300, 600	Palmer-a et al.,1975
Rabbit	Gavage	Day 2-16	135	135	22.5, 45 ,135	Nolen et al.,1975
Rabbit	Drinking water	Day 6-18	3330 (**LOAEL**)	3330 (**LOAEL**)	3030	Endo et al.,1980
Rat	Dermal	Day 2-15	6	60	0.6, 6, 60	Palmer-b et al.,1975
Rat	Dermal	Day 0-21	20	400	20, 100, 400	Daly et al.,1980
Mouse	Dermal	Day 0-13	110	110	110	Sato et al.,1972
Mouse	Dermal	Day 6-15	150	1500	15, 150, 1500	Imahori et al.,1976
Rabbit	Dermal	Day 1-16	0.9	90	0.9, 9, 90	Palmer-b e4t al.,1975
Mouse	SC	Day 0-3 or Day 8-11	20	200	20, 200	Takahashi et al., 1975

Conclusion

LAS was evaluated for developmental/teratogenic effects on rats, mice and rabbits. Some findings of maternal toxicity were found at low or relatively low doses, administered to rats and mice dermally and by gavage, but they are associated with the irritation effects of LAS, either on the skin or the gastrointestinal tract.

Two studies, one with rabbits administered by gavage (Palmer-a et al.,1975) and one with mice administered dermally (Palmer-b et al.,1975), although well documented and conducted according to standard guidelines, did not allow determination of reliable NOAELs, due to dose ranges that are too large between the doses with no effects (2 and 50 mg/kg bw/day, respectively) and maternal toxic doses (300 and 500 mg/kg bw/day, respectively) which resulted in high mortality rates of dams and litter losses.

In two studies a clear decrease in the pregnancy rate of mice was noted, associated with the toxic doses of 400 mg/kg bw/day administered by gavage (Takahashi et al.,1975) and 1500 mg/kg bw/day administered dermally (Imahori et al.,1976), but no effects on the litters parameters or malformations were found. In other studies no effects were found both in parental animals and litters at oral doses up to 780 mg/kg bw/day and at dermal doses up to 400 mg/kg bw/day for litters. The most reliable are those by Nolen and Palmer.

In a study LAS at 20% in aqueous solution was applied to the dorsal skin of pregnant mice during the pre-implantation period (Nomura et al.,1980). Some dead, deformed and growth-retarded embryos were observed in the treated group. This was interpreted as a secondary effect due to maternal toxicity

at this high LAS concentration and its irritation effects, also corroborated by a study in which LAS was not detected in the uterus of pregnant ICR mice administered a single oral dose of 350 mg/kg bw on day 3 of gestation (Koizumi et al.,1985) (see 5.2.1.10).

To sum up: some effects, such as embryo death or deformities, decrease in pregnancy rate and litter loss were noted in some studies at maternal toxic doses. However, no decreases in the litter size, no changes in the litter parameters, no malformations or significant differences in skeletal defects were observed at oral doses up to 780 mg/kg bw/day and dermal doses up to 1500 mg/kg bw/day.

5.2.2 Identification of critical endpoints

5.2.2.1 Overview on hazard identification

LAS shows an oral LD_{50} of 1080 mg/kg bw (this value is adjusted for 86% activity) and a dermal LD_{50} of > 2000 (undiluted substance). The usual concentration sold to formulators is 50%. According to CLP-Regulation, the test substance is a Category IV toxicant (H302: Harmful if swallowed).

LAS did not show any irritation effects on rabbit's skin at concentrations from 1% to 2.5%, while it is moderately irritating at a concentration of 5%. In the range from 47% to 50% it is irritating to skin, according to the EU criteria. Irritation symptoms worsened after exposure, and desquamation, necrosis and hyperkeratinization were noted by day 4 in all animals. These resolved in one animal by day 12, but in the other two animals symptoms continued through the end of the observation period. Therefore, LAS is considered a Category 2 skin irritant.

The substance is non-irritating at 1% and moderately irritating at 5% (not classifiable as an irritant, according to the CLP criteria), while it is severely irritating to eye at the concentration of about 50%. Severe irritation was noted in the animals whose eyes were not rinsed and was not resolved by day 21. Milder irritation was observed in animals that had the test substance rinsed from their eye after 4 or 30 seconds, and effects seen in these rinsed animals were reversible within 7 or 14 days. Based on the irreversible irritation observed in the unrinsed animals, LAS is considered a Category 1 eye irritant. Reliable data on acute inhalation are not available, but given the irritant nature of LAS, it is expected that high LAS aerosol concentrations may be irritating to the respiratory tract.

LAS is not a contact sensitiser, on the basis of both animal and human volunteer tests.

LAS was tested for toxicity in several repeated dose toxicity experiments by the oral and dermal routes in rodents (rats, mice) and non-rodents (monkeys).

In monkeys dosed by gavage and subcutaneous injection, the observed effects were diarrhoea at 150 mg/kg bw/day and vomiting at 300 mg/kg bw/day, but effects of systemic toxicity were not found.

Ultra-structural changes in liver cells were observed at the dose of 20 mg/kg bw/day in one 6 months study in mice which were dosed orally (drinking water), but effects were not seen at higher doses in other studies. These changes seem to be reversible as they disappeared in the course of the study (as did liver effects reported at higher doses in two 24-month carcinogenicity studies in rats in which proliferation of hepatic cells and other effects were observed after one and six months and later disappeared). Since these alterations later disappeared, they are considered to represent adaptation to the administration of LAS.

Increased weight of the cecum and slight degeneration of the renal tubes were seen in a 9-month rat study at the dose of 115 mg/kg bw/day administered by oral feed.

In another 9-month study in rats, a significant decrease in renal Na, K-ATPase was seen at the oral dose (drinking water) of 145 mg/kg bw/day, while no effects were seen at 85 mg/kg bw/day.
Oral administration (in diet or drinking water) for 9 months of higher doses in other studies with mice and rats (from 250 to 780 mg/kg bw/day) resulted in suppressed body weight gain, changes in weight of spleen, heart, thymus, cecum, liver, and degeneration of renal tubes. Also haematological, serum-biochemical and enzymatic alterations were seen in liver and kidneys.

Repeated dermal application on rats of 280 mg/kg bw/day of LAS for 15 days caused local irritation effects and, as a consequence, suppression of the body weight gain.

In view of the available information it is not possible to determine which single study among those summarized above is the most reliable or appropriate for the determination of a NOAEL. On the basis of data from all the studies a NOAEL of 85 mg/kg bw/day is proposed, which is the closest value to the lowest available LOAEL (115 mg/kg bw/day).

In all *in vitro* and *in vivo* assays there is no indication of genetic toxicity for LAS.

The oral long term studies performed did not indicate any potential for carcinogenicity of LAS and showed no effects or histopathological findings at doses up to 300 mg/kg bw/day.

Results of studies on reproduction fail to show any adverse effects at any of the doses tested. Based on these studies, a NOAEL of 350 mg/kg bw/day, corresponding to the highest tested dose, is estimated.

For the developmental toxicity/teratogenicity, some findings of maternal toxicity were found at low or relatively low doses, administered dermally and by gavage to rats, mice and rabbits, but they are associated with irritation effects of LAS, either on the skin or the gastrointestinal tract. In other oral studies no effects were found in parental animals up to 780 mg/kg bw/day. Some effects, such as embryo death or deformities, decrease in pregnancy rate and litter loss, were noted in some studies at maternal toxic doses, but in general no decreases in the litter size, no changes in the litter parameters, no malformations or significant difference of skeletal defects were observed at oral doses up to 780 mg/kg and dermal doses up to 1500 mg/kg bw/day.

5.2.2.2 Adverse effects related to accidental exposure

The oral toxicity is greater than 1080 mg/kg bw (adjusted for 86% activity) and the dermal toxicity is greater than 2000 mg/kg bw (undiluted substance) for LAS. LAS is present in detergent formulations at 30% as a maximum.

LAS is severely irritating to the eye at concentrations of about 50%, while is moderately irritating at 5% and non-irritating at 1%. The irritating effects diminished with rinsing after the exposure.
LAS is irritating to skin at a concentration of about 50% after 4 hours of exposure, while it is moderately irritating at a concentration of 5%, and not irritating at 2.5%, after 24 hours exposure.

5.2.3 Determination of NOAEL or quantitative evaluation of data

Repeated dose toxicity

Many studies are available for the repeated dose oral toxicity. In view of the available information it is not possible to determine which single study is the most reliable or appropriate for the determination of a NOAEL. Because of that, based on data from all the studies, a NOAEL of 85 mg/kg bw/day is proposed, which is the NOAEL value closest to the lowest available LOAEL (115 mg/kg bw/day). This NOAEL is the dose with no effects on renal biochemical parameters that has been observed in a 9-month study of oral toxicity in rats.

Carcinogenicity
The oral long-term studies performed did not indicate any potential for carcinogenicity of LAS and showed no effects or histopathological findings at doses up to 300 mg/kg bw/day.

Reproductive toxicity
Results of studies on reproduction fail to show any adverse effects at any of the doses tested. Based on these studies, an oral NOAEL of 350 mg/kg bw/day, corresponding to the highest tested dose, is assessed**.**

Developmental toxicity and teratogenicity
Some findings of maternal toxicity were found at low or relatively low doses, administered dermally and by gavage to rats, mice and rabbits, but they are associated with irritation effects of LAS, either on the skin or the gastrointestinal tract.

In other oral studies no effects were found in parental animals up to 780 mg/kg bw/day.

To sum up, some effects, such as embryo death or deformities, decrease in pregnancy rate and litter loss were noted in some studies at maternal toxic doses, but in general no decreases in the litter size, no changes in the litter parameters, no malformations or significant difference in skeletal defects were observed at oral doses up to 780 mg/kg bw/day and at dermal doses up to 1500 mg/kg bw/day.

5.3 Risk assessment

5.3.1 Margin of exposure calculation

The Margin of Exposure (MOE) is the ratio of the No Observed Adverse Effect Level (NOAEL) or an appropriate substitute to the estimated or actual level of human exposure to a substance. A systemic NOAEL for LAS was determined using the 9 months oral NOAEL of 85 mg/kg bw/day in the rat (see 5.2.3) and a bioavailability of 80% (Michael,1968) following gastrointestinal absorption. The resulting value of **68 mg/kg bw/day** was used as the **systemic NOAEL** to calculate the MOE values in the different exposure scenarios detailed below.

Conversion from oral NOAEL to **inhalation NOAEC** results in a NOAEC of **74 mg/m^3/day**, which was used to calculate the MOE values for inhalation exposure.

Exposure scenario: direct skin contact from hand washed laundry
For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of 0.83 mg/kg bw/day estimated for the dermal exposure to LAS from hand washed laundry.

$$\mathbf{MOE_{direct\ skin}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/0.83 = \mathbf{82}$$

Exposure scenario: direct skin contact from pre-treatment of clothes

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of 0.49 mg/kg bw/day estimated for the dermal exposure to LAS from pre-treatment of clothes.

$$\mathbf{MOE_{direct\ skin}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/0.49 = \mathbf{139}$$

Exposure scenario: direct skin contact from hand dishwashing

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of 0.18 mg/kg bw/day estimated for the dermal exposure to LAS from hand dishwashing.

$$\mathbf{MOE_{direct\ skin}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/0.18 = \mathbf{378}$$

Other possible direct skin contact scenarios, such as short direct contact with laundry powder or laundry tablets result in even lower estimated systemic doses and will give larger MOE. These are not further considered in this risk assessment.

Exposure scenario: indirect skin contact from wearing clothes

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of 28,31 mg/kg bw/day estimated for the dermal exposure to LAS from wearing fabrics washed in laundry detergents.

$$\mathbf{MOE_{indirect\ skin}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/28.31 = \mathbf{2.40}$$

Exposure scenario: inhalation of and skin contact with aerosols from cleaning sprays

For calculation of the MOE, the systemic NOAEC of 75 mg/kg bw/day was divided by the daily systemic dose of $1.31 \cdot 10^{-5}$ mg/kg bw/day estimated for the exposure to LAS from inhalation of aerosols generated with surface cleaning sprays.

$$\mathbf{MOE_{inhalation\ aerosols}} = \text{systemic oral NOAEL /estimated systemic dose} = 74/1.31 \cdot 10^{-5} = \mathbf{5.65 \cdot 10^{6}}$$

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of $3.78 \cdot 10^{-2}$ mg/kg bw/day estimated for the exposure to LAS from skin of aerosols generated with surface cleaning sprays.

$$\mathbf{MOE_{skin\ contact}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/3.78 \cdot 10^{-2} = \mathbf{1.80 \cdot 10^{3}}$$

Exposure scenario: inhalation of detergent dust during washing processes; powder detergents

The dose of LAS from inhalation of detergent dust during the washing process was estimated to amount to $1.03 \cdot 10^{-8}$ mg/kg bw/day. The MOE that could be calculated from this low exposure is higher than 10^{9}. Such low exposure does not contribute significantly to the total LAS exposure and will therefore not be considered in the risk assessment.

Exposure scenario: oral route from residues left on dishware

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of $1.94 \cdot 10^{-3}$ mg/kg bw/day estimated for the oral route from residues left on dishware.

$$\mathbf{MOE_{oral\ route}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/1.94 \cdot 10^{-3} = \mathbf{3.51 \cdot 10^{4}}$$

Exposure scenario: inhalation and skin contact from laundry pretreatment products: Spray spot removers

The dose of LAS from inhalation from laundry pretreatment products (spray spot removers) was estimated to amount to $3.51 \cdot 10^{-6}$ mg/kg bw/day. The MOE that could be calculated from this low exposure is higher than 10^{7}. Such low exposure does not contribute significantly to the total LAS exposure and will therefore not be considered in the risk assessment.

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of $1.74 \cdot 10^{-3}$ mg/kg bw/day estimated for the exposure to LAS from skin of aerosols generated with surface cleaning sprays.

$$\mathbf{MOE_{skin\ contact}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/1.74 \cdot 10^{-3} = \mathbf{3.91 \cdot 10^{4}}$$

Exposure scenario: skin contact from laundry pretreatment products: Liquid spot removers

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of 0.49 mg/kg bw/day estimated for the exposure to LAS from skin of aerosols generated with surface cleaning sprays.

$$\mathbf{MOE_{skin\ contact}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/0.49 = \mathbf{139}$$

Exposure scenario: inhalation and skin contact from liquid cleaners: Oven cleaners (spraying)

The dose of LAS from inhalation from liquid cleaners (oven cleaners (spraying)) was estimated to amount to $1.90 \cdot 10^{-6}$ mg/kg bw/day. The MOE that could be calculated from this low exposure is higher than 10^7. Such low exposure does not contribute significantly to the total LAS exposure and will therefore not be considered in the risk assessment.

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of $2.52 \cdot 10^{-3}$ mg/kg bw/day estimated for the exposure to LAS from skin of aerosols generated with surface cleaning sprays.

$$\mathbf{MOE_{skin\ contact}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/2.52 \cdot 10^{-3} = \mathbf{2.70 \cdot 10^4}$$

Exposure scenario: skin contact from liquid cleaners: Oven cleaners (cleaning)

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of $2.19 \cdot 10^{-2}$ mg/kg bw/day estimated for the exposure to LAS from skin of aerosols generated with surface cleaning sprays.

$$\mathbf{MOE_{skin\ contact}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/2.19 \cdot 10^{-2} = \mathbf{3.11 \cdot 10^3}$$

Exposure scenario: skin contact from liquid cleaners: Bathroom cleaners (mixing & loading)

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of $3.71 \cdot 10^{-5}$ mg/kg bw/day estimated for the exposure to LAS from skin of aerosols generated with surface cleaning sprays.

$$\mathbf{MOE_{skin\ contact}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/3.71 \cdot 10^{-5} = \mathbf{1.83 \cdot 10^6}$$

Exposure scenario: skin contact from liquid cleaners: Bathroom cleaners (cleaning)

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of $7.04 \cdot 10^{-2}$ mg/kg bw/day estimated for the exposure to LAS from skin of aerosols generated with surface cleaning sprays.

$$\mathbf{MOE_{skin\ contact}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/7.04 \cdot 10^{-2} = \mathbf{9.66 \cdot 10^2}$$

Exposure scenario: skin contact from liquid cleaners: Floor cleaners (mixing)

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of $2.19 \cdot 10^{-3}$ mg/kg bw/day estimated for the exposure to LAS from skin of aerosols generated with surface cleaning sprays.

$$\mathbf{MOE_{skin\ contact}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/2.19 \cdot 10^{-3} = \mathbf{3.11 \cdot 10^{4}}$$

Exposure scenario: skin contact from liquid cleaners: Floor cleaners (cleaning)

For calculation of the MOE, the systemic NOAEL of 68 mg/kg bw/day was divided by the daily systemic dose of 4.16 mg/kg bw/day estimated for the exposure to LAS from skin of aerosols generated with surface cleaning sprays.

$$\mathbf{MOE_{skin\ contact}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/4.16 = \mathbf{16.3}$$

Exposure scenario: oral route from accidental ingestion and accidental contact with the eyes

Occasional ingestion of a few milligrams of LAS as a consequence of accidental ingestion of laundry and cleaning products is not expected to result in any significant adverse health effects to humans given the low toxicity profile of LAS. This view is reinforced by the fact that poison control centers, such as for example those in Germany, have not reported a case of lethal poisoning with detergents containing LAS.

Contact of hand wash solutions containing LAS with the skin is not a cause of concern given that LAS is not a contact sensitiser and that the concentrations of LAS in such solutions are well below 1%. As reported in section 5.2.1.2 of this assessment, aqueous solutions of LAS at concentrations up to 2.5% failed to show any irritation effects on rabbit skin after 24 hours of occlusive application.

Accidental contact of hand wash solutions containing LAS with the eyes is not expected to cause more than a mild irritation on the basis of the experimental data as reported in section 5.2.1.3.

Total consumer exposure

The consumer exposure from direct and indirect skin contact as well as from inhalation and from oral route in drinking water and dishware results in an estimated total body burden of 34.6 mg/kg bw/day. Comparison with the systemic NOAEL of 68 mg/kg bw/day yields an MOE of 1.97.

$$\mathbf{MOE_{total}} = \text{systemic oral NOAEL /estimated systemic dose} = 68/34.6 = \mathbf{1.97}$$

5.3.2 Risk characterization

5.3.2.1 Systemic toxicity

Scenarios relevant to the consumer exposure to LAS have been identified and assessed using the margin of exposure or equivalent assessments. The Margin of Exposure for the combined estimated systemic dose is 1.97.

The estimated Margin of Exposure is based on conservative estimations of both exposure and NOAEL (which is a systemic NOAEL given the existence of oral toxicokinetic data). The critical adverse effect identified associated to the NOAEL was a change in renal biochemical parameters. Other than that, the toxicological data show that LAS was not genotoxic in vitro or in vivo, did not induce tumors in rodents after two years daily dosing, and failed to induce either reproductive toxicity or developmental or teratogenic effects at the highest doses tested. Based on the above, the presence of LAS in consumer products does not raise any safety concerns associated to systemic toxicity.

5.3.2.2 Local effects

Neat LAS is an irritant to skin and eyes. The irritation potential of aqueous solutions of LAS depends on the concentration.

Contact of hand wash solutions containing LAS with the skin is not a cause of concern given that LAS is not a contact sensitiser and that the concentrations of LAS in such solutions are well below 1%. As reported in section 5.2.1.3 of this assessment, aqueous solutions of LAS at concentrations up to 2.5% failed to show any irritation effects on rabbit skin after 24 hours of occlusive application.

Accidental contact of hand wash solutions containing LAS with the eyes is not expected to cause more than a mild irritation on the basis of the experimental data as reported in section 5.2.1.4.

In the course of laundry pre-treatment, skin contact with concentrated powder paste or neat liquid detergent (in the worst case containing up to 14% LAS) may occur. If it does, contact is confined to a fraction of the skin of the hands (palms or fingers), is of very short duration (typically a few minutes at most) and the initial high LAS concentration is usually diluted out rapidly in the course of the pre-treatment task. Failing to rinse hands in water after contact with the laundry pre-treatment paste or liquid may result in transient skin irritation in the hands, which is expected to be mild in nature and effectively avoided by prompt washing with water.

Potential irritation of the respiratory tract is not a concern given the very low levels of airborne LAS generated as a consequence of cleaning sprays aerosols or laundry powder detergent dust (see sections 5.1.3.6 and 5.1.3.7).

LAS is present in household liquid detergent products at concentrations that range from 1% to 30%. Accidental spillage of neat product into the eye is to be avoided as can be expected to result in likely irritation. Immediate rinsing of the eyes with water for several minutes should follow accidental spillage of neat product. The experience from many years of marketing of household liquid detergent products containing LAS is that accidental eye spillage results at worst in transient irritation, which heals after a few days with no irreversible effects to the eye.

5.3.2.3 Acute effects

Occasional ingestion of a few milligrams of LAS as a consequence of accidental ingestion of laundry and cleaning products is not expected to result in any significant adverse health effects to humans given the low toxicity profile of LAS. This view is reinforced by the fact that poison

control centers, such as for example those in Germany and UK, have not reported any case of lethal poisoning with detergents containing LAS.

5.3.3 Summary and conclusions

The presence of LAS in many commonly used household detergents gives rise to a variety of possible consumer contact scenarios including direct and indirect skin contact, inhalation, and oral ingestion derived either from residues deposited on dishes, from accidental product ingestion, or indirectly from drinking water.

The consumer aggregate exposure from direct and indirect skin contact as well as from inhalation and from oral route in drinking water and dishware results in an estimated total body burden of 34.6 mg/kg bw/d.

The toxicological data show that LAS was not genotoxic *in vitro* or *in vivo*, did not induce tumors in rodents after two years daily dosing, and failed to induce either reproductive toxicity or developmental or teratogenic effects at the highest doses tested. The critical adverse effect identified after repeat long term dosing of LAS to animals was a change in renal biochemical parameters. A systemic NOAEL of 68 mg/kg bw/day was established.

Comparison of the aggregate consumer exposure to LAS with the systemic NOAEL results in an estimated Margin of Exposure of 1.97. The estimated Margin of Exposure is based on conservative estimations of both exposure and NOAEL (which is a systemic NOAEL given the existence of oral toxicokinetic data).

Neat LAS is an irritant to skin and eyes. The irritation potential of aqueous solutions of LAS depends on concentration. Local effects of hand wash solutions containing LAS do not cause concern given that LAS is not a contact sensitiser and that the concentrations of LAS in such solutions are well below 1% and therefore not expected to be irritating to eye or skin. Laundry pre-treatment tasks, which may translate into brief hand skin contact with higher concentrations of LAS, may occasionally result in mild irritation easily avoided by prompt rinsing of the hands in water. Potential irritation of the respiratory tract is not a concern given the very low levels of airborne LAS generated as a consequence of cleaning sprays aerosols or laundry powder detergent dust.

In view of the extensive database on toxic effects, the low exposure values calculated and the resulting large Margin of Exposure described above, it can be concluded that use of LAS in household laundry and cleaning products raises no safety concerns for the consumers.

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Yoneyama M, T Fujii, M Ikawa, H Shiba, Y Sakamoto, N Yano, H Kobayashi, H Ichikawa, K Hiraga (1976), Studies on the toxicity of synthetic detergents.(II) Subacute toxicity of linear and branched alkylbenzene sulphonates in rats, *Ann. Rep. Tokyo Metr. Res. Lab.* 24: 409 Yoneyama M, Y Mabuchi, M Icawa, H Kobayashi, H Ichicawa, Subacute toxicity of LAS, *Ann. Rep. Tokyo Metrop. Res. Lab. Public Health* 27(2): 105-112 (in Japanese), see: IPCS, 1996.

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7. Contributors to this report

7.1 Substance team

- **Manufacturers of LAS**

- ECOSOL (European Center of Studies on LAB-LAS), a CEFIC sector group formed by:
  - PETRESA
  - SASOL Italy
  - WIBARCO

- **Formulators**
  - PROCTER & GAMBLE

The substance team is in debt with the members of HERA Human Health and Environmental Task Forces as well as with the Industry coalition for the OECD/ICCA SIDS assessment of LAS for their valuable comments and suggestions during the preparation of the report.

7.2 HERA environmental task force

- AISE
- BASF
- CIBA Speciality Chemicals
- Clariant
- Dow Corning
- Henkel
- Petresa.
- Procter & Gamble, Eurocor.
- Rhodia
- Sasol Germany
- Sasol Italy.
- Shell Chemicals
- Solutia Services International
- Solvay
- Unilever

7.3 HERA human health task force

- BASF
- Bayer
- CIBA
- Clariant
- Colgate-Palmolive
- Degussa-Hüls
- Henkel
- McBride
- Procter & Gamble, Eurocor.
- Shell Chemicals
- Unilever

7.4 Industry coalition for the OECD/ICCA SIDS assessment of LAS

- Colgate
- Crompton
- Dial
- Huntsman

- John Adams Associates
- Kao
- Petresa
- Procter & Gamble
- Sasol It
- Sasol N.A.
- Stepan
- Venoco
- Weinberg Group
- YPF

FOREWORD **INTRODUCITON**

LINEAR ALKYLBENZENE SULFONATE (LAS)

1322-98-1 Decylbenzene sulfonic acid, sodium salt
25155-30-0 Dodecylbenzene sulfonic acid, sodium salt
26248-24-8 Tridecylbenzene sulfonic acid, sodium salt
27636-75-5 Undecylbenzene sulfonic acid, sodium salt
68081-81-2 C_{10-16} Monoalkylbenzene sulfonic acid, sodium salt
68411-30-3 C_{10-13} Alkylbenzene sulfonic acid, sodium salt
69669-44-9 C_{10-14} Alkyl deriv benzene sulfonic acid, sodium salt
85117-50-6 C_{10-14} Monoalkylbenzene sulfonic acid, sodium salt
90194-45-9 C_{10-13} Alkyl deriv benzene sulfonic acid, sodium salt
127184-52-5 4-C_{10-13}-sec Alkyl deriv benzene sulfonic acid, sodium salt

SIDS INITIAL ASSESSMENT REPORT

For

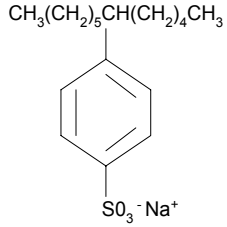
20th SIAM

Paris, France, 19-21 April, 2005

1.	**Chemical Name:**	Linear Alkylbenzene Sulfonate (LAS)
2.	**CAS Numbers:**	1322-98-1 Decylbenzene sulfonic acid, sodium salt 25155-30-0 Dodecylbenzene sulfonic acid, sodium salt 26248-24-8 Tridecylbenzene sulfonic acid, sodium salt 27636-75-5 Undecylbenzene sulfonic acid, sodium salt 68081-81-2 C_{10-16} Monoalkylbenzene sulfonic acid, sodium salt 68411-30-3 C_{10-13} Alkylbenzene sulfonic acid, sodium salt 69669-44-9 C_{10-14} Alkyl deriv benzene sulfonic acid, sodium salt 85117-50-6 C_{10-14} Monoalkylbenzene sulfonic acid, sodium salt 90194-45-9 C_{10-13} Alkyl deriv benzene sulfonic acid, sodium salt 127184-52-5 4-C_{10-13}-sec Alkyl deriv benzene sulfonic acid, sodium salt
3.	**Sponsor Country:**	United States National SIDS Contact Point in Sponsor Country: Oscar Hernandez, Director U.S. Environmental Protection Agency Risk Assessment Division (7403 M) 1200 Pennsylvania Avenue, NW Washington DC 20460 Phone: (202) 564-7461
4.	**Shared Partnership with:**	Industry Coalition for the SIDS Assessment of LAS
5.	**Roles/Responsibilities of the Partners:**	Industry was the main preparer; U.S. EPA was the main reviewer. It should be noted, however, that U.S. EPA did not review the exposure modelling that appears in Annex 1 and cannot make any conclusions regarding the exposure results of this modelling exercise.
•	Name of industry sponsor /consortium	Industry Coalition for the SIDS Assessment of LAS
•	Process used	Consortium member companies contributed in-house studies of physical-chemical properties, environmental fate and transport, ecotoxicity, and test organism toxicity for the chemicals and mixtures in the category. To supplement the industry data, literature searches were conducted employing a strategy utilizing databases available from the U.S. Chemical Information Systems and the European International Uniform Chemical Information Database (IUCLID) and Institute for Systems, Informatics And Safety (ISIS) Environmental Chemicals Data Information Network (ECDIN) databases. These databases include: Registry of Toxic Effects of Chemical Substances (RTECS) Hazardous Substances Database (HSDB)

	Aquatic Toxicity Information Retrieval (AQUIRE) Toxic Substances Control Act Test Submissions (TSCATS) Integrated Risk Information System (IRIS) The Environmental Teratology Information Center (ETIC) The Developmental and Reproductive Toxicology Database (DART) The Catalog of Teratogenic Agents (CTA) ENVIROFATE, DATALOG, AQUIRE, PHYOTOX and TERRATOX Chemical Carcinogenesis Research Information (CCRIS) The Environmental Mutagen Information Center (EMIC) GENETOX Sax's Dangerous Properties of Industrial Materials Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles International Uniform Chemical Information Database (IUCLID) Environmental Chemical Data Information Network (ECDIN) TOXLINE www.chemfinder.com standard scientific data compendia such as Verschueren (1996), CRC Handbook of Chemistry and Physics and The Merck Index. CAS Registry Numbers in dossier section 1.01 were used to match records available in each database. All reports identified were subject to a reliability check for determining adequacy in developing the Robust Summaries. U.S. EPA reviewed and edited drafts to come to consensus.
6. Sponsorship History	
• How was the chemical or category brought into the HPV Chemicals Programme ?	The industry coalition agreed to sponsor LAS in the SIDS-ICCA program, with the U.S. EPA being the country sponsor.
7. Review Process Prior to the SIAM:	Prepared by Industry. Reviewed by U.S. EPA to come to a consensus document. Human health portion of SIAP accepted at SIAM 17, Arona, Italy, November 2003. Environmental portion of SIAP accepted at SIAM 20, Paris, France, April 2005. U.S. EPA did not evaluate the exposure annex and therefore, can make no conclusions regarding these values.
8. Quality Check Process:	Industry coalition members developed the documents, which were then reviewed by outside third parties.
9. Date of Submission:	Revised document submitted August 15, 2005.

SIDS INITIAL ASSESSMENT PROFILE

CAS Nos.	1322-98-1 Decylbenzene sulfonic acid, sodium salt 25155-30-0 Dodecylbenzene sulfonic acid, sodium salt 26248-24-8 Tridecylbenzene sulfonic acid, sodium salt 27636-75-5 Undecylbenzene sulfonic acid, sodium salt 68081-81-2 C_{10-16} Monoalkylbenzene sulfonic acid, sodium salt 68411-30-3 C_{10-13} Alkylbenzene sulfonic acid, sodium salt 69669-44-9 C_{10-14} Alkyl deriv benzene sulfonic acid, sodium salt 85117-50-6 C_{10-14} Monoalkylbenzene sulfonic acid, sodium salt 90194-45-9 C_{10-13} Alkyl deriv benzene sulfonic acid, sodium salt 127184-52-5 4-C_{10-13}-sec Alkyl deriv. benzene sulfonic acid, sodium salt
Category Name	Linear Alkylbenzene Sulfonate (LAS)
Structural Formula	This structure of a C_{12}-LAS is representative of the category. 

SUMMARY CONCLUSIONS OF THE SIAR

Category Identification/ Justification

The LAS molecule contains an aromatic ring sulfonated at the para position and attached to a linear alkyl chain at any position except the terminal carbons. The alkyl carbon chain typically has 10 to 14 carbon atoms and the linearity of the alkyl chains ranges from 87 to 98%. While commercial LAS consists of more than 20 individual components, the ratio of the various homologs and isomers, representing different alkyl chain lengths and aromatic ring positions along the linear alkyl chain, is relatively constant in currently produced products, with the weighted average carbon number of the alkyl chain based on production volume per region between 11.7-11.8. LAS are supported as a category because of the close consistency of the mixtures, their commercial uses, fate, and health and environmental effects. LAS is the primary cleaning agent used in many laundry detergents and cleaners at concentrations up to 25 percent in consumer products, and up to 30 percent in commercial products, with the exception of one reported product at 45% percent in concentrated solid form that is mechanically dispensed into diluted solution for dishwashing.

Human Health

Substantial data exist for mammalian toxicity. The available data indicate that LAS exhibits slight acute toxicity. Oral LD_{50} values for rats range from 1,080 to 1,980 mg/kg bw. Oral LD_{50} values for mice are 2,160 and 2,250 mg/kg bw for males and females, respectively. The rat dermal LD_{50} value was greater than 2,000 mg/kg bw. The oral and dermal acute toxicity data for LAS generally indicate low hazard potential when all studies are considered together. Acute inhalation toxicity data indicate that LAS is moderately toxic, with mortality occurring at respirable particle concentrations of 310 mg/m^3 (MMAD = 2.5 microns).

In a series of studies on rabbits, LAS was not irritating to the skin or eyes at low concentrations (0.5-2.5%), moderately irritating at 5%, and more severely irritating at higher (about 50%) concentrations. In studies that

included rinsing, eye irritation effects diminished with rinsing after 30 seconds of exposure and were slight with rinsing after 4 seconds of exposure. In a low volume eye test (LVET) using a 35% LAS solution, rabbits experienced moderate irritation that was completely reversible by day 35. (Note that the maximum concentration of LAS is 25 percent in consumer products and normally less than 30 percent in commercial products.) Accidental eye exposure in 231 manufacturing employee incidents and 284 consumer incidents established that eye irritation effects of exposure during manufacturing and use of products containing LAS and other surfactants are moderate, transient and reversible.

In 15 repeated dose studies with rats, mice, and monkeys exposed to LAS via oral and dermal routes, LOAELs ranged from 115 to 750 mg/kg bw/day. The corresponding NOAELs ranged from 40 to 250 mg/kg bw/day. Effects commonly observed included suppressed body weight gain, diarrhea, increases in relative liver weight, differences in enzymatic and serum-biochemical parameters, and mild degeneration and desquamation of the tubular epithelium in the kidneys.

In four well designed *in vitro* bacterial (*Salmonella*) mutagenicity studies, LAS shows no evidence of mutagenicity either with or without S9 metabolic activation. LAS showed no evidence of causing increased cell transformation in an *in vitro* cell transformation assay. In *in vivo* studies, no significant differences in chromosome aberrations were seen when mice were given either oral doses up to 800 mg/kg bw/day or dietary doses up to 1170 mg/kg bw/day. In a mouse micronucleus study, LAS did not induce a clastogenic effect. Rats given dietary doses up to 450 mg/kg bw/day also showed no significant differences in chromosome aberrations. Collectively, these data support that LAS is not genotoxic.

The highest dose tested in four carcinogenicity studies with rats was 300 mg/kg bw/day. In the most documented study, rats were administered up to 250 mg LAS/kg body weight/day in the diet for two years. Results of this study indicate no gross or histopathological evidence of a carcinogenic effect. No evidence of tumorigenesis was observed in any of the carcinogenicity studies. While the quality and focus of the studies precludes a definitive assessment, the results of the genetic toxicology and rodent bioassay studies collectively provide strong weight-of-evidence support that LAS is not genotoxic and is not a rodent carcinogen.

Similarly, no evidence of reproductive or fertility effects was observed in any of the three available reproductive toxicity studies in which rats were given dietary doses over three to four generations. NOAELs from these reproductive studies ranged from 70 to 350 mg/kg bw/day, which were the highest doses tested. In 17 developmental toxicity studies, effects such as embryo death or deformities, and litter loss were most often observed only at maternally toxic doses and were associated with the irritation effects of LAS on skin or the gastrointestinal tract. No decreases in litter size, no changes in litter parameters, no malformations or significant differences in skeletal defects were observed at oral doses up to 780 mg/kg bw/day in rats and at dermal doses of 500 mg/kg bw/day in mice and 90 mg/kg bw/day in rabbits.

All of the studies included in the dossier are considered reliable, but all with limitations. The results are consistent with each other and these data are used in a weight-of-evidence approach. Based on these considerations, the highest NOAEL value below the lowest LOAEL from all of the mammalian toxicity studies is the most appropriate. Therefore, the NOAEL is 85 mg/kg bw/day. This value comes from a rat drinking water, 9-month repeated dose toxicity study. The lowest LOAEL (115 mg/kg/day) was associated with increased weight of the cecum and slight degeneration of the renal tubules.

Environment

Pure LAS is a solid at ambient temperatures with a melting point of 198.5°C. The boiling point for LAS could not be determined experimentally due to decomposition beginning at 444°C. LAS has a low vapor pressure (calculated as 3-5 x 10^{-13} Pa). LAS is water soluble, with a critical micelle concentration (CMC) value of 0.1 g/L and forms a clear solution in water at concentrations up to 250 g/L. Although it is impossible to accurately measure an octanol-water partition coefficient for surface-active agents like LAS, an octanol-water partition coefficient of log 3.32 has been calculated for $C_{11.6}$ LAS. K_d values for LAS in activated sludge and sediment increased with increasing alkyl chain length of LAS homologues with K_d values for C_{12} LAS of 3210 L/kg in activated sludge and 330 L/kg in river sediment. In activated sludge, sorption and desorption equilibria for LAS were achieved very rapidly, and comparison of the extent of sorption and biodegradation shows that the absorbed fraction as well as the soluble fraction of LAS is available for biodegradation. Based on Fugacity III modeling results using the most relevant input parameters, more than 99 percent of the residual (non-biodegraded) fraction of LAS distributes to the soil. LAS does not undergo significant degradation by abiotic mechanisms under environmentally relevant conditions as photolyzable and hydrolyzable groups are absent from the chemical structure.

An extensive database of studies demonstrates rapid and complete (ultimate) biodegradation of LAS in many of the available aerobic biodegradation tests, including soil and the aqueous environment. In several tests, LAS has been shown to be readily biodegradable, and has passed the 10-day biodegradation window in mineralization tests for most ready tests. LAS is removed in biological wastewater treatment at percentages ranging from 77-82% for trickling filters up to 99%+ for activated sludge. The biodegradation kinetics of the longer alkyl chain lengths are generally faster, and their sorption coefficients larger. The primary degradation intermediates are sulfophenyl carboxylates (SPCs), which further degrade to CO_2, SO_4^{2-}, and water. LAS does not generally degrade under anaerobic conditions. The measured bioconcentration factors of pure homologues and isomers decrease with decreasing average alkyl chain lengths (from almost 1000 for 2-phenyl-C_{13} LAS to 2 for 6-phenyl-C_{10} LAS), all with rapid clearance. The calculated BCF for currently produced $C_{11.6}$ LAS is 87 and was 22 for filtered Mississippi River water (average alkyl chain length of surface water fingerprint = $C_{10.8}$).

Ecotoxicity data are extensively available for LAS, with several comprehensive reviews having been completed. The lowest reliable acute $LC_{50}/EC_{50}/ErC_{50}$ values based on a review of the aquatic toxicity data on commercially representative LAS ($C_{11.6}$-$C_{11.8}$) were 1.67, 1.62 and 29.0 mg/L for fish, *Daphnia magna*, and algae, respectively. Acute toxicity is greater for individual LAS homologues with longer alkyl chain lengths. LAS biodegradation intermediates are significantly less toxic than the parent LAS with L/EC_{50} values >1000 mg/L for fish and *D. magna*. Chronic freshwater toxicity studies following guideline exposures (28-30 days for fish, 21 days for invertebrates and 3-4 days for algae provided the following NOEC values: fish NOEC = 1 mg/L (two studies, two species); Daphnia, NOEC = 1.18-3.25 mg/L (six values, two studies, one with 5 diets); algae, NOEC = 0.4-18 mg/L (four studies, two species). In addition all of the available, reliable chronic single species aquatic toxicity data on LAS have been evaluated, including three freshwater species in which multiple studies were reported and nine freshwater species for which single studies were reported. Single NOEC values and geometric mean NOEC values (calculated for species with multiple results) were normalized to $C_{11.6}$ LAS. These NOEC values range from 0.25 to 6.1 mg/L for freshwater species, including fish, invertebrates, algae and higher plants. Geometric mean NOEC values for marine species ranged from 0.025 to 5.0 mg/L. Based on the model ecosystem studies, a NOEC of 0.27 mg/L (0.37 if normalized to $C_{11.6}$ LAS) was determined for the freshwater ecosystem. This value is based on model stream ecosystem studies of over 250 species, and is consistent with the single species chronic freshwater data.

NOEC values for sediment exposures were greater than or equal to 81 mg/kg dry matter based on studies in four species, including GLP studies in *L. variegates* (survival, reproduction and growth over 28 days) and *C. elegans* (egg production, 3 days). Field studies indicate no adverse effects of LAS in sludge-amended soil from LAS levels of 15 mg/kg dry matter in the soil (9 microbial functions/processes and abundance/diversity of microarthropods and earthworms, short-term and 4 years) or 31,300 mg/kg dry matter in sludge (function of microbial community, short-term and 1 year).

In laboratory studies in which young trees are exposed to artificial sea spray, LAS concentrations of 10 mg/L lead to increased foliar penetration of NaCl, a hypothesized mechanism of defoliation.

A health and environmental risk assessment is available (heraproject.com).

Exposure

Current LAS production is approximately 390,000 metric tons in the North America, 400,000 metric tonnes in Europe, and 85,000 metric tonnes in Japan. Global production was 2.6 million metric tonnes in 1995. In the production phase, manufacturing processes have been designed to maximize production yield and minimize potential releases. Worker exposure is possible during the detergent formulation stage by inhalation of powders or dermal contact of powders and liquids. Good manufacturing design practices (e.g., enclosed production in agglomeration processes, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) in place at facilities that manufacture liquid and dry (granular/powder) materials are anticipated to mitigate worker exposure to LAS. Any LAS that is not incorporated into a product is captured by dust-handling equipment for recycling back into the production process. A limited amount of LAS in aqueous solution may be released as a dilute solution from washing and rinsing operations in the manufacturing process and is discharged to wastewater treatment. Incidental quantities of the dry (granular/powder) product (e.g., from floor sweepings) may be disposed in landfills.

Labeling of consumer products containing LAS and other surfactants include warnings of the potential for eye irritation and first aid instructions to rinse with water.

Data suggest that inhalation of LAS products during use will be low. Spray products containing LAS are designed to produce the large particle sizes needed for efficient delivery of the spray to the surface being cleaned. In laboratory simulations with six spray nozzles representing those used in spray cleaning products, less than 0.1% of the total volume sprayed consists of respirable particles (particles under 10 microns in diameter) and air concentrations in the breathing zone are in the 0.13-0.72 mg/m^3 range. Inhalation of detergent dusts during washing processes, modeled by HERA (2004), was 10-fold lower than inhalation of aerosols from cleaning product sprays. This estimate is based on a published study reporting an average of 0.27 µg dust per cup of product used for machine laundering. This is a conservative (protective) estimate as exposure from modern compact/granular detergent formulations produced in agglomeration processes, which produce larger particle sizes, would be expected to be much less. Based on these data, it is expected that exposures to respirable particles from inhalation are low.

Results of extensive environmental monitoring evaluations in the United States indicate that measured surface water concentrations were generally below 50 µg/L for river water samples collected under low dilution (worst case) conditions below treatment plant mixing zones. Values in the 2800 km reach of the Mississippi River from Minneapolis to New Orleans range from non-detect (<0.1 µg/L) to 28 µg/L (362 samples). LAS river water concentrations similar to those in the US were observed in monitoring studies conducted in Europe and Japan.

Measured LAS concentrations in river sediments were generally less than 1-2 mg/kg dry weight. Mississippi River sediments were <1 mg/kg dry matter with one exception. LAS levels in sediments of the receiving waters of the Tiber River (Italy) were 1.8 mg/kg dry matter. Higher LAS concentrations have been observed near untreated or poorly treated wastewater discharges, e.g. LAS in sediments of a small river (Rapid Creek, USA) below a trickling filter treatment plant averaged 190 mg/kg just below the outfall, 11.2 mg/kg less than 5 miles downstream and 5.3 mg/kg greater than 5 miles downstream

RECOMMENDATION AND RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

Human Health: The chemicals in the LAS category are currently of low priority for further work because of their low hazard potential except for skin and eye irritation and acute inhalation. Based on data presented by the Sponsor Country, exposure to respirable particles is anticipated to be low. Other countries may desire to investigate any exposure scenarios that were not presented by the Sponsor Country.

Environment: The chemicals in the LAS category possess properties indicating a hazard for the environment (fish, invertebrates and algae). However, they are of low priority for further work due to ready and/or rapid biodegradation and limited potential for bioaccumulation.

SIDS Initial Assessment Report

1 IDENTITY

1.1 Identification of the Substance Category

CAS Number:	1322-98-1	Decylbenzene sulfonic acid, sodium salt
	25155-30-0	Dodecylbenzene sulfonic acid, sodium salt
	26248-24-8	Tridecylbenzene sulfonic acid, sodium salt
	27636-75-5	Undecylbenzene sulfonic acid, sodium salt
	68081-81-2	C_{10-16} Monoalkylbenzene sulfonic acid, sodium salt
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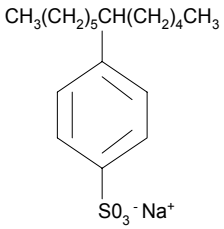
	85117-50-6	C_{10-14} Monoalkylbenzene sulfonic acid, sodium salt
	90194-45-9	C_{10-13} Alkyl deriv benzene sulfonic acid, sodium salt
	127184-52-5	4-C_{10-13}-sec Alkyl deriv benzene sulfonic acid, sodium salt
Chemical Name:	Linear Alkylbenzene Sulfonate (LAS)	
Description	LAS is the primary cleaning agent used in many laundry detergents and cleaners at concentrations up to 25 percent in consumer products, somewhat higher in industrial/commercial products. The LAS molecule contains an aromatic ring sulfonated at the *para* position and attached to a linear alkyl chain at any position except the terminal carbons (Valtorta et al., 2000). The linear alkyl carbon chain typically has 10 to 14 carbon atoms, with the approximate mole ratio varying somewhat regionally with weighted averages of 11.7-11.8. The alkyl chains are >95% linear. The structure of C_{12}-LAS, representative of the category, is shown in the figure. While commercial LAS consists of more than 20 individual components, the ratio of the various homologues and isomers, representing different alkyl chain lengths and aromatic ring positions along the linear alkyl chain, is relatively constant across the various detergent and cleaning applications. Because of the close consistency of the mixtures, their commercial uses, fate and effects, LAS is discussed as a category rather than as individual CAS numbers in this assessment.	



Molecular Weight	Range depending on alkyl chain length from 338 ($C_{11.3}$) to 356 ($C_{12.6}$)	
	The approximate weight percentage of the alkyl chain varies somewhat regionally as shown below.	

Region	<C_{10}	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	>C_{14}	Range of Averages	Weighted Average*
Canada 68081-81-2	≤1	<16	19-39	20-50	5-27	<3	<1	11.8	11.8
Europe 25155-30-0 68081-81-2 68411-30-3 85117-50-6 90194-45-9 127184-52-5	≤1	8-20	19-39	20-50	5-27	<1-3	<1	11.6-11.8	11.7
Japan 68081-81-2 68411-30-3 69669-44-9	≤1	7-16	19-39	20-50	5-27	<1-3	<1	11.7-11.8	11.8
United States 1322-98-1** 25155-30-0 26248-24-8** 27636-75-5** 68081-81-2 69669-44-9 85117-50-6 90194-45-9	<2	1-25	7-50	20-50	5-45	<1-10	<1	11.3-12.6	11.7

* Weighted by production volume for each region.
**Manufacture of LAS under these CAS numbers has recently been discontinued.

As shown in the table, all the LAS category members (CAS numbers) have the alkyl chain distributions for the LAS category. All of the data in this assessment, except for data identified as such, is on LAS category materials having the alkyl chain distribution shown in the table.

1.2 Production/Purity/Impurities

LAS is manufactured from linear alkylbenzene (LAB) in self-contained, enclosed systems (see Annex, Format A, Section VI(1), for more information). LAB is produced by reacting paraffins with benzene and a catalyst and isolating the LAB by distillation. The LAB is then sulfonated, which in turn is then neutralized to sodium salts of LAS.

Commercial LAS is exclusively manufactured as mixtures of C10 to C13 or C14 alkyl chain homologues, having average alkyl chain lengths ranging from C11.3 to C12.6, with the predominant materials having average alkyl chain lengths ranging from C11.7 to C11.8 (Table above). Each alkyl chain homologue consists of a mixture of all the possible sulfophenyl isomers except for the 1-phenyl isomer, which is not found in the commercial material. The catalyst used to make the LAB determines the distribution of the phenyl isomers in commercial LAS with the proportion of the 2-phenyl isomers ranging from 18 to 28% (Valtorta et al., 2000). Consequently,

commercial LAS consists of a mixture of 20 or more compounds, the 2-phenyl to 5-phenyl isomers of the C10 homologue, the 2-phenyl to 6-phenyl isomers of the C11 and C12 homologues and the 2-phenyl to 7 phenyl isomers of the C13 homologue, etc.

The commercial material is >95% pure LAS. Some methyl-substituted (i.e., iso-branched) LAS may be present in the mixtures (Nielsen et al. 1997). The amount of the iso-LAS component is small (1-6%) and was shown not to limit biodegradation relative to pure linear component (Nielsen et al. 1997; Cavalli et al. 1996). Non-linear components such as dialkyltetralin sulfonates (DATS) can be present at levels of less than 1 to 8% depending on the manufacturing process (Nielsen et al. 1997). DATS, like iso-LAS, have been shown to be biodegradable (Nielsen et al. 1997). Improvements in processing techniques in the U.S., Europe, and Japan incorporated to increase LAS yields also reduce the amount of DATS present.

While historically LAS has ranged from 87-98% pure, recent market information (LAS SIDS Consortium, unpublished, 2005) indicates that less than 5% of the global LAS production contains high levels of DATS.

1.3 Physico-Chemical properties

Table 1 Summary of physico-chemical properties

Property	Value	Method	Reference (Reliability)
Physical state	Solid		Dossier 1.1B
Melting point	198.5ºC	Experimental ($C_{12.0}$)	Dossier 2.1a (2)
	274ºC	Calculated as C_{10}*	Dossier 2.1b (2)
	279ºC	Calculated as C_{11}*	Dossier 2.1c (2)
	284ºC	Calculated as C_{12}*	Dossier 2.1d (2)
	290ºC	Calculated as C_{13}*	Dossier 2.1e (2)
Boiling point	Decomposition onset at 444ºC	Experimental ($C_{12.0}$)	Dossier 2.2a (2)
	630ºC	Calculated as C_{10}*	Dossier 2.2b (2)
	642ºC	Calculated as C_{11}*	Dossier 2.2c (2)
	654ºC	Calculated as C_{12}*	Dossier 2.2d (2)
	665ºC	Calculated as C_{13}*	Dossier 2.2e (2)
Relative density	1.06 g/cm^3	Experimental ($C_{11.6}$)	Dossier 2.3a (4)
Bulk density	450-550 kg/m^3	Experimental ($C_{11.6}$, $C_{12.0}$)	Dossier 2.3b,c (4)
Vapor pressure (at 25ºC)	3 x 10^{-13} Pa	Calculated as C_{12} *[using all phenyl position isomers]*	Dossier 2.4a (4)
	2.88 x 10^{-12} Pa	Calculated as C_{10}*	Dossier 2.4b (2)
	1.22 x 10^{-12} Pa	Calculated as C_{11}*	Dossier 2.4c (2)
	5.13 x 10^{-13} Pa	Calculated as C_{12}*	Dossier 2.4d (2)
	2.16 x 10^{-13} Pa	Calculated as C_{13}*	Dossier 2.4e (2)
Partition coefficient n-octanol/water (log value)	3.32	Calculated as $C_{11.6}$ *[using all phenyl position isomers]*$_1$	Dossier 2.5a (2)
	1.94	Calculated as C_{10}*	Dossier 2.5b (2)
	2.43	Calculated as C_{11}*	Dossier 2.5c (2)
	2.92	Calculated as C_{12}*	Dossier 2.5d (2)
	3.42	Calculated as C_{13}*	Dossier 2.5e (2)
Critical micelle concentration	0.1 g/L	Experimental (C_{12})	Dossier 2.6Aa (2)
Water solubility	250 g/L	Experimental ($C_{11.6}$)	Dossier 2.6Ab (2)
pH	10.0 ± 1	1% solution ($C_{12.0}$)	Dossier 2.6Ba (4)
pKa	<1	Based on structural analogue (benzene sulfonic acid)	Dossier 2.6Bb (4)
Henry's law constant	6.35 x 10^{-3} Pa m^3/mole	Calculated as C_{12}	Dossier 2.13A (2)

* Structure modelled is the pure homologue, 2-phenyl isomer, not the commercial material.

Table 1 summarizes the representative physico-chemical properties of LAS. Pure LAS is a solid at ambient temperatures. The melting point for LAS has been experimentally determined. EPI Suite calculations (dossier 2.1b-e), which are reliable for predicting trends, indicate that the melting point and boiling point increase with increasing alkyl chain length as expected. The boiling point for LAS could not be determined experimentally due to decomposition. EPI Suite calculations indicate that vapour pressure and log Kow also increases with increasing alkyl chain length. Since surfactants such as LAS preferentially partition to the octanol-water interface, it is impossible to accurately measure a log Kow. However, Roberts (1991) found that QSARS developed to calculate log Kow have shown a high correlation to measured acute toxicity data for multiple species and multiple surfactants, including LAS. The most reliable calculated value for C11.6 LAS (log Kow = 3.32) takes into account the various phenyl position isomers of LAS. LAS is water soluble, with a critical micelle concentration (CMC) value of 0.1 g/L and forms a clear solution in water at concentrations up to 250 g/L.

1.4 Category Justification

The LAS molecule contains an aromatic ring sulfonated at the para position and attached to a linear alkyl chain at any position except the terminal carbons. The alkyl carbon chain typically has 10 to 14 carbon atoms and the linearity of the alkyl chains ranges from 87 to 98%. While commercial LAS consists of more than 20 individual components, the ratio of the various homologues and isomers, representing different alkyl chain lengths and aromatic ring positions along the linear alkyl chain, is relatively constant in currently produced products, with the weighted average carbon number of the alkyl chain based on production volume per region between 11.7-11.8. LAS is supported as a category because of the close consistency of the mixtures, their commercial uses, fate, and health and environmental effects. LAS is the primary cleaning agent used in many laundry detergents and cleaners at concentrations up to 25 percent in consumer products, and up to 30 percent in commercial products, with the exception of one reported product at 45% percent in concentrated solid form that is mechanically dispensed into diluted solution for dishwashing.

2 GENERAL INFORMATION ON EXPOSURE

2.1 Production Volumes and Use Pattern

LAS is manufactured from linear alkylbenzene (LAB) in self-contained, enclosed systems (see Annex 1 for more information). LAB is produced by reacting paraffins with benzene and a catalyst and isolating the LAB by distillation. The LAB is then sulfonated, which in turn is then neutralized to sodium salts of LAS.

Data on LAS production and consumption volumes, uses, releases and potential exposures were collected from published sources and surveys of member companies of the Industry Coalition for the SIDS Assessment of LAS, representing about 75% of the North American production of LAS. Approximately 390,000 metric tons of LAS were consumed in North America (United States and Canada combined) in 2000 (Colin A. Houston, 2002). Production in Europe in 2000 was approximately 400,000 metric tons (as reported in HERA 2004). Production in Japan in 2001, where all of the LAS producers are members of the consortium, was approximately 85,000 metric tons based on the results of the Coalition survey. Global production was 2.6 million metric tons in 1995, the most recent data available (EU Risk Assessment Report for LAB, 1997).

Based on the results of the survey of consortium members (LAS SIDS Coalition Survey 2002), about 78-97% of the LAS consumption worldwide is in liquid and powder consumer and industrial laundry and fine fabric detergents. Another 2-10% of the LAS produced is used in consumer and industrial dishwashing liquids, with the remainder used in other consumer and industrial cleaners. Following use, the predominant disposal route for these products is via the wastewater. Tables 2 and 3 show the percentage of LAS that occurs in various types of consumer and industrial detergent products.

Table 2. Percentage of LAS in Different Types of Consumer Products[1]

Consumer Product Type	Range of Percent Composition that is LAS		
	North America	Europe	Japan
Laundry Detergents			
Powders	5-25%	5-25%	5-25%
Liquids	1-25%	5-10%	5-25%
Tablets	5-25%	10-25%	5-25%
Liquid Fine Fabric Detergents	-	-	1-5%
Bleaches	-	-	0.1-0.5%
Pre-Washes	-	-	5-10%
Fabric Conditioners (sheets)	0.1-0.5%	-	-
Dishwashing Detergents (liquids)	5-25%	10-25%	1-5%
General Cleaners (dilutable)	1-5%	1-5%	-
Hard Surface Cleaners	1-5%	0.1-0.5%	0.5-10%
Other Cleaners	-	-	0.1-0.5%
Face & Hand Soaps (bar)	1-5%	-	-

[1] LAS SIDS Coalition Survey 2002

Table 3. Percentage of LAS in Different Types of Institutional and Industrial Products[1]

Industrial Product Type	Range of Percent Composition that is LAS		
	North America	Europe	Japan
Laundry Detergents			
Powders	5-25%	5-10%	5-10%
Liquids	-	10-25%	-
Pre-Washes	-	10-25%	-
Dishwashing Detergents (liquids)	5-10%	25-30%	5-30%
General Cleaners			
Dilutable	1-5%	-	-
Spray	1-5%	-	-
Hard Surface Cleaners	-	-	1-10%
Disinfectants (liquids)	5-10%	-	-
Other Uses	25-30%[2]	10-25%	10-25%

[1] LAS SIDS Coalition Survey 2002

[2] The only exception is a product containing 45% LAS that is a concentrated solid mechanically dispensed into diluted solution for dishwashing.

2.2 Environmental Exposure and Fate

2.2.1 Sources of Environmental Exposure

Based on the results of the survey of members of the Coalition (LAS SIDS Coalition Survey 2002; year 2000 data), there is a potential for releases to the environment from manufacturing and formulation, although processes have been designed to maximize production yield and minimize potential releases. In the US, LAS that is not incorporated into a product is captured by dust-handling equipment for recycling back into the production process. A limited amount of LAS in aqueous solution may be released as a dilute solution from washing and rinsing operations in the manufacturing process and discharged to wastewater treatment. Incidental quantities of the dry (granular/powder) product (e.g., from floor sweepings) may be disposed in landfills.

Environmental releases from down-the-drain discharges following product use could lead to potential ecological exposures in surface waters and possibly in agricultural soils. Products containing LAS disposed of down-the-drain are transported to wastewater treatment plants or discharged to the environment. LAS not biodegraded in wastewater treatment will be discharged in effluent or in the biosolids (sludge) produced by wastewater treatment. LAS in sludge may enter the environment from land application of sludge to agricultural soil or in leachate from landfills. Based on its temperature of decomposition, LAS is unlikely to enter the environment from incineration of sludge.

2.2.2 Photodegradation

LAS has low vapor pressure (3×10^{-13} Pa for C_{12} LAS) indicating significant amounts of LAS are unlikely to be present in the atmosphere for photodegradation. Data are available on the photodegradation of LAS in water but not for other environmental compartments. There is no evidence of LAS photodegradation in water under environmental conditions and the absence of photolyzable groups suggests that LAS is unlikely to undergo significant degradation by this mechanism. However, LAS photodegradation in water has been demonstrated in the presence of photoactivating materials (and typically high intensity light spectrum). Matsuura and Smith (1970) found >95% photolytic degradation after 20 minutes for aqueous LAS solutions exposed to a 1200-watt mercury vapor lamp using ferric perchlorate as a sensitizer. Hidaka et al. (1985) found rapid (<1-2 hours) decomposition of the aromatic ring followed by slower oxidation of the aliphatic chain for LAS in aqueous TiO_2 solutions under a xenon lamp. Hermann et al. (1997) found that the presence of humic substances delayed the mercury lamp photodegradation of LAS in aqueous solutions by factor of two or more.

2.2.3 Stability in Water

Cross and Dekker (1977) reported degradation of LAS by abiotic hydrolysis under extreme conditions (e.g., elevated temperatures, presence of inorganic acids) not likely to be encountered in the environment. Based on the results from extreme conditions and professional judgment, it is concluded that LAS does not degrade significantly by non-biological mechanisms. The reliability of this study could not be assigned because the original data were not available for review. However, the absence of readily hydrolysable groups in the chemical structure and the use pattern in shelf-stable liquid cleaning products supports this conclusion.

2.2.4 Stability in Soil

Several measurements of LAS in sludge-amended soil from both laboratory and field studies have been reported. Figge and Schoberl (1989) conducted a laboratory study using ^{14}C LAS (mixture not defined), and thus measuring ultimate biodegradation, showing LAS mineralization rates in soil corresponding to half lives ($t_{0.5}$) of 13-26 days. Knaebel et al. (1990) observed more rapid mineralization (half lives of 1.1-3.7 days) of C_{13} LAS in 10 soil types. Ward and Larson (1989) observed similar rates of mineralization (half lives of 15.8 to 25.7 days) as Figge and Schoberl using pure C_{10} to C_{14} LAS homologues and two different soil types. In the most recent laboratory study, Elsgaard et al. (2001b) showed more than 73% primary biodegradation for nominal LAS concentrations of 8 to 62 mg/kg and a 15% depletion for nominal concentrations of 488 mg/kg after two weeks in soil spiked with aqueous LAS and LAS-spiked sewage sludge.

Field investigations in the U.K. in which the annual sludge spreading averaged 6 ton/ha (Holt et al.,1989; Waters et al., 1989) demonstrated LAS removal (primary biodegradation) corresponding to half lives in the range of 7-22 days. At a landfilling operation in Spain in which very high levels of sludge were blended with soil (15% sludge, 85% soil), an LAS half live of 19.3 days was observed (de Ferrer et al., 1997). At sludge application rates within those currently recommended in Europe (equal or below 5 ton/ha/y), a field study estimated $t_{0.5}$ values, due to primary biodegradation, in the range of 3-7 days (Küchler and Schnaak,1997). Mortensen et al. (2001) also reported data for degradation of LAS in sludge-amended soil under realistic field conditions. LAS was not taken up by plants and its degradation in soil increased by the presence of crop plants with concentration decreasing from 27 mg/kg (dry soil) to 0.7-1.4 mg/kg (dry soil) at harvesting time after 30 days ($t_{0.5}$ <4 d). During degradation, the relative fractions of homologues C_{10}, C_{11}, and C_{12} decreased, while C_{13} increased.

2.2.5 Transport between Environmental Compartments

Games (1982; reliability not assignable) reported that Kd values for LAS increased with increasing alkyl chain length of LAS homologues. Kd values (L/kg) for activated sludge ranged from 220 (C10 LAS), 1000 (C11 LAS), 3070 (C12 LAS) to 9330 (C13 LAS). Kd values for river sediment ranged from 41 (C10 LAS), 100 (C11 LAS), 330 (C12 LAS), 990 (C13 LAS) to 2950 (C14 LAS). Traina et al. (1996) also reported that log Koc values (L/kg) for LAS and dissolved humic substances increased with increasing alkyl chain length: 4.02 (C10 LAS), 4.83 (C12 LAS) and 5.49 (C14 LAS). Based on the C11 and C12 LAS-activated sludge data, Feijtel et al. (1999) estimated the Kd value for commercially representative C11.6 LAS and activated sludge as 2512 L/kg. Very recently, Temmink and Klapwijk (2004) determined the sorption properties of LAS using activated sludge from a pilot-scale treatment plant. The Kd value (L/kg) for C12 LAS was 3210 L/kg, virtually identical to the value reported by Games (1982). Applying the same estimation procedures as used by Feijtel et al. (1999; reliability not assignable) results in a Kd value for C11.6 LAS and activated sludge of 2500 L/kg. Painter and Zabel (1988) estimated Kd values of between 6 and 300 L/kg in water-river sediments and between 2 and 20 L/kg in water-soil, in both cases dependent on organic carbon content and other characteristics of the solid phase. Tolls and Sijm (2000) report that sorption affinity decreases with increasing LAS concentrations, which suggests that concentration dependency should be taken into account when assessing sorption of surfactants such as LAS.

Temmink and Klapwijk (2004) also reported that sorption and desorption equilibria were achieved very rapidly for LAS in activated sludge, with sorption equilibrium achieved within 5-10 minutes. In other experiments conducted in a pilot scale treatment plant, 92-98% of the LAS was adsorbed to the sludge with only 2-8% present as dissolved LAS. Despite this high degree of sorption, more

than 99% of the LAS load was removed by biodegradation, showing that the adsorbed fraction as well as the soluble fraction of LAS is readily available for biodegradation.

Mackay et al. (1996) conducted five-stage Level III fugacity modelling that included evaluative, regional and local-scale models. The level I and II models each resulted in LAS partitioning in air, water, soil and sediment at percentages of 0, 26, 56 and 18%, respectively. The overall residence time of LAS is predicted to be 100 hours with removal primarily by biodegradation in water (76%) and partitioning to sediment (13%). Impacts of LAS are predicted to be restricted to local receiving waters and their sediments and biota. In the Level III Fugacity Model, when discharges are directly to water, the residence time is predicted to be 33 hours and more than 99% remains in the water. However, in shallower receiving water more partitioning to sediments might be expected. When discharge is to soil, the residence time is predicted to be 28 days because of the slower biodegradation rate (compared to water) and little transfer to other media. Using the ChemCAN 4 model and assuming 90% LAS discharge to soil and 10% to water, LAS partitioning in air, water, soil and sediment is predicted to be 0, 0.64, 99.35 and 0.004%.

Level III fugacity modelling was also conducted by ECETOC (1993; reliability not assigned due to uncertainty regarding the input parameters) to predict LAS concentrations in air, biota, sediment, arable soil, suspended solids and water. LAS concentrations were predicted to be highest in soil and suspended solids.

2.2.6 Biodegradation

Biodegradation is the primary mechanism by which LAS is transformed, with the formation of sulfophenyl carboxylates (SPCs) as biodegradation intermediates (Swisher 1987; Schoeberl 1989; Huddleston and Allred 1963; dossier 3.5w). Longer alkyl chain LAS homologues undergo more rapid primary biodegradation to SPCs than shorter chain homologues (Bock and Wickbold 1966). SPC toxicities are several orders of magnitude lower than that of the parent material (Kimerle and Swisher 1977; dossier 4.1r, 4.2Af). SPCs also biodegrade as demonstrated by the rapid and complete biodegradation of LAS (to CO2, SO42-, and water) under aerobic conditions documented below.

An extensive database of studies is available demonstrating rapid and complete biodegradation of LAS in freshwater under aerobic conditions (e.g., Ruffo et al. 1999; Nielsen and Huddleston 1981; dossier section 3.5). The studies summarized in Table 4 demonstrate that LAS passes standard tests for ready biodegradability, including the 10-day biodegradation window (Add refs). Rapid biodegradation of the iso-LAS components of LAS was also demonstrated by Cavalli et al. (1996) in a modified OECD 301E biodegradation study in which C11.6 LAS containing 5-6% iso-LAS was the sole source of carbon and the bacterial biomass was obtained from soil. Preliminary tests showed that more than 90% of the LAS disappeared within 4 days so additional LAS was added to the test system every fourth day over a 80-day test period. No accumulation of iso-LAS was observed in this study demonstrating that the iso-LAS components are just as biodegradable as LAS. Rapid biodegradation of LAS has also been demonstrated in marine systems, as shown by measured loss of LAS in salt water samples collected off the coast of Spain in which half-lives ranged from 3.4 to 13.8 days, with 4-9 days being the most frequent values (Vives-Rego et al. 2000).

Table 4. Results of Aerobic Ready Biodegradation Studies on LAS

Study, Protocol	Endpoint	Test Material Description (Average Alkyl Chain Length)	Degradation	Duration (days)	Reference
DOC Die-Away, Directive 79/83/EEC, Appendix V, C.4-A (OECD 301A)	DOC Removal	$C_{11.6}$	93%; meets 10-day window criterion	28	Schoeberl 1993b, dossier 3.5e; reliability = 1
DOC Die-Away, Directive 79/83/EEC, Appendix V, C.4-A (OECD 301A)	DOC Removal	$C_{11.6}$	94%; meets 10-day window criterion	28	Schoeberl 1993c, dossier 3.5f; reliability = 1
OECD 301B, Modified Sturm Test	CO_2 Production	$C_{11.6}$	66.7%; 10-day window not met	28	Ruffo et al., 1999, dossier 3.5b; reliability = 1
OECD 301B, Modified Sturm Test	CO_2 Production	$C_{11.6}$	83%; meets 10-day window criterion	28	Enste-Diefenbach, 2002, dossier 3.5z; reliability = 1
Modified OECD Screening Test, Directive 84/449/EEC, C.3 (OECD 301E)	DOC Removal	$C_{11.6}$	76%; meets 10-day window criterion	28	European Commission 2000, dossier 3.5g; reliability = 4
OECD Screening Test according to "Verordnung ueber die Abbaubarkeit anionischer und nichtionischer grenzflaechenaktiver Stoffe in Wasch- und Reinigungsmittel vom 30.1.1977". Bundesgesetzblatt Teil I, S. 244. 1977	DOC Removal	$C_{11.6}$	95%; meets 10-day window criterion	19	European Commission 2000, dossier 3.5i; reliability = 4

While LAS degrades rapidly under aerobic conditions, it does not degrade under anaerobic conditions, except under special conditions. Denger and Cook (1999) showed that strains of anaerobic bacteria capable of degrading LAS (using it as a sulfur source) under sulfur-limiting conditions are present in nature. Sanz et al. (1999) were the first to demonstrate that LAS anaerobic biodegradation does occur under conditions that are not sulfur-limited, using anaerobic digester sludge and specific HPLC methods to measure the loss of the parent material. Prats et al. (2000) confirmed with specific HPLC analysis (loss of LAS) that LAS biodegrades anaerobically in the ECETOC-28 test, although increased gas production (mineralization) was not observed. Angelidaki et al. (2000a) demonstrated that degradation (loss of LAS) occurred under anaerobic conditions when exposed to inocula obtained from lake sediments or aerobic environments such as compost and activated sludge from a wastewater treatment plant. Anaerobic stabilized sewage sludge in continuous stirred reactors also showed a capacity to anaerobically degrade LAS, as measured by loss of parent material (Angelidaki et al. 2000b). Measurement of radiolabeled biogas and/or intermediates would be required for confirmation of these preliminary results.

Degradation of LAS in soils has also been reported – see section 2.2.4 above.

2.2.7 Bioaccumulation

The bioaccumulation potential of LAS has been investigated. Early studies, e.g., Kimerle et al. 1981, used 14C-ring labelled LAS and measured only total radiolabeled materials, likely including LAS metabolites, and thus limiting the conclusions that can be drawn specific to LAS. Tolls et al. (1997) conducted a series of experiments with fathead minnows (Pimephales promelas) according to OECD Guideline 305E protocols in which the limitations of the earlier studies were overcome. Individual LAS homologues were tested in flow-through exposures for up to 192 hours for the uptake phase, followed by a depuration phase in which fish were transferred to unspiked water. The resulting bioconcentration factors (BCFs) ranged from 2 L/kg (6-phenyl-C10 LAS) to almost 1000 L/kg (2-phenyl-C13 LAS), with BCF generally increasing with increasing alkyl chain length. BCF values were also calculated for a standard mixture (typical of LAS in European detergent formulations, average alkyl chain length = C11.6) and a representative environmental sample (filtered Mississippi river water, average alkyl chain length = C10.8). The respective BCFs were 87 and 22 L/kg, indicating that the bioconcentration potential of LAS is decreased by environmental processes such as biodegradation and absorption, which reduce aquatic concentrations (Tolls et al. 1997). These processes, as documented above, also preferentially remove longer alkyl chain length components, reducing the bioconcentration potential of the mixture fingerprint since the remaining lower alkyl chain materials have lower BCFs.

2.2.8 Other Information on Environmental Fate

In the US, monitoring in 50 wastewater treatment facilities in 11 states showed average LAS levels in raw sewage ranged from 4.2 to 5.7 mg/L (McAvoy et al. 1993) while levels in raw sewage from five European countries ranged from 4.0-15.1 mg/L (DiCorcia et al. 1994, Waters and Feijtel 1995).

US monitoring data indicated that LAS is largely removed in wastewater treatment plants, averaging over 99% removal in activated sludge, 98% for lagoons/oxidation ditches, 96% for rotating biological contactors and 77-82% for trickling filters (McAvoy et al. 1993, Trehy et al. 1996). Monitoring data from five European countries showed LAS removal in activated sludge treatment ranged from 98.5-99.9% (DiCorcia et al. 1994, Waters and Feijtel 1995) and averaged 92.9% in four trickling filter plants in the U.K. (Holt et al. 2000). Results of a mass balance study of an activated sludge treatment plant indicate that removal is primarily due to biodegradation with only about 20% of the influent LAS removed with the sludge (DiCorcia et al. 1994).

In the US, average concentrations in river water below treatment plant mixing zones were generally below 50 µg/L for samples collected under low dilution conditions (McAvoy et al. 1993, Trehy et al. 1996). Tabor and Barber (1996) reported LAS at concentrations ranging from non-detect (<0.1 µg/L) to 28.2 µg/L in 362 water samples collected in an intensive sampling effort over the 2,800 km reach of the Mississippi River from Minneapolis to New Orleans. The alkyl chain length of the LAS in the water samples averaged 11.1 carbons, indicating preferential loss of the longer alkyl chain molecules, consistent with the sorption and biodegradation data discussed above.

LAS river water concentrations similar to those in the US were observed in monitoring studies conducted in Europe and Japan. DiCorcia et al. (1994) found the LAS level in the Tiber River (Italy) below the Roma Nord treatment plant was 9.7 µg/L. Waters and Feijtel (1995) reported that LAS levels in river water below activated sludge treatment plants in five European countries ranged from <2.1 to 47 µg/L. Matthijs et al. (1999) found a mean LAS concentration of 14.2 µg/L in surface waters downstream, just past the mixing zone, of activated sludge treatment plants in the Netherlands**.** Fox et al. (2000) reported an LAS concentration, corrected for dilution, of 70 µg/L 4.8 km (6 hours flow time) from the outfall of trickling filter treatment plant in the U.K. Gandolfi et al. (2000) found the mean LAS concentration in the Lambro River (Italy), where 40% of the local

wastewater was discharged untreated, was 28 µg/L. Nishiyama et al. (2003) reported that the median LAS concentration in water from 4 rivers (7 sites) in Japan was 6 µg/L (range <4-81).

In river sediments, LAS concentrations were generally less than 1-2 mg/kg dry weight. LAS concentrations in Mississippi River sediments were generally <1 mg/kg, ranging from 0.01 to 0.95 mg/kg (mean = 0.23 ± 0.19 mg/kg), with one outlier, a value of 20 mg/kg observed in an effluent transport canal (Tabor and Barber 1996). The average alkyl chain length of the sediment associated LAS was $C_{11.5}$ (range $C_{10.7\text{-}11.9}$). LAS concentrations in sediments of a small river (Rapid Creek, USA) below a trickling filter treatment plant averaged 190 mg/kg just below the outfall, 11.2 mg/kg less than 5 miles downstream and 5.3 mg/kg greater than 5 miles downstream (Rapaport and Eckoff 1990). LAS levels in the receiving waters of the Tiber River (Italy) were 1.8 mg/kg in the sediments (DiCorcia et al. 1994). LAS concentrations in sediment below poorly functioning treatment plants or treatment plants having only primary treatment may be higher.

LAS has been detected in seawater and marine sediments near the outfalls of untreated urban wastewaters or in highly polluted harbors (Bester et al. 2001, Leon et al. 2001, Temara et al. 2001, DelValls et al. 2002, Folke et al. 2002, Petrovic et al. 2002). LAS levels in three sets of seawater samples were less than or equal to 0.03 µg/L, 1-9 µg/L and 2.4-92 µg/L. In marine sediments, the absence of macrofauna and the presence of other components of wastewater, including other highly biodegradable compounds such as soap, indicate the impact of untreated wastewater discharge on these local environments.

LAS concentrations (mean ± standard deviation) in sludge from US sewage treatment plants ranged from 150 (±120) mg/kg dry matter for aerobic digesters to 10,500 (±5,200) mg/kg dry matter for anaerobic digesters (McAvoy et al. 1993). Maximal LAS sludge levels reported in European monitoring studies were also generally less than 20,000 mg/kg (Berna et al. 1989, DiCorcia et al. 1994, Waters and Feijtel 1995, Cavalli and Valtorta 1999, Carlsen et al. 2002). The one exception was an activated sludge plant treating wastewater with high hardness (500 ppm as $CaCO_3$) in which the LAS levels in the digested sludge (30,200 mg/kg) likely represents calcium-precipitated LAS (Berna et al. 1989).

In sludge-amended agricultural soils, LAS concentrations are generally less than 15 mg/kg dry weight, even immediately after sludge spreading. LAS concentrations in the U.K. in four fields spread within days of sludge application were 4.5, 7.8, 10.6 and 19.8 mg/kg, ranged from 0.2-2.1 mg/kg in four fields spread two to three months previously and were less than 1 mg/kg (maximum concentration = 2.5 mg/kg) in 83% of the fields (n=42) spread the previous year (Waters et al. 1989). In Denmark, a cultivated field spread with medium amounts of sludge (not further defined) had LAS concentrations of 1.12 mg/kg in the 0-10 cm depth and lower concentrations at lower depths (Carlsen et al. 2002). In the US, the presence of crop plants (barley, rape, or carrot) increased the degradation of LAS in soil (Mortensen et al. 2001). During degradation, the relative fraction of homologues C_{10}, C_{11}, C_{12} decreased, while C_{13} increased.

E-FAST modeling of U.S. manufacturing facility effluent discharges (see Annex 1, Format C, Modeling Evaluation #1) resulted in estimated mean and low flow (7Q10) stream concentrations of 4.8 µg/L and 13 µg/L, respectively. E-FAST modeling of down-the-drain disposal in the U.S. (see Annex 1, Format C, Modeling Evaluation #2) resulted in estimated median and 7Q10 (low flow) stream concentrations of 0.099 and 1.3 µg/L, respectively.[1]

[1] US EPA did not evaluate the EFAST modeling results and therefore can make no conclusions regarding these values.

2.3 Human Exposure

2.3.1 Occupational Exposure

LAS is manufactured from linear alkylbenzene (LAB) in self-contained, enclosed systems (see Annex for more information). LAB is produced by reacting paraffins with benzene and a catalyst and isolating the LAB by distillation. The LAB is then sulfonated, which in turn is then neutralized to sodium salts of LAS. Exposure to industrial workers is limited because this is an enclosed manufacturing process designed to minimize losses and the potential for release (see Annex). Worker exposure is possible during the detergent formulation stage by inhalation of powders or dermal contact of powders and liquids. However, good manufacturing design practices (e.g., enclosed production, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) are in place at facilities that manufacture liquid and dry (granular/powder) materials to mitigate worker exposure to LAS. No special engineering controls or additional personal protective equipment are uniquely specified for LAS (LAS SIDS Coalition Survey 2002).

2.3.2 Consumer Exposure

The greatest potential for exposure of humans to LAS is associated with consumer use of laundry and cleaning products. Consumer exposure could result from direct or indirect skin or eye contact, inhalation of aerosols from cleaning sprays, and oral ingestion of residues deposited on dishes, accidental product ingestion, or indirectly from drinking water. Based on exposure modeling (Annex 1), the greatest potential of LAS exposure is from pretreatment of laundry, due to direct hand and forearm contact with neat product formulations, and from residual product on laundry clothing due to the large surface area of the body in contact with clothing.

Exposure to LAS in these formulated laundry or cleaning products is mitigated by following use and precaution instructions on product labels. Product labels reflect the hazard potential of the ingredients in the product under foreseeable use conditions. These product labels also include first aid instructions to accompany each hazard warning. For example, products may include eye and/or skin irritancy warnings along with instructions to rinse thoroughly if dermal or other exposure occurs.

Laundry and cleaning products may be used as is, or diluted prior to or during use. Human exposure will be further mitigated by the fact that residues on skin from cleaning products are usually washed or rinsed off. Actual dermal absorption is less than 1% of product (Schaefer and Redelmeier 1996).

Modeling of exposure potential from use of consumer products (see Annex) resulted in estimated exposures of 5.6×10^{-2} to 4.7×10^{-5} mg/kg/day. Modeling of potential aquatic exposures and human exposures from down-the-drain releases from consumer use of products containing LAS resulted in estimated exposures of 1.9×10^{-6} mg/kg/day and 7.2×10^{-7} mg/kg/day for drinking water and fish consumption, respectively. These human exposure evaluations include conservative (protective) input assumptions, e.g. all dermal modeled exposures use a default assumption of 100% absorption vs. a measured value of <1%.

It is important to note that the laboratory exposure from the summarized inhalation study (Kinney 1985; see SIAR section 3.1.2) is not representative of the possible LAS exposure during actual production or use. In the Kinney study, animals were given high exposures to respirable-sized particles (MMAD = 2.5 microns). However, spray products containing LAS are designed to

produce large particle sizes. These large particles are needed for efficient delivery of the spray to the surface being cleaned. This results in particle sizes that are much larger than the respirable particle sizes used in testing and therefore would not be able to reach far into the lungs where effects could occur. A study conducted for the Soap and Detergent Association (Battelle 1999) measured the under 10 micron fraction delivered from 6 consumer product spray nozzles. The overall mean (n=30) is 0.11% particles under 10 microns and the standard deviation is 0.21. The very highest observation was 0.80% particles under 10 microns. This testing only captured the spray particles that are under 600 microns, so the actual mean respirable particle percent of total volume sprayed is less than 0.1%. The Battelle (1999) study also reported that for consumer spray products in normal use conditions, the peak breathing zone concentration under 10 microns ranged from 0.13-0.72 mg/m^3. HERA (2004) reported that measurements of aerosol particles under 6.4 microns in size generated upon spraying with typical surface cleaning spray products resulted in a product concentration of 0.35 mg/m^3.

Inhalation of detergent dust during washing processes was modelled by HERA (2004) and found to be 10-fold lower than the exposure from inhalation of aerosols from cleaning sprays. This estimate is based on a study reporting an average release of 0.27 µg dust per cup of product used for machine laundering (Hendricks, 1970). This is a conservative (protective) estimate as exposure from modern compact/granular detergent formulations produced in agglomeration processes would be expected to be much less.

These estimates of exposure to respirable particles from consumer and industrial products indicate that inhalation is not a likely route of concern for human exposure (see SIAR Annex 1 and dossier section 1.10B(b) and (c) for more information).[2]

3 HUMAN HEALTH HAZARDS

3.1 Effects on Human Health

3.1.1 Toxicokinetics, Metabolism and Distribution

Studies in Animals

The absorption, distribution, metabolism and elimination of LAS has been studied in several species, including rats, mice, guinea pigs, pigs, and rhesus monkeys (Debane 1978; Michael 1968; Havermann and Menke 1959; Cresswell et al. 1978; Sunakawa et al. 1979). LAS was administered either topically (i.e., dermally) or orally. Results showed that LAS can be absorbed from the gastrointestinal tract. Absorbed LAS is then metabolized and excreted without accumulation in the major tissues or fat.

Debane (1978) found that when 0.2 to 0.5% LAS was topically applied once to the back skin of rats and guinea pigs, approximately 0.1 to 0.6% was absorbed. No accumulation was observed in specific organs and LAS was quickly excreted in the urine after being metabolized. IPCS (1996) notes that prolonged contact with the skin may compromise the integrity of the epidermal barrier, thereby potentially permitting greater absorption from this route. Michael (1968) found that LAS administered orally as an aqueous solution was readily absorbed from the gastrointestinal tract (80-90% of the dose). Most of the absorbed dose was eliminated within 72 hours and 60-65% was

[2] US EPA did not evaluate the modeling results in Annex 1 and therefore can make no conclusions regarding these values.

eliminated via the urine, with sulfophenyl butanoic and sulfophenyl pentatonic acid as metabolites. Approximately 35% of the absorbed dose was excreted in the bile. Although the metabolites in the bile were not identified, it was shown that no unchanged LAS was eliminated via this pathway. In oral studies with pigs, Havermann and Menke (1959) found that at 200 hours after oral administration, the radiolabeled LAS was relatively high in bristles and bones, while low in liver, kidney and spleen. After 10 weeks only traces of radioactivity were still in the body. At 40 hours after administration, 40% of the dose was excreted into the urine and 60% of the dose via the feces. In another study (Sunakawa et al. 1979), rats were dosed orally with 14C-LAS and radioactivity was detected 0.25 hours after administraton, reaching a maximum at 2 hours. The biological half-life was calculated to be 10.9 hours. The distribution was high in the digestive tract and in the bladder at 4 hours after administration, with high concentrations also found in the liver, kidney, testis, spleen and lung. At 168 hours after administration, the rates of excreted radioactivity were 47% in the urine and 50% in the feces.

Toxicokinetics has also been studied in adult rhesus monkeys (Cresswell et al. 1978). Two male and two female monkeys were given single or repeated oral (30, 150 or 300 mg/kg) or subcutaneous (0.1, 0.5 or 1 mg/kg) doses of 14C-LAS. For example, after single 30 mg/kg oral doses, the radioactivity was rapidly excreted, mostly during the first 24 hours. Means of 71.2% and 23.1% of the dose were excreted in the urine and feces, respectively, during 5 days. During seven consecutive daily (30 mg/kg/day) or subcutaneous (1 mg/kg/day) doses, there was no accumulation of radioactivity in plasma. Mean peak concentrations and biological half-lives were similar after the first and seventh doses. No unchanged LAS was detected in the urine after oral or subcutaneous doses. Five metabolites were excreted but they were not identified.

Studies in Humans

Studies were conducted with isolated human skin preparations using two solutions of C12 LAS (Howes 1975). The results demonstrated that penetration through the skin and subsequent absorption does not occur to any significant extent (less than 1%) at 24 to 48 hours.

3.1.2 Acute Toxicity

Acute mammalian toxicity data are available for all three potential routes of exposure (inhalation, dermal, oral), as summarized below and in Table 5.

Studies in Animals

Oral

Eight acute oral toxicity studies are available for LAS using rats, and one acute oral study is available using mice (Murmann 1984a,b,c; Ito et al. 1978; Kynoch 1986a; Monsanto 1971, 1972a,b). All of the studies were conducted on the low average chain length LAS (C11.2-C11.7). The resultant LD50 values ranged from 1,080 up to 1,980 mg/kg bw for rats and greater than 2000 mg/kg bw for mice, with no significant difference between sexes. Mortality and symptoms of toxicity occurred at the high doses tested in each study, and usually within the first few hours or days, after which surviving animals generally recovered. Symptoms noted in most of the studies included piloerection, hunched posture, abnormal gait (waddling), lethargy, reduced appetite, decreased respiratory rate, ptosis, pallor of the extremities, and diarrhea. All oral studies are reliability 1 or 2, except for those by Ito et al. (1978), which were rated unassignable (4) since the original reports were not available for review. However, these studies were considered reliable because they have been reviewed by the International Program on Chemical Safety.

Dermal

The acute dermal toxicity of LAS was studied in rats under OECD Guideline 402 and GLP conditions (Kynoch 1986b). The LAS used in this study was $C_{11.2}$ LAS, which has an average alkyl chain length slightly shorter than the range of chain lengths currently used in the United States ($C_{11.2}$-$C_{12.6}$). There were no deaths or systemic reaction to five male and five female rats following a single dermal application of 2000 mg/kg bw of LAS at 47% active matter. Well defined or slight erythema and slight edema were observed at all test sites after removal of the occlusive dressing on Day 2. All test sites were entirely covered by scab formation from Day 7. Sloughing from the scabbed skin began at various times between Day 7 and Day 12 and was completed before termination. Low bodyweight gains or loss of body weight were recorded for one male and three females in Day 8. Two of the same females and a third female also showed low bodyweight gain between Days 8 and 15. Terminal necropsy findings were normal. Additional dermal toxicity studies (Monsanto 1971, 1972a, b) are included in Table 5 but the reliability was rated unassignable (4) due to deficiencies in the number of animals per dose.

Inhalation

Acute inhalation data are available for LAS (CAS #25155-30-0; Kinney 1985). In this reliability 2 study, groups of six 8-week old rats underwent nose-only exposures to aerosol atmospheres containing 65, 120, 260 or 310 mg/m^3 respirable-sized particulate LAS (MMAD = 2.5 microns) for 4 hours, followed by 14 days of observations for clinical signs. No mortality occurred at concentrations up to 260 mg/m^3. At 310 mg/m^3, one rat died during the exposure and two rats died one day post exposure. Given these results C_{12}-LAS is considered moderately toxic by inhalation (see SIAR section 2.3.2 for discussion of inhalation exposure).

Conclusion

The available acute toxicity data by the oral route of exposure indicate that LAS exhibits slight acute oral toxicity, with symptoms of toxicity and mortality at high doses but not at lower doses. LD_{50} values for rats and mice range from 1,080 to 1,980 mg/kg bw. No effects were observed in dermal exposure studies with rats at 2,000 mg/kg bw, indicating low dermal hazard potential. Inhalation toxicity data indicate that LAS is moderately toxic, with mortality occurring at respirable particle concentrations of 310 mg/m^3 (MMAD = 2.5 microns). However, less than 0.1% of the total volume sprayed from consumer product spray nozzles consists of respirable particles. Estimates of exposures from consumer spray products indicate that inhalation is not a route of concern.

Table 5. Acute Toxicity to Mammalian Species

Species	Route of Exposure	LD_{50} (mg/kg bw unless otherwise specified)	Doses (mg/kg bw)	Reference (Reliability)
Rat	Oral	1080	1075, 1220, 1360, 1710	Murmann 1984a (2)
Rat	Oral	1630	1260, 1580, 1785, 1990	Murmann 1984b (2)
Rat	Oral	1410	1190, 1500, 1890	Murmann 1984c (2)
Rat	Oral	1460 (males) 1470 (females)	-	Ito et al. 1978 (4)
Rat	Oral	1980	1500, 2350, 3760	Kynoch 1986a (1)
Rat	Oral	1320	1000, 1260, 1580	Monsanto 1971 (2)
Rat	Oral	1430	1000, 1260, 1580, 2000	Monsanto 1972a (2)
Rat	Oral	1360	1000, 1260, 1580, 2000	Monsanto 1972b (2)
Mouse	Oral	2160 (males) 2250 (females)	-	Ito et al. 1978 (4)
Rat	Inhalation	310 mg/m^3 *	65, 120, 260, 310 mg/m^3	Kinney 1985 (2)
Rat	Dermal	> 2000	2000	Kynoch 1986b (1)
Rabbit	Dermal	> 200 and < 316	126, 200, 316, 501, 794, 1260, 2000, 3160, 5010	Monsanto 1971 (4)
Rabbit	Dermal	> 631 and < 1000	200, 316, 631, 1000, 1260, 2000, 3160	Monsanto 1972a (4)
Rabbit	Dermal	> 631 and < 1000	200, 398, 631, 1000, 1260, 2000, 3160	Monsanto 1972b (4)
Rat	subcutaneous	840 (males) 810 (females)	-	Ito et al. 1978 (4)
Mouse	subcutaneous	1250 (males) 1400 (females)	-	Ito et al. 1978 (4)
Rat	intravenous	119 (males) 126 (females)	-	Ito et al. 1978 (4)
Mouse	intravenous	207 (males) 298 (females)	-	Ito et al. 1978 (4)
Mouse	intravenous	115 (C_{10}-LAS) 105 (C_{12}-LAS)	-	Hopper et al. 1949 (2)

* Value is Approximate Lethal Concentration

3.1.3 Irritation

Skin Irritation

Several skin irritation studies have been conducted on rabbits for LAS at a concentration of about 50% (Liggett and Parcell 1986a; Biolab 1989a; Kaestner 1997; Murmann 1983a). Findings in all the studies were consistent and showed similar irritation effects, as would be expected with a surface active agent.

In the most reliable study (Liggett and Parcell 1986a), conducted under OECD protocols and GLP conditions, a 47% LAS concentration was applied to the clipped intact skin of three rabbits. Well defined to moderate skin reactions were observed in all three animals, as was desquamation of the stratum corneum. These reactions gradually ameliorated from days 5, 10, and 11, respectively, and had resolved completely in one animal by day 12. Similar results were observed in studies of 50% concentration LAS reported by Biolab (1989a), Kaestner (1997), and Murmann 1983a. Several older studies conducted on a neat commercial LAS material (0.5 g moistened with water) resulted in a classification as a severe skin irritant (Monsanto 1971, 1972a,b).

Additional skin irritation studies have been conducted with lower concentrations of LAS (Biolab 1989b,c,d). At 1% and 2.5% LAS, no skin irritation was observed in rabbits following exposure under OECD Guidelines. At 5%, LAS was classified as a moderate skin irritant.

Eye Irritation

Several eye irritation studies on rabbits are available for LAS at a concentration of about 50% (Liggett and Parcell 1986b; Biolab 1989d; Murmann 1983b; and Kaestner 1987). All studies had consistent findings and showed significant irritation effects.

The most reliable study (Liggett and Parcell 1986b) was performed under OECD Guidelines and GLP conditions in which each of three rabbits received LAS at 47% placed into the lower everted lid of one eye. Significant conjunctivae chemosis was observed in all animals, with minor effects on cornea opacity and conjunctivae redness in two animals. One animal showed significant ocular reactions in all sites, which had not cleared at day 14. Concurrent with this study, the eyes of other rabbits were rinsed following 4 or 30 second eye exposures. Irritation was still present but diminished after the 30 second rinsing and only slight after the 4 second rinsing. Other studies of 50% LAS conducted on rabbits using OECD Guidelines also resulted in a classification of irritating with effects noted in the iris and conjunctivae that were persistent at day 6 (Biolab 1989d; Murmann 1983b).

In two Japanese studies conducted on LAS tested at low concentrations (Oba et al. 1968; Iimori et al. 1972), no abnormalities were seen at 0.01% but slight congestion was seen at 0.05% and considerable congestion was seen at 0.1% that disappeared within 24 hours. Marked responses were observed at 0.5% LAS and higher, including severe congestion and edema, increased secretion, turbidity of the cornea, and disappearance of the corneal reflex. These effects disappeared completely after 120 hours. The results of two additional rabbit studies conducted under OECD Guidelines indicated no irritation at 1% LAS but marked reactions for conjunctival redness and chemosis at 5% (Biolab 1984). Finally, three older non-standard studies are available in which 100 mg of finely ground solid commercial LAS sample was placed in the eyes of rabbits (Monsanto 1971, 1972a,b). The resultant scores ranged from 10 to 19 out of 110, which classifies this as a mild irritant.

Comparisons between animal test results and human eye irritation experiences indicate that the rabbit eye irritation test is not well correlated to human responses for 29 surfactant-based cleaning products. Human experience with eye exposure to surfactants was reported by Freeberg et al (1984)

and coworkers (Freeberg et al. 1986, Cormier et al. 1995). These studies investigated exposure of manufacturing employees and consumers to laundry, household and personal cleaning products containing LAS and other chemicals. While concentrations were not reported in the Freeberg et al. publications, the coalition survey indicates that LAS concentrations in US consumer products range from 0.1-25% and in commercial products from 1-30%, with the exception of one reported product at 45% in concentrated form that is mechanically dispensed into dilution for dishwashing. The results of the Freeberg et al. studies indicate that in accidental exposure situations, the effects were moderate, transient and reversible. In the Freeberg et al. (1984) study (n=514), 88.1% of the eyes cleared in 4 days or less with no reported permanent eye damage. All eyes cleared in 28 days. Labeling of consumer products containing LAS and other surfactants include warnings of the potential for eye irritation and with first aid instruction to rinse with water.

Conclusion (Skin and Eye Irritation)

LAS was found to be not irritating to skin at concentrations of 1% and 2.5%, moderately irritating at 5%, and more severely irritating at higher concentrations of about 47-50%. LAS is generally not irritating to the eyes of rabbits at concentrations up to about 1% (some congestion does occur at 0.05-0.5%), moderately irritating at 5%, and more severely irritating at 47-50%. At these higher concentrations the irritation may be present for up to 14 days. In studies that included rinsing, irritation effects diminished with rinsing after 30 seconds of exposure and were slight with rinsing after 4 seconds of exposure. Human experience has established that irritation effects of consumer products containing LAS and other surfactants are moderate, transient and reversible.

3.1.4 Sensitization

Studies in Animals

Three studies are reported in which skin sensitization in guinea pigs was examined (RBM 1985 [dossier section 5.3c]; Murmann 1988 [dossier section 5.3b]; European Commission 2000 [dossier section 5.3a]). Studies were conducted according to OECD Guidelines and used induction concentrations of 1, 3 or 25% LAS. No sensitization was observed. A.D. Little (1991) reported that LAS may be a weak sensitizer in guinea pigs under exaggerated exposure conditions (e.g., injection induction), but that clear no-effect levels were well below anticipated exposure levels.

Studies in Humans

Human exposure studies, with volunteers who provided informed consent, are also available for LAS. In a repeat insult patch test, LAS was applied at 0.10% to the upper arms of 95 volunteers (Procter & Gamble, unpublished data). The 24 hour exposure was repeated 3 times a week for 3 weeks during the induction period. After a 14-17 day rest, a 24-hour challenge patch was applied. No evidence of skin sensitization occurred in any of the 95 volunteers. Nusair et al. (1988) conducted extensive patch tests in which 2,294 volunteers were exposed to LAS as a raw material and 17,887 were exposed to LAS in formulations. Again, no evidence of sensitization was observed. In a study reported in the IUCLID Data Set, LAS was found to be sufficiently compatible with the skin after it was applied as a 1% solution to the skin of middle Europeans (Matthies 1989).

Conclusions

Skin sensitization studies with guinea pigs showed no sensitization at either lower (6.7%) or higher (50%) concentrations. Results of animal studies, human exposure studies and actual use support the conclusion that LAS does not have significant skin sensitization properties.

3.1.5 Repeated Dose Toxicity

Numerous repeated dose toxicity studies are available, and include studies on rats, mice, and rhesus monkeys and oral, dermal, and drinking water exposures. The results are summarized in Table 6.

Studies in Animals

Oral

Many studies have investigated the effects of repeated doses of LAS via the oral exposure route, mainly in the feed but also by gavage and through the drinking water. In a key study, groups of 8 or 9 rats of each sex were given LAS in drinking water at equivalent doses of 85, 145, and 430 mg/kg bw/day for 9 months (Yoneyama et al. 1976). Body weight gain was suppressed in the male 430 mg/kg bw/day group. Hematological examination revealed no significant change in any of the experimental groups, but a dose-related decrease in cholesterol level was seen in males. Significant decreases in the activities of glutamate-oxalate transaminase and lactate dehydrogenase were seen in males at the middle dose and a dose-related increase in the activity of glutamate-oxalate transaminase in females. A significant decrease in renal Na,K-ATPase was seen in the middle-dose group. No organ weight changes were observed. The NOAEL is 85 mg/kg bw/day.

Other studies show similar responses, with commonly reported effects at higher doses including diarrhea, suppression of body weight gain, increases in relative weight of the liver, changes in other organ weights, differences in enzymatic and serum-biochemical parameters (e.g., ATPase, LDH, G6Pase), and mild degeneration and desquamation of the tubular epithelium in the kidneys. Occasionally, other effects have been observed, including marked degeneration of renal tubes, proteinaceous degeneration in the liver, and effects on subcellular components (Yoneyama et al. 1972; Gupta et al. 1986; Mathur et al. 1986; Watari et al., 1977).

Dermal

LAS was applied for 15 days to the backs of male Wistar rats at daily doses of 0.5 g of solutions at 20 and 30% (about 286 and 427 mg/kg bw/day) (Sadai and Mizuno 1972). Body weight gain was suppressed in the 20% group and the body weight was decreased in the 30% group. An infiltrating, yellowish-reddish brown crust was observed 2-3 days in the 20% group, and at 1-2 days in the 30% group. At 4-6 days the crust was abraded and erosion occurred at the abraded site. Histological examinations of the application site revealed severe necrosis of the region from the epidermis cuticle to the upper layer of the dermis, severe infiltration of leukocytes in the necrotic site, diffuse inflammatory cell infiltration of all layers of the corium. No changes were observed in the tongue, but the oral mucosa revealed atrophy and slight degeneration of the epithelium. No systemic effects were observed. The effects on body weight are considered to be related to LAS irritation. Therefore, the local LOAEL for dermal exposure from this study in rats is 286 mg/kg bw/day.

Inhalation

No long term studies on LAS inhalation are available. Based on its irritant nature, it is expected that repeat inhalation of LAS might be irritating to the respiratory tract.

Conclusion

LAS has been tested for toxicity resulting from repeated exposures via the oral and dermal routes in rodents (rats and mice) and non-rodents (monkeys). Test durations ranged from 15 days up to 9 months and exposure doses ranged from 8.8 up to 1,030 mg/kg bw/day. LOAELs ranged from 115 to 750 mg/kg bw/day and the highest NOAEL (below the lowest LOAEL) is 85 mg/kg bw/day. This overall NOAEL was selected as the most appropriate value based on the study duration (9 months) and the data from all the studies.

It should be noted that several of the key studies are given a reliability score of 4. This score was assigned because the original reports were not available for review; however, these studies were evaluated and included in the IPCS review of LAS (IPCS 1996) and therefore are considered to be reliable for the purposes of this SIDS assessment. A weight of evidence approach was used to consider the data from all studies. The Yoneyama et al. (1976) study was highlighted because it reports the highest NOAEL below the lowest LOAEL from all the studies.

Table 6. Summary of Repeated Dose Toxicity Tests

Species	Route of Exposure	Study Duration	NOAEL (mg/kg bw/day)	LOAEL (mg/kg bw/day)	Doses (mg/kg bw/day)	Reference
Rat	Oral feed	12 weeks	50	250	50, 250	Oser and Morgareidge 1965
Rat	Oral feed	90 days	220	-	8.8, 44, 220	Kay et al. 1965
Rat	Gavage	30 days	125	250	125, 250, 500	Ito et al. 1978
Rat	Oral feed	Up to 12 weeks	-	750	750	Ikawa et al. 1978
Rat	Oral feed	6 months	40	115	40, 115, 340, 1030	Yoneyama et al 1972
Rat	Gavage	10 weeks	-	50*	50, 100, 250	Gupta et al. 1986; Mathur et al. 1986
Rat	Oral feed	9 months	-	260	260, 780	Yoneyama et al. 1976
Rat	Drinking water	9 months	85	145	85, 145, 430	Yoneyama et al. 1976
Rat	Oral feed	2 years	250	-	10, 50, 250	Buehler et al. 1971
Rat	Drinking water	2 years	200	-	20, 100, 200	Tiba 1972
Mouse	Drinking water	6 months	-	20#	20	Watari et al. 1977
Mouse	Oral feed	9 months	-	500	500, 1000	Yoneyama et al. 1976
Mouse	Drinking water	9 months	250	600	100, 250, 600, 900	Yoneyama et al. 1976
Monkey	Gavage + sc injection	28 days	30 (oral) + 0.1 (sc)	150 (oral) + 0.5 (sc)	30, 150, 300 (oral) + 0.1, 0.5, 1.0 (sc)	Heywood et al. 1978
Rat	Dermal	15 days	-	286	286, 427	Sadai and Mizuno 1972

*Although ultrastructural changes in liver cells were observed in the study, the changes were considered minimal and reversible. Effects have not been seen at similar doses in other studies that used techniques that are commonly applied in standard toxicity study protocols; in this study additional techniques were applied. Therefore, this value was considered a LOEL rather than an LOAEL.

Watari et al. (1977) administered LAS to mice (number and sex not reported) for 6 months at an equivalent dose of 20 mg/kg bw day in drinking water. Atrophy of the golgi apparatus, degeneration of the mitochondria, and increased appearance of lysosomes were observed in liver cells. Effects on the rough endoplasmic reticulum were observed. The severity of these cellular effects was dependent on the length of the administration. After six months, some liver cells showed degenerative cytoplasm and indications of cell necrosis. Some animals still showed cellular effects after the two months post administration while other animals showed full recovery. No other effects were reported. It is unclear how often these effects would be observed in other studies, if those studies also used electron microscopy. However, based on the use of a single dose (i.e., no dose response information) and the likelihood of dehydration in the dosed animals it was decided that 20 mg/kg bw day was better presented as a LOEL.

3.1.6 Genetic Toxicity

In vitro Studies

Several in vitro bacterial (Ames) tests have been conducted on LAS using Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, and TA 1538 strains with and without metabolic activation at test material concentrations up to 5000 µg/plate (Schoeberl 1993a; Inoue et al. 1980; Sunakawa et al. 1981). Results were negative in all studies, while the positive and negative controls gave the expected results. Similarly, results with and without activation were negative in a recombination assay using Bacillus subtilis at concentrations up to 50 µg/plate and in an E. coli reverse mutation assay (Inoue and Sunakawa 1979).

A transformation test with Syrian hamster embryo (SHE) cells without metabolic activation also showed negative results (Inoue et al. 1980).

In vivo Studies

In vivo mammalian bone marrow cytogenetic studies on LAS exposure are available in which mice received either oral gavage doses up to 800 mg/kg bw/day (Inoue et al. 1977) or dietary doses up to 1170 mg/kg (Masabuchi et al. 1976). Rats were also given dietary doses up to 450 mg/kg bw/day (Masabuchi et al. 1976). In all studies, there was no significant difference in the incidence of chromosomal aberrations between the treated groups and the control groups. A dominant lethal assay with mice is also available in which male mice received LAS in the diet at a dose of 300 mg/kg bw/day for 9 months before being mated with untreated females (Masabuchi et al. 1976). There were no significant differences in fertility, the mortality of ova and embryos, the number of surviving fetuses, or the index of dominant lethal induction between the experimental groups and the control group. Three male mice each given a single intraperitoneal injection of 100 mg/kg bw LAS showed no differences in the incidences of polychromatic erythrocytes with micronuclei in the bone marrow between the control and treatment group (Kishi et al. 1984). The reliability of each of the in vivo studies reported here was not assignable because the original study reports were not available for review. However, they had been evaluated by the International Program of Chemical Safety (IPCS 1996) and therefore are considered reliable.

Conclusion

No indication of genetic toxicity for LAS is evident in any of the studies conducted.

3.1.7 Carcinogenicity

Several studies looked at the potential for tumorigenicity in rats. In the most documented study (Buehler et al. 1971), four groups of Charles River weanling rats, divided by sex, were given 0.5, 0.1, and 0.02% (10, 50, 250 mg/kg bw/day) LAS in their food for 2 years. Following completion of those studies, five male and five female rats from each of the parental groups (F_{1b} and F_{2b}) and all survivors were selected for necropsy. Gross examination of all animals for pathology did not reveal any abnormalities. No consistent dietary induced changes that could be considered a toxic response were observed. Animals that showed significant loss of weight, development of tumors, or other evidence of abnormalities were sacrificed and tissues examined. The incidence of tumors and the common incidental diseases were similar in all dieting groups.

Other rat studies had similar results with drinking water exposures up to 200 mg/kg bw/day for 24-26 months (Tiba 1972; Endo et al. 1980) or dietary exposures up to 300 mg/kg bw/day for up to 24 months (Fujii et al. 1977; Yoneyama et al. 1977). No effects were observed on survival, body weight gain, or general histopathology and hematological endpoints. Slight increases in liver and

cecum weight, biochemical activity (GOT, GTP, ALP, bilirubin), and looseness, atrophy and fatty change of hepatic cells in the liver were sometimes reported. No evidence of tumorigenesis was observed. Note that the IPCS report (1996) concluded that these studies were inadequate to evaluate the carcinogenic potential of LAS.

Conclusion

Several studies investigated the tumorigenic potential of LAS. While the quality and focus of the studies preclude a definitive assessment, the results do not show evidence of carcinogenicity

3.1.8 Reproductive Toxicity

Three separate reproductive toxicity studies are available in which rats were exposed to LAS for up to four generations. One publication (Buehler et al. 1971) reported the results of the carcinogenicity study discussed above plus a separate three-generation reproductive study.

In that three-generation study, rats were given the sodium salt of C_{10-14} LAS in the diet for approximately 2 years (Buehler et al. 1971). Four groups of male and female weanling rats received dietary doses equivalent to 14, 70 and 350 mg/kg bw d, with 50 animals of each sex per dose group. All reproductive parameters, including fertility, gestation, parturition, neonatal viability, lactation, and post-weaning growth were normal for all test groups. In addition, no definitive adverse effects in hematology and pathology or gross abnormalities were noted. Therefore, the reproductive NOAEL is 350 mg/kg bw/day. Similarly, a commercial light duty liquid detergent (CLD) containing 17% LAS and 7% alkyl ether sulfate was administered in the diet to three generations of CD strain rats at doses equivalent to 40, 200 and 1000 mg/kg bw/day CLD (Palmer et al. 1974). Again, no treatment-related effects on general parental toxicity or toxicity to the offspring was observed over the course of the study, and the NOAEL is 1000 mg/kg bw/day CLD (corresponding to 170 mg/kg bw LAS). In the third available study, two groups of 20 Wistar rats of each sex were given a dose equivalent to 70 mg/kg bw/day in their drinking water and evaluated for reproductive performance over 4 generations (Endo et al. 1980). The administration of LAS had no adverse effects on fertility, parturition, gestation period, or lactation in any of the generations. The corresponding NOAEL for this study is therefore 70 mg/kg bw/day. Note that the IPCS report (1996) concluded that many of these studies had some inadequacies and recommended definitive studies to be carried out; however, the data are adequate for a weight of evidence approach.

In support of this data, two repeated dose studies (Kay et al. 1966 (dossier 5.4b; Buchler et al. 1971; dossier 5.4k) examined organ weights and histopathology of various organs including the gonads and reported that no adverse effects were observed in a 90-day oral feed study in rats at doses as high as 220 mg/kg bw/day (highest dose tested) or in a 2-year oral feed study in rats at doses as high as 250 mg/kg bw/day (highest dose tested). The absence of reproductive organ effects in these studies adds to the weight of evidence that LAS is not a reproductive toxicant.

Conclusion

No effects on reproduction were observed in any of the three available reproductive toxicity studies in which rats were given dietary doses over three to four generations. No effects on gonadal weights or histopathology were observed in 90-day and 2-year repeated dose studies. The results of the repeated dose and reproductive toxicity studies collectively provide strong weight-of evidence support that LAS is not a reproductive toxicant. Given the consistent lack of effects, the highest dose tested (350 mg/kg bw/day) should be considered the highest NOAEL. The range of NOAELs was 70 to 350 mg/kg bw/day for the five studies.

3.1.9 Developmental Toxicity

A substantial number of studies have been conducted to determine the developmental toxicity and teratogenicity characteristics of LAS. These studies have included exposures to several species (rats, rabbits, mice) by the oral route via gavage, in the diet, or in the drinking water, and by the dermal exposure route. Table 7 summarizes the maternal and fetal data from the available developmental studies.

Oral exposure

In one representative oral exposure study, LAS at a dose of 0.1% was administered to 40 female rats and 22 female rabbits in drinking water from day 6 to 15 (rats) and day 6 to 18 (rabbits) of pregnancy (Endo et al. 1980; European Commission 2000). This dose corresponds to 70 and 250 mg/kg bw/day for rats and rabbits, respectively. The only effect on the dams was a slight inhibition of body weight gain in the rabbits. No significant effects were observed in the litter parameters of both species as compared to the controls. Delayed ossification was observed in rabbits, but there was no increase in malformations in either the rabbits or the rats. Consequently, the fetal LOAEL for the rabbit is 250 mg/kg bw/day, which is also the maternal LOAEL. The NOAELs (maternal and fetal) for the rat are 70 mg/kg bw/day.

Maternal effects in other oral exposure studies ranged from no effects to severe toxicity and death in some studies. Common effects included decreased body weights, gastrointestinal effects, and diarrhea. Some studies resulted in anorexia. In two oral feed studies, no maternal effects were observed (Nolen et al., 1975; Tiba et al., 1976). However, in four gavage studies, deaths occurred at higher doses tested. Specifically, 1 CD rat died at 600 mg/kg bw/day, although this effect was not conclusively related to treatment (Palmer et al., 1975a). In a study with Charles-River pathogen-free mice of the CD-1 strain, 35% of the animals died at 300 mg/kg bw/day and 90% died at 600 mg/kg bw/day (Palmer and Lovell, 1971b). A study in New Zealand white rabbits also resulted in severe maternal toxicity and 85 and 100% deaths at 300 and 600 mg/kg bw/day, respectively (Palmer and Neuff, 1971; Palmer et al., 1975a). Finally, in a study in ICR mice, two animals died at 300 mg/kg bw/day (Shiobara and Imahori, 1976). In studies where maternal toxicity was observed, LOAELs ranged from 100-400 mg/kg bw/day, similar to the results of repeated-dose toxicity studies (section 3.1.5) where LOAELs from oral exposures ranged from 115-750 mg/kg bw/day.

In nine other oral exposure studies the results on offspring were similar to those of Endo et al. (1980) reported above, with litter effects, where observed, only occurring at maternally toxic doses (Palmer and Lovell 1971a; Palmer et al. 1975a; Nolen et al. 1975; Tiba et al., 1976; Palmer and Lovell 1971b; Takahashi et al. 1975; Shiobara and Imahori 1976; Palmer and Neuff 1971). In a drinking water study in rats, a dose of 600 mg/kg bw/day that produced maternal toxicity resulted in marginal retardation of sternebral ossification in offspring (Palmer and Lovell, 1971a). In another study in which maternal toxicity was observed, effects in mice and rabbit offspring included increased fetal loss (at 300 and 600 mg/kg bw/day), and reduced litter size and minor skeletal or visceral anomalies (mice at 300 mg/kg bw/day) (Palmer et al., 1975a). In a third study (mice, gavage) in which maternal toxicity was observed, there was delayed ossification among living fetuses and decreased body weights at the highest dose tested (300 mg/kg bw/day) but no increase in malformations (Shiobara and Imahori, 1976). In three other studies with maternal toxicity, no offspring effects were observed at the highest doses tested, 600 mg/kg bw/day in a gavage study in rats (Palmer et al., 1975a), 600 mg/kg bw/day in drinking water study in mice (Palmer and Lovell, 1971b) or 400 mg/kg bw/day in a gavage study in mice (Takahashi et al. 1975). Three other oral studies reported no maternal or offspring effects at the highest doses tested, 225 mg/kg bw/day in a rat feeding study (Nolen et al. 1975), 780 mg/kg bw/day in a second rat feeding study (Tiba et al. 1976) or 135 mg/kg bw/day in a rabbit feeding study (Nolen et al. 1975).

In addition, the three multigenerational studies reported in section 3.1.8 (Buehler et al. 1971; Palmer et al. 1974; Endo et al. 1980) all reported no affects on various reproductive and developmental parameters at doses as high as 350 mg/kg bw/day.

Dermal Exposure

In a representative dermal exposure study, an aqueous solution of LAS was applied to the shaved skin on the backs of pregnant female rats on days 2 to 15 of gestation (Palmer et al. 1975b). Doses were 0.03, 0.3 and 3% (0.6, 6, and 60 mg/kg bw/day). At the high dose, local irritation was observed resulting in a slightly lower body weight gain and hypersensitivity (increased irritability). No differences from the control groups were reported at any dose for number of litters, viable young, litter weight, fetal weight, embryonic deaths, implantations, corpora lutea, or pre- and postimplantation embryonic loss. No differences in major malformations or visceral and skeletal anomalies were observed. The resultant maternal NOAEL was 6 mg/kg bw/day and the NOAEL for developmental toxicity was 60 mg/kg bw/day.

Similar results were obtained in six other dermal exposure studies, with LOAELs for maternal toxicity ranging from 9-1500 mg/kg bw/day (Daly et al. 1980; Palmer et al. 1975b; Sato et al. 1972; Imahori et al. 1976; Takahashi et al. 1975). In all cases toxicity was associated with the irritancy effects of LAS on skin resulting in reduced body weight as observed in the dermal repeated dose study (section 3.1.5). No maternal toxicity was observed at the only concentration tested (110 mg/kg bw/day) in the mouse study of Sato et al. (1972).

Effects on developmental parameters were observed in one study in which maternal toxicity was also observed (Palmer et al. 1975b). The effects included significant fetal loss and consequent reduction in litter size at 500 mg/kg bw/day in mice. Some fetal loss was also observed at the next highest dose tested (50 mg/kg bw/day) but the reduction in litter size was not statistically significant. Significant offspring effects were not observed in the other dermal exposure studies at the highest doses tested, which ranged from 90-1500 mg/kg bw/day (Table 7).

Conclusion

LAS has been evaluated for developmental effects with rats, mice and rabbits. In oral studies, findings of maternal toxicity were observed at doses of 100-400 mg/kg bw/day, consistent with the results of oral repeated dose studies. In dermal studies, findings of maternal toxicity were observed at doses of 9-1500 mg/kg bw/day and were associated with the irritancy effects of LAS on skin resulting in reduced body weight as observed in the dermal repeated dose study.

With regard to developmental toxicity/teratogenicity, effects such as embryo death or deformities and litter loss were observed only at maternally toxic doses. In two drinking water studies, delayed ossification in rabbits was observed at 250 mg/kg bw/day and in rats at 600 mg/kg bw/day. Mice and rabbits exhibited fetal loss at 300 and 600 mg/kg bw/day. Decreased litter size and minor skeletal/visceral anomalies were observed in mice at 300 mg/kg bw/day oral exposure. In another oral study, mice had delayed ossification and decreased body weight at 300 mg/kg bw/day. In a dermal study in mice, significant fetal loss and decreased litter size was observed at 500 mg/kg bw/day.

It should be noted that several of the key studies are given a reliability score of 4. This score was assigned because the original reports were not available for review; however, these studies were evaluated and included in the IPCS review of LAS (IPCS 1996) and therefore are considered to be reliable for the purposes of this SIDS assessment.

Table 7. Results from Developmental Toxicity Studies on LAS

Animal	Route	Exposure in Pregnancy	NOAEL Maternal (mg/kg bw/day)	NOAEL Fetal (mg/kg bw/day)	Doses (mg/kg bw/day)	Reference
Oral Exposure						
Rat	Drinking water	Days 6-15	70	70	70	Endo et al. 1980
Rat	Drinking water	Days 6-15	300	300	0.2, 2, 300, 600	Palmer & Lovell 1971a
Rat	Gavage	Days 6-15	300	600	0.2, 2, 300, 600	Palmer et al. 1975a
Rat	Oral feed	Continuous or Days 6-15	225	225	22.5, 112.5, 225	Nolen et al. 1975
Rat	Oral feed	Days 0-20	780	780	80, 780	Tiba et al. 1976
Mouse	Drinking water	Days 6-15	2	600	0.2, 2, 300, 600	Palmer & Lovell 1971b
Mouse	Gavage	Days 6-15	2	300	0.2, 2, 300, 600	Palmer et al. 1975a
Mouse	Gavage	Days 0-6 or Days 7-13	40	400	40, 400	Takahashi et al. 1975
Mouse	Gavage	Days 6-15	10	300	10, 100, 300	Shiobara & Imahori 1976
Rabbit	Drinking water	Days 6-18	250 (LOAEL)	250 (LOAEL)	250	Endo et al. 1980
Rabbit	Gavage	Days 6-18	2	2	0.2, 2, 300, 600	Palmer et al. 1975a; Palmer and Neuff 1971
Rabbit	Oral feed	Days 2-16	135	135	22.5, 45, 135	Nolen et al. 1975
Dermal Exposure						
Rat	Dermal	Days 2-15	6	60	0.6, 6, 60	Palmer et al. 1975b
Rat	Dermal	Days 0-21	20	400	0.1, 2, 10, 20, 100, 400	Daly et al. 1980
Mouse	Dermal	Days 2-13	5	50	5, 50, 500	Palmer et al. 1975
Mouse	Dermal	Days 0-13	110	110	110	Sato et al. 1972
Mouse	Dermal	Days 6-15	150	1500	15, 150, 1500	Imahori et al. 1976
Mouse	SC Injection	Days 0-3 or 8-11	20	200	20, 200	Takahashi et al. 1975
Rabbit	Dermal	Days 1-16	0.9	90	0.9, 9, 90	Palmer et al. 1975b

3.2 Initial Assessment for Human Health

Substantial data exist for mammalian toxicity. The available data indicate that LAS exhibits slight acute toxicity. Oral LD_{50} values for rats range from 1,080 to 1,980 mg/kg bw. Oral LD_{50} values for mice are 2,160 and 2,250 mg/kg bw for males and females, respectively. The rat dermal LD_{50} value was greater than 2,000 mg/kg bw. The oral and dermal acute toxicity data for LAS generally

indicate low hazard potential when all studies are considered together. Acute inhalation toxicity data indicate that LAS is moderately toxic, with mortality occurring at respirable particle concentrations of 310 mg/m^3 (MMAD = 2.5 microns).

In a series of studies on rabbits, LAS was not irritating to the skin or eyes at low concentrations (0.5-2.5%), moderately irritating at 5%, and more severely irritating at higher (about 50%) concentrations. In studies that included rinsing, eye irritation effects diminished with rinsing after 30 seconds of exposure and were slight with rinsing after 4 seconds of exposure. In a low volume eye test (LVET) using a 35% LAS solution, rabbits experienced moderate irritation that was completely reversible by day 35. (Note that the maximum concentration of LAS is 25 percent in consumer products and normally less than 30 percent in commercial products.) Accidental eye exposure in 231 manufacturing employee incidents and 284 consumer incidents established that eye irritation effects of exposure during manufacturing and use of products containing LAS and other surfactants are moderate, transient and reversible.

In 15 repeated dose studies with rats, mice, and monkeys exposed to LAS via oral and dermal routes, LOAELs ranged from 115 to 750 mg/kg bw/day. The corresponding NOAELs ranged from 40 to 250 mg/kg bw/day. Effects commonly observed included suppressed body weight gain, diarrhea, increases in relative liver weight, differences in enzymatic and serum-biochemical parameters, and mild degeneration and desquamation of the tubular epithelium in the kidneys.

In four well designed *in vitro* bacterial (*Salmonella*) mutagenicity studies, LAS shows no evidence of mutagenicity either with or without S9 metabolic activation. LAS showed no evidence of causing increased cell transformation in an *in vitro* cell transformation assay. In *in vivo* studies, no significant differences in chromosome aberrations were seen when mice were given either oral doses up to 800 mg/kg bw/day or dietary doses up to 1170 mg/kg bw/day. In a mouse micronucleus study, LAS did not induce a clastogenic effect. Rats given dietary doses up to 450 mg/kg bw/day also showed no significant differences in chromosome aberrations. Collectively, these data support that LAS is not genotoxic.

The highest dose tested in four carcinogenicity studies with rats was 300 mg/kg bw/day. In the most documented study, rats were administered up to 250 mg LAS/kg body weight/day in the diet for two years. Results of this study indicate no gross or histopathological evidence of a carcinogenic effect. No evidence of tumorigenesis was observed in any of the carcinogenicity studies. While the quality and focus of the studies precludes a definitive assessment, the results of the genetic toxicology and rodent bioassay studies collectively provide strong weight-of-evidence support that LAS is not genotoxic and is not a rodent carcinogen.

Similarly, no evidence of reproductive or fertility effects was observed in any of the three available reproductive toxicity studies in which rats were given dietary doses over three to four generations. NOAELs from these reproductive studies ranged from 70 to 350 mg/kg bw/day, which were the highest doses tested. In 17 developmental toxicity studies, effects such as embryo death or deformities, and litter loss were most often observed only at maternally toxic doses and were associated with the irritation effects of LAS on skin or the gastrointestinal tract. No decreases in litter size, no changes in litter parameters, no malformations or significant differences in skeletal defects were observed at oral doses up to 780 mg/kg bw/day in rats and at dermal doses of 500 mg/kg bw/day in mice and 90 mg/kg bw/day in rabbits.

All of the studies included in the dossier are considered reliable, but all with limitations. The results are consistent with each other and these data are used in a weight-of-evidence approach. Based on these considerations, the highest NOAEL value below the lowest LOAEL from all of the mammalian toxicity studies is the most appropriate. Therefore, the NOAEL is 85 mg/kg bw/day. This value comes from a rat drinking water, 9-month repeated dose toxicity study. The lowest

LOAEL (115 mg/kg/day) was associated with increased weight of the cecum and slight degeneration of the renal tubules.

Current LAS production is approximately 390,000 metric tons in the North America, 400,000 metric tons in Europe, and 85,000 metric tons in Japan. Global production was 2.6 million metric tons in 1995. In the production phase, manufacturing processes have been designed to maximize production yield and minimize potential releases. Worker exposure is possible during the detergent formulation stage by inhalation of powders or dermal contact of powders and liquids. Good manufacturing design practices (e.g., enclosed production in agglomeration processes, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) in place at facilities that manufacture liquid and dry (granular/powder) materials are anticipated to mitigate worker exposure to LAS. Any LAS that is not incorporated into a product is captured by dust-handling equipment for recycling back into the production process. A limited amount of LAS in aqueous solution may be released as a dilute solution from washing and rinsing operations in the manufacturing process and is discharged to wastewater treatment. Incidental quantities of the dry (granular/powder) product (e.g., from floor sweepings) may be disposed in landfills.

Labelling of consumer products containing LAS and other surfactants include warnings of the potential for eye irritation and first aid instructions to rinse with water.

Data suggest that inhalation of LAS products during use will be low. Spray products containing LAS are designed to produce the large particle sizes needed for efficient delivery of the spray to the surface being cleaned. In laboratory simulations with six spray nozzles representing those used in spray cleaning products, less than 0.1% of the total volume sprayed consists of respirable particles (particles under 10 microns in diameter) and air concentrations in the breathing zone are in the 0.13-0.72 mg/m^3 range. Inhalation of detergent dusts during washing processes, modeled by HERA (2004), was 10-fold lower than inhalation of aerosols from cleaning product sprays. This estimate is based on a published study reporting an average of 0.27 μg dust per cup of product used for machine laundering. This is a conservative (protective) estimate as exposure from modern compact/granular detergent formulations produced in agglomeration processes, which produce larger particle sizes, would be expected to be much less. Based on these data, it is expected that exposures to respirable particles from inhalation are low.

4 HAZARDS TO THE ENVIRONMENT

4.1 Aquatic Effects

The aquatic toxicity of LAS has been extensively studied, and several comprehensive reviews have been prepared (e.g., Arthur D. Little (SDA) 1991; BKH 1993; ERASM 2000; IPCS 1996; van de Plassche et al. 1999). The data cover a wide range of taxonomic groups and exhibit a predictable degree of intra- and inter-species variability attributable to differences in test design, differences in species sensitivity, and the use of different chain length mixtures of LAS.

Factors Affecting Toxicity

Aquatic toxicity is greater for individual homologues of LAS with longer carbon chains and would therefore be expected to be greater for commercial LAS products with longer average chain lengths. Although the 48 hour study was shorter than normal and less than the standard number of fish were used, the Kimerle and Swisher (1977) study clearly demonstrates the increase in toxicity to fathead

minnows and to *Daphnia magna* with increasing homologue chain length. These data are shown in Table 8.

Table 8. Aquatic Toxicity for Individual LAS Homologues[1]

	48-hour LC_{50} (mg/L)	
	D. magna **(Dossier, section 4.2Af)**	**Fathead minnow (Dossier, section 4.1r)**
Individual LAS Homologues		
C_{10}	12.3	43.0
C_{11}	5.7	16.0
C_{12}	3.5	4.7
C_{13}	2.0	0.4
C_{14}	0.7	0.4

[1] Reliability of Study = (2)

As discussed in section 2.2.6, the longer alkyl chain homologues biodegrade faster (Bock and Wickbold, 1966). Toxicity of the biodegradation intermediates is significantly less than the parent LAS. Acute toxicity tests conducted on LAS degradation intermediates (i.e., SPCs) yielded 48-hour LC_{50} values >1000 mg/L for fathead minnows and *D. magna* using the same procedures as for the data reported in the above table (Kimerle and Swisher 1977).

The trend of increasing toxicity with increasing alkyl chain length has also been demonstrated with algae. In one study, three different LAS materials with average chain lengths of C_{11}, $C_{11.6}$, and C_{13} were tested in accordance with the OECD 201 protocol under GLP conditions (Verge and Moreno 1996a, dossier section 4.3d,e). The resultant EC_{50} values were 240, 163, and 54 mg/L, respectively, for the three materials. Similarly, the authors tested five pure homologue cuts and determined the EC_{50} values to be 270, 111, 48, 30, and 18 mg/L for the pure C_{10}, C_{11}, C_{12}, C_{13}, and C_{14}, respectively.

Qualitative Structure-Activity Relationships (QSARs) have been developed for LAS and other surfactants (Roberts 2004). These QSARs are based on correlations to the log K_{ow} and supported by considerable experimental data. Although it is extremely difficult to accurately measure log K_{ow}s for surfactants because of their strong preference for the oil-water interface, log K_{ow}s may be reliably calculated using the Leo and Hansch method as modified Roberts. This method takes into account all the structural elements of the surfactant molecule including for LAS, the alkyl chain length and the position of attachment of the sulfophenyl group to the alkyl chain. For LAS category materials (and many other surfactants), the alkyl chain length is the major structural element that varies and thus the major factor causing the log K_{ow} for LAS to vary. The QSAR for LAS is described more fully in Annex 3, where it is used to calculate chronic NOEC values for $C_{11.6}$ LAS.

Acute Toxicity Test Results

Freshwater Fish

LAS toxicity has been evaluated on a variety of freshwater fish species in many studies. Van de Plassche et al. (1999) reviewed the acute fish data compiled by BKH (1993) for LAS and related materials, including many materials with average alkyl chain lengths outside the range of current commercial LAS (section 1.1), and for alkyl chain homologs from C_{10} to C_{14} (original studies not reviewed). Van de Plassche et al. commented that the range of LC_{50} values was very large due to

the range of materials tested (including many materials not representative of commercial LAS) and the differences in test design (not necessarily following standard guidelines). Consequently, the range of LC_{50} values for fish presented by Van d Plassche et al. was only provided for one species (*Pimephales promelas,* 0.40-100 mg/L) as an example of the wide ranges found. These values include mixtures of chemicals in addition to commercial LAS products. It is unclear which values within the range refer to the commercial LAS products and the individual records were not available for validation.

Van de Plassche et al. (1999) did calculate the geometric mean values for seven species of fish, as shown in Table 9 below, and found the interspecies variation decreases considerably when the geometric mean value per species is calculated. This comparison indicates that the large variation found (e.g., *P. promelas* LC_{50} values ranged from 0.4-100 mg/L; geometric mean = 3.2 mg/L) is due primarily to the wide range of materials tested and differences in test designs.

Table 9. Geometric Mean Fish LC_{50} Toxicity Results[1]

Species	Geometric Mean (Range) LC_{50} (mg/L)	Number of Records
Lepomis macrochirus (bluegill sunfish, dossier section 4.1c)	3.0	88
Pimephales promelas (fathead minnow, dossier section 4.1d)	3.2 (0.4-100 mg/L)	35
Leusiscus idus melanotus (golden orfe, dossier section 4.1e)	2.9	11
Carassius auratus (goldfish, dossier section 4.1f)	9.5	46
Oncorhynchus mykiss (rainbow trout, dossier section 4.1f)	3.0	10
Oryzias latipes (medaka, dossier section 4.1f)	13	5
Poecilia reticulata (guppy, dossier section 4.1f)	3.8	9

[1]Reliability of Studies = (4); Original Data Not Reviewed

HERA (2004) conducted an extensive search of the data previously compiled by BKH (1993) and the published and unpublished literature since this data compilation for studies on commercial LAS and on species for which standardized test methodologies are available. As described in Appendix 2, a total of 18 fish studies were identified. Of these 11 studies were found to have been conducted using currently relevant LAS ($C_{11.6}$-$C_{11.8}$) and valid test methods. LC_{50} values ranged from 1.67-7.7 mg/L with no values below 1 mg/L. A robust summary for the study representing the lowest value for fish (critical study) was prepared and the study reference is provided in Table 10.

Table 10. Acute Aquatic Toxicity Results (lowest value for each taxon) [1]

Taxon	$LC_{50}/EC_{50}/IC_{50}$ (mg/L)	Reference
Fish (*Lepomis macrochirus*), LC_{50} (dossier, section 4.1a) [96 hr. exposure]	1.67	Lewis and Perry 1981
Daphnia magna, EC_{50} (dossier, section 4.2Aa) [48 hr. exposure]	1.62	Hooftman and van Drongelen-Sevenhuijsen 1990
Algae (Selenastrum capricornutum), IC_{50} (dossier, section 4.3a) [96 hr. exposure]	29.0	Lewis 1986; Lewis and Hamm 1986

[1]The reliability of studies = (2)

Freshwater Invertebrates

LAS toxicity has also been evaluated on a variety of freshwater invertebrate species in many studies. Van de Plassche et al. (1999) reviewed the acute invertebrate data compiled by BKH (1993) for LAS and related materials, including many materials with average alkyl chain lengths outside the range of current commercial LAS (section 1.1), and for alkyl chain homologs from C_{10} to C_{14}. Similar to the results with fish, the range of invertebrate EC_{50} values was very large due to the range of materials tested (including many materials not representative of commercial LAS) and the differences in test design (not necessarily following standard guidelines). The range of EC_{50} values was only provided for one invertebrate species (*Daphnia magna,* 0.26-55 mg/L). These values include chemicals in addition to commercial LAS products. It is unclear which values within the range refer to commercial LAS products and the individual records were not available for validation.

Van de Plassche et al. (1999) also calculated the geometric mean value for *Daphnia magna* and other aquatic invertebrates. The geometric mean EC_{50} for *Daphnia magna* based on 139 records was determined to be 4.7 mg/L (dossier, section 4.2Ac). The geometric mean EC_{50} values for *Gammarus pulex*, *Mysidopsis bahia*, and *Panaeus duorarum* were 6.2 mg/L (25 records), 1.7 mg/L (6 records), and 49 mg/L (5 records), respectively (dossier, section 4.2Ba). Because this is a review article and the individual studies were not reviewed independently, the reliability of these studies is not assignable. Lewis and Surprenant (1983) also reported an LC_{50} of 16 mg/L for the nematode *Rhabditis* sp. for C_{12} LAS (dossier, section 4.2Bf; reliability = 2).

The HERA search (HERA 2004) also found 20 daphnid studies on commercial LAS, of which 11 studies were on currently relevant LAS ($C_{11.6}$-$C_{11.8}$) and followed standardized test methods (Annex 2). EC_{50} values on *Daphnia magna* ranged from 1.62 to 9.3 mg/L. A robust summary for the study representing the lowest value has been prepared and the study is referenced in Table 10 above.

Freshwater algae

LAS toxicity has also been evaluated on a variety of freshwater algae species although van de Plassche et al. (1999) did not provide geometric mean or range data on acute algae data.

The HERA search (HERA 2004) found 13 algae studies on commercial LAS, of which 5 studies were on currently relevant LAS (C11.6-C11.8) and followed standardized test methods (Annex 2). The range of ErC_{50} values on algae ranged from 29-163 mg/L. A robust summary for the study representing the lowest value has been prepared and the study is referenced in Table 10 above.

Marine Species

Acute aquatic toxicity data for marine species have been summarized by van de Plassche et al. (1999). Geometric mean EC_{50} values were 6.2 mg/L (25 records), 1.7 mg/L (6 records), and 49

mg/L (5 records) for *Gammarus pulex* (amphipod), *Mysidopsis bahia* (mysid), and *Panaeus duorarum* (pink shrimp), respectively (dossier, section 4.2Ba). Temara et al. (2001) also summarized acute aquatic toxicity data, as shown in Table 11.

Table 11. Aquatic Toxicity for Marine Species[1,2]

Taxon	Geometric Mean LC_{50} (mg/L)	Alkyl Chain Length	Number of Records
All spp.[3]	4.36 (SD = 0.79)	$C_{11.7\text{-}12.0}$	36
Crustacea	17.0 (SD=0.68)	$C_{11.7\text{-}12.0}$	14
Fish	1.58 (SD = 0.16)	$C_{11.7\text{-}12.0}$	6

[1] From Dossier 4.1g, 4.2Bb
[2] Reliability of Studies = (4); Original Data Not Reviewed
[3] Data from fish, crustacea, algae and other species.

Chronic Toxicity Test Results

Freshwater Species

Table 12 in the SIAR includes all available, reliable chronic freshwater NOEC values obtained in studies following guideline exposure periods (28-30 days for fish, 21 days for invertebrates and 3-4 days for algae). These studies result in the following NOEC values: fish NOEC = 1 mg/L (two studies, two species); Daphnia, NOEC = 1.18-3.25 mg/L (six values, two studies, one with 5 diets); algae, NOEC = 0.4-18 mg/L (four studies, two species).

Table 12 - Chronic NOEC Values for Freshwater Species Following Guideline Exposure Periods[1]

Species, Reference (Reliability)	Endpoint (Exposure Period)	NOEC (mg/L)	LAS Alkyl Chain Length
Fish (28-30 day exposure period)			
Lepomis macrochirus, dossier 4.5.1m (2)	Juvenile Growth[2] (28 d)	1.0	11.6
Pimephales promelas, dossier 4.5.1b (2)	Fry Survival (30 d)	1	12.3
Invertebrates (21 day exposure period)			
Daphnia magna, dossier 4.5.2c (2)	Reproduction (21 d)	1.18	11.8
Daphnia magna, dossier 4.5.2e (2)	Reproduction (21 d)	1.25-3.75[3]	11.8
Algae (3-4 day exposure period)			
Scenedesmus subspicatus, dossier 4.3e (2)	Population Growth Rate (3 d)	18	12.0
Scenedesmus subspicatus, dossier 4.3f (1)	Population Growth Rate (3 d)	2.4	11.6
Scenedesmus subspicatus, dossier 4.3g (1)	Population Growth Rate (3 d)	0.4	11.6
Selenastrum capricornutum, dossier 4.3a (2)	Population Growth Rate (4 d)	0.5	11.8

[1] Reliability of Studies = (2) or (1)
[2] Most sensitive endpoint.
[3] Range of NOECs of 5 diets.

The chronic toxicity to freshwater aquatic organisms of commercial LAS with $C_{10\text{-}13}$ alkyl chains and average carbon lengths close to $C_{11.6}$ has been reviewed by van de Plassche et al. (1999) and the

geometric mean NOEC values, normalized to $C_{11.6}$ LAS, from this review are provided in Table 12A. These values are based on the earlier data compilation of BKH (1993) but the archive of studies for this data compilation is no longer available and a new compilation was undertaken. The available freshwater chronic toxicity studies were retrieved and robust summaries prepared on all the available studies. The reliable chronic studies are shown in Table 12A. Additional studies in the dossier were not included in the table either because the duration of the test was too short for a reliable chronic study or because the reliability of the study could not be assessed. Available NOEC values from individual studies ranged from 0.25 to 54.3 mg/L. The endpoints affected included behavior, growth, mobility, mortality, and reproduction, depending on the species tested.

Table 12A. Chronic Aquatic Toxicity for Freshwater Species*

Species, Reference (Reliability)	Endpoint (Exposure Period)	Avail-able NOEC (mg/L)	LAS Alkyl Chain Length	Available NOEC Normalized to $C_{11.6}$ LAS[1]	Van de Plassche et al. (1999) Geometric Mean NOEC (mg/L), Normalized to $C_{11.6}$ LAS, (range[2]), [Number Studies]
Fish					
Brachydanio rerio[4]					2.3 [1]
Lepomis macrochirus, dossier 4.5.1m (2)	Juvenile Growth[8] (28 d)	1.0	11.6	1.0	--[3]
Oncorhynchus mykiss[4]					0.34 (0.19-0.89) [7]
Pimephales promelas, dossier 4.5.1b (2)	Fry Survival (30 d)	1	12.3	1.87	
Pimephales promelas, dossier 4.5.1j (2)	Fry Survival (196 d)	0.63	12.0	0.9	
Pimephales promelas, geometric mean				1.3	0.87 (0.3-2) [14]
Poecilia reticulata[4]					3.2 [1]
Tilapia mossambica, dossier 4.5.1e (2)	Reproduction (90 d)	0.25	N/A[5]	0.25	0.25 [1]
Aquatic Invertebrates					
Ceriodaphnia sp., dossier 4.5.2b (2)	Reproduction (7 d)	0.7[9]	11.8	0.84	3.2 [1]
Chironomus riparius, dossier 4.5.2o (2)	Emergence (24 d)	2.4	11.8	2.87	2.8 [1]
Daphnia magna, dossier 4.5.2c (2)	Reproduction (21 d)	1.18	11.8	1.41	
Daphnia magna, dossier 4.5.2e (2)	Reproduction (21 d)	1.99[10]	11.8	2.38	
Daphnia magna, geometric mean				1.83	1.4 (0.3-10) [12]
Paratanytarsus parthenogenica, dossier 4.5.2h (2)	Survival & Population Size (28 d)	3.4	N/A[5]	3.4	3.4 [1]
Algae					
Chlamydomonas reinhardi[4]					12 [1]

Chlorella kessleri[4]					3.5[1]
Microcystis aeruginosa, dossier 4.3s (2)	Population Growth Rate (4 d)	0.3[6]	11.6	0.3	0.80 (0.3-10.7[7]) [4]
Plectonema boryanum[4]					15 [1]
Scenedesmus subspicatus, dossier 4.3d (2)	Population Growth Rate (3 d)	54.3[6]	11.6	54.3	
Scenedesmus subspicatus, dossier 4.3e (2)	Population Growth Rate (3 d)	18	12.0	26	
Scenedesmus subspicatus, dossier 4.3f (1)	Population Growth Rate (3 d)	2.4	11.6	2.4	
Scenedesmus subspicatus, dossier 4.3g (1)	Population Growth Rate (3 d)	0.4	11.6	0.4	
Scenedesmus subspicatus, geometric mean				6.1	7.7 (0.8-105[7]) [4]
Selenastrum capricronutum, dossier 4.3a (2)	Population Growth Rate (4 d)	0.5	11.8	0.58	3.8 (1-39[7]) [9]
Higher Plants					
Elodea canadensis, dossier 4.3o (2)	Growth, Productivity (28 d)	4	11.6	4	--[3]
Lemna minor, dossier 4.3p (2)	Frond Count (7 d)	0.9[6]	11.8	1.1	--[3]

*Reliability of Studies = (2) or (1), except for Van de Plassche et al. (1999), where Reliability = (4), Original Data Not Reviewed

[1] The normalization procedure is described in SIAR Annex 3.

[2] Feijtel & van de Plassche, 1995.

[3] Not reviewed by van de Plassche et al. 1999.

[4] No valid chronic study identified.

[5] Not available.

[6] EC_{50} value divided by 3; as documented in Annex 3, the average EC_{50}/NOEC ratio for LAS is 3.

[7] Ranges include EC_{50}/3.

[8] Most sensitive endpoint.

[9] Geometric mean of trout chow/algae NOEC (0.5 mg/L) and yeast diet EC_{10} (0.99 mg/L).

[10] Geometric mean of 5 diets considered by the authors of the study to be equivalent to 5 replications of the same diet.

Table 12A also provides the available NOEC values normalized to $C_{11.6}$ LAS by the QSAR procedures used by van de Plassche et al. (1999) and described in detail in Annex 3. Geometric mean normalized NOEC values are provided for species (*P. promelas, D. magna* and *S. subspicatus*) for which multiple studies are available. These normalized NOEC values range from 0.25 to 6.1 mg/L for the 12 species for which we were able to document reliable values. The similarity of these values, as shown in Table 12A, to those of van de Plassche et al. (1999) supports the validity of the BKH (1993) data compilation and the van de Plassche et al. (1999) assessment of the data despite the fact that not all of the studies cited by these authors could be retrieved and validated.

Van de Plassche et al. (1999) used statistical methods to estimate the lowest 5% of the NOEC distribution, the HC_5. The HC_5 value calculated by van de Plassche et al., from the NOEC data shown in Table 12A, was 0.32 mg/L. This value is based on a fit of the data to a log-normal distribution. As described in Annex 3, an improved estimate can be obtained by comparing the goodness of fit of various distributions. The best distribution to the van de Plassche data was found with the log-logistic distribution, which gave an HC_5 value of 0.36 mg/L (Annex 3). Applying these same methods to the available NOEC data, normalized to $C_{11.6}$ LAS (Table 12A), gave an HC_5 value of 0.24 mg/L (Annex 3). Because these values are based on NOEC data from 12 or more species of fish, algae, several groups of invertebrates, and higher plants (for the available data), these values are all considered to be valid estimates of the HC_5 for LAS. Based on goodness of fit, the best HC_5 values are 0.24 mg/L for the available NOEC data and 0.36 mg/L for the van de Plassche et al. (1999) data.

Marine Species

Chronic aquatic toxicity data are available for marine species and have been summarized by van de Plassche et al. (1999) and Temara et al. (2001). Because these are review articles the reliability of the individual studies could not be independently assessed. Geometric mean results are shown in Table 13.

Table 13. Chronic Aquatic Toxicity Data for Marine Species (dossier 4.5.2t)[1]

Genus (and species)	Geometric mean NOEC (mg/L)
Fish	
Limanda (*yokohamae*)*	0.05
Aquatic Invertebrates	
Arbacia	0.45
Arcatia	0.30
Asterias	0.35
Botrylloides	1.94
Botryllus	0.75
Chaetopterus	0.45
Crassostrea (*virginica*)*	0.025
Crassostrea	0.04
Molgula	0.90
Mysidopsis (*bahia*)*	0.12
Mysidopsis	0.20
Mytilus (*edulis*)*	0.025
Mytilus	0.04
Spisula	0.80
Algae	
Dunaliella	0.11
Laminaria	5.00

[1]Reliability of Studies = (4); Original Data Not Reviewed

*Normalized to $C_{11.6}$ LAS (van de Plassche et al. 1999); all others are for LAS with average alkyl chain lengths of 11.6-12.0 (Temara et al. 2001)

Toxicity to Microorganisms

Three LAS mixtures (average chain lengths of C11, C11.6 and C13) and five pure homologues were used to evaluate inhibition to activated sludge using OECD Guideline 209 (Verge and Moreno 1996b, dossier section 4.4a,b). Results showed EC50 values of 760, 550 and 650 mg/L for the C11, C11.6, and C13 commercial materials, respectively, and 1042-1200, 740-782, 500-723, 700-795, and 900-1045 mg/L for the C10, C11, C12, C13, and C14 pure homologues, respectively. In all of these studies, an extended contact time of 3 hours (instead of the standard 15 minutes) was used to better simulate the normal residence time in wastewater treatment plants. An older study using the standard 15-minute exposure reported EC50 values of 107-152 mg/L for a commercial LAS sample (dossier 4.4c; reliability not assignable). Studies with C11.6/C11.8 LAS and the bacterium Pseudomonas putida reported EC50 values of 350 mg/L (30-min. exposure, dossier 4.4e), 150 mg/L (16-hr exposure, dossier 4.4f) and 60.9-63.5 mg/L (18-hr. exposure, dossier 4.4d) and EC0/EC10/NOEC values of 64 and 250 mg/L (30 min. exposures, dossier 4.4e,g), 30 and 50 mg/L (16-hr. exposure, dossier 4.4f,h) and 52.7-56.6 (18-hr. exposure, dossier 4.4d). While there is variability in the values, the data are consistent in showing LAS toxicity to activated sludge or a bacterium only at LAS concentrations considerably above those observed in the aquatic environment.

Normal operation of an activated sludge digester was observed even in the presence of high and atypical concentrations of LAS (30 g/kg dry matter) in anaerobic sludge indicating that the microbial population present was not inhibited (Berna et al., 1989, dossier 4.4i). The treatment plant operational records were not directly available for review, so these conclusions are based on the evaluation of Berna et al. (1989). Sanz et al. (1999, dossier 3.5p) determined that concentrations of LAS usually found in anaerobic digesters are an order of magnitude lower than concentrations that may be inhibitory to anaerobic microbial populations (40-150 mg C11.54 LAS/L). Based on the sludge partition coefficient for C11.6 LAS (dossier 3.3.1a) of 2500 L/kg, aqueous phase concentrations inhibitory to anaerobic microbial populations (40-150 mg/L) would require LAS levels in sludge of 100-375 g/kg, fully supportive of the results of Berna et al (1989) above showing no inhibition of anaerobic microbial populations in activated sludge digesters at LAS concentrations of 30 g/kg dw sludge.

Sediment Toxicity Test Results

Several studies have investigated the toxicity to organisms exposed to LAS in the sediment, as summarized in Table 14. Midge larvae (*Chironomus riparius*) were exposed for 24 days to natural stream sediment spiked with commercial LAS with an average alkyl chain length $C_{11.8}$ (Pittinger et al. 1989). The resultant LOEC was 993 mg/kg and the NOEC 319 mg/kg, based on emergence success. A fresh water bivalve mollusk, *Anodonta cygnea*, was exposed to commercial LAS sorbed to natural pond sediment by repeated additions for 80 days (Bressan et al. 1989). All animals survived and were actively filter-feeding at sediment concentrations measured to be 750 mg/kg at the beginning of the test and 200 mg/kg at the end of the test. Similarly, a tubificid, *Branchiura sowerbyi*, was exposed for 220 days to sediment spiked with an undefined LAS (Casellato et al. 1992). No effects were observed at mean measured concentrations that were initially 26 mg/kg and decreased to 7.18 mg/kg by the end of the study. While the absence of reported toxicity is reassuring, it appears that the range of exposure concentrations was too low to derive a useful NOEC value. In addition, the reliability of the study could not be assessed so it is not included in Table 14. According to Marin et al. (1994), no effects were observed in the marine mussel, *M. galloprovinciallis*, at 132 mg/kg (initial measured concentration) of $C_{11.6}$ LAS. The LAS concentration decreased by 90% by the end of the exposure to 7.85 mg/kg, which is the value reported as the NOEC in Table 14. Most recently, GLP studies have been conducted with *Lumbriculus variegates* (an oligochaete worm) and *Caenorhabditis elegans* (a nematode worm) to finalize the effects assessment of sediment associated $C_{11.4}$ LAS (Comber et al. 2004). After 28

days of exposure to artificial sediment spiked with radiolabeled LAS, the resultant survival, reproduction and growth NOEC for *L. variegates* was 81 mg/kg based on the average concentrations measured at 0 and 28 days. For *C. elegans*, the NOEC was 100 mg/kg after 3 days exposure to artificial sediments spiked with non-radiolabeled LAS based on effects on egg production.

Table 14. Results of Sediment Exposures[1]

Species	Endpoint	Test Duration (days)	NOEC (mg/kg)	Reference (Reliability)
Freshwater				
Chironomus riparius	Emergence	24	319	Pittinger et al. 1989, dossier 4.5.2v
Anodonta cygnea	Survival, Behavior	80	≥200*	Bressan et al. 1989, dossier 4.5.2p
Lumbriculus variegatus	Reproduction, Growth	28	81	Comber et al. 2004, dossier 4.5.2r
Caenorhabditis elegans	Fertility, Egg Production	3	100	Comber et al. 2004, dossier 4.5.2s
Marine				
Mytilus galloprovincialis	Survival, Physiological Response	7	≥7.85**	Marin et al. 1994, dossier 4.5.2u

[1] Reliability of Studies = (2)
* The measured concentration in the test chamber was 750 mg/kg at test initiation and 200 mg/kg at test completion (highest concentration tested).
** The measured concentration in the test chamber was 132 mg/kg at test initiation and 7.85 mg/kg at test completion (highest concentration tested).

Model Ecosystem Test Results

A variety of model ecosystem and mesocosm studies have been conducted on LAS. Many of these studies have been evaluated and summarized in two recent review papers (van de Plassche et al. 1999; Belanger et al. 2002). NOEC values for standing (lentic) and flowing (lotic) water model ecosystems range from about 0.12 to 9.8 mg/L (Table 15). The lowest NOEC value (0.12 mg/L) was observed in an artificial stream study (Tattersfield et al., 1995, 1996) in which river water was seeded from field collections and a hydrocyclone used to prevent colonization of biota throughout the study. Drift therefore comprised only emigration and not immigration. This is an ecologically restrictive study design that ignores the importance of recovery vectors present in natural systems. In addition, the reliability could not be adequately assessed so this study is not included in Table 15. An integrated model stream ecosystem (Experimental Stream Facility, ESF) without these design limitations was used to test a C_{12}LAS homologue with a high content (35.7%) of its most hydrophobic and toxic 2-phenyl isomer (Belanger et al. 2002). The 56-day ESF study included a representative community encompassing over 250 taxa and resulted in an NOEC value of 0.27 mg/L. The Belanger et al. (2002) review of the mesocosm studies, including the Tattersfield et al. study, concluded that a NOEC of 0.27 mg/L for C_{12} LAS (0.37 mg/L if normalized to $C_{11.6}$ LAS) was the most reliable, defensible, and robust value for the aquatic ecosystem. This value is based on model stream ecosystem studies of over 250 species, and is consistent with the single-species chronic freshwater data (Table 12A), and the resultant HC_5 values (0.24-0.36 mg/L for $C_{11.6}$ LAS).

Table 15. Results of Model Ecosystem Studies[1]

Type of Ecosystem	Avg. Alkyl Chain Length	Exposure Duration	Most Sensitive Endpoint (Species)	NOEC (mg/L)	Reference (Reliability)
Experimental Stream	C_{12}	56 days	Increased drift, reduced benthic abundance (Invertebrates)	0.27	Belanger et al. 2002, dossier 4.7a (1)
Experimental Stream	$C_{11.9}$	45 days	No effects observed (Periphyton, detritus, invertebrates, snails, amphipods and fish)	>0.36	Fairchild et al. 1993, dossier 4.7f (2)
Outdoor Ponds	C_{12}	56 days	Reduced egg production (Cyclopedia)	3.5	Huber 1989; Huber et al. 1987, dossier 4.7 g (2)
Aquaria with sediment and activated sludge effluent	$C_{11.9}$	28 days	Microbial function	0.5	Larson and Maki 1982, dossier 4.7h (2)
Aquaria with sediment and activated sludge effluent	$C_{11.9}$	28 days	Growth (Bluegill sunfish)	1.0	Maki 1981, dossier 4.7i (2)
In Situ River	$C_{11.9}$	21 days	Photosynthesis inhibition (phytoplankton)	9.8	Lewis et al. 1993, dossier 4.7j (2)
Bottles filled with lake water	$C_{11.8}$ $C_{13.3}$	3 hours/ month for 6 months	Photosynthesis inhibition (phytoplankton)	3.4* 1.9*	Lewis and Hamm 1986, dossier 4.7k (2)

[1]Reliability of Studies = (2) or (1)

* EC_{50} values

4.2 Terrestrial Effects

A large amount of ecotoxicity data are available for terrestrial organisms (e.g., Carlsen et al. 2002). Many of the studies, both laboratory and field, have been conducted recently in Denmark on soil organisms including plants, soil invertebrates, and microorganisms (Jensen and Krogh 1999; Jensen et al. 2001; Holmstrup and Krogh 2001; Elsgaard et al. 2001a,b; Brandt et al., 2003).

Terrestrial Toxicity – Soil Invertebrates

The data from studies evaluating the effects of LAS on soil dwelling organisms have recently been summarized in Jensen et al. (2001). However, the reliability of the individual studies could not be directly assessed so they are not included in Table 16. Additional information is available from other investigations of LAS toxicity on terrestrial invertebrates with test durations ranging from 14 days to 6 weeks (Holmstrup and Krogh 2001; Mieure et al. 1990). These additional data are summarized in Table 16. All studies used natural agricultural soil, with the exception of Mieure et al. (1990), who used artificial soil. In all studies, $C11.5/C_{11.6}$ LAS was added as aqueous solutions and not associated with sludge, which would be the normal route of exposure for agricultural soil. The bioavailability of LAS is greatly affected by interaction with sludge (Elsgaard et al. 2001a, b) and the toxicity in Table 16 below may or may not reflect exposure to free LAS in soil interstitial water. It is not known whether the data appropriately account for bioavailability in sludge-amended soils. (See Dossier section 4.6.1 for more information.)

Table 16. Results of LAS Exposures on Soil Invertebrates (in mg/kg dry weight)[1]

Species (test duration)	Endpoint	NOEC	LOEC	L/EC_{10}	L/EC_{50}	Reference (Reliability)
Aporrectodea caliginosa (28 d)	Adult Survival Juvenile Survival Juvenile Growth	278 >397 278	793 >397 397	329 >397 105	535 >397 354	Holmstrup and Krogh 2001, dossier 4.6.1b (2)
Aporrectodea longa (28 d)	Adult Survival Juvenile Survival Juvenile Growth	278 397 79	793 793 278	329 296 84	535 517 349	Holmstrup and Krogh 2001, dossier 4.6.1b (2)
Enchytraeus albidus (6 wks)	Adult survival Reproduction	<750 750	750 1500	511 447	1400 1143	Gejlsbjerg et al., 2001; dossier 4.6.1f (2)
Enchytraeus albidus (21 d)	Adult Survival Reproduction	198 20	397 40	194 6	430 41	Holmstrup and Krogh 2001, dossier 4.6.1b (1)
Eisenia foetida (14 d)	Body Weight	250	500		>1000	Mieure et al. 1990, dossier 4.6.1c (2)
Folsomia candida (4 wks)	Adult survival Reproduction	1000 500	2500 1000	750 480	1338 1143	Gejlsbjerg et al., 2001; dossier 4.6.1f (2)
Folsomia fimetaria (21 d)	Adult Survival Reproduction	>793 278	>793 278	>793 85	>793 424	Holmstrup and Krogh 2001, dossier 4.6.1b (1)
Folsomia fimetaria (21 d)	Adult survival Juvenile survival Reproductive output Juvenile growth Molting frequency	>1000 500 500 <200 <300	>1000 700 1000 200 300	>1000 196 147 163 185	>1000 570 737 896 923	Holmstrup and Krogh, 1996, dossier 4.6.1e (2)
Hypoaspis aculeifer (21 d)	Adult Survival Reproduction	>793 278	>793 793	>793 82	>793 236	Holmstrup and Krogh 2001, dossier 4.6.1b (2)
Hypogastrura assimilis (21 d)	Reproduction	79	278	99	421	Holmstrup and Krogh 2001, dossier 4.6.1b (1)
Lumbricus terrestris (14 d)	Body Weight/ Burrowing	667	1333		>1333	Mieure et al. 1990, dossier 4.6.1d (2)

[1]Reliability of Studies = (2) or (1)

Terrestrial Toxicity – Plants

Several studies have been conducted in which terrestrial plants have been exposed to LAS-spiked soils. These studies are summarized in Table 17 and presented in Dossier section 4.6.2. Windeat (1987) evaluated the effect of C_{11} LAS on three crop species (sorghum, sunflower, mung bean). The laboratory standard procedure, based on OECD Guideline 208, was conducted in an artificial soil consisting of potting compost and sand for up to 21 days. Growth (shoot fresh weight) was the

most sensitive endpoint and resulted in NOEC value of 100 mg/kg dw for all three species. The EC_{50} values were 167, 289 and 316 mg/kg dw for the sorghum, sunflower and mung bean, respectively. Figge and Schoberl (1989) tested the effects of a defined mixture of LAS (composition not reported) to several crop species. Studies were conducted in a "plant metabolism box" consisting of natural soil cores taken from two different ecosystems. Radiolabeled LAS absorbed to digested sludge was incorporated into the soils, which were then planted with either grass, bush beans, radishes, or potatoes and maintained for either 76 or 106 days. The resulting NOEC values were 27.2 mg/kg dw for grass, beans and radishes, and 16.2 mg/kg dw for potatoes.

Table 17. Results of LAS Exposure on Terrestrial Plants (in mg/kg dry weight)[1]

Species	Endpoint	EC_{10}	EC_{50}	NOEC	Reference
Grass, Beans, Radishes	Biomass			27.2*	Figge and Schoberl 1989, dossier 4.6.2b
Potatoes	Biomass			16.2*	Figge and Schoberl 1989, dossier 4.6.2b
Sorghum bicolour (crop sorghum)	Growth		167	100	Windeat 1987
Helianthus annuus (sunflower)	Growth		289	100	Windeat 1987
Phaseolus aureus (mung bean)	Growth		316	100	Windeat 1987

[1]Reliability of Studies = (2)
* Highest concentration tested.

Additional terrestrial plant studies are included in the LAS dossier. The reliability of the NOEC and EC_{10} values for these additional studies could not be adequately assessed because the original studies were not available for review. Therefore, they are not included in Table 17.

The potential for LAS and other surfactants to influence defoliation in coastal trees was reviewed in a literature review (Hamwijk 2002). In laboratory studies in which young trees are exposed to artificial sea spray, it has been demonstrated that the presence of surfactants at a concentration that causes a dynamic surface tension < 30 mN/m lead to an increased foliar penetration of NaCl via the stomata. For example, Grieve and Pitman (1978) examined the influence of surfactants on foliar NaCl uptake in Norfolk Island Pines (*Araucaria heterophylla*). Plants were exposed to seawater with different concentrations of LAS. At 10 mg/L of LAS, which corresponds with a reduced surface tension of 32 mN/m, the Na^+ content in the foliage increased almost tenfold to a level of approximately 500 µmol/g dw and damage symptoms were recorded. It was found that a low surface tension increases the contact angle with the leave and makes it possible for an aqueous solution to enter the stomata. Richard et al. (1996) reported the results of a 2-minute exposure of pine trees (*Pinus halepensis*) to ^{14}C-LAS (58 mg/L). LAS was primarily absorbed in the epicuticular waxes of the pine needles with very little in other plant material. The amount of absorption, and changes in wax fine structure (SEM), was much greater for LAS in seawater (where surface tension = 29 mN/m) than in distilled water (surface tension = 45 mN/m). However, the concentrations of LAS in seawater (section 2.2.8) are much lower than those required to increase foliar penetration in these studies, suggesting that this mechanism may not be relevant to coastal tree defoliation.

Terrestrial Toxicity – Avian

One non-guideline study is available in which the effects of commercial LAS (not specified) on Leghorn chicken hens is evaluated (Lopez-Zavalla et al. 1975). Ten month old hens were given a 200 ppm dose in drinking water for 45 days, during which mortality and egg quality were measured. No effects were observed and, while non-traditional, the study does indicate that up to 200 mg/kg in the drinking water does not adversely affect hen survival or egg-laying. See Dossier section 4.6.3 for more information.

Terrestrial Toxicity – Field Studies

Jensen and Krogh (1999; dossier section 4.7d) did not observe any short-term or long-term (4 years) adverse effects on 9 different microbial functions/processes or the abundance or diversity of microanthropods and earthworms after sludge application resulting in LAS soil concentrations of 15 mg/kg dry weight. Brandt et al. (2003; dossier section 4.7c) found that $C_{11.6}$ LAS spiked into sludge at levels of 7.1 or 31.3 g/kg dry matter did not adversely effect the function of the microbial community in sludge-amended, well-drained (and thus primarily aerobic) agricultural soils. The study should be considered a worst-case due to the application of high LAS concentrations only occasionally encountered in sewage sludge (Cavalli and Valtorta 1999, Waters et al. 1989; dossier section 3.2p,o), the use of LAS-spiked sludge possible overestimating the actual bioavailability relative to aged surfactants in natural sludge, the application of relatively large (4 x 4 cm) two dimensional sludge bands possible retarding oxygen intrusion and consequently LAS degradation in the sludge relative to smaller spherical sludge clumps present under more realistic field conditions, and the use of a coarse, sandy soil with relatively low organic matter content.

4.3 Other Environmental Effects

Evaluation of Estrogenic Effects

LAS has been evaluated to determine whether it could be an endocrine disrupter using a recombinant yeast screen (Routledge and Sumpter 1996: Navas et al. 1999) and a vitellogenin assay using cultured trout hepatocytes (Navas et al. 1999). No signs of estrogenic effects were observed for LAS or its sulfophenyl carboxylate (SPC) biodegradation intermediates, as expected from the absence of any structural alert.

4.4 Initial Assessment for the Environment

Pure LAS is a solid at ambient temperatures with a melting point of 198.5°C. The boiling point for LAS could not be determined experimentally due to decomposition beginning at 444°C. LAS has a low vapor pressure (calculated as 3-5 x 10^{-13} Pa). LAS is water soluble, with a critical micelle concentration (CMC) value of 0.1 g/L and forms a clear solution in water at concentrations up to 250 g/L. Although it is impossible to accurately measure an octanol-water partition coefficient for surface-active agents like LAS, an octanol-water partition coefficient of log 3.32 has been calculated for $C_{11.6}$ LAS. K_d values for LAS in activated sludge and sediment increased with increasing alkyl chain length of LAS homologues with K_d values for C_{12} LAS of 3210 L/kg in activated sludge and 330 L/kg in river sediment. In activated sludge, sorption and desorption equilibria for LAS were achieved very rapidly, and comparison of the extent of sorption and biodegradation shows that the absorbed fraction as well as the soluble fraction of LAS is available for biodegradation. Based on Fugacity III modeling results using the most relevant input parameters, more than 99 percent of the residual (non-biodegraded) fraction of LAS distributes to the soil. LAS does not undergo significant degradation by abiotic mechanisms under

environmentally relevant conditions as photolyzable and hydrolyzable groups are absent from the chemical structure.

An extensive database of studies demonstrates rapid and complete (ultimate) biodegradation of LAS in many of the available aerobic biodegradation tests, including soil and the aqueous environment. In several tests, LAS has been shown to be readily biodegradable, and has passed the 10-day biodegradation window in mineralization tests for most ready tests. LAS is removed in biological wastewater treatment at percentages ranging from 77-82% for trickling filters up to 99%+ for activated sludge. The biodegradation kinetics of the longer alkyl chain lengths are generally faster, and their sorption coefficients larger. The primary degradation intermediates are sulfophenyl carboxylates (SPCs), which further degrade to CO_2, SO_4^{2-}, and water. LAS does not generally degrade under anaerobic conditions. The measured bioconcentration factors of pure homologues and isomers decrease with decreasing average alkyl chain lengths (from almost 1000 for 2-phenyl-C_{13} LAS to 2 for 6-phenyl-C_{10} LAS), all with rapid clearance. The calculated BCF for currently produced $C_{11.6}$ LAS is 87 and was 22 for filtered Mississippi River water (average alkyl chain length of surface water fingerprint = $C_{10.8}$).

Ecotoxicity data are extensively available for LAS, with several comprehensive reviews having been completed. The lowest reliable acute $LC_{50}/EC_{50}/ErC_{50}$ values based on a review of the aquatic toxicity data on commercially representative LAS ($C_{11.6}$-$C_{11.8}$) were 1.67, 1.62 and 29.0 mg/L for fish, *Daphnia magna*, and algae, respectively. Acute toxicity is greater for individual LAS homologues with longer alkyl chain lengths. LAS biodegradation intermediates are significantly less toxic than the parent LAS with L/EC_{50} values >1000 mg/L for fish and *D. magna*. Chronic freshwater toxicity studies following guideline exposures (28-30 days for fish, 21 days for invertebrates and 3-4 days for algae provided the following NOEC values: fish NOEC = 1 mg/L (two studies, two species); Daphnia, NOEC = 1.18-3.25 mg/L (six values, two studies, one with 5 diets); algae, NOEC = 0.4-18 mg/L (four studies, two species). In addition all of the available, reliable chronic single species aquatic toxicity data on LAS have been evaluated, including three freshwater species in which multiple studies were reported and nine freshwater species for which single studies were reported. Single NOEC values and geometric mean NOEC values (calculated for species with multiple species) were normalized to $C_{11.6}$ LAS. These NOEC values range from 0.25 to 6.1 mg/L for freshwater species, including fish, invertebrates, algae and higher plants. Geometric mean NOEC values for marine species ranged from 0.025 to 5.0 mg/L. Based on the model ecosystem studies, a NOEC of 0.27 mg/L (0.37 if normalized to $C_{11.6}$ LAS) was determined for the freshwater ecosystem. This value is based on model stream ecosystem studies of over 250 species, and is consistent with the single species chronic freshwater data.

NOEC values for sediment exposures were greater than or equal to 81 mg/kg dry matter based on studies in four species, including GLP studies in *L. variegates* (survival, reproduction and growth over 28 days) and *C. elegans* (egg production, 3 days). Field studies indicate no adverse effects of LAS in sludge-amended soil from LAS levels of 15 mg/kg dry matter in the soil (9 microbial functions/processes and abundance/diversity of microarthropods and earthworms, short-term and 4 years) or 31,300 mg/kg dry matter in sludge (function of microbial community, short-term and 1 year).

In laboratory studies in which young trees are exposed to artificial sea spray, LAS concentrations of 10 mg/L lead to increased foliar penetration of NaCl, a hypothesized mechanism of defoliation.

A health and environmental risk assessment is available (heraproject.com); the risk assessment has not been reviewed by the U.S. Environmental Protection Agency.

Results of extensive environmental monitoring evaluations in the United States indicate that measured surface water concentrations were generally below 50 µg/L for river water samples

collected under low dilution (worst case) conditions below treatment plant mixing zones. Values in the 2800 km reach of the Mississippi River from Minneapolis to New Orleans range from non-detect (<0.1 µg/L) to 28 µg/L (362 samples). LAS river water concentrations similar to those in the US were observed in monitoring studies conducted in Europe and Japan.

Measured LAS concentrations in river sediments were generally less than 1-2 mg/kg dry weight. Mississippi River sediments were <1 mg/kg dry matter with one exception. LAS levels in sediments of the receiving waters of the Tiber River (Italy) were 1.8 mg/kg dry matter. Higher LAS concentrations have been observed near untreated or poorly treated wastewater discharges, e.g. LAS in sediments of a small river (Rapid Creek, USA) below a trickling filter treatment plant averaged 190 mg/kg just below the outfall, 11.2 mg/kg less than 5 miles downstream and 5.3 mg/kg greater than 5 miles downstream.

5 RECOMMENDATIONS

Human Health: The chemicals in the LAS category are currently of low priority for further work because of their low hazard potential except for skin and eye irritation and acute inhalation. Based on data presented by the Sponsor Country, exposure to respirable particles is anticipated to be low. Other countries may desire to investigate any exposure scenarios that were not presented by the Sponsor Country.

Environment: The chemicals in the LAS category possess properties indicating a hazard for the environment (fish, invertebrates and algae). However, they are of low priority for further work due to ready and/or rapid biodegradation and limited potential for bioaccumulation.

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Annex 1 – Use and Exposure Information

Linear Alkylbenzene Sulfonate (LAS)

Member countries did not evaluate the exposure annex and therefore, can make no conclusions regarding these values.

Annex 1 – Use and Exposure Information

Linear Alkylbenzene Sulfonate (LAS)

Industry Coalition for the SIDS Assessment of LAS

August 11, 2003

Purpose

To provide high end to bounding estimates of the potential environmental and human exposure to LAS from its manufacture and its use in consumer, commercial and industrial products in the United States to complement an OECD SIDS Programme review of this category.

Coverage

The report covers exposure from manufacturing and consumer/commercial/industrial use for all LAS volumes produced and used in the United States.

Synthesis of Key Assessment Results

Background: LAS is a mixture of closely related isomers and homologues covering several CAS numbers, each containing an aromatic ring sulfonated at the para position and attached to a mostly linear (87-98%) alkyl chain. It is an anionic surfactant that has been widely used since its 1964 introduction as the primary cleaning agent in consumer/commercial/industrial laundry detergents and cleaning products. This chemistry replaced branched alkylbenzene sulfonate (BABS), eliminating excessive foaming of sewage treatment plants and receiving waters caused by the poor biodegradability of BABS.

Results Summary: Approximately 390,000 metric tons of LAS are consumed annually in North America (United States and Canada combined). Production in Europe is approximately 400,000 metric tons. Production in Japan is approximately 85,000 metric tons. About 78-97% of the LAS consumption worldwide is in liquid, dry and tablet forms of laundry and fine fabric detergents. Another 2-10% is used in dishwashing liquids, with the remainder used in other cleaners. The predominant disposal route for these products is via wastewater. LAS is water soluble (250 g/L) and has low vapor pressure (3E-13 Pa). The low volatility and production of LAS in tablet, powder/granular and liquid forms minimize the potential for inhalation. It is effectively removed in biological wastewater treatment (up to 99+%) and is rapidly and completely biodegraded (70-90+% in ≤28 days). It has low potential for bioaccumulation (BCF - 87 L/kg), with rapid clearance. These characteristics help to minimize the potential for human and environmental exposure. Engineering controls (e.g., exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) in place at facilities that manufacture liquid and dry materials sufficiently mitigate worker exposure to LAS. The aquatic NOEC is 270 µg/L based on the Belanger et al. (2002) review of mesocosm studies, which concluded that a NOEC of 0.27 mg/L (0.37 mg/L if normalized to $C_{11.6}$ LAS) was the most reliable, defensible and robust value for LAS in the aquatic ecosystem. Results of extensive environmental monitoring evaluations in the United States indicate that measured surface water concentrations were generally below 50 µg/L for river water samples collected under low dilution (worst case) conditions below treatment plant mixing zones and range from non-detect (< 0.1 µg/L) to 28 µg/L in the 2800 km reach of the Mississippi River. An appropriate NOAEL from animal studies for use as a comparison is 85 mg/kg (see reasons stated in the main text of the SIAR). Modeled estimates of environmental exposure leading to indirect human exposure from drinking water and fish consumption range from 3.5×10^{-5} to 9.3×10^{-7} mg/kg/day. Similarly, the results of the dermal exposure modeling for various activities range from 5.6×10^{-2} to 4.7×10^{-5} mg/kg/day. These human exposure evaluations include conservative

(protective) input assumptions (e.g. all modeled exposures are conservative by a factor of at least 100 due to use of a default assumption of 100% absorption vs. a measured value of 1%).

Format A: General Information

I. Identification Information

(1) Date of Submission 2003-11-06

(2) Identity of Organization

Industry Coalition for the SIDS Assessment of LAS
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Washington, DC 20045, USA
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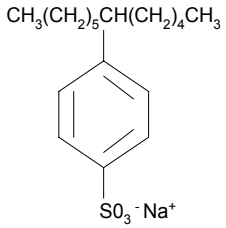
(3) Table of Contents

II. Substance information

(1) Category name
Linear Alkylbenzene Sulfonate (LAS)

(2) Substance Name(s) and CAS RN

1322-98-1	Decylbenzene sulfonic acid, sodium salt
25155-30-0	Dodecylbenzene sulfonic acid, sodium salt
26248-24-8	Tridecylbenzene sulfonic acid, sodium salt
27636-75-5	Tridecylbenzene sulfonic acid, sodium salt
68081-81-2	C_{10-16} Monoalkylbenzene sulfonic acid, sodium salt
68411-30-3	C_{10-13} Alkylbenzene sulfonic acid, sodium salt
69669-44-9	C_{10-14} Alkylbenzene sulfonic acid, sodium salt
85117-50-6	C_{10-14} Monoalkylbenzene sulfonic acid, sodium salt
90194-45-9	C_{10-13} Alkyl derivatives benzene sulfonic acid, sodium salt
127184-52-5	4-C_{10-13}-sec Alkyl derivatives benzene sulfonic acid, sodium salt



(3) Substance Formula and Structure
The LAS molecule contains an aromatic ring sulfonated at the *para* position and attached to a linear alkyl chain at any position except the terminal carbons (Valtorta et al., 2000). The alkyl carbon chain typically has 10 to 14 carbon atoms. The linearity of the alkyl chains ranges from 87-98%. While commercial LAS consists of more than 20 individual components, the ratio of the various homologues and isomers, representing different alkyl chain lengths and aromatic ring positions along the linear alkyl chain, is relatively constant across the various detergent and cleaning applications, with the average carbon number of the alkyl chain varying between 11.7-11.8. Because of the close consistency of the mixtures, their commercial uses, fate and effects, LAS is discussed as a category rather than as individual CAS numbers in this assessment. The structure of a C_{12}-LAS, representative of the category, is shown in the figure.

(4) Physical Form
All members of the category are solid at room temperature; melting point >198.5°C.

(5) Other Constituents
Some methyl-substituted (i.e., iso-branched) LAS may be present in the mixtures (Nielsen et al. 1997). The amount of the iso-LAS component is small (1-6%) and was shown not to limit biodegradation relative to pure linear component (Nielsen et al. 1997; Cavalli et al. 1999). Non-linear components such as dialkyltetralin sulfonates (DATS) can be present at levels of less than 1 to 8% depending on the manufacturing process (Nielsen et al 1997). The presence of these amounts of DATS does not significantly affect the biodegradation of LAS (Nielsen et al 1997). Improvements in processing techniques in the US, Europe and Japan incorporated to increase LAS yields also reduce the amount of DATS present in LAS.

III. Purpose and Coverage of this Report

(1) Purpose
To provide high end to bounding estimates of the potential environmental and human exposure to LAS from its manufacture and its use in consumer, commercial and industrial products in the United States to complement an OECD SIDS Programme review of this category.

(2) Coverage
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IV. Summary

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(2) Summary of Data Collection Efforts
Information in this assessment was assembled from a number of sources:

1) Surveys of member companies of the Industry Coalition for the SIDS Assessment of LAS, representing about 75% of LAS producers and users, collected data on LAS production volumes, uses, releases, and potential exposures. To protect proprietary information, independent counsel compiled the resulting data. Two recent economic reviews, published by Colin A Houston and SRI international, were used to confirm the compiled results for the U.S. Additional information was also derived from a report prepared by the "Human and Environmental Risk Assessment on ingredients of European household cleaning products" (HERA 2004).

2) Environmental monitoring data were collected via two comprehensive US studies. The first determined LAS surface water and sediment concentrations over 3 separate research vessel cruises on the 2800 kilometer reach of the Mississippi River between Minneapolis and New Orleans in three seasons of 1991-92. The second determined concentrations of LAS in wastewater plants and surface waters, at 50 locations in 11 states. These data are summarized in Format B attachments.

3) Potential LAS exposures estimated via modeling are summarized in Format C attachments. Potential exposures resulting from manufacturing facility effluent discharges are modeled using US EPA's E-FAST model. This modeling includes estimates of aquatic exposure based on modeled surface water concentrations. Potential human exposure is estimated based on modeled drinking water concentrations and fish consumption from sources downstream from effluent discharges. Similarly, potential aquatic exposures and human exposures from drinking water and fish consumption are modeled using E-FAST following consumer use of products containing LAS (i.e., down-the-drain releases). Finally, dermal exposures from consumer uses of products are examined using general exposure models for three exposure scenarios: 1) use of diluted and undiluted laundry and cleaning products (laundry pre-treatment, hand-wash of laundry, hand-wash of dishes, washing of hands with dishwashing liquid) and diluted and undiluted hard surface cleaning products; 2) exposure to laundry and fabric conditioning product residual on clothing (liquid, dry and tablet laundry detergents, dryer sheet fabric conditioner); and 3) exposure to face and hand soap residual after use.

(3) Discussion of Key Uncertainties, Limitations, Data Gaps

a) Manufacturers representing about 75% of the US volume were involved in the industry survey. Thus, it is possible that there may be minor uses and potential consumer exposures beyond those estimated here. However two recently published economic reviews and a published European assessment support the uses presented. In the assessment, the estimated volume encompassing all US producers was used and exposure estimates are presented for all known uses.

b) This exposure assessment takes a conservative (protective) approach to modeling, selecting inputs based on conservative values for each parameter; thus modeled estimates are likely to significantly exceed actual exposures. For predicted environmental exposures, this is supported by a comparison of monitoring results to modeling estimates. For consumer exposure, actual dermal absorption is less than 1% of product (Schaefer and Redelmeier 1996), whereas all modeled exposures include a default assumption of 100% absorption. Therefore, the modeled exposure is conservative by a factor of at least 100.

c) Several scenarios are not modeled—direct and indirect oral, inhalation, and sediment—but information is presented to establish that exposure from these scenarios are not significant compared to the scenarios that are discussed in detail.

(4) Exposure Results
The following table shows the estimated exposure for the scenarios assessed, and the NOEC or NOAEL values.

Exposure Scenario	Estimated Exposure (µg/L) or (mg/kg/day)	NOEC (µg/L)* or NOAEL (mg/kg/day)**
Surface Water Monitoring		
Mississippi River	2.21	270*
50 U.S. Rivers	43 to 46	270*
Manufacturing Effluent Modeling		
Aquatic **Mean stream conc.** 7Q10 Stream conc.	50th percentile facility 4.8 13	 270* 270*
Drinking Water Consumption 50th percentile facility	9.3E-7	85**
Fish Consumption 50th percentile facility	3.5E-5	85**
Consumer Use Modeling		
Aquatic Median flow 7Q10 flow	 9.9E-2 1.3	 270* 270*
Drinking Water Consumption 7Q10 flow	1.9E-6	85**
Fish Consumption 7Q10 flow	7.2E-7	85**
Consumer Use – Dermal Modeling		
Diluted and undiluted laundry and dishwashing products and hard surface cleaning products		
Laundry pre-treatment (diluted)	3.0E-3 to 6.0E-3	85**
Neat Laundry pre-treatment (undiluted)	5.0E-3 to 1.0E-2	85**
Hand-wash of laundry (diluted)	4.7E-5 to 1.2E-3	85**
Hand-wash of dishes (diluted)	5.0E-4 to 2.3E-3	85**
Hand-wash (dishwashing liquids) of hands (diluted)	1.0E-4 to 7.4E-4	85**
Hard surface cleaners (diluted)	1.0E-3 to 5.0E-4	85**
Hard surface cleaners (undiluted)	5.0E-3 to 1.0E-3	85**
Laundry product residual on clothing		
Liquid detergents	2.0E-3 to 5.0E-2	85**
Dry detergents	1.0E-2 to 5.0E-2	85**
Tablet laundry detergent	1.1E-2 to 5.6E-2	85**
Fabric conditioning (dryer sheets)	5.0E-5 to 3.0E-4	85**
Face and Hand Soap product residual after washing		
Bar soap - hand	3.6E-3 to 1.8E-2	85**
Bar soap - face	5.0E-4 to 2.3E-3	85**

The dermal exposures are also summarized below aggregated by product category use. The aggregation was accomplished by adding the modeled exposures within a product category, e.g., three scenarios for liquid detergent exposures were modeled – hand-washing, neat pre-treatment, and residual on clothing. These human exposure evaluations include conservative (protective) input assumptions (e.g. all modeled exposures are conservative by a factor of at least 100 due to use of a default assumption of 100% absorption vs. a measured value of 1%).

Product Type	Estimated Exposure (mg/kg/day)	NOAEL (mg/kg/day)
Laundry Detergent – Liquid	7.0E-3 to 6.1E-2	85
Laundry Detergent – Dry	1.4E-2 to 6.3E-2	85
Dish Detergent	6.0E-4 to 3.0E-3	85
Hard Surface Cleaners	1.0E-3 to 5.0E-4	85
Fabric Conditioning (dryer sheet)	5.0E-5 to 3.0E-4	85
Bar Soap	4.1E-3 to 2.0E-2	85

V. Production, Import and Use

(1) Estimated Volume (tonnes/year) US/Canada – 390,000 tonnes/yr (2000 data, Colin A. Houston 2002) Europe – 400,000 tonnes/yr (2001 data, HERA 2004) Japan – 85,000 tonnes/yr (2000 data, LAS SIDS Coalition Survey 2002)
(2) Function/ Product Use Categories and Percent Volume to Each LAS is a surfactant, used as the primary cleaning agent in a variety of consumer/commercial/industrial laundry and cleaning products. About 78-97% of LAS consumption worldwide is in liquid, dry and tablet laundry and fine fabric detergents. Another 2-10% is used in dishwashing liquids, with the remainder used in other cleaners.

VI. Activities, Releases and Exposures, and Factors that Mitigate or Exacerbate Exposures by Activity

Manufacture
(1) Process Description LAS is produced from the sulfonation of linear alkylbenzene (LAB) to make an intermediate, LAB sulfonic acid. The acid is produced primarily by oleum or air/SO_3 sulfonation, in batch or continuous processing equipment in enclosed sulfonation facilities. The entire production of LAB sulfonic acid is used in the production of LAS. LAS is formed when the LAB sulfonic acid is neutralized to the sodium salt with sodium hydroxide or other base. LAS is produced in a closed system process as both dry product and as an aqueous solution. There are 22 LAS manufacturing facilities in the US. (Colin Houston, 2000). The following manufacturing and mitigation measures apply to all of the manufacturing facilities operated by members of the Coalition in Canada, Europe, Japan and the United States (LAS SIDS Coalition Survey, 2002).
(2) General Description of Potential Releases and Exposures Potential releases to the environment are minimal due to manufacturing processes that have been designed to maximize production yield and minimize potential releases. Extensive engineering controls are in place to minimize releases to the environment. These controls include SO_2/SO_3 monitoring devices, spill containment dikes for rail unloading, leak inspections, high level tank alarms, and auto shut off valves. Emissions controls include line cyclones, electrostatic precipitation and passing through caustic scrubbers and scrubbing demisters. Any LAS that is not incorporated into a product is captured by dust-handling equipment for recycling back into the production process. A limited amount of LAS in aqueous solution may be released as a dilute solution from washing and rinsing operations in the manufacturing process. Any minimal LAS released from manufacturing plants that produce or formulate LAS is discharged to wastewater treatment. Incidental quantities of the dry product (e.g., from floor sweepings) may be disposed in landfills. Potential workplace exposures include inhalation of dust, dermal contact with powders, granules and liquids; there is the potential for incidental or accidental ingestion, and/or eye contact with the product during handling in the manufacturing process.
(3) Discussion of Factors that Mitigate or Exacerbate Releases and Exposures LAS is water soluble (250 g/L) and has low vapor pressure (3E-13 Pa). The low volatility and production of LAS in tablet, powder/granular (e.g., use of Good Manufacturing Practices, personal protective equipment) and liquid (e.g., droplet size controls) forms minimize the potential for inhalation. It is effectively removed in biological wastewater treatment (up to 99+%) and is rapidly and completely biodegraded (70-90+% in ≤28 days). It has low potential for bioaccumulation (BCF - 87 L/kg), with rapid clearance. These characteristics help to minimize the potential for human and environmental exposure. LAS environmental releases are not regulated independently, but as part of overall facility emissions. Mitigation includes use of good manufacturing practices, best available technology and engineering controls. Engineering controls (e.g., exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) in place at facilities that manufacture liquid and dry materials sufficiently mitigate worker exposure to LAS. All processing of LAB, LAB sulfonic acids and LAS takes place in closed systems that significantly minimize worker exposure. Workers also wear standard personal protective equipment including safety goggles, face shields, safety shoes, impervious nitrile gloves, long sleeved clothing, and rubber boots. Workers may also employ cartridge-type respirators equipped with organic vapor cartridges and acid-resistant suits, for example, during steaming and washing. The closed production process and use of personal protective equipment effectively eliminates exposure to production workers. No special engineering controls and no additional personal protective equipment are uniquely specified for LAS.
(4) Remarks Product formulation, the blending of LAS with other ingredients, is not expected to result in workplace exposures that exceed those for LAS manufacturing facilities. In some cases, LAS is blended into finished products in the same facilities where it is produced, in other cases the facilities are separate. In all cases, engineering controls and personal protective equipment are similar.

Industrial Use
(5) Function/Product Use Description A minor amount of LAS production (0.003%) has industrial uses. The vast majority of the production used for industrial purposes are as plasticizers in masonry admixtures (~60%) and air entraining agents in concrete admixtures (~40%). Polymer stabilizers in food packing films and dispersing agents in sealant materials for can ends, pail lids, and drums make up no more than about 3% of total Industrial uses.
(6) General description of Potential Releases and Exposures There is a low potential for incidental dermal, ingestion, inhalation or eye contact with the product during handling and use. There is also a low potential for environmental release from industrial uses of LAS.
(7) Discussion of Factors that Mitigate or Exacerbate Releases and Exposures Exposure to LAS in industrial products is mitigated by following use and precaution instructions on product labels.
(8) Remarks Industrial uses make up an insignificant portion of the total LAS production. LAS is manufactured for use in consumer and commercial/institutional laundry and cleaning product formulations and is not used as an intermediate/derivative for further chemical manufacturing processes.

Commercial Use
(9) Function/Product Use Description LAS is a surfactant used in commercial laundry and cleaning products that are either used as supplied or diluted prior to use. Uses include institutional and industrial products; for example: Product Type — Concentration in Products in US/Canada (range) Laundry detergents (dry) 5-25 % Dishwashing detergents (liquids) 5-10 % General cleaners 1-5 % Disinfectant cleaners (liquids) 5-10 % Product Type — Concentration in Products in Europe (range) Laundry detergents (dry) 5-10 % Laundry detergents (liquids) 10-25 % Pre-washes 10-25 % Dishwashing detergents (liquids) 25-50 % Product Type — Concentration in Products in Japan (range) Laundry detergents (dry) 5-10 % Dishwashing detergents (liquids) 5-50 % Hard surface cleaners 1-10%

(10) General description of Potential Releases and Exposures
Laundry and cleaning products may be used as is, or diluted prior to or during use.

Dermal contact may occur with commercial products. There is a low potential for incidental or accidental ingestion of, inhalation of, and/or eye contact with the product during handling and use.

Environmental releases from down-the-drain discharges following product use could lead to potential ecological exposures in surface waters and indirect human exposures via drinking water and fish consumption. These potential exposures are quantified in the following pages based on monitoring data (Format B) and modeling data (Format C).

(11) Discussion of Factors that Mitigate or Exacerbate Releases and Exposures
Exposure to LAS in formulated commercial laundry or cleaning products is mitigated by following use and precaution instructions on product labels. Product labels reflect the hazard potential of the chemical ingredients in the product. These product labels also include first aid instructions to accompany each hazard warning. For example, commercial products may include eye and skin irritancy warnings along with instructions to rinse thoroughly if dermal or other exposure occurs.

LAS is water soluble (250 g/L) and has low vapor pressure (3E-13 Pa). Commercial products containing LAS are disposed of down-the-drain and transported to wastewater treatment plants where LAS is effectively removed (up to 99+%). Residual LAS entering the environment is rapidly and completely biodegraded (70-90+% in ≤28 days in standard tests). It has a low potential for bioaccumulation (BCF – 87 L/kg) and studies indicate that it is rapidly metabolized and eliminated from the bodies of aquatic organisms. These characteristics help to minimize the potential for environmental and human exposure.

(12) Remarks: Estimates of inhalation exposure apply to both consumer and commercial products as both use the same type of spray nozzles (for spray cleaners) and the same type of equipment to make powder/granulated products. The human experience with eye irritation covers both manufacturing and use of consumer and commercial products.

Consumer Use

(13) Function/ Product Use Description
LAS has wide-spread and dispersive use as a surfactant in the following consumer products.

Product Type	Concentration in Products in US/Canada (range)
Laundry detergents (dry)	5-25 %
Laundry detergents (liquids)	1-25 %
Laundry detergents (tablets)	5-25 %
Fabric conditioners (sheets)	0.1-0.5 %
Dishwashing detergents (liquids)	5-25 %
General cleaners (dilutable)	1-5 %
Hard surface cleaners	1-5 %
Face and hand soaps (bars)	1-5 %

Product Type	Concentration in Products in Europe (range)
Laundry detergents (dry)	5-25 %
Laundry detergents (liquids)	5-10 %
Laundry detergents (tablets)	10-25 %
Dishwashing detergents (liquids)	10-25 %
General cleaners (dilutable)	1-5 %
Hard surface cleaners	0.1-0.5 %

Product Type	Concentration in Products in Japan (range)
Laundry detergents (dry)	5-25 %
Laundry detergents (liquids)	5-25 %
Laundry detergents (tablets)	5-25 %
Fine fabric detergents (liquid)	1-5 %
Bleaches	0.1-0.5 %
Pre-washes	5-10 %
Dishwashing detergents (liquids)	1-5 %
Hard surface cleaners	0.5-10 %
Other cleaners	0.1-0.5 %

The level (%) in products shown above is in the formulated product and does not take into account any dilution prior to or during use.

(14) General Description of Direct Exposures to Consumer Products and of Potential Releases to the Environment Leading to Environmental Exposures and Indirect Human Exposures
Laundry and cleaning products may be used as is, or diluted prior to or during use.

Dermal contact may occur with laundry and/or cleaning products. There is some potential for incidental or accidental ingestion of, inhalation of, and/or eye contact with products during handling and use.

Environmental releases from down-the-drain discharges following product use may lead to potential environmental exposures in surface waters and indirect human exposures via drinking water and fish consumption.

These potential exposures are discussed in the following pages and quantified in monitoring data (Format B) and modeling data (Format C).

(15) Discussion of Factors that Mitigate or Exacerbate Releases and Exposures

Exposure to LAS in formulated consumer laundry and cleaning products is mitigated by following use and precaution instructions on product labels. Product labels reflect the hazard potential of the chemical ingredients in the product. These product labels also include first aid instructions to accompany each hazard warning. For example, commercial products may include eye and skin irritancy warnings along with instructions to rinse thoroughly if dermal or other exposure occurs.

Human exposure will be mitigated by the fact that residues from cleaning products are usually washed or rinsed off. Actual dermal absorption is only about 1% of product (Schaefer and Redelmeier 1996), whereas all modeled exposures include a default assumption of 100% absorption. Therefore, the modeled exposure is conservative by a factor of at least 100.

LAS is water soluble (250 g/L) and has low vapor pressure (3E-13 Pa). Consumer products containing LAS are disposed of down-the-drain and transported to wastewater treatment plants where LAS is effectively removed (up to 99+%). Residual LAS entering the environment is rapidly and completely biodegraded (70-90+% in ≤28 days in standard tests). It has a low potential for bioaccumulation (BCF – 87 L/kg) and studies indicate that it is rapidly metabolized and eliminated from the bodies of aquatic organisms. These characteristics help to minimize the potential for environmental and human exposure.

(16) Remarks:

Direct oral exposures are not modeled in this evaluation since these would only occur via accidental ingestion, and result in temporary, acute symptoms. None of the uses of LAS are in products intended for human consumption. Potential oral indirect exposure via drinking water and fish ingestion are included in Modeling Evaluations 1 and 2.

Estimates of inhalation exposure apply to both consumer and commercial products as both use the same type of spray nozzles (for spray cleaners) and the same type of equipment to make the powder/granulated products. Trigger spray systems used for spray cleaners are designed to deposit the vast majority of the product on the surface to be cleaned and the respirable fraction of the amount sprayed is very small. A study conducted for the Soap and Detergent Association (Battelle 1999) measured the under 10 micron (respirable particle size) fraction delivered from 6 consumer product spray nozzles. The overall mean (n=30) is 0.11% particles under 10 microns and the standard deviation is 0.21. The very highest observation was 0.80%. This testing only captured the spray particles that are under 600 microns (maximum resolution of the test equipment), so the actual respirable particle percent of total volume sprayed is less than 0.1%. The Battelle (1999) study also reported that for consumer spray products in normal use conditions, the peak breathing zone concentration under 10 microns ranged from 0.13-0.72 mg/m^3. HERA (2004) reported an air concentration of 0.35 mg/m^3 in experimental measurements of aerosol particles under 6.4 microns that are generated upon spraying with typical surface cleaning spray products. Using this data and assuming a worst case scenario, HERA modeled potential consumer exposures via inhalation of aerosols from cleaning sprays, predicting an exposure of 4.0E-5 mg/kg/day from this pathway, which is several orders of magnitude below the 5.0E-3 to 1.0E-3 predicted for total dermal exposure to spray cleaners. This information, considered together with low volatility of LAS and infrequent use of spray products in comparison to products involving dermal contact, indicates that inhalation exposures do not contribute significantly to total exposure.

Indirect oral exposure from deposition of LAS on dishes washed with products containing LAS is not modeled. Due to the use of dilute solutions and the rinsing of dishes following wash, any exposure from this source would be very low compared to the direct dermal exposures that are modeled.

Also not modeled is sediment exposure. Monitoring of sediments in a 2800 km reach of the Mississippi river indicates sediment concentrations of 0.01 to 0.95 mg/kg (mean = 0.23 ± 0.19 mg/kg) while NOEC values for sediment exposure are ≥81 mg/kg.

Format B: Monitoring Evaluation #1

I. Identification Information

(1) Activity associated with Monitoring Information Sampling of surface waters and sediments of the Mississippi River between Minneapolis and New Orleans during 1991-1992.
(2) Citation Tabor, C.F. and Barber, L.B., II. 1996. Fate of linear alkylbenzene sulfonate in the Mississippi River. Environ. Sci. Technol. 30:161-171.

II. Monitoring Study Design

(1) Monitoring Study Objective Determination of the LAS concentrations in surface waters and sediments to provide data on the water quality of the river.
(2) Description of Scenario Monitored Samples were collected on a 2800 kilometer reach of the Mississippi river between Minneapolis and New Orleans during three research vessel cruises conducted in the summer (June 23-August 7) and fall (September 24-November 13) of 1991 and the spring (March 25-May 10) of 1992.

III. Sampling and Analytical Methods

(1) Sampling Surface water cross-channel composite grab samples were collected on the upstream leg of each cruise (beginning at New Orleans). Discharge-averaged composite water samples were collected on the downstream leg of each cruise (beginning at Minneapolis). Composite bottom sediment samples were collected in shallow areas off the main navigation channel during the downstream leg of each cruise.
(2) Method/ Procedure This monitoring study included extensive sampling of surface waters and sediments for the 2800 kilometer length of the Mississippi River. Dissolved LAS was isolated by passing water samples through a silica cartridge and eluted with acetonitrile followed by methylene chloride. LAS was extracted from sediments by centrifugation followed by methanol extractions. Extracts from both water and sediment were derivatized to form the trifluoroethyl ester of LAS. The derivatized extracts were then analyzed by GC/MS. Samples were collected with substantial attention to data quality and included quality control samples. The analytical method was chemical specific for LAS, with a detection limit of 0.1 µg/L for dissolved LAS. No contamination of field blanks or sample degradation during storage was observed.

IV. Description and Results

(1) Media Sampled Surface water and bottom sediments

(2) Results
LAS was identified in 21% of the surface water samples and 100% of the bottom sediment samples.

Where detected, surface water concentrations ranged from 0.1 to 28.2 µg/L (mean = 2.21 ± 3.77 µg/L), with the highest concentrations occurring near cities such as Minneapolis and St. Louis and concentrations decreasing with increasing distance downstream. The average alkyl chain length for the dissolved LAS was $C_{11.1}$ (range $C_{10.2\text{-}12.0}$).

Bottom sediment concentrations ranged from 0.01 to 0.95 mg/kg (mean = 0.23 ± 0.19 mg/kg) [one outlier of 20 mg/kg from an effluent transport canal was excluded], with the highest concentrations occurring downstream from Minneapolis, a large city located on a relatively small river. The average alkyl chain length of the sediment associated LAS was $C_{11.5}$ (range $C_{10.7\text{-}11.9}$).

The data indicate that biodegradation and sorption are the main removal processes affecting dissolved LAS.

(3) Remarks
The aquatic NOEC is 270 µg/L, a conservative value based on C_{12} LAS which is the top end of the range found in the environment. The mean surface water concentration measured in the Mississippi River in this study is 2.21 µg/L.
NOEC values for sediment exposure are ≥81 mg/kg while sediment concentrations ranged from 0.01 to 0.95 mg/kg (mean = 0.23 ± 0.19 mg/kg).

V. Reliability

(1) Reliability Score 2 (Reliable with restrictions) because OECD standard test methods do not exist for monitoring studies. However, this is a high quality study carried out with strict attention to accepted analytical and sample collection procedures.

Format B: Monitoring Evaluation #2

I. Identification Information

(1) Activity associated with Monitoring Information Sampling of wastewater treatment plant influents, effluents, and surface river waters from 50 locations in 11 U.S. States.
(2) Citation McAvoy, D.C., Eckhoff, W.S., and Rapaport, R.A. 1993. Fate of linear alkylbenzene sulfonate in the environment. Environ. Toxicol. Chem. 12:977-987.

II. Monitoring Study Design

(1) Monitoring Study Objective Determination of real-world concentrations of LAS in wastewater treatment plants and surface waters.
(2) Description of Scenario Monitored Samples were collected from a national distribution of drainage basins across the U.S. and from a variety of treatment plant types. Sites were selected based on low effluent dilution and samples were collected during the periods of lowest flow. Influent and effluent samples were collected from each wastewater treatment plant. Receiving water samples were collected above and below the outfalls from each treatment plant. The monitoring results were also used to verify mathematical modeling predictions.

III. Sampling and Analytical Methods

(1) Sampling Twenty-four hour composite samples of influent and effluent were collected from each treatment plant over a 3-5 day period, then further composited to represent the average concentration of LAS over the period. Receiving water samples were collected midchannel above the wastewater treatment plant outfalls and below the effluent mixing zones as a three-sample transect.
(2) Method/ Procedure This monitoring study included sampling of wastewater treatment plant influents and effluents, as well as surface waters above and below the mixing zone in 50 river locations across the U.S. Dissolved LAS was isolated from solution by solid-phase separation using a SAX column and concentrations determined by HPLC/fluorescence analysis. The analytical method was chemical specific for LAS, with a detection limit of 2 μg/L for total LAS.

IV. Description and Results

(1) Media Sampled Wastewater treatment influent and effluent, and river surface water samples above and below the mixing zone.
(2) Results Average LAS influent concentrations ranged from 4.2-5.7 mg/L. Based on effluent concentrations, removal rates averaged 99.3% for activated sludge plants. LAS concentrations in samples collected under low flow conditions below the mixing zone were generally below 50 μg/L. The average alkyl chain length ranged from $C_{11.8-11.9}$

(3) Remarks
The aquatic NOEC is 270 µg/L. The mean surface water concentrations measured in 50 river locations across the U.S. ranged from <10 to 330 µg/L with mean values of 42 to 46 µg/L. The highest concentration was observed in a low (less than 3-fold) dilution effluent canal below a trickling filter plant. All other values were <180 µg/L with more than 80% of the sites below 50 µg/L. Since several of the wastewater treatment plants included in this study have dilution factors less than 3, these values represent worst case estimates.

Results from this study were used to validate the water-quality model PG-GRiDS under low flow conditions. Measured concentrations of LAS agreed well with model predictions.

V. Reliability

(1) Reliability Score 2 (Reliable with restrictions) because OECD standard test methods do not exist for monitoring studies. However, this is a high quality study carried out with strict attention to accepted analytical and sample collection procedures.

Format C: Modeling Evaluation #1

I. Identification Information

(1) Activity associated with Modeling Information Manufacturing Facility Effluent Discharge - Environmental Exposure Including Indirect Human Exposure

II. Modeling Objective

(1) Modeling Study Objective High end to bounding estimate of surface water concentration (including drinking water and fish consumption exposure) as a result of manufacturing facility effluent discharge.
(2) Description of Modeled Scenario Daily release estimated from a hypothetical manufacturing facility anywhere in the US producing 20% of annual US volume. Accounts for wastewater treatment, in-stream dilution and bioaccumulation potential. Assumes 365 days of operation per year.

III. Description of Model and Model Validation

(1) Tool or Model E-FAST – Provides screening level estimates of the concentrations of chemicals released to the environment from industrial discharge. Designed to provide high end to bounding estimates of exposure. Chemical-specific and facility-specific data or defaults can be used. Modeling conducted February 2003.
(2) Validation/ Peer Review Standard model (beta release) used by USEPA Office of Pollution Prevention and Toxics in screening level assessments
(3) Availability and Documentation www.epa.gov/oppt/exposure/docs/efast.htm

IV. Inputs, Outputs, and Quality Description

(1) Media Modeled Surface water, drinking water and edible fish tissue
(2) Inputs Pre-treatment facility release (process loss) – 290 kg/day; estimated as follows: -350,000 tonnes/yr – annual production in US - 958 tonnes/day– daily production assuming 365 days/yr - 1.4 tonnes/day – daily process loss assuming 0.15% loss USEPA default value - 0.29 tonnes/day (290 kg/day) plant release assuming hypothetical facility produces one-fifth the total annual production, (there are 22 production sites in the US, Colin A. Houston 2002), a conservative assumption is that the maximum daily process loss for a single facility is 0.29 tonnes/day (290 kg/day) SIC Code is Soaps, Detergents, etc. Manufacture (2841-2844) Release days – 365 Wastewater treatment removal – 99%—reasonable based on monitoring data and likelihood that microbes downstream of LAS production facilities will be well acclimated BCF – 87 L/kg—maximum value based on Tolls et al. 1997 (22-87 L/kg for C10.6-C11.6 LAS) and recently published mean values of 23-80 L/kg for four species for C12 LAS by Versteeg and Rawlings 2003. NOEC = 270 µg/L Thus, conservative estimates are used in the determination of several of the input parameters and the

estimation does not account for biodegradation during transport to the wastewater treatment plant (HERA 2004).

(3) Model Outputs
Results following wastewater treatment; where 50th percentile represents a facility on a mid-size stream with average flow.

Aquatic exposure -
50th percentile facility -
Mean stream concentration = 4.8 µg/L
7Q10 stream concentration = 13 µg/L
[7Q10 is the lowest 7-day average flow in a year that occurs on an average once every 10 years]

Drinking water exposure -
50th percentile facility -
Average Daily Dose (ADD) =
9.3E-07 mg/kg/day (chronic non-cancer)

Fish consumption exposure –
50th percentile facility -
Average Daily Dose (ADD) =
3.5 E-05 mg/kg/day (chronic non-cancer)

(4) Reliability Score 2 (Reliable with restrictions) The model has not been validated but is sufficiently conservative and accepted by authorities. Appropriate inputs have been selected reflecting best available information and conservative estimates where applicable.

Modeling can be useful in first tier approach for exposure assessment. Model outputs reflect E-FAST model assumptions that are designed to provide high end to bounding estimates of exposure.

(5) Remarks
The aquatic NOEC = 270 µg/L. The estimated mean and low flow (7Q10) stream concentrations are 4.8 µg/L and 13 µg/L, respectively, for the 50th percentile scenario.

An appropriate NOAEL from animal studies for comparison is 85 mg/kg (see reasons stated in the SIAR). Estimated exposures in consumer products for the 50th percentile facility scenario are 9.3E-07 mg/kg/day (drinking water) and 3.5E-05 mg/kg/day (fish consumption).

Product formulation facilities are not expected to have environmental releases that exceed those for LAS manufacturing facilities.

Format C: Modeling Evaluation #2

I. Identification Information

(1) Activity associated with Modeling Information Consumer Use (i.e., down-the-drain release) - Environmental Exposure Including Indirect Human Exposure

II. Modeling Objective

(1) Modeling Study Objective High end to bounding estimate of surface water concentration (including drinking water and fish consumption exposures) as a result of daily consumer usage of laundry and cleaning products.
(2) Description of Modeled Scenario Down-the-drain release of total USA annual production volume into total volume of USA municipal wastewater system. Accounts for wastewater treatment and in-stream dilution. Accounts for bioaccumulation potential.

III. Description of Model and Model Validation

(1) Tool or Model E-FAST
(2) Validation/ Peer Review Standard model (beta release) used by USEPA Office of Pollution Prevention and Toxics in screening level assessments
(3) Availability and Documentation www.epa.gov/oppt/exposure/docs/efast.htm

IV. Inputs, Outputs, and Quality Description

(1) Media Modeled Surface water, drinking water and edible fish tissue
(2) Inputs Release – 350,000 tonnes (total US annual production) Wastewater treatment removal – 99% BCF estimate – 87 L/kg NOEC – 270 µg/L
(3) Model Outputs Results following wastewater treatment; **Aquatic exposure -** Mean stream flow concentration = 0.099 µg/L 7Q10 stream flow concentration = 1.3 µg/L [7Q10 is the lowest 7-day average flow in a year that occurs on average once every 10 years] Indirect human exposure estimates under low stream flow (7Q10) conditions are: **Drinking water exposure -** Average Daily Dose (ADD) = 1.9E-06 mg/kg/day (chronic non-cancer) **Fish consumption exposure** – Average Daily Dose (ADD) = 7.2E-07 mg/kg/day (chronic non-cancer)

(4) Reliability Score 2 (Reliable with restrictions) The model has not been validated but is sufficiently conservative and accepted by authorities. Appropriate inputs have been used reflecting best available information and conservative estimates where applicable.
(5) Remarks The aquatic NOEC = 270 µg/L. The estimated median and 7Q10 (low flow) exposures are 0.099 and 1.3 µg/L, respectively. The NOAEL chosen for LAS for this assessment is 85 mg/kg/day. Estimated exposures in consumer products under 50th percentile conditions are 1.9E-06 mg/kg/day and 7.2E-07 mg/kg/day for drinking water and fish consumption, respectively.

Format C: Modeling Evaluation #3

I. Identification Information

(1) Activity associated with Modeling Information
Dermal Exposures from Use of Consumer Products

II. Modeling Objective

(1) Modeling Study Objective

To provide estimates of human dermal exposure (in daily dose, i.e., mg/kg/day) to the general population from use of consumer products containing LAS.

(2) Description of Modeled Scenario

Dermal exposures to LAS that are modeled include:

Exposure during the activity/use of products --

Laundry detergent: hand washing laundry
Laundry detergent: pretreatment
Dishwashing liquid detergents: hand washing dishes
Dishwashing liquid: hand washing hands
Hard surface cleaners (diluted and undiluted)

Exposure from residuals on clothing –

Laundry detergents on clothing following washing
Fabric conditioner on clothing

Exposure from residuals after using products

Face and hand soap (bars)

III. Description of Model and Status of Peer Review and Validation

(1) Tool or Model

The modeling presented here uses simple, first principle equations, which err on the side of being protective.

General Exposure Model

Potential Chemical Exposure (PE) =
Exposure to Product (EXP) x Chemical Concentration in Product Formulation (PF)

Dermal Route – Product Specific Models

1. **Exposure during the activity/use of diluted and undiluted laundry and dishwashing products, and diluted and undiluted hard surface cleaning products**

$$\frac{[FQ \times CA \times PC \times FT \times CF \times TF \times DA]}{BW} \times PF$$

2. **Exposure to laundry and fabric conditioning product residual on clothing**

$$\frac{[A \times PR \times PT \times DA \times CF]}{BW} \times PF$$

["FQ" frequency of use is 1 wash load/day for clothing]

3. **Exposure to face and hand soap residual after use**

$$\frac{[FQ \times A \times PR \times DA \times CF]}{BW} \times PF$$

Where:

FQ: frequency of use (use/day)
CA: body surface contact area (cm^2)
PC: product concentration (g/cm^3)
FT: film thickness on skin (cm)
CF: conversion factor (1000 mg/g)
TF: time scaling factor (unitless)
DA: dermal absorption (%)
BW: female body weight (kg)
PF: LAS concentration in product formulation (%)
A: amount per use (g/day or g/wash)
T: transfer to skin (%)
PR: percent retained on clothing or on skin (%)
PT: percent transferred from clothing to skin (%)

(2) Validation/Peer Review

These exposure calculations use first principle equations and are mathematically consistent with the EPA Exposure Guidelines (1992) with regard to modeling dermal doses.

(3) Availability and Documentation

USEPA 1992. Guidelines for Exposure Assessment. [FRL-4129-5]

IV. Inputs, Outputs, and Quality Description

(1) Media Modeled
The exposure media are the LAS-containing products used by consumers. The LAS Coalition fielded a survey among producers and formulators to establish the range of LAS concentrations in each of the product forms. For each product category containing LAS, the minimum and maximum of the range were utilized as inputs for the dermal exposure models.

(2) Inputs
The dermal exposure scenarios encompass conservative, screening-level inputs including: the high-end frequency of product use, the high-end amount of product per use, the high-end percent of product retained on skin or clothes following use. Also, actual dermal absorption is only about 1% of product (Schaefer and Redelmeier 1996), whereas all modeled exposures include a default assumption of 100%. Thus, the modeled exposure is conservative by a factor of at least 100 based on absorption alone. LAS coalition member companies provided formulation information on the range of LAS concentrations in specified product types to be used in this assessment.

Exposure during the activity/use of diluted and undiluted laundry and dishwashing products, and diluted and undiluted hard surface cleaning products

$$\frac{[FQ \times CA \times PC \times FT \times CF \times TF \times DA]}{BW} \times PF$$

	Laundry Pre-treatment (diluted)	Neat Laundry Pre-treatment (undiluted)	Hand-wash of Laundry (diluted)	Hand-wash of Dishes (diluted)	Hand-wash of hands with dish liquid (diluted)	Hard Surface Cleaners (diluted)	Hard Surface Cleaners (undiluted)
Frequency (FQ) (use/day)	1 [h]	1 [h]	1 [h]	3 [h]	0.14 [h]	1 [h]	1 [h]
Contact Area (CA) (cm^2)	360 [b]	360 [b]	1680 [f]	1680 [f]	1680 [f]	1680 [f]	180 [j]
Product Concentration (PC) (g/cm^3)	0.6 [a]	1 [a]	0.01 [a]	0.0015 [a]	0.9 [g]	0.01 [a]	1 [a]
Film Thickness (FT) (cm)	0.0024 [c]	0.0024 [c]	0.0024 [c]	0.0024 [c]	0.0024 [c]	0.0024 [c]	0.0024 [c]
Conversion Factor (CF) (1000 mg/g)	1000	1000	1000	1000	1000	1000	1000
Time Scaling Factor (TF) (unitless)	0.007 [d]	0.007 [d]	0.007 [d]	0.03 [d]	.00035 [d]	0.014 [h]	0.014 [h]
Dermal Absorption (DA) (%)	100% [i]	100% [i]	100% [i]	100% [i]	100% [i]	100% [i]	100% [i]
Female body weight (BW) (kg)	60 [e]	60 [e]	60 [e]	60 [e]	60 [e]	60 [e]	60 [e]
LAS concentration in product formulation (PF) [g] (%)	5-10%	5-10%	1-25%	5-25%	5-25%	1-5%	1-5%

References:
a: LAS Coalition survey
b: Palms surface area (EPA Exposure Factors Handbook)
c: EPA 560/5-85-007, Methods of assessing exposure to chemical substances, Vol.7, Versar, 1985
d: HERA project
e: Female body weight (EU Technical Guidance Document, 1996)
f: Hands and forearms (EPA Exposure Factors Handbook)
g: LAS Coalition survey, Min-Max values
h: SDA Habit and Practice Survey

i: Default assumption
j: Surface area of the palm of one hand (EPA Exposure Factors Handbook)

Exposure to laundry and fabric conditioning product residual on clothing

$$\frac{[A \times PR \times PT \times DA \times CF]}{BW} \times PF$$

	Liquid Laundry Detergent	Dry Laundry Detergent	Tablet Laundry Detergent	Fabric conditioner (dryer-sheet)
Amount Per Use (A) (g/day or g/wash)	121 [a]	121 [a]	135 [a]	3 [a]
Percent Retained on Clothing (PR) (%)	1% [a]	1% [a]	1% [a]	10% [a]
Percent Transferred from Clothing to Skin (PT) (%)	1% [a]	1% [a]	1% [a]	1% [a]
Dermal Absorption (DA) (%)	100% [b]	100% [b]	100% [b]	100% [b]
Conversion Factor (CF) (1000 mg/g)	1000	1000	1000	1000
Female body weight (BW) (kg)	60 [c]	60 [c]	60 [c]	60 [c]
LAS concentration in product formulation (PF) [g] (%)	1-25% [d]	5-25% [d]	5-25% [d]	0.1 – 0.5% [d]

References:
a: SDA Habit and Practice Survey
b: Default assumption
c: EU Technical Guidance Document, 1996
d: LAS Coalition Survey, Min-Max values

Exposure to face and hand soap residual after use

$$\frac{[FQ \times A \times PR \times DA \times CF]}{BW} \times PF$$

	Bar Soap Hand	Bar Soap Face
Frequency of Use (FQ) (use/day)	6 [a]	1 [a]
Amount Per Use (A) (g/use)	0.36 [a]	0.27 [a]
Percent Retained on Skin (PR) (%)	1% [e]	1% [e]
Dermal Absorption (DA) (%)	100% [b]	100% [b]
Conversion Factor (CF) (1000 mg/g)	1000	1000
Female body weight (BW) (kg)	60 [c]	60 [c]
LAS concentration in product formulation (PF) [g] (%)	1-5% [d]	1-5% [d]

References:
a: SDA Habit and Practice Survey
b: Default assumption
c: EU Technical Guidance Document, 1996
d: LAS Coalition Survey, Min-Max values
e: CTFA 2003 data

(3) Model Outputs

Exposure during the activity/use of diluted and undiluted laundry and dishwashing products and diluted and undiluted hard surface cleaning products

	Potential Dermal Exposure (mg/kg/day) [a]
Laundry Pre-Treatment (diluted)	3.0E-3 to 6.0E-3
Neat Laundry Pre-Treatment (undiluted)	5.0E-3 to 1.0E-2
Hand-wash of Laundry (diluted)	4.7E-5 to 1.2E-3

Hand-wash of Dishes (diluted)	5.0E-4 to 2.3E-3
Hand-wash (dishwashing liquids) of hands (diluted)	1.0E-4 to 7.4E-4
Hard Surface Cleaners (diluted)	1.0E-3 to 5.0E-4
Hard Surface Cleaners (undiluted)	5.0E-3 to 1.0E-3

[a] range based on minimum and maximum product concentration values

Exposure to laundry and fabric conditioning product residual on clothing

	Potential Dermal Exposure (mg/kg/day) [a]
Liquid Laundry Detergent	2.0E-3 to 5.0E-2
Dry Laundry Detergent	1.0E-2 to 5.0E-2
Tablet Laundry Detergent	1.1E-2 to 5.6E-2
Fabric conditioning (dryer sheets)	5.0E-5 to 3.0E-4

[a] range based on minimum and maximum product concentration values

Exposure to face and hand soap residual after use

	Potential Dermal Exposure (mg/kg/day) [a]
Bar Soap – Hand	3.6E-3 to 1.8E-2
Bar Soap - Face	5.0E-4 to 2.3E-3

[a] range based on minimum and maximum product concentration values

(4) Reliability Score 1 (Reliable without restrictions) The models used are first principle equations, which are sufficiently conservative, have undergone peer review and are generally accepted by authorities. Appropriate inputs have been used, reflecting best available information and conservative estimates where applicable.

(5) Remarks

An appropriate NOAEL from animal studies for use as a comparison is 85 mg/kg. Estimated dermal exposures in consumer products range from a low of 0.000047 to a high of 0.056 mg/kg/day.

These human exposure evaluations include conservative (protective) input and model assumptions (e.g. all modeled exposures are conservative by a factor of at least 100 due to use of a default assumption of 100% absorption vs. a measured value of <1%).

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Annex 2 – Commercial LAS (C11.6 – C11.8) Acute Toxicity Data

This Annex provides the results of an extensive review of the data previously compiled by BKH (1993) and of the published and unpublished literature since this data compilation (HERA 2004). The purpose of this review is to identify the lowest valid acute toxicity values on commercially representative LAS, having average alkyl chain lengths of C11.6 to 11.8 (Table, SIAR Section 1.1). Valid studies on commercial LAS on test species for which there are OECD acute toxicity guidelines are listed in the tables below. References to the published studies follow the tables. Studies that were not valid, or were not conducted on commercial LAS, are listed in the table of rejected studies along with the reasons for rejection.

Lowest valid values for each taxon are identified in the table. Robust summaries of these studies are included in the dossier. The location of other studies provided in the dossier are noted under Remarks.

Note that all non GLP studies date before the implementation of OECD GLP guidelines. Studies noted as QA are those whose report mentioned a specific Quality Assurance program.

Fish, 96h. Lepomis macrochirus

Reference and year	LC50 (mg/L)	Lab	Test Procedure	GLP	Static/flow through	# replicates	Indiv./rep	Nominal conc (mg/L)	Test T range (°C)	Hard. (mg CaCO3/L)	Measured conc.	Control mortality	Remarks/deviation from protocol
1. 22852, P&G 1979	3.7	Bionomics	US EPA 1975 EPA-660/3-75-009	QA	Static	3	10	Control, 1.3, 2.2, 3.6, 6.0, 10	22±1	43	Nominal conc active	0%	6 and 10 mg/L solutions were cloudy; dossier 4.1(m)
2. 23613,P&G 1980	4.4	UCES	US EPA 1975 EPA-660/3-75-009	QA	Static	Not reported	10	Control, 0.86, 1.4, 2.4, 4.0, 6.7	20-23	30	Nominal conc active	0%	Dossier 4.1(m)
3. 23612, P&G 1980	4.6	Bionomics	US EPA 1975 EPA-660/3-75-009	QA	Static	3	10	Control, 0.78, 1.3, 2.2, 3.6, 6.0, 10	22±1	48	Nominal conc active	0%	6 and 10 mg/L solutions were cloudy; dossier 4.1(m)
4. 23617, P&G 1980	4.6	Bionomics	US EPA 1975 EPA-660/3-75-009	QA	Static	3	10	Control, 0.78, 1.3, 2.2, 3.6, 6.0, 10	22±1	45	Nominal conc active	0%	Dossier 4.1(m)
5. 23722, P&G 1980	4.6	UCES	US EPA 1975 EPA-660/3-75-009	QA	Static	5	10	Control, 1.0, 1.8, 3.2, 5.6, 10	21-22	38	Nominal conc active	0%	Dossier 4.1(m)
6. 22824, P&G 1978	6.3	UCES	US EPA 1975 EPA-660/3-75-009	No	Static	Nortreported	10	Control, 1.4, 2.2, 3.6, 6.0, 10	22±0.5	46	Nominal conc active	0%	Dossier 4.1(m)
7. 28661, P&G 1982	6.4	Biospherics	US EPA 1975 EPA-660/3-75-009	QA	Static	Nortreported	10	Control, 01.3, 2.2, 3.6, 6.0, 10	21-22	47	Nominal conc active	0%	Dossier 4.1(m)
8. 27917, P&G 1980	7.7	Bionomics	US EPA 1975 EPA-660/3-75-009	No	Static	3	10	Control, 1.3, 2.2, 3.6, 6.0, 10	22±1	42	Nominal conc active	0%	10 mg/L solution was cloudy; dossier 4.1(m)

Reference and year	LC50 (mg/L)	Lab	Test Procedure	GLP	Static/flow through	# replicates	Indiv./rep	Nominal conc (mg/L)	Test T range (ºC)	Hard. (mg CaCO3/L)	Measured conc.	Control mortality	Remarks/deviation from protocol
9. 23603, P&G 1979	7.1	UCES	US EPA 1975 EPA-660/3-75-009	QA	Static	Not reported	10	Control, 1.0, 1.8, 3.2, 5.6, 10	20.5-21	42	Nominal conc active	0%	
10. Lewis and Perry, 1981	1.67		US EPA 1975 EPA-660/3-75-009	No	Static	Not reported	10		22±1	137	Nominal conc active		Low value; dossier 4.1(a)

Fish, 96h. Pimephales promelas

Reference and year	LC50 (mg/L)	Lab	Test Procedure	GLP	Static/flow through	# replicates	Indiv./rep	Nominal conc (mg/L)	Test T range (ºC)	Hard. (mg CaCO3/L)	Measured conc.	Control mortality	Remarks/deviation from protocol
11. Holman and Macek, 1980	4.1		US EPA 1975 EPA-660/3-75-009	No						40	MBAS		$C_{11.7}$; dossier 4.1(q)

Daphnia magna: 48 h

Reference and year	LC50 (mg/L)	Lab	Test Procedure	GLP	Static/flow through	# replicates	Indiv./rep	Nominal conc	Test T range (°C)	Hard. (mg CaCO3/L)	Measured conc.	Control mortality	Remarks/deviation from protocol
12. 23618, P&G 1980	4.4	Bionomics	US EPA 1975 EPA-660/3-75-009	QA	Static	3	5	Control, 0.78, 1.3, 2.2, 3.6, 6.0, 10	21-22	175	nominal active	0%	White foam formed on surface of test solution containing 10 mg/L but dissipated within 24 h; dossier 4.2A(e)
13. 22853, P&G 1979	4.9	Bionomics	US EPA 1975 EPA-660/3-75-009	No	Static	3	5	Control, 1.4, 2.2, 3.6, 6.0, 10	22±1	162	nominal active	0%	Dossier 4.2A(e)
14. 23611,P&G 1980	7.1	UCES	US EPA 1975 EPA-660/3-75-009	QA	Static	4	5	Control, 1.9, 3.2, 5.4, 9.0, 15	21-22	220	nominal active	0%	Dossier 4.2A(e)
15. 28793, P&G 1982	9.3	Biospherics	US EPA 1975 EPA-660/3-75-009	No	Static	4	10	Control, 4.9, 6.1, 9.6, 12, 15	20.5-21	120	nominal active	2.5%	Lab practice to use 10 instead of recommended 5 daphnid per replicate to enhance statistical validity
16. Taylor, 1985	4.6		US EPA 1975 EPA-660/3-75-009	No	Static	3	5		21±1	300	Nominal		
17. Lewis and Perry, 1981	3-5.6		US EPA 1975 EPA-660/3-75-009	No	Static	3	5				Measured as MBAS		
18. Lewis and Suprenant, 1983	1.8-5.6		US EPA 1975 EPA-660/3-75-009	No	Static						Nominal		
19. Maki and Bishop, 1979	2.5-4.3		US EPA 1975 EPA-660/3-75-009	No	Static	3	5		21±1	120	Measured as MBAS		

Reference and year	LC50 (mg/L)	Lab	Test Procedure	GLP	Static/flow through	# replicates	Indiv./rep	Nominal conc	Test T range (ºC)	Hard. (mg CaCO3/L)	Measured conc.	Control mortality	Remarks/deviation from protocol
20. Lewis, 1983	4.8		ASTM	No	Static	3	5			131	Measured as MBAS		
21. Verge & Moreno, 2000	6.3		OECD 202, 1984	No	Static	4	5		20±1	200	Nominal		
22. Hooftman and van Drongelen-Sevenhuijsen 1990	1.62	TNO	OECD 202, 1984	Yes	Static	4	5	Control, 3.2, 5.6, 10, 18, 32, 56, 100	20±1		Measured		Low value; dossier 4.2A(a)

Algae, Selenastrum capricornutum and Scenedesmus subspicatus

Reference and year	ErC50 (mg/L)	Exposure period	Test species	Lab	Test Procedure	GLP	# replicates	# cells./rep	Nominal conc., mg/L	Test T range (ºC)	Hard. (mg NaHCO3/L)	Measured conc.	Control 96h count	Remarks/deviation from protocol
23. 43235, P&G 1991	35.5	96 Hr	*Selenastrum capricornutum*	Bio-nomics	OECD 201	Yes	Duplicate tests and quadriuplicate controls	10^4 cells/ml	Control, 1.0, 3.1, 10, 32, 99, 180, 320, 560	21-22	150	measured	3.610^6 cells/ml	White precipitate at 2 highest concentrations.
24. Lewis, 1986; Lewis and Hamm, 1986	29	96 Hr	*Selenastrum capricornutum*		ASTM, 1984	No				21.2-25.6	137			Low value; dossier 4.3(a)
25. Verge and Moreno, 1996	163	72 Hr	*Scenedesmus subspicatus*		OECD, 1984	No	Triplicate test concentrations and six control replicates	10^4		21-22		Nominal		Dossier 4.3(d)
26. Scholz, 1992	127.9	72 Hr	*Scenedesmus subspicatus*		Dir 88/302/EEC, 1988	Yes		20,000 cells/ml	Control, 0.6, 2.4, 10, 40, 160	24+/-2		Nominal		Dossier 4.3(f)
27. Scholz, 1994	82	72 Hr	*Scenedesmus subspicatus*		Dir 92/69/EEC, 1992	Yes		20,000 cells/ml	Control, 0.1, 0.4, 1.6, 6.4, 25, 160	24+/-2		Nominal		Dossier 4.3(g)

List of Published References

10. Lewis, M.A., and Perry, R.L., 1981; Acute Toxicities of Equimolar and Equitoxic Surfactant mixtures to *Daphnia magna* and *Lepomis macrochirus*.

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19. Maki, A. and Bishop, W., 1979; Acute Toxicity Studies of Surfactants to *Daphnia magna* and *Daphnia pulex*. Arch. Environm. Contam. Toxicol. 8, 599-612 (1979).

20. Lewis, M.A., 1983; Effect of loading density on the acute toxicities of Surfactants, Copper, and Phenol to *Daphnia magna* Straus. Arch. Environ. Contam. Toxicol. 12, 51-55.

21. Verge, C. and Moreno A.; 2000; Effect of Anionic Surfactants on *Daphnia magna*. Tenside Surf. Det. 37 (2000) 3.

24. Lewis, M.A., 1986; Comparison of the effects of surfactants on freshwater phytoplankton communities in experimental enclosures and on algal population growth in the laboratory. Environ. Toxicol. Chem., Vol. 5, pp 319-322; Lewis, M.A., and Hamm, B.G., 1986; Environmental modification of the photosynthetic response of lake plankton to surfactants and significance to a laboratory-field comparison. Water Res. 20:1575-1582.

25. Verge, C., and Moreno A., 1996; Toxicity of anionic surfactants to green microalgae *Scenedesmus subspicatus* and *Selenastrum capricornutum*. Tenside Surf. Det. 33 , 166-169.

List of Rejected References

Paper	Reason
Fish – *Lepomis macrochirus*	
Dolan and Hendricks, 1976. The lethality of and intact and degraded LAS mixture to bluegill sunfish and a snail. Journal WPCF, Vol. 48, No.11, November 1976, pp.2570-2577.	Test product is not commercial LAS (C13 sulfonic acid)
Procter & Gamble 22581, 28361, 1991; dossier 4.1(n)	Study not available
Fish – *Pimephales promelas*	
Kimerle and Swisher, 1977; dossier 4.1(r)	Test product is not commercial LAS (C13.3); exposure period 48 Hr
Swisher et al., 1978; dossier 4.1(p)	Test product is not commercial LAS (C11.1)
McKim, Arthur and Thorslund, 1979. Toxicity of a Linear Alkylate Sulphonate detergent to larvae of four species of freshwater fish. Bull. Environ. Contam. Toxicol., 14(1), 1-7.	Test product is not commercial LAS; it is a detergent formulation
Macek and Sleight, 1977. Utility of toxicity tests with embryos and fry of fish in evaluating hazards associated with the chronic toxicity of chemicals to fishes. Aquatic Toxicology and Hazard Evaluation, ASTM STP 634, P.L. Mayer and J.L. Hamelink, Eds., American Society for Testing and Materials, 1977, pp. 137-146.	Fish were larvae, not the age recommended in OECD Method
Daphnia magna	
Hüls, 1986. 7/86, N. Sholz, unpublished	LC50 24 Hr determined for *Daphnia magna*
Maki, 1979. Correlations between *Daphnia magna* and Fathead minnow (*Pimephales promelas*) Chronic Toxicity values for several classes of test substances. J. Fish.Res. Board Can., vol 36, 1979, pages 411-420.	Chronic test
Kimerle and Swisher, 1977; dossier 4.2A(g)	Test product is not commercial LAS (C13.3)
Canton and Sloof, 1982. Substitutes for phosphate containing washing products: their toxicity and biodegradability in the aquatic environment. Chemosphere, Vol.11, No.9, pp 891-907.	Test product is not commercial LAS (C11)

Barera and Adams, 1983. "Resolving some practical questions about Daphnia Acute Toxicity Tests". Aquatic Toxicology and Hazard Assessment: Sixth Symposium, ASTM STP 802, W.E. Bishop, R.D. Cardwell and B.B. Heidolph, Eds. American Society for Testing and Materials, Philadelphia, 1983, pp 509-518.	Test product is not commercial LAS (C13.3)
Lal , Misra, Viswanathan and Murti, 1983. Comparative studies on Ecotoxicology of Synthetic Detergents. Ecotoxicology and Environmental Safety, 7, 538-545.	Test product not specified Mode of culturing Daphnia not clear Test method not specified Test conditions not clearly explained Calculations not clear. Median Tolerance Limit is the parameter assessed.
Gard-Terech and Palla, 1986. Comparative kinetics study of the evolution of freshwater aquatic toxicity and biodegradability of linear and branched alkylbenzene sulfonates. Ecotoxicology and Environmental Safety 12, 127-140 (1986).	Toxicity determined for effluent of biodegradation test
Huels, unpublished; dossier 4.2A(d)	Study not available
Procter & Gamble, 1991, 23276; dossier 4.2A(f)	Study conducted as part of QA program to qualify various labs and the result is not considered reliable
Algae	
Canton and Sloof, 1982. Substitutes for phosphate containing washing products: their toxicity and biodegradability in the aquatic environment. Chemosphere, Vol.11, No.9, pp. 891-907.	Test product is not commercial LAS (C11)
Henkel, unpublished (Registry No. 5929) ; dossier 4.3(h)	Study not available
Huls AG, 1/90 N. Scholz; dossier 4.3(i)	Study not available
Procter & Gamble AL/12, 1991; dossier 4.3(j)	Mis-cited; not available and not a P&G study
Procter & Gamble 29101, 1991; dossier 4.3(k)	Mis-cited; values and protocol do not match report; report invalid
Procter & Gamble AL/10, 1991; dossier 4.3(l)	Mis-cited; not available and not a P&G study
Procter & Gamble P2636.01, 1991; dossier 4.3(m)	Test product is not commercial LAS (C12.3)
Yamane et al., 1984; dossier 4.3(n)	Exposure period: 48 Hr

ANNEX 3 – DERIVATION OF THE HC_5 VALUE

Linear Alkylbenzene Sulfonate (LAS)
Industry Coalition for the SIDS Assessment of LAS

Introduction

Extrapolation procedures are commonly used to evaluate the available laboratory-generated single-species toxicity test data. For data sets in which toxicity data are available for a reasonably large number of species, the species sensitivity distribution approach is often used. In this approach, the concentration protection of most single species (generally 5%, i.e., 95% of the species NOECs are greater) is calculated. This value, called the HC_5, is the lower 5^{th} percentile of a distribution of single-species NOEC tests and thus is protective of the environment (Aldenberg and Slob 1993).

For the current evaluation of LAS data, the HC_5 for aquatic species was calculated for LAS using the available single-species chronic freshwater data including the data summarized by van de Plassche et al. (1999).

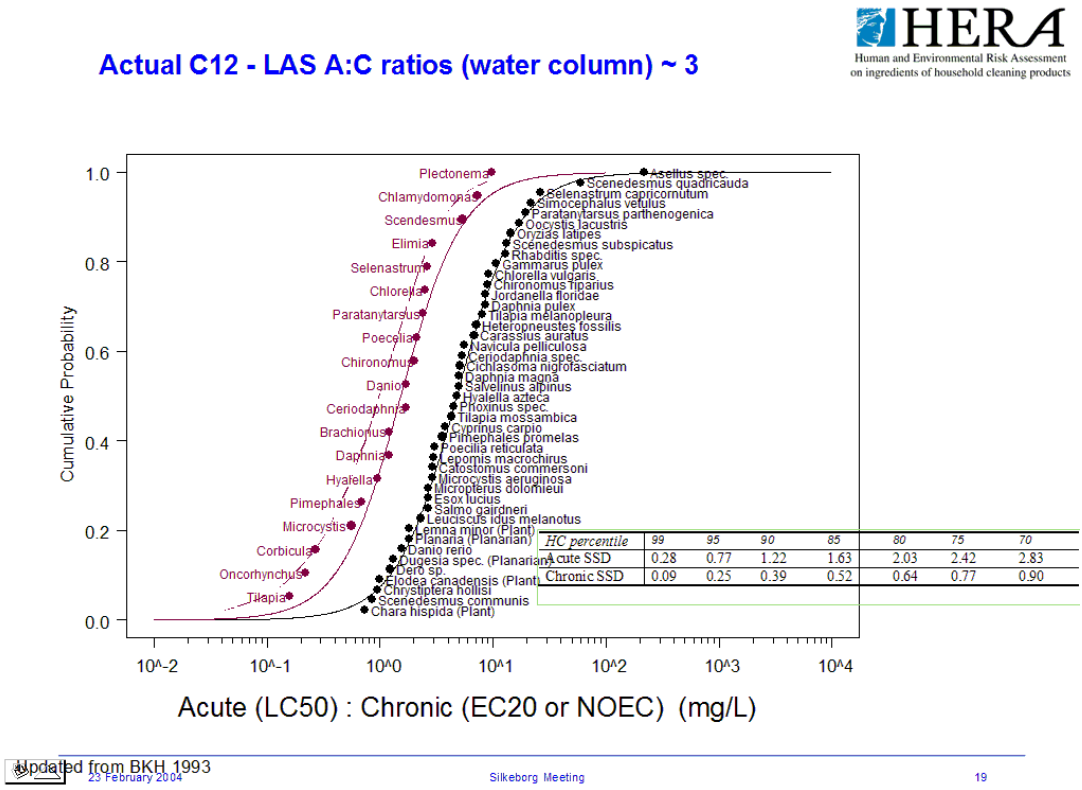
Method

The van de Plassche et al. (1999) data were analyzed using several types of distributions as described in Versteeg et al. (1999). The goodness-of-fit for each distribution was evaluated by the one-sample Cramer-vom Mises statistical test, which was used to compare the relative goodness-of-fit with the various distributions. Based on higher p-values, the log-logistic distribution was a better fit to the data than the log normal distribution used by van de Plassche et al. (1999).

Consequently, the available chronic data and the van de Plassche et al data were plotted using log-logistic distributions. The fitted NOEC distribution is shown by the solid line in the distribution function. Lower 95% confidence limits on the fitted NOEC distribution function (dashed lines) were calculated analogous to the methods of Aldenberg and Slob (1993), with the exception that here the maximum likelihood estimators were used as opposed to moment estimators to measure goodness-of-fit. The maximum likelihood estimators are generally less biased and have better precision than moment estimators (Schafer and Sheffield 1973).

The Kolmogorov-Smirnov (K-S) statistical test was used to determine the goodness-of-fit and calculate the HC_5 ($HC_{5,\ 50\%\ confidence\ interval}$) value.

The available chronic toxicity data and the data of van de Plassche et al. (1999) are presented in Table 12A of this SIAR. For *Microcystis aeruginosa*, dossier 4.3s, the NOEC was calculated by dividing the EC_{50} value by 3. As documented below (data from BKH 1993), the average EC_{50}/NOEC ratio for LAS is 3, and thus this calculation of the NOEC value from the EC_{50} is supported by a large database of information.



All NOEC values were normalized to $C_{11.6}$ as this was considered the structure most typically produced and used globally. The normalization procedure (van de Plassche et al. 1999) was based on the use of quantitative structure-activity relationships (QSARs). Since no long-term QSARs were available for LAS, QSARs for short-term toxicity were used. Normalization was carried out using the following procedure.

The log K_{ow} was calculated for $C_{11.6}$ LAS and the tested structure using the Leo and Hansch method (1979) with the modification for phenyl isomer position by Roberts (1991), which calculates log K_{ow} values for LAS using a position-dependent branching factor (PDBF). An increment of 0.54 is used for a CH_2 unit (Leo and Hansch 1979).

The EC_{50} values were calculated using the following QSAR for LAS:

$$\text{Log}(1/EC_{50}) = 0.63 \log K_{ow} + 2.52$$

The ratio between the predicted EC_{50}s for the normalized and the tested structure was calculated. The NOEC of the tested structure was then multiplied by this ratio to obtain the NOEC for the normalized structure. The normalized NOECs were then used to calculate the geometric mean for each species for which data were available.

For example, for a NOEC of 0.9 mg/L for $C_{12.6}$ LAS, the procedure is as follows. The calculated log K_{ow} and molecular weight for $C_{12.6}$ LAS are 3.86 and 356, respectively. Using the QSAR given above, this leads to an EC_{50} of 4.0 mg/L. For $C_{11.6}$ LAS, the calculated log K_{ow} and molecular weight are 3.32 and 342, respectively, leading to an EC_{50} of 8.4 mg/L. The ratio between the predicted EC_{50} values for $C_{11.6}$ LAS and $C_{12.6}$ LAS is 2.1. Multiplying the NOEC of 0.9 mg/L by 2.1 leads to a normalized NOEC of 1.9 mg/L for $C_{11.6}$ LAS.

Results

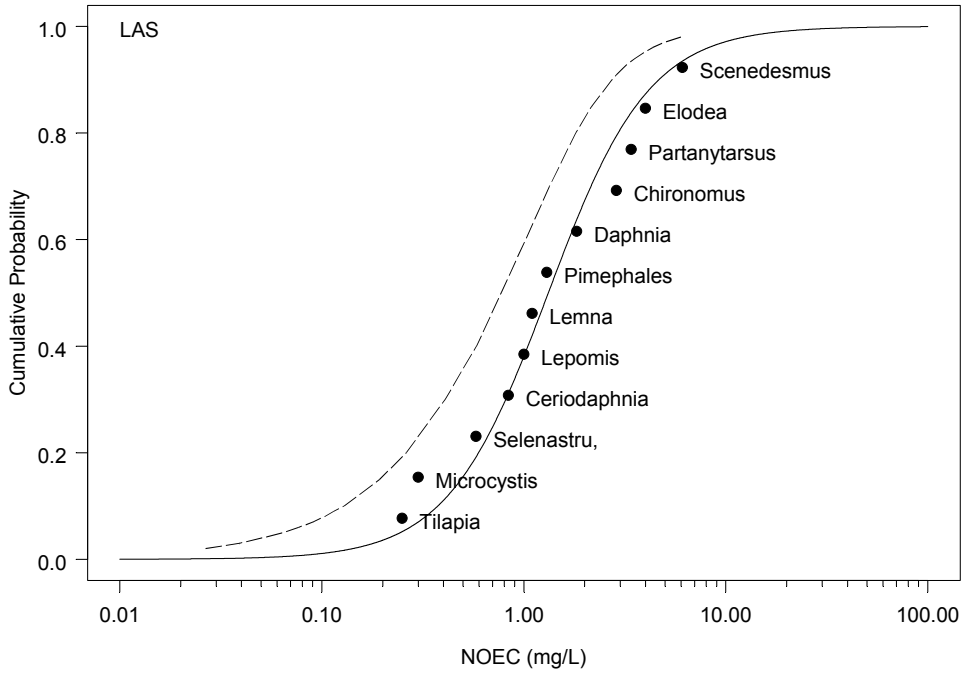
The single-species chronic toxicity data summarized by van de Plassche et al. (1999) resulted in a calculated HC_5 value of 0.32 mg/L. This value is based on a fit of the data to a log-normal distribution. Using the goodness-of-fit comparisons as described above, the best fit with the van de Plassche et al. data was found with the log-logistic distribution (Versteeg et al. 1999). A HC_5 value of 0.36 mg/L was determined for $C_{11.6}$ LAS with the log-logistic distribution. The data used ("Original VdP Values"), the cumulative probability distribution of the data and the HC_5 calculation are shown below.

These same methods were also applied to the available chronic data provided in the dossier and summarized in Table 12A of this SIAR. Using the log-logistic distribution of the normalized NOEC data, the HC_5 value calculated is 0.24 mg/L. The data used ("Available Chronic Values"), the cumulative probability distribution of the data and the HC_5 calculation are shown below.

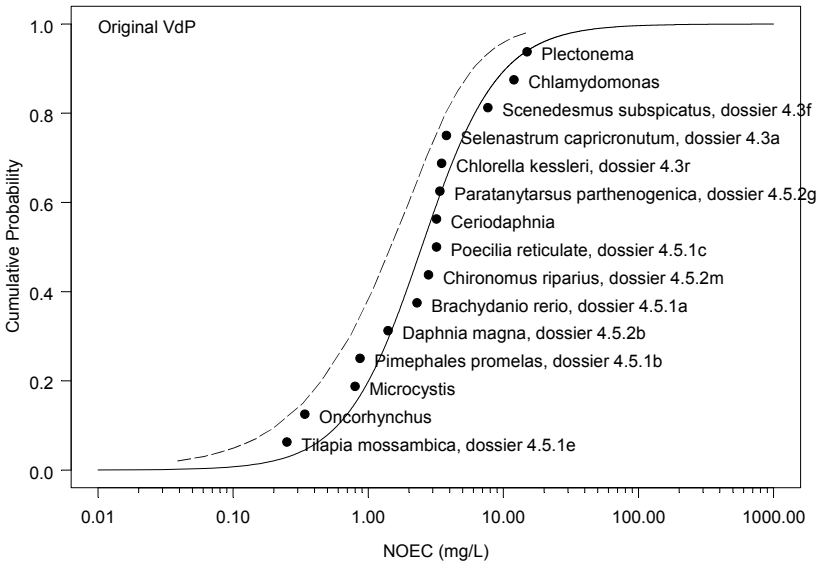
Original VdP Values (Table 12A)	NOEC (mg/L)	Available Chronic Values	NOEC (mg/L)
Fish		**Fish**	
Brachydanio rerio (Not reviewed by van de Plassche et al.)	2.3	(No valid study identified)	
		Lepomis macrochirus, dossier 4.5.1m	1
Oncorhynchus mykiss (geometric mean)	0.34	(No valid study identified)	
Pimephales promelas (geometric mean)	0.87	Pimephales promelas, geometric mean	1.3*
Poecilia reticulata	3.2	(No valid study identified)	
Tilapia mossambica	0.25	Tilapia mossambica, dossier 4.5.1e	0.25
Aquatic Invertebrates		**Aquatic Invertebrates**	
Ceriodaphnia sp.	3.2	Ceriodaphnia sp., dossier 4.5.2b	0.84
Chironomus riparius	2.8	Chironomus riparius, dossier 4.5.2o	2.87
Daphnia magna (geometric mean)	1.4	Daphnia magna, geometric mean	1.83*
Paratanytarsus parthenogenica	3.4	Paratanytarsus parthenogenica, dossier 4.5.2h	3.4
Algae		**Algae**	
Chlamydomonas reinhardi	12	(No valid study identified)	
Chlorella kessleri	3.5	(No valid study identified)	
Microcystis sp. (geometric mean)	0.8	Microcystis aeruginosa, dossier 4.3s	0.3**
Plectonema boryanum	15	(No valid study Identified)	
Scenedesmus subspicatus (geometric mean)	7.7	Scenedesmus subspicatus, geometric mean	6.1*
Selenastrum capricronutum (geometric mean)	3.8	Selenastrum capricronutum, dossier 4.3a	0.58*
Higher Plants		Higher Plants	
(Not reviewed by van de Plassche et al.)		Elodea canadensis, dossier 4.3o	4
(Not reviewed by van de Plassche et al.)		Lemna minor, dossier 4.3p	1.1

*Geometric mean of available valid studies (see Table 12A)
** $EC_{50}/3$

Available Chronic Data Distribution



Original VdP Values



Compound Group	Log-Logistic Calculation Statistical Parameters Intercept (u) (mean)	Scale (sigma) Variability	K-S Test p-value	HC5
Available Chronic Values	**0.279**	**0.5736**	**0.9756**	**0.244**
Original VdP Values	**0.911**	**0.6531**	**0.8655**	**0.363**

Discussion

The HC_5 values for LAS are considered to be valid estimates of the NOEC since all three meet the OECD criteria for statistical extrapolation methods (OECD 2002). These include:

1) QSAR method – The approach used to normalize the NOEC data is clearly described (above). The approach is considered reliable because it's application to LAS and other major surfactants is well documented in the scientific literature (Leo and Hansch 1979, Roberts 1991, van de Plassche et al. 1999).

2) Clear input data – Reliable NOEC values from freshwater single-species chronic studies are used as described in Table 12A of the SIAR and listed above.

3) Mode of action – LAS has a nonspecific mode of action described as "narcosis toxicity" (Roberts 1991). As expected from this mode of action, sensitivity of the tested species follows a log –normal and log-logistic distribution with a high degree of goodness of fit. The best fit of the data is to the log-logistic distribution.

4) Minimum species requirements – Represented species include fish, crustaceans, insects, a rotifer, algae, and higher plants.

5) Minimum sample size – The database consists of NOEC values on at least 12 freshwater species.

6) Use of multiple data for same species – In the van de Plassche et al. (1999) review, the geometric mean value is used for species with multiple values (number of species indicated in Table 12A). For the available data set, the geometric mean value of the valid studies is provided.

7) Statistical fitting procedure – The specified Kolmogorov-Smirnov test was used as described above. Goodness of fit across distributions (i.e. log-normal versus log-logistic) was compared using the Cramer-von Mises statistical test as described by Versteeg et al. (1999).

8) Estimation parameter – The reported value is as specified, the HC_5 value with 50% confidence limits.

9) Estimation of NOEC – The HC_5 values support the conclusion of the mesocosm studies that no uncertainty (assessment) factor is needed to determine the NOEC value for LAS. The NOEC for LAS is derived from the entire database of freshwater chronic data, including the HC_5 values and the mesocosm data, as discussed in the SIAR, section 4.1 Aquatic Effects.

References

Aldenberg, T., and Slob, W. 1993. Confidence limits for hazardous concentrations based on logistically distributed NOEC toxicity data. Ecotoxicol. Environ. Saf. 25:48-63.

BKH. 1993. The use of existing data for estimation of the maximum tolerable environmental concentration of LAS. Part I: main report. Part II: data list, BKH, Delft (NL).

Leo, A.J., and Hansch, C. 1979. Substituent Constants for Correlation Analysis in Chemistry and Biology. John Wiley & Sons, New York, NY (USA).

Organization for Economic Cooperation and Development (OECD). 2002. Manual for Investigation of HPV Chemicals. Chapter 4: Initial Assessment for the Environment. Section 4.2. Guidance for the Initial Assessment of Aquatic Effects. October 2002.

Roberts, D.W. 1991. QSAR issues in aquatic toxicity of surfactants. Sci. Total Environ. 109/110:557-568.

Schafer, R.E., and Sheffield, T.S. 1973. Inferences on the parameters of the logistic distribution. Biometrics 29:449-455.

van de Plassche, E.J., de Bruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J., and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: Linear alkylbenzene sulfonate, alcohol ethoxylates, alcohol ethoxylated sulfates, and soap. Environ. Toxicol. Chem. 18:2653-2663.

Versteeg, D.J., Belanger, S.E., and Carr, G.J. 1999. Understanding single-species and model ecosystem sensitivity: Data-based comparison. Environ. Toxicol. Chem. 18:1329-1346.

SIDS DOSSIER

LINEAR ALKYLBENZENE SULFONATE (LAS)

CAS NOs. 1322-98-1
25155-30-0
26248-24-8
27636-75-5
68081-81-2
68411-30-3
69669-44-9
85117-50-6
90194-45-9
127184-52-5

Sponsor Country : United States of America
Date: August 15, 2005

TABLE OF CONTENTS

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

A. CAS number The information provided in this dossier refers to various individual compounds and mixtures of sulfonated linear alkyl benzenes which are identified by the following CAS numbers and names:

CAS No.	EINECS No.	Name
1322-98-1	215-347-5	Decylbenzene sulfonic acid, sodium salt
25155-30-0	246-680-4	Dodecylbenzene sulfonic acid, sodium salt
26248-24-8	247-536-3	Tridecylbenzene sulfonic acid, sodium salt
27636-75-5	248-583-2	Undecylbenzene sulfonic acid, sodium salt
68081-81-2	268-356-1	C_{10-16} Monoalkylbenzene sulfonic acid, sodium salt
68411-30-3	270-115-0	C_{10-13} Alkylbenzene sulfonic acid, sodium salt
69669-44-9	274-070-8	C_{10-14} Alkyl derivatives benzene sulfonic acid, sodium salt
85117-50-6	285-600-2	C_{10-14} Monoalkylbenzene sulfonic acid, sodium salt
90194-45-9	290-656-6	C_{10-13} Alkyl derivatives benzene sulfonic acid, sodium salt
127184-52-5		4-C_{10-13}-sec Alkyl derivatives benzene sulfonic acid, sodium salt

B. Name *(IUPAC name)* See A.

C. Name *(OECD name)* Linear alkylbenzene sulfonate (LAS)

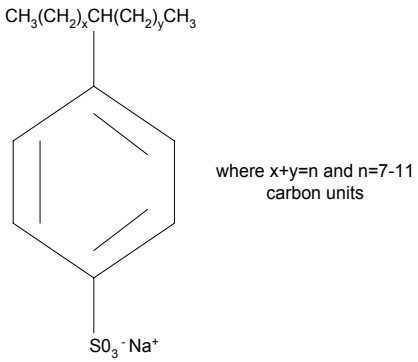
D. CAS Descriptor

Relatively consistent mixture of homologues with predominately linear (currently >95% for most products) varying alkyl chain lengths (from C_{10} to C_{14}) and phenyl isomers with attachment of the *para* sulfonate (sodium salt) benzene ring to the alkyl chain at non-terminal positions. This description applies to all of the CAS numbers listed in 1.01A as shown by the alkyl chain distribution in the table in 1.01G.

E. EINECS-Number See A.

F. Molecular Formula See G.

G. Structural Formula



The linear alkyl carbon chain typically has 10 to 14 carbon units, with the approximate mole ratio varying somewhat regionally, as shown in the following table:

Region	<C_{10}	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	>C_{14}	Range of Averages	Weighted Average*
Canada 68081-81-2	≤1	<16	19-39	20-50	5-27	<3	<1	11.8	11.8
Europe 25155-30-0 68081-81-2 68411-30-3 85117-50-6 90194-45-9 127184-52-5	≤1	8-20	19-39	20-50	5-27	<1-3	<1	11.6-11.8	11.7
Japan 68081-81-2 68411-30-3 69669-44-9	≤1	7-16	19-39	20-50	5-27	<1-3	<1	11.7-11.8	11.8
United States 1322-98-1** 25155-30-0 26248-24-8** 27636-75-5** 68081-81-2 69669-44-9 85117-50-6 90194-45-9	<2	1-25	7-50	20-50	5-45	<1-10	<1	11.3-12.6	11.7

*Weighted by production volume for each region.
**Manufacture of LAS under these CAS numbers has recently been discontinued.

The molecular weights depend on alkyl chain length and range from 338 ($C_{11.3}$) to 356 ($C_{12.6}$). As shown in the table, all the LAS category members (CAS numbers) have the alkyl chain distributions for the LAS category. All of the data in this assessment, except for homologue data identified as such, is on LAS category materials having the alkyl chain distribution shown in the table. The available information on the test substances is provided in the robust summary for each test. All results have been corrected for 100% activity.

Commercial LAS is exclusively manufactured as mixtures of C_{10} to C_{13} or C_{14} alkyl chain homologues, having average alkyl chain lengths ranging from $C_{11.3}$ to $C_{12.6}$, with the predominant materials having average alkyl chain lengths ranging from $C_{11.7}$ to $C_{11.8}$ (Table above). Each alkyl chain homologue consists of a mixture of all the possible sulfophenyl isomers except for the 1-phenyl isomer which is not found in the commercial material. The catalyst used to make the LAB determines the distribution of the phenyl isomers in commercial LAS with the proportion of the 2-phenyl isomers ranging from 18 to 28% (Valtorta et al., 2000). Consequently, commercial LAS consists of a mixture of 20 or more compounds, the 2-phenyl to 5-phenyl isomers of the C_{10} homologue, the 2-phenyl to 6-phenyl isomers of the C_{11} and C_{12} homologues and the 2-phenyl to 7 phenyl isomers of the C_{13} homologue, etc.

H. **Substance Group** Not applicable

I. **Substance Remark** Not applicable

J. **Molecular Weight** Range depending on alkyl chain length

1.02 OECD INFORMATION

A. **Sponsor Country:** United States of America

B. **Lead Organization:**

Name of Lead Organization: United States Environmental Protection Agency
Contact person: Mr. Oscar Hernandez
Address:
1200 Pennsylvania Avenue, N.W.
Washington, D.C. 20460
USA
Tel: (202) 564-7641
Email: hernandez.oscar@epa.gov

C. Name of responder

Name: John Heinze Ph.D., Consortium Manager
Address:
Industry Coalition for the SIDS Assessment of LAS
c/o Council for LAB/LAS Environmental Research
529 14th Street, N.W., Suite 807
Washington, D.C. 20045
USA
Tel: (202) 737-0171
Fax: (202) 737-8406

Consortium Participants
Center for LAB Environmental and Technical Studies for Asia (CLETSA)
Cognis Deutschland GmbH&Co.KG
Colgate-Palmolive Company
Huntsman Corporation
Kao Corporation
Lion Corporation
Petresa International N.V.
Quimica Venoco, CA
YPF SA
Sasol North America
Stepan Company
TAYCA Corporation
The Dial Corporation
The Procter & Gamble Company
Unilever Household and Personal Care North America

Additional Participants
Mitsubishi Chemical Corporation
Nippon Petrochemicals Co., Ltd.
W.R. Grace & Company

1.03 CATEGORY JUSTIFICATION

The LAS molecule contains an aromatic ring sulfonated at the para position and attached to a linear alkyl chain at any position except the terminal carbons. The alkyl carbon chain typically has 10 to 14 carbon atoms and the linearity of the alkyl chains ranges from 87 to 98%. While commercial LAS consists of more than 20 individual components, the ratio of the various homologues and isomers, representing different alkyl chain lengths and aromatic ring positions along the linear alkyl chain, is relatively constant in currently produced products, with the weighted average carbon number of the alkyl chain based on production volume per region between 11.7-11.8. LAS is supported as a category because of the close consistency of the mixtures, their commercial uses, fate, and health and environmental effects. LAS is the primary cleaning agent used in many laundry detergents and cleaners at concentrations up to 25 percent in consumer products, and up to 30 percent in commercial products, with the exception of one reported product at 45% percent in concentrated solid form that is mechanically dispensed into diluted solution for dishwashing.

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [**X**]; organometallic [ ]; petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [ ]; solid **[X]** for pure substance

C. Purity 87-98%

Purity refers to the percent LAS, with iso-branched LAS and DATS considered to be impurities. The "activity" may also be stated, and represents the percent of active LAS in the solution (e.g., 50% active LAS is half strength LAS, the LAS of which will be 87-98% pure, with the remaining 50% consisting of water).

D. Manufacturing Process

LAS is manufactured from linear alkylbenzene (LAB) in self-contained, enclosed systems (see SIAR Annex, Format A, Section VI(1), for more information). LAB is produced by reacting paraffins with benzene and a catalyst and isolating the LAB by distillation. The LAB is then sulfonated, which in turn is then neutralized to sodium salts of LAS.

1.2 SYNONYMS

Linear alkylbenzene sulfonates
LAS
Sodium-n-alkyl (C_{10-13}) Benzene Sulfonate
Numerous trade names, e.g. Marlon A

1.3 IMPURITIES

Remarks: Dialkyltetralin Sulfonates (DATS) and single methyl-branched alkyl chain LAS (iso-LAS) make up minor components in commercial LAS. Concentrations range from <1 to 8% for DATS and <1 to 6% for iso-LAS, depending on the manufacturing process used. Recent market information (LAS SIDS Consortium, unpublished, 2005) indicates that less than 5% of the global LAS production contains high levels of DATS. Consequently, the average (based on production volume) linearity and purity of LAS worldwide is greater than 95%. The presence of DATS and iso-LAS did not significantly affect the biodegradation of LAS relative to the pure linear component, as both DATS and iso-LAS are biodegradable substances. This is discussed in detail in the summaries at section 3.5(x) and 3.5(y).

References:
1) Nielsen, A.M., Britton, L.N., Beall, C.E., McCormick, T.P. and Russell, G.L. 1997. Biodegradation of coproducts of commercial linear alkylbenzene sulfonate. Environ. Sci. Technol. 31L3397-3404.
2) Cavalli, L., Cassani, G., Lazzarin, M., Maraschin, C., Nucci, G., and Valtorta, L. 1996b. Iso-branching of linear alkylbenzene sulphonate (LAS). Tenside Surf. Det. 33:393-398.
3) LAS SIDS Consortium, unpublished, 2005.

1.4 ADDITIVES

Value: None
Remarks: No additives

1.5 QUANTITY

(a)
Remarks: Year 2000 data, as reported in a Colin A. Houston report, indicate an estimated volume of LAS consumption in North America (United States and Canada combined) as 390,000 metric tonnes.
Reference: Colin A. Houston. 2002. Surfactant Developments. Forecast to 2010. A Multiclient Study. Colin A. Houston & Associates, Inc., August 2002.

(b)
Remarks: In a market survey completed by ECOSOL in 2000, companies in Europe reported a total consumption of LAS of approximately 400,000 metric tonnes. This includes CAS numbers 1322-98-1, 25155-30-0, 68411-30-3, 85117-50-6 and 90194-45-9.
Reference: HERA. 2004. HERA-LAS Human and Environmental Risk Assessment: Linear Alkylbenzene Sulphonates, LAS. CAS No. 68411-30-3, Version 2.0, May 2004; available at www.heraproject.com.

(c)
Remarks: Total LAS production for the companies surveyed in the most recent year for which data are available (generally 2002) was approximately 430,000 metric tonnes. Almost half of this production (198,000 metric tonnes) occurred in North America (United States and Canada combined). Production in Europe, as reported by the member companies surveyed, was approximately 152,000 metric tonnes. Data cited above in (a) and (b) for LAS consumption in the United States and Europe are viewed as the more reliable estimates, because all LAS producers are not included in the coalition member survey. Production in Japan, where all the LAS producers are members of the consortium, was 85,000 metric tonnes and is considered a reliable estimate.
Reference: Industry Coalition for the SIDS Assessment of LAS Survey conducted in 2002 (LAS SIDS Consortium Survey, 2002).

(d)
Remarks: More than 1 million tonnes per annum produced globally based on: (1) 364 to 415 ktonnes produced annually in U.S. from 1987 to 199l; (2) 400 ktonne produced in Western Europe and 2570 ktonnes world-wide in 1995; (3) 950 ktonnes produced in Europe, North America and Japan in 1994; (4) 2 million tonnes consumed world-wide in 1990; (5) 410 ktonne produced in Western Europe, 2.6 million tonnes worldwide in 1995.
Reference: (1) CHIMICA OGGI, Sept. 1998
(2) EU Risk Assessment Report for LAB, May 1997
(3) IPCS Environmental Health Criteria 169, WHO, 1996
(4) Nielsen et al. 1997
(5) Soap and Detergent Association, 1996

1.6 LABELLING AND CLASSIFICATION

Labelling

Remarks: None designated

Classification
Remarks: None designated

1.7 USE PATTERN

A. General

Type of Use:	Category:
main	Wide dispersive use
industrial	Personal and domestic use
use	Cleaning/Washing agent

Remarks: About 78-97% of the LAS consumption worldwide is in liquid and powder consumer and industrial laundry and fine fabric detergents. Another 2-10% of the LAS produced is used in consumer and industrial dishwashing liquids, with the remainder (1-5%) used in other consumer and industrial cleaners.

B. Uses in Consumer Products

Function	Amount present	Physical state
detergent	up to 25% of formulation	powder or liquid

Remarks: LAS is an anionic surfactant that lowers the surface tension of water, enabling soils and stains to loosen and release from fabrics and surfaces. LAS is the primary cleaning agent used in many liquid and powder laundry detergents and speciality household cleaners at concentrations up to 25 percent of the total formulation.

The following table shows the percentage of LAS that occurs in various types of consumer detergent products.

Consumer Product Type	Range of Percent Composition that is LAS		
	North America	Europe	Japan
Laundry Detergents			
- Powders	5-25%	5-25%	5-25%
- Liquids	1-25%	5-10%	5-25%
- Tablets	5-25%	10-25%	5-25%
Liquid Fine Fabric Detergents	-	-	1-5%
Bleaches	-	-	0.1-0.5%
Pre-Washes	-	-	5-10%
Fabric Conditioners (sheets)	0.1-0.5%	-	-
Dishwashing Detergents (liquids)	5-25%	10-25%	1-5%
General Cleaners (dilutable)	1-5%	1-5%	-
Hard Surface Cleaners	1-5%	0.1-0.5%	0.5-10%
Other Cleaners	-	-	0.1-0.5%
Face & Hand Soaps (bar)	1-5%	-	-

Reference: 1) Soap and Detergent Association 1996
2) Survey data for Industry Coalition for the SIDS Assessment of LAS. 2002.

C. Uses in Institutional and Industrial Products

The following table shows the percentage of LAS that occurs in various types of institutional and industrial detergent products.

Industrial Product Type	Range of Percent Composition that is LAS		
	North America	**Europe**	**Japan**
Laundry Detergents			
- Powders	5-25%	5-10%	5-10%
- Liquids	-	10-25%	-
Pre-Washes	-	10-25%	-
Dishwashing Detergents (liquids)	5-10%	25-30%	5-30%
General Cleaners			
- Dilutable	1-5%	-	-
- Spray	1-5%	-	-
Hard Surface Cleaners	-	-	1-10%
Disinfectants (liquids)	5-10%	-	-
Other Uses	25-30%*	10-25%	10-25%

6.1 * *The only exception is a product containing 45% LAS that is a concentrated solid mechanically dispensed into diluted solution for dishwashing.*

Reference: 1) Soap and Detergent Association 1996
2) Survey data for Industry Coalition for the SIDS Assessment of LAS. 2002.

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

Exposure limit value
Type: None established by OSHA, ACGIH or NIOSH

Short term exposure limit value
Value: None established by OSHA, ACGIH or NIOSH

1.9 SOURCES OF EXPOSURE

Remarks: Exposure to industrial workers is limited because this is an enclosed manufacturing process designed to minimize losses and the potential for release. Worker exposure is possible during the detergent formulation stage by inhalation of powders or dermal contact of powders and liquids. However, good manufacturing design practices (e.g. enclosed production, exhaust ventilation, dust collection) and personal protective equipment (e.g. protection clothing, eyewear, and glove) in place of at facilities that manufacture liquid and dry (granular/powder) materials sufficiently mitigate worker exposure to LAS. No special engineering controls or additional personal protective equipment are uniquely specified for LAS.

LAS is used primarily in household laundry and dishwashing cleaning products. After use, LAS is discharged into the wastewater treatment system. The exposure of the general human population and of environmental organisms depends on the application of LAS, the local sewage treatment practices, and on the characteristics of the receiving environment.

It is reasonable to consider that the tasks with the greatest exposure to the consumer are hand dishwashing and hand washing of clothing.

Reference: 1) EU Risk Assessment Report for LAB, May 1997.
2) IPCS Environmental Health Criteria 169, WHO, 1996.

1.10 ADDITIONAL REMARKS

A. Options for disposal

Remarks: Unused LAS may be recovered for reprocessing or disposed of by incineration or landfill or by flushing to sewage system; used material enters sewage system and is treated at WWTP. Spills may be recovered for reprocessing or disposal.
Reference: MSDS.

B. Other remarks

(a)
Remarks: The majority of LAS is disposed of in sewage during use as cleaning/washing agents.
Reference: Soap and Detergent Association 1996.

(b)
Methods: A study conducted for the Soap and Detergent Association (Battelle 1999) measured the under 10 micron fraction delivered from 6 consumer product spray nozzles. The six standard trigger sprayers (TS800) were manufactured by Calmar Dispensing System, Inc. The specified average output of the sprayers, based on water at 90 strokes per minute, is no less than 0.75 mL per stroke. The specified spray pattern is a nearly circular pattern with a diameter of no less than four inches at a distance of approximately eight inches. The six trigger sprayers were evaluated to determine emitted aerosol size distribution, output per stroke and spray pattern in order to avoid choosing a trigger sprayer with abnormal characteristics for the experiment. Size distribution of aerosols generated from the six sprayers was measured using a laser diffraction particle sizer (Mastersizer Model X, Malvern Intruments Ltd).
Remarks: The overall mean (n=30) is 0.11% particles under 10 microns and the standard deviation is 0.21. The very highest observation was 0.80% particles under 10 microns. This testing only captured the spray particles that are under 600 microns, so the actual mean respirable particle percent of total volume sprayed is less than 0.1%. The Battelle (1999) study also reported that for consumer spray products in normal use conditions, the peak breathing zone concentration under 10 microns ranged from 0.13-0.72 mg/m^3. HERA (2004) reported that measurements of aerosol particles under 6.4 microns in size generated upon spraying with typical surface cleaning spray products resulted in a product concentration of 0.35 mg/m^3. These estimates of exposure to respirable particles from consumer spray products indicate that inhalation is not a likely route of concern for human exposure (see SIAR Annex 1 for more information). Estimates of inhalation exposure apply to both consumer and commercial products as both use the same type of spray nozzles (for spray cleaners) and the same type of equipment to make powder/granulated products. The human experience with eye irritation covers both manufacturing and use of consumer and commercial products.
References: 1) Battelle, Inc. 1999. Measurement and characterization of aerosols generate from a consumer spray product-pilot study. Final report to the Soap and Detergent Association. Battelle Study No. N003043A. January.

2) HERA. 2004. Linear Alkylbenzene Sulphonate, LAS. Human & Environmental Risk Assessment on ingredients of European household cleaning products. Version 2.0, May 2004. http://www.heraproject.com/RiskAssessment.cfm

(c)

Methods: A comprehensive testing program was undertaken to evaluate consumer exposure to dust from powdered enzyme detergent use in comparison with worker exposure at factories. Airborne dust was collected in consumers' homes during normal use of laundry detergents. Consumer use of laundry products was then simulated in the laboratory to permit collection of sufficient samples for analysis of the amount of enzyme in detergent dust, and for detergent dust particle size distribution determinations and persistence measurements. Representative commercial products sold by Procter & Gamble were tested. Air sampling was carried out using an electrostatic precipitator using a battery powered source and was conducted continuously from the time each housewife began to pour laundry product for use until she left the laundry area. The entry orifice of the sampling device was located at a point spatially equivalent to the direction and distance from the housewife's nose from the point of dust generation. Laboratory simulation of consumer practices was based on extensive consumer habits developed by a variety of conventional techniques.

Remarks: The results of the in-home studies indicate that detergents contribute only 5% of the dust present during the time detergents are dispensed for laundering, with the rest of the dust believed to be mainly lint. Virtually all detergent dust (95%) settled in less than 2 minutes. On average, there is 0.27 µg detergent dust exposure per cup of product used for double-pour machine laundering.

Based on this amount, HERA (2004) calculated the amount of LAS exposure from laundry detergent use. Up to 22% (0.06 µg/use) of the detergent dust can be expected to be LAS. Assuming a worst case exposure (all dust is inhaled and laundry is done 3 times a day), the exposure to LAS of an average adult is estimated to be 0.003 µg/kg bw/day. This amount does not contribute significantly to the total exposure of LAS as compared to the amount from inhalation of aerosols from cleaning sprays, which is approximately 10-fold higher (0.04 µg/kg bw/day).

References:

1) Hendricks, M.H. 1970. Measurement of enzyme laundry detergent product dust levels and characteristics in consumer use. J. Am. Oil Chem. Soc. 47:207-211.

2) HERA. 2004. Linear Alkylbenzene Sulphonate, LAS. Human & Environmental Risk Assessment on ingredients of European household cleaning products. Version 2.0, May 2004. http://www.heraproject.com/RiskAssessment.cfm

2. PHYSICAL-CHEMICAL DATA

2.1 MELTING POINT

(a)

Value:	198.5°C
Decomposition:	Onset at 444°C (47% weight loss at 500°C)
Method:	Thermal analysis was performed on the Netzsch DSC 204C and TG209C with N_2 atmosphere.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	C_{10-14} Monoalkylbenzene sulfonic acid, sodium salt (CAS #85117-50-6); mean molecular weight = 348, average alkyl chain length = $C_{12.0}$. The test material is a commercial product, contains 85% active matter and is a coarse, cream-colored powder at 25°C.
Remarks:	This measured melting point value is significantly lower than the EPI Suite estimated values for other LAS materials. Note that the activity represents the total percent active materials (LAS, iso-LAS and DATS) in the test substance. The nonactive material in a powdered sample of LAS is likely sodium sulfate and other salts which have very high melting points (e.g., sodium sulfate = 884°C) and would not interfere with the measurement of the LAS melting point.
Reference:	Huntsman. 2002. Report of melting point analysis for NANSA HS 85/5. Cover memo from A. Ashworth to K.B. Sellstrom dated April 12, 2002.
Reliability:	2 Valid with restrictions

(b)

Value:	274°C
Decomposition:	Not identified
Method:	Estimation: EPI Suite (Mean or Weighted MP)
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	C_{10} LAS (CAS #1322-98-1)
Remarks:	Structure modeled is the pure C_{10} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference:	USEPA. 2000. EPI Suite v3.10.
Reliability:	2 Valid with restrictions. Standard EPA estimation software.

(c)

Value:	279°C
Decomposition:	Not identified
Method:	Estimation: EPI Suite (Mean or Weighted MP)
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	C_{11} LAS (CAS #27636-75-5)
Remarks:	Structure modeled is the pure C_{11} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference:	USEPA. 2000. EPI Suite v3.10.
Reliability:	2 Valid with restrictions. Standard EPA estimation software.

(d)

Value:	284°C
Decomposition:	Not identified
Method:	Estimation: EPI Suite (Mean or Weighted MP)
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	C_{12} LAS (CAS #25155-30-0)
Remarks:	Structure modeled is the pure C_{12} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference:	USEPA. 2000. EPI Suite v3.10.

Reliability: 2 Valid with restrictions. Standard EPA estimation software.

(e)
Value: 290°C
Decomposition: Not identified
Method: Estimation: EPI Suite (Mean or Weighted MP)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{13} LAS (CAS #26248-24-8)
Remarks: Structure modeled is the pure C_{13} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

2.2 BOILING POINT

(a)
Decomposition: Onset at 444°C (47% weight loss at 500°C)
Method: Thermal analysis was performed on the Netzsch DSC 204C and TG209C with N_2 atmosphere.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: $C_{10\text{-}14}$ monoalkylbenzene sulfonic acid, sodium salt (CAS #85117-50-6); mean molecular weight = 348, average alkyl chain length = $C_{12.0}$. The test material is a commercial product, contains 85% active matter and is a coarse, cream-colored powder at 25°C.
Remarks: Note that the activity represents the total percent active materials (LAS, iso-LAS and DATS) in the test substance. The nonactive material in a powdered sample of LAS is likely sodium sulfate and other salts which have very high melting points (e.g., sodium sulfate = 884°C) and would not interfere with the measurement of the LAS melting point.
Reference: Huntsman. 2002. Report of melting point analysis for NANSA HS 85/5. Cover memo from A. Ashworth to K.B. Sellstrom dated April 12, 2002.
Reliability: 2 Valid with restrictions

(b)
Value: 630°C
Method: Estimation: EPI Suite (Adapted Stein & Brown method)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{10} LAS (CAS #1322-98-1)
Remarks: Structure modeled is the pure C_{10} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

(c)
Value: 642°C
Method: Estimation: EPI Suite (Adapted Stein & Brown method)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{11} LAS (CAS #27636-75-5)
Remarks: Structure modeled is the pure C_{11} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

(d)
Value: 654°C
Method: Estimation: EPI Suite (Adapted Stein & Brown method)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{12} LAS (CAS #25155-30-0)
Remarks: Structure modeled is the pure C_{12} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

(e)
Value: 665ºC
Method: Estimation: EPI Suite (Adapted Stein & Brown method)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{13} LAS (CAS #26248-24-8)
Remarks: Structure modeled is the pure C_{13} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

2.3 DENSITY

(a)
Type: Bulk density **[ ]**; Density **[ ]**; Relative Density **[X]**
Value: 1.06 g/cm^3
Temperature: 20°C
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: Marlon A 390 (CAS #68411-30-3) $C_{10\text{-}13}$ LAS, average alkyl chain length = $C_{11.6}$
Remarks: Source cited in IUCLID is Sicherheitsdatenblatt "Marlon A 390; Huels Ag. vom 03.12.93
Reference: Cited in IUCLID Data Sheet for CAS #68411-30-3.
Reliability: 4 Not assignable. Original report not available for review.

(b)
Type: Bulk density **[X]**; Density **[ ]**; Relative Density **[ ]**
Value: 0.45 g/cm^3 (450 kg/m^3)
Temperature: 20°C
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test Substance: $C_{10\text{-}14}$ monoalkylbenzene sulfonic acid, sodium salt (CAS #85117-50-6); mean molecular weight = 348, average alkyl chain length = $C_{12.0}$. The test material is 85% active matter and is a coarse, cream-colored powder at 25°C.
Reference: Huntsman 2002. Report on the melting point analysis for NANSA HS 85/S. Attached technical bulletin dated 04-01-1994. Cover memo from A. Ashworth to K.B. Sellstrom dated April 12, 2002.
Reliability: 4 Not assignable. Original report not available for review.

(c)
Type: Bulk density **[X]**; Density **[ ]**; Relative Density **[ ]**
Value: ca. 550 kg/m^3
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: Marlon A 390 (CAS #68411-30-3) $C_{10\text{-}13}$ LAS, average alkyl chain length = $C_{11.6}$
Remarks: Source cited in IUCLID is Sicherheitsdatenblatt "Marlon A 390; Huels Ag. vom 03.12.93

Reference: Cited in IUCLID Data Sheet for CAS #68411-30-3.
Reliability: 4 Not assignable. Original report not available for review.

2.4 VAPOR PRESSURE

(a)
Value: 3×10^{-13} Pa
Method: Calculation
Test Substance: C_{12} LAS (CAS #25155-30-0)
Remarks: Cites estimates calculated by Lyman (see References).
Reference: 1) HERA. 2002. HERA-LAS Human and Environmental Risk Assessment: Linear Alkaylbenzene Sulphonates, LAS. CAS No. 68411-30-3, Draft #6, May 2002.
2) Lyman, W.J. 1985. Environmental exposure from chemicals, V.I, p.31, Neely, W.B., and Blau, G.E., editors. CRC Press. Boca Raton.
Reliability: 4 Not assignable. Original report not available for review.

(b)
Value: 2.88×10^{-12} Pa
Temperature: 25° C
Method: Estimation: EPI Suite (Modified Grain Method)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{10} LAS (CAS #1322-98-1)
Remarks: Structure modeled is the pure C_{10} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v.3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

(c)
Value: 1.22×10^{-12} Pa
Temperature: 25ºC
Method: Estimation: EPI Suite (Modified Grain Method)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{11} LAS (CAS #27636-75-5)
Remarks: Structure modeled is the pure C_{11} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v.3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

(d)
Value: 5.13×10^{-13} Pa
Temperature: 25ºC
Method: Estimation: EPI Suite (Modified Grain Method)
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{12} LAS (CAS #25155-30-0)
Remarks: Structure modeled is the pure C_{12} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v.3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

(e)
Value: 2.16×10^{-13} Pa
Temperature: 25ºC
Method: Estimation: EPI Suite (Modified Grain Method)
GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test Substance: C_{13} LAS (CAS #26248-24-8)
Remarks: Structure modeled is the pure C_{13} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v.3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

2.5 PARTITION COEFFICIENT $log_{10}P_{ow}$ ($log_{10}K_{ow}$)

(a)
Log Pow: 3.32
Method: Calculation
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: $C_{11.6}$ LAS
Remarks: Calculated for $C_{11.6}$ LAS using the QSAR method of Leo and Hansch (1979) as modified by Roberts (1991) for surfactant structures. This takes into account the various phenyl positions along the linear alkyl chain. See the Roberts (1991) summary at 2.5(g) for a full description of the method modifications.
Reference: 1) HERA. 2002. HERA-LAS Human and Environmental Risk Assessment: Linear Alkylbenzene Sulphonates, LAS. CAS No. 68411-30-3, Draft #6, May 2002.
2) Leo, A.J. and Hansch, C. 1979. Substituent Constants for Correlation Analysis in Chemistry and Biology. J. Wiley & Sons, N.Y.
3) Roberts, D.W. 1991. QSAR issues in aquatic toxicity of surfactants. Sci. Total Environ. 109/110:557-568.
Reliability: 2 Valid with restrictions. These results are considered reliable because a standard calculation technique was employed.

(b)
Log Pow: 1.94
Method: Estimation: EPI Suite
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{10} Decylbezene sulfonic acid, sodium salt (CAS #1322-98-1)
Remarks: Structure modeled is the pure C_{10} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

(c)
Log Pow: 2.43
Method: Estimation: EPI Suite
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{11} LAS (CAS #27636-75-5)
Remarks: Structure modeled is the pure C_{11} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

(d)
Log Pow: 2.92
Method: Estimation: EPI Suite
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{12} LAS (CAS #25155-30-0)

Remarks: Structure modeled is the pure C_{12} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

(e)
Log Pow: 3.42
Method: Estimation: EPI Suite
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{13} LAS (CAS #26248-24-8)
Remarks: Structure modeled is the pure C_{13} sodium salt homologue, 2-phenyl isomer, not the commercial material.
Reference: USEPA. 2000. EPI Suite v3.10.
Reliability: 2 Valid with restrictions. Standard EPA estimation software.

(f)
Remarks: In its review of LAS and related compounds, IPCS notes that while the octanol-water partition coefficient can be calculated in practice, it is impossible to measure P_{ow} for surface-active compounds like LAS. This has been confirmed by Roberts (2000).
Reference: 1) IPCS. 1996. Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates and Related Compounds. World Health Organization, Geneva, Switzerland.
2) Roberts, D.W. 2000. Use of octanol/water partition coefficient as hydrophobicity parameters in surfactant science. 5th World CESIO Congress 2:1517-1524, May-June 2000, Firenze, Italy.

(g)
Methods: Acute lethal toxicity data for a range of anionic and non-ionic surfactants were analyzed with the objective of determining whether QSARs can be developed relating toxicity to calculated log P values. Approaches to dealing with the deficiencies in the Leo and Hansch (1979) fragment method for calculating log P of surfactants (related to mixtures and phenyl isomer position) were developed and applied to the general narcosis QSAR of Könemann (1981) as represented by Equation 1:

$$\text{Log } (1/LC_{50}) = 0.87\log P + 1.13 \qquad \text{(EQ 1)}$$

(for 14-d LC_{50} tests on guppies; n = 50, r = 0.998, s = 0.237)

Mixtures
Two approaches were taken in this paper to address mixtures. In the first approach, P was calculated for each component individually then multiplied by the mole fraction and summed to give a weighted average log P. Alternatively, when only the overall average composition was known, log P was calculated for the average structure.

Phenyl isomer position
Since the fragment method gives values for log P that are independent of branch (i.e., phenyl isomer) position, a position-dependent branch factor (PDBF) was defined. Branching results in a decrease in the number of water molecules required to solvate the hydrocarbon chain by allowing water molecules to be shared between the two branches. Where both branches are long the water sharing effect should continue, although to a decreasing extent with increasing distance from the branching position, as long as the branches can be paired. To model this, a water sharing function log (CP + 1) was

defined in which CP is found by pairing off carbon atoms along the two branches up to the terminus of the shorter branch. Regression analysis correlating log ($1/LC_{50}$) to goldfish with a combination of ALP [representing log P calculated without a branch factor] and log (CP + 1) [representing the water sharing function]:

$$\text{Log } (1/LC_{50}) = 0.78\text{ALP} - 1.13 \log (\text{CP} + 1) + 2.06 \quad \text{(EQ 2)}$$

(for LC_{50} tests on guppies; n = 20, r = 0.997, s = 0.041)

Further, dividing the first two terms on the right of EQ 2 by 0.78 gave, assuming the role of the second term to be solely that of the branching factor, the following equation:

$$\text{Log P} = \text{ALP} - 1.44 \log (\text{CP} + 1) \quad \text{(EQ 3)}$$

Thus, the PDBF was defined as -1.44 log (CP + 1). Further details on this method are described in Roberts (1989).

Log P values calculated using EQ 3 were found to give good correlations with published river sediment sorption partition coefficients for LAS compounds, supporting the applicability and validity of the PDBF. Log P values calculated using EQ 3 were also used successfully in regression of toxicity data for pure LAS homologues and isomers to *Daphnia magna* and *Gammarus pulex*. The basic equation is similar to EQ 1 and has the general form:

$$\text{Log } (1/LC_{50}) = a\log \text{P} + b \quad \text{(EQ 4)}$$

with the values for a, b and regression data shown in the following table:

	***Daphnia* (H)**	***Daphnia* (S)**	***Gammarus* (H)**	***Gammarus* (S)**
Value of *a*	0.7	0.64	0.76	0.71
Value of *b*	2.23	2.44	2.46	2.27
Regression data				
n	9	12	9	11
r	0.987	0.955	0.966	0.950
s	0.07	0.15	0.13	0.16
F	263	103	98	83

Notes: H = hard water (250 mg/L $CaCO_3$); S = soft water (25 mg/L $CaCO_3$). Strongly negative outliers omitted.

The log P coefficients and intercepts for goldfish, *Daphnia*, and *Gammarus* are all intermediate between those of Könemann's QSAR equation (EQ 1), suggesting that a narcosis (possibly polar) mechanism applies to LAS acute toxicity.

Results: Agreement between observed and calculated toxicities for LAS is good. The fact that QSARs derived from compounds whose log P values are calculated with the PDBF give good predictions for unbranched compounds supports the validity of the PDBF for the type of branching encountered in LAS.

Remarks: The analyses presented in this paper indicates that the problems of calculating log P for surfactants can be overcome. The case for the applicability of the PDBF appears compelling, although it is based on indirect evidence. In terms of acute aquatic toxicity, anionic surfactants like LAS do not seem greatly different from unreactive non-surfactant organic chemicals. Anionic surfactants of various types have log ($1/LC_{50}$) values

which are well predicted on the basis of their calculated log P values by QSAR equations resembling those associated with the polar narcosis mechanism.

Reference: 1) Roberts, D.W. 1991. QSAR issues in aquatic toxicity of surfactants. The Science of the Total Environment 10/110:557-568.

2) Roberts, D.W. 1989. Aquatic toxicity of linear alkyl benzene sulphonates (LAS) – A QSAR Approach. Communicaciones presentadas a las Jornada del Comite Espanol de la Detergencia 20:35-43. Also in J.E. Turner, M.W. England, T.W. Schulz and N. J. Kwaak (Eds) QSAR 88. Proc. Third Int. Workshop on Quantitative Structure-Activity Relationships in Environmental Toxicology 22-26 May 1988, Knoxville, TN, pp. 91-98. Available from NTIS.

3) Könemann, H. 1981. Quantitative structure-activity relationships in fish toxicity studies: Part I. Relationships for 50 industrial pollutants. Toxicology 19:209-221.

4) Leo, A.J. and Hansch, C. 1979. Substituent Constants for Correlation Analysis in Chemistry and Biology, New York.

Reliability: 2 Valid with restrictions. Well documented QSAR analysis.

2.6 WATER SOLUBILITY

A. Solubility

(a)

Value: CMC = 0.1 g/L (C_{12} LAS)

Description: Miscible in water

Method: Surface tension of aqueous solutions of NaLAS was measured by an automated Lauda TE IC by the duNouy ring method. All solutions were prepared with water passed through a Nanopure water filter system and with sufficient salt to equalize the ionic strength. Solubility of commercial NaLAS was determined by slowly lowering the temperature in a Fisher Isotemp incubator over several days and recording the temperature at which the solutions first turned cloudy (cloud point). Clear points were determined by raising the temperature slowly over several days and recording when the solution cleared. The solubility of the C_{12} narrow-distribution phenyl isomers was determined by heating a saturated solution to 70°C for 0.5-3 h and then cooling to 5°C. After equilibrating to room temperature overnight, the cloudy mixture was centrifuged, and the clear supernatant drawn off, weighed, and dehydrated to determine percentage solids. The percentage dissolved was then calculated from the weight loss to the supernatant.

GLP: Yes **[ ]** No **[ ]** ? **[?]**

Test Substance: C_{12} LAS and commercial C_{11-13} LAS (sodium salts)

Remarks: Surface activity increased with increasing average alkyl chain length. Some decrease in surface tension was observed with increasing phenyl isomer number, but the range of phenyl isomer distribution of commercial products is not large enough to significantly alter the surface tension vs. log concentration plot. Increasing the average alkyl chain length of LAS decreases solubility (i.e., increases cloud point). The following table shows the critical micelle concentration (CMC) for various chain lengths LAS tested.

Chain length, isomer composition, dialkyltetralin sulfonate content	CMC (g/L)
C_{11} high 2-phenyl, low dialkyltetralinsulfonate	0.120
C_{11} high 2-phenyl, high dialkyltetralinsulfonate	0.120

C_{11} low 2-phenyl, low dialkyltetralinsulfonate	0.120
C_{12} low 2-phenyl, low dialkyltetralinsulfonate	0.105
C_{13} low 2-phenyl, low dialkyltetralinsulfonate	0.038

Reference: Smith, D.L. 1997. Impact of composition on the performance of sodium linear alkylbenzenesulfonate (NaLAS). JAOCS 74:837-845.
Reliability: 2 Valid with restrictions

(b)
Value: >250 g/L
Description: Miscible in water
GLP: Yes **[ ]** No **[ ]** ? **[?]**
Test Substance: Various LASs made from four commercial LABs, average alkyl chain length = 11.6
Remarks: The study shows that 25% solutions (250 g/L) of various LASs have cloud clear points (i.e., form clear solutions at rising temperatures) at temperatures of 2-21°C, depending on LAS composition. Cloud and clear points decrease dramatically with increasing 2-phenyl isomer composition. The results demonstrate that 25% solutions of LAS are soluble at room temperature.
Reference: Cohen, L., Vergara, R., Moreno, A. and Berna, J.L. 1995. Influence of 2-phenyl alkane and telralin content on solubility and viscosity of linear alkylbenzene sulfonate. JAOCS 72:115-122.
Reliability: 2 Valid with restrictions

(c)
Value: ca. 250 g/L
Temperature: 20°C
Description: Miscible in water
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: Marlon A 390 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks: Miscible with water at 20°C. Depending on the concentration, clear solutions (up to ~25% w/w) or inhomogeneous, viscous pastes were obtained. Sources cited are two reports by Huels AG dated 1988 and 1993.
Reference: Cited in IUCLID Data Sheet for CAS #68411-30-3.
Reliability: 4 Not assignable. Original report not available for review.

B. pH Value, pKa Value

(a)
pH Value: 10.0 ± 1.0 (1% solution)
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Remarks: C_{10-14} monoalkylbenzene sulfonic acid, sodium salt (CAS #85117-50-6); mean molecular weight = 348, average alkyl chain length = $C_{12.0}$
Reference: Huntsman 2002. Report on the melting point analysis for NANSA HS 85/S. Attached technical bulletin dated 04-01-1994. Cover memo from A. Ashworth to K.B. Sellstrom dated April 12, 2002.
Reliability: 4 Not assignable. Original report not available for review.

(b)
pKa Value: <1 for aromatic sulfonic acids such as benzosulfonic acid
Reference: Hodgman, C.D. 1961. Handbook of Chemistry and Physics, 43rd edition. The Chemical Rubber Publishing Company, Cleveland, Ohio.
Reliability: 4 Not assignable. Original data not available for review.

2.7 FLASH POINT *(liquids)*

Remarks: Not applicable.

2.8 AUTO FLAMMABILITY *(solid/gases)*

Remarks: Not applicable.

2.9 FLAMMABILITY

Remarks: Not applicable.

2.10 EXPLOSIVE PROPERTIES

Remarks: Not applicable.

2.11 OXIDISING PROPERTIES

Remarks: Not applicable.

2.12 OXIDATION: REDUCTION POTENTIAL

Remarks: Not applicable.

2.13 ADDITIONAL DATA

A. Henry's law constant

Value:	6.37 x 10^{-3} Pa m^3/mole
Method:	Estimation: EPI Suite
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test Substance:	LAS (CAS #25155-30-0)
Remarks:	Calculated using the bond method detailed in Meylan and Howard (1991) and the input parameters resident in the EPI Suite database. Assumes 25°C, molecular weight 348.48. Data reported in EPI Suite as 6.29 x 10^{-8} atm-m^3/mole and converted to Pa m^3/mole.
Reference:	1) USEPA. 2000. EPI Suite v3.10. 2) Meylan, W.M. and Howard, P.H. 1991. Bond contribution method for estimating Henry's law constant. Environ. Toxicol. Chem. 10:1283-1293.
Reliability:	2 Valid with restrictions. Standard EPA estimation software.

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

3.1.1 PHOTODEGRADATION

(a)

Type:	Air **[ ]**; Water **[X]**; Soil **[ ]**; Other **[ ]**
Light source:	Sunlight **[ ]**; Xenon lamp **[ ]**; Other **[X] Mercury vapor lamp**
Light spectrum:	200-350 nm
Concentration:	Initial LAS concentration 60 to 182 mg/1
Temperature:	28°C
Direct photolysis Degradation:	>95 % (weight/weight) after 20 minute (exposure time)
Indirect Photolysis Degradation:	Rapid photodegradation
Method:	A series of photodegradation studies were conducted. Aqueous solution of LAS (pH 6.75) were passed through an irradiated tubular flow reactor. Reaction rates were obtained for both non-sensitized conditions and when ferric perchlorate (0.04 to 3.15 x 10^{-4} g-mole/L) was used as a sensitizer. A Hanovia 1200-watt mercury-vapor lamp was the source of radiation. The LAS concentration was determined by the methylene blue method. Appropriate controls were used.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	LAS; activity: 95% (CAS #25155-30-0)
Remarks:	Complete conversion of LAS to intermediates at an average residence time as low as 1 minute. The maximum conversion to CO_2 was obtained at a residence time of 20 minutes and corresponded to 7 moles CO_2 per mole of LAS. Reaction rate increases by two orders of magnitude in presence of ferric perchlorate. Half order kinetics with respect to light intensity and LAS concentration explained the data for nonsensitized conditions. An appropriate rate equation could be derived by assuming a second-order deactivation of light-activated LAS molecules. The sensitized reaction was believed to occur by abstraction of hydrogen atoms from LAS by hydroxyl radicals. Hydroxyl radicals presumably are produced by an electron-transfer reaction involving light-activated ferric ions. The mechanism is complex; over-all kinetics indicated a first-order effect of (Fe^{+3}), 1.2 order in light intensity, and maxima in the rate for intermediate LAS and O_2 concentrations.
Reference:	Matsuura, T. and Smith, J.M. 1970. Kinetics of photodecomposition of dodecyl benzene sulfonate. Ing. Eng. Chem. Fund. 9:252-260.
Reliability:	2 Valid with restrictions

(b)

Type:	Air **[ ]**; Water **[X]**; Soil **[ ]**; Other **[ ]**
Light source:	Sunlight **[ ]**; Xenon lamp **[X]**; Other **[ ]**
Spectrum:	>330 nm
Concentration:	50 mg/L
Temperature:	25°C; during photolysis the solution temperature reached 35-40°C.
Indirect Photolysis:	
Type of sensitizer:	TiO_2 suspension
Degradation:	Rapid photodegradation of LAS (<1 to 2 hours)
Method:	A study was conducted to determine the photodegradation of LAS in aqueous TiO_2 dispersions. Experiments were carried out with 25 mL solutions containing LAS surfactant with TiO_2. Some experiments used open vessels (37 mL Pyrex glass reaction vessels) under aerobic conditions. Others used

vessels sealed with a rubber septum, the solution purged with argon and a fixed volume of oxygen injected. Spectrophotometric analysis was performed at regular intervals.

GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: LAS (CAS #25155-30-0)
Remarks: The reaction involves fast decomposition of the aromatic ring followed by slower oxidation of the aliphatic chain.
Reference: Hidaka, H., Kubata, H., Gratzel, M., Serpone, N. and Pelizzetti, E. 1985. Photodegradation of surfactants. I. Degradation of sodium dodecyl sulfonate in aqueous semiconductor dispersions. Nouveau J. Chemie 9:67-69.
Reliability: 2 Valid with restrictions

(c)
Type: Air **[ ]**; Water **[X]**; Soil **[ ]**; Other **[ ]**
Light source: Sunlight **[ ]**; Xenon lamp **[ ]**; Other **[X] Mercury lamp**
Light spectrum: 400-580 nm
Spectrum: 223 nm
Concentration: 100 mg/L H_20
Temperature: 20°C
Indirect Photolysis:
Type of sensitizer: Humic substances
Results: Photodegradation of LAS was reduced by humic substances by a factor of 2 or more. The aliphatic side chains are degraded first, followed by aromatic ring cleavages. Degradation follows first order kinetics both with and without the presence of humics.
Method: The effects of humics on the photolytic degradation of LAS was studied. Soil humic substances were extracted by a cationic exchange resin/water suspension from a humic podzol. Water-soluble synthetic humic substances were prepared by autoxidation of pyrogallol in alkaline solution. Aqueous solutions of 15 mg/L humic substance and 100 mg/L LAS were irradiated with a mercury lamp. Photometric measurements were performed with a spectrophotometer for recording the changes caused by photolysis at definite times at 223 nm for LAS.
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: LAS (CAS #25155-30-0)
Remarks: The presence of humic substances delays photodegradation of LAS, primarily because they act as UV-absorbers. The reaction between humics and LAS is dominated by electrostatic repulsion because of the negatively charged components at the given pH. The hydrophobic interaction between humics and LAS is relatively weak compared to the electrostatic repulsion. Possibly the sulfonic groups from LAS may be bound by metal bridges to humic surfaces. The study used humic substance with a relatively high proportion of aromatic carbon; whereas a lower proportion is more typical in natural environments. Therefore, the difference in photolysis rate is likely to be less pronounced.
Reference: Hermann, R., Gerke, J. and Ziechmann, W. 1997. Photodegradation of the surfactants LAS and dodecylpyridinium-chloride as affected by humic substances. Water, Air, and Soil Pollution 98:45-55.
Reliability: 2 Valid with restrictions

3.1.2 STABILITY IN WATER

Type: Abiotic (hydrolysis) **[X]** ; biotic (sediment)**[ ]**
Results: LAS is stable in water.
GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance:	C_{10-13} alkylbenzene sulfonic acid, sodium salt (CAS #68411-30-3)
Remarks:	LAS can be decomposed at extreme conditions such as elevated temperatures in the presence of inorganic acids such as phosphoric, sulphuric and hydrochloric acid, e.g.: 60-70% sulphuric acid at 140 - 190 degree C or with concentrated HCl in a sealed container at 150 - 200 degree C. Information as cited in IUCLID Data Sheet for CAS #68411-30-3 and in an analytical textbook.
Reference:	Cross, J. and Dekker, M. (ed.). 1977. Anionic surfactants: Chemical analysis. Vol.8. Pp. 111-115.
Reliability:	4 Not assignable. Original studies not available for review.

3.1.3 STABILITY IN SOIL

(a)

Type:	Laboratory
Radiolabel:	Yes **[X]** No **[ ]** ? **[ ]**
Concentration:	27.2 mg/kg (Ecosystem Section I) and 16.2 mg/kg (Ecosystem Section II) (initial amounts in dry soil); 0.44 mg/kg (I) and 0.19 (II) (at end of trials)
Temperature:	Room temperature
Dissipation Time:	DT_{50} = 13-26 days
Method:	Soil cores taken from two ecosystems were collected and placed in a climate controlled "plant metabolism box". Ecosystem Section I consisted of a heavy clay-like soil. Ecosystem Section II consisted of loose, sandy soil. Radiolabeled LAS (a defined mixture) absorbed to digested sludge was incorporated into the soils, after which the soils were planted with either grass, bush beans and radishes (Section I) or potatoes (Section II). The test systems were maintained under a defined standard climate (i.e., an average day in June in Northern Germany) for the vegetative period (76 and 106 days, respectively for Sections I and II). At the end of the growing season samples were collected from plants and soil and subjected to radioanalysis.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test Substance:	LAS. The authors state that they tested a defined mixture of LAS, but do not report the composition in this paper.
Remarks:	Correponding to Ecosystem Sections I and II, 63.6% and 72.3% of initial radioactivity went to the atmosphere (primarily as CO_2), 26.8% and 18.3% were detected in soil cores, 6.6% and 5.9% were present in biomass, and 0.99% and 1.4% leached out with percolated water. The study shows that LAS adsorbed to digested sludge is relatively rapidly converted to CO_2 and, to a lesser extent, polar organic secondary products in the upper soil layers. LAS and the secondary products are strongly adsorbed to the topsoil. LAS introduced into the topsoil by repeated application of sludge did not accumulate in the soil. Growth of crops is not impaired; the use of LAS-containing sludge had no adverse effect on the biomass yield (crop yield) under regulated use conditions.
Reference:	Figge, K. and Schoberl, P. 1989. LAS and the application of sewage sludge in agriculture. Tenside Surf. Det. 26:122-128.
Reliability:	2 Valid with restrictions

(b)

Type :	Field trial **[ ]**; Laboratory **[X]**; Other **[ ]**
Radiolabel:	Yes **[X]** No **[ ]** ? **[ ]**
Concentration:	0.05 mg/kg
Soil temperature:	Probably room temperature
Soil humidity:	80% of water holding capacity
Soil classification:	DIN19863 **[ ]**; NF X31-107 **[ ]**; USDA **[ ]**; Other **[X]** mainly U.S. Soil

	Conservation Service soil type designation, by Howard Laboratories, Dayton, Ohio
Organic Carbon:	1.4 - 50%
Soil pH:	4.9 - 8.4
Cation exchange capacity:	0.15 meg/100 g soil dry weight
Microbial biomass:	Activity in dpm/h/gdw soil varied from 11,327 to 51,683
Dissipation time:	DT_{50} : 1.1 - 3.7 days
Method:	other: described in reference
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{13} LAS (CAS #26248-24-8); activity 98%
Remarks:	Half-lives ranged from 1.1 to 3.7 days (mineralization). First order dissipation rate constants ranged from 0.14 - 0.63/day. Mineralization occurred without a lag-period in every soil tested. Cycles of wetting and drying in the lab prior to testing resulted in more rapid and extensive mineralization. Community microbial activity did not correlate with rate or extent of mineralization. Microbial communities have indigenous ability to degrade low LAS concentrations, the ability is present in a wide array of soil types from various locations. 1. Soil Alpine, sand, pH 5.5, CEC 0.15, TOC 50 (mg/g) 2. Soil Bonnell, sandy loam, pH 8.4, CEC 29, TOC 31.6 3. Soil Brashear, silt loam, pH 7.7, CEC 37, TOC 24.9 4. Soil Eden, silt loam, pH 7.4, CEC 33, TOC 45.1 5. Soil Eden, loamy sand, pH 6.1, CEC 41, TOC 19.6 6. FL soil, sand, pH 4.9, CEC 6.3, TOC 13.8 7. GA soil, loamy sand, pH 4.9, CEC 15.5, TOC 1.4 8. Soil Huntington, loam, pH 7.3, CEC 24, TOC 20.1 9. Soil Lakin, loam, pH 6.5, CEC 24, TOC 34.6 10. Soil Pate, silt loam, pH 7.7, CEC 46, TOC 48.0.
Reference:	Knaebel, D.B., Federle, T.W. and Vestal, J.R. 1990. Mineralisation of linear alkylbenzene sulfonate (LAS) and linear alcohol ethoxylate (LAE) in 11 contrasting soils. Envir. Toxicol. Chem. 9:981-988.
Reliability:	2 Valid with restrictions
(c)	
Type :	Field trial **[X]**; Laboratory **[ ]**; Other **[ ]**
Radiolabel:	Yes **[ ]** No **[X]** ? **[ ]**
Dissipation time:	DT_{50} : 7 - 22 days
Results:	In fields not recently spread with sludge, the concentrations of LAS found in the sludge amended soil were generally less than 1 mg/kg. This represents an estimated loss of LAS from soil of >98%. In fields recently spread, the concentrations in soil are in the range of <0.2 to 20 mg/kg, representing losses of LAS between 70 and 99% of the estimated total cumulative load. The authors conclude that overall the data indicate that an adequate safety margin exists between the concentrations of LAS in sludge-amended soils and those likely to affect the growth of crop plants.
Method:	The disappearance of LAS from sludge-amended soils was investigated from 51 fields on 24 farms in the Thames Water Authority, U.K. Annual sludge spreading averaged 6 ton/ha. Application of sludge was made by subsurface injection, surface spreading onto arable land with or without ploughing, or surface spreading onto pasture land. Regular sampling was conducted for up to 122 days. LAS concentrations in the soil were analyzed with HPLC.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	Commercial LAS as present in primary sludge or anaerobically digested sludge from WWTPs in the United Kingdom.

Remarks:	Half-lives compare well with those for ultimate degradation in lab soil tests (with .....14-C-evolution), indicating that the degradation of LAS does not lead to the ... formation of significant levels of break-down intermediates in soil. The homologue distribution of LAS in soil suggests that removal represents biodegradation rather than leaching.
Reference:	1) Holt, M.S., Matthijs, E. and Waters, J. 1989. The concentrations and fate of linear alkylbenzene sulphonate in sludge amended soils. Wat. Res. 23:749-759. 2) Waters, J., Holt, M.S., Matthijs, E. 1989. Fate of LAS in sludge amended soils. Tenside Surfactants Detergents 26(2):129-135.
Reliability:	2 Valid with restrictions

(d)

Type:	Laboratory
Radiolabel:	Yes **[ ]** No **[X]** ? **[ ]**
Concentration:	8 to 488 mg/kg
Soil Composition:	Coarse sand 67%, fine sand 16%, silt 8.6%, clay 6.2% and humus 2.7%
Organic Carbon:	1.5%
Method:	LAS mixed with sewage sludge was applied to sandy agricultural soil and incubated for up to 8 weeks. Various microbial soil parameters were measured (see Section 4.4). LAS was quantified after methanol extraction using HPLC.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test Substance:	C_{10-13} LAS obtained as an aqueous sodium salt solution with a LAS content of 16.1% (w/w), NA-LAS average molecular weight = 342 g/mol, distribution: C_{10} 14%, C_{11} 34%, C_{12} 31%, and C_{13} 21%.
Results:	For nominal concentrations of 8 to 62 mg/kg, the depletion of LAS after 2 weeks was more than 73%. At 488 mg/kg, only 15% depletion occurred. It is possible that this high LAS level may have inhibited microbial activity or caused a prolonged log phase to occur.
Reference:	Elsgaard, L. Petersen, S.O. and Debosz, K. 2001b. Effects and risk assessment of linear alkylbenzene sulfonates in agricultural soil. 2. Effects on soil microbiology as influenced by sewage sludge and incubation time. Environmental Toxicology and Chemistry. 20:1664-1672.
Reliability:	2 Valid with restrictions

(e)

Type :	Field trial **[X]**; Laboratory **[X]**; Other **[ ]**
Radiolabel:	Yes **[ ]** No **[X]** ? **[ ]**
Soil Content:	Clay 1.8 - 4%, Silt 7.6 - 18.5 %, Sand 77.1 - 95.5%
Organic Carbon:	Ranged from 0.9 - 1.79%
Soil pH:	5.2 – 6.8
Dissipation time:	DT_{50}: 3 days (lysimeters) DT_{50}: 7 days (field trials)
Method:	Sewage sludge containing LAS was added to four cultivated sandy soils with low amounts of organic matter in field trials and lysimeter studies. The field trial lasted one year. For the lysimeter studies, undisturbed soil columns were taken from the corresponding field sites.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	Marlon A350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = 11.6; activity: 50%
Remarks:	LAS are mobile in all four soils tested. They were detected down to a depth of 30-40 cm after being applied at the surface. After one week, a concentration of 500 mg/kg was measured in the 0-5 cm layer, which corresponds to 23% of the the total LAS. In the 5-10 cm layer, the

concentration was measured at 9.5 mg/kg (approximately 4%). Very little reached the 30-40 cm layer, although a value significantly above the limit of detection (0.050 mg/kg) was determined. No leaching was observed out of the soil columns and disappearance of LAS in the field trials was attributed to rapid biodegradation in the soil (approximately 99% of the total LAS was biodegraded after 42 days). The half-life was determined to be 3 days. There was a noticeable shift to shorter alkyl chain length homologues in the percolating water (i.e., longer alkyl chains were retained more strongly). These shorter chain length homologues have a lower toxicity.

Reference: Kuchler, T. and Schnaak, W. 1997. Behaviour of linear alkylbenzene sulfonates (LAS) in sandy soils with low amounts of organic matter. Chemosphere. 35:153-167.

Reliability: 2 Valid with restrictions

(f)

Type : Field trial **[ ]**; Laboratory **[X]**; Other **[ ]**

Radiolabel: Yes **[X]** No **[ ]** ? **[ ]**

Concentration: 250 mg/kg

Soil temperature: 20°C

Soil humidity: 35 g water/100g soil dry weight

Soil pH: 6.9 - 7.1

Dissipation time: DT_{50} : 15.8 - 25.7 day

Method: Assays were conducted in flow-through microcosms with 15 g (dry wt) of soil adjusted to a 35% moisture level. The test substances were ^{14}C ring labelled LAS pure homologues (C_{10}, C_{11}, C_{12}, C_{13}, C_{14}) which were premixed with digester sludge and added to flasks at an initial concentration of 2.5, 25 or 250 mg/kg. $^{14}CO_2$ evolution was determined by LSC. The first-order biodegradation rate constant was estimated using non-linear regression techniques. The study was conducted in both sandy loam and loamy sand soil types.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: Pure LAS homologues C_{10-14} tested concurrently.

Results: The biodegradation rates followed first order kinetics over a wide range of concentrations and chain lengths. Half-lives (mineralization) were reported as C_{10} 21 days; C_{11} 25.7 d; C_{12} 23.1 d; C_{13} 18.2 d; C_{14} 17.8 d in sandy loam; C_{10} 16.5 d and C_{14} 15.8 d in loamy sand. The degradation rate constants were C_{10} 0.033/d; C_{11} 0.027/d, C_{12} 0.030/d, C_{13} 0.038/d, C_{14} 0.039/d in sandy loam; C_{10} 0.042/d C_{14} 0.044/d in loamy sand Mineralisation efficiency averaged 65%. The remaining radiolabel was incorporated into microbial biomass or soil humic material.

Remarks: Half-lives for mineralization of the benzene ring, the rate-limiting step for LAS degradation, ranged from 18 to 26 days.

Reference: Ward, T.E. and Larson, R.J. 1989. Biodegradation kinetics of LAS in sludge-amended agricultural soils. Ecotox. and Environ. Safety 17:119-130.

Reliability: 2 Valid with restrictions

(g)

Type: Field trial **[ ]**; Laboratory **[ ]**; Other **[X] Greenhouse pot**

Radiolabel: Yes **[ ]** No **[X]** ? **[ ]**

Concentration: 3.7 to 5.1 g/kg dry wt

Soil composition: Clay 3.7 %, Silt 3.1 %, Fine Sand 19.5 %, Coarse Sand 71.4 %

Organic Carbon: 1.3%

Soil pH: 5.9

Cation exchange capacity: 10.7 cm/kg

Microbial biomass: not stated

Method: Sewage sludge was incorporated into a sandy soil to give a range of very low to very high applications (0.4 to 90 mg/ha dry weight). LAS was added as water solutions to this mixture. The soil was transferred to pots and sown with barley, rape, or carrot and allowed to grow for 19, 85, and 30 days, respectively in a greenhouse. Plant-free controls were also established. Samples were collected of the soil and analyzed for total LAS and for individual homologues.
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: LAS C_{10-13}, Approximate composition at start of study: C_{10} 3%, C_{11} 22%, C_{12} 40%, C_{13} 35%
Results: LAS was not taken up by plants and its degradation in soil increased by the presence of crop plants with concentration decreasing in rape from 27 mg/kg (dry soil) to 0.7 - 1.4 mg/kg (dry soil) at harvesting after 30 days. During degradation, the relative fraction of homologues C_{10}, C_{11}, and C_{12} decreased, while C_{13} increased.
Reference: Mortensen, G.K., Elsgaard, H., Ambus, P., Jensen, E.S., and Gron, C. 2001. Influence of plant growth on degradation of linear alkylbenzene sulfonate in sludge-amended soil. J. Environ. Qual. 30:1266-1270.
Reliability: 2 Valid with restrictions

(h)
Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X]**
Medium: Sludge modified soils
Method: LAS biodegradation and its kinetic parameters were studied in a land filling operation using sludges (15%) blended with soil (85%) at a site in Spain. Once the soil was blended with the sludges, grab samples were taken in three different zones of the plot. All samples were blended every day in order to have a daily composite sample. Immediately after sampling, all samples were frozen and then sieved to a 2 mm particle size. The sampling was conducted on 10 different days over a period of 62 days. LAS determination in sludge-modified soils was carried out by HPLC-UV. Degradation was determined based on LAS concentrations measured on the 10 sampling days.
Results: Average LAS concentrations on the 10 sampling days were 155, 55.6, 28.0, 30.2, 35.2, 28.2, 31.6, 35.1, 19.3 and 16.7 for days 0, 6, 15, 20, 27, 34, 41, 48, 55 and 62, respectively. The biodegradation level reached after 62 days was 89.2%. Assuming first order kinetics, the half-life is 19.3 days.
Remarks: LAS adsorbed or precipitated on anaerobic sludges is biodegraded during soil amendment operations by commonly occurring micro organisms. The table shows a shift in the percent homologue distribution on days 0 and 62, demonstrating that higher molecular weight homologues exhibit stronger soil adsorption.

% phenyl homologue	Day 0	Day 62
C_{10}	3.7	1.2
C_{11}	29.4	18.7
C_{12}	41.4	48.9
C_{13}	25.5	31.2

Reference: de Ferrer, J., Moreno, A., Vaquero, M.T. and Comellas, L. 1997. Monitoring of LAS in direct discharge situations. Tenside Surf. Det. 34:278-283.
Reliability: 2 Valid with restrictions

3.2 MONITORING DATA (ENVIRONMENTAL)

(a)
Type of Measurements: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Mississippi River**
Medium: Surface Water
Results: LAS was detected in 16% of the 323 mainstem samples collected during the upstream sampling cruises at concentrations ranging from 0.1 to 10.3 μg/L, and in 15% of the 39 tributary samples at concentrations ranging from 0.1 to 2.8 μg/L. LAS was detected in 21% of the 38 mainstem composite samples collected during the downstream cruises at concentrations ranging from 0.1 to 2.8 μg/L and was not detected in any of the 16 tributary composite samples. LAS was detected in 85% of the 34 samples collected from the Thebes time-series site at concentrations ranging from 0.4 to 28.2 μg/L.
Remarks: The 2,800 km reach of the Mississippi River between Minneapolis and New Orleans was examined for the occurrence of LAS. River water was sampled in the summer and fall of 1991 and in the spring of 1992 during upstream and downstream sampling cruises. LAS was analyzed using solid-phase extraction and gas chromatography/mass spectrophotometry. The range of average chain length for all dissolved LAS was 10.2-12.0, with an average of 11.1. The removal of the higher LAS homologues and external isomers indicates that sorption and biodegradation are the principle processes affecting dissolved LAS.
Reference: Tabor, C.F. and Barber, L.B. 1996. Fate of linear alkylbenzene sulfonate in the Mississippi River. Environ. Sci. Technol. 30:161-171.
Reliability: 2 Valid with restrictions

(b)
Type of Measurements: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Mississippi**
Medium: Sediment
Results: LAS was present on all bottom sediments (33 locations) at concentrations ranging from 0.01 to 20 mg/kg dry matter. It should be noted that all concentrations were <0.1 mg/kg with the exception of the one extremely high level of 20 mg/kg. The 20 mg/kg sample was found at Pig's Eye Slough, the canal carrying the Minneapolis STP effluent to the the Mississippi River. All concentrations are dry weight.
Remarks: The 2,800 km reach of the Mississippi River between Minneapolis and New Orleans was examined for the occurrence of LAS. Bottom sediment was sampled in the summer and fall of 1991 and in the spring of 1992. Composite samples were collected at 25 locations during the downstream leg of each cruise. These samples consisted of 5-7 individual sediment samples on each of 2-3 transects in each pool. In addition, grab samples were taken at 8 other locations during the downstream cruise. LAS was analyzed using solid-phase extraction and gas chromotography/mass spectrophotometry. The average chain length for sorbed LAS ranged from 10.7 to 12.5, with an average of 11.5. Sorbed LAS appears to degrade slowly.
Reference: Tabor, C.F. and Barber, L.B. 1996. Fate of linear alkylbenzene sulfonate in the Mississippi River. Environ. Sci. Technol. 30:161-171.
Reliability: 2 Valid with restrictions

(c)
Type of Measurements: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Rivers in USA**
Medium: Influents, effluents, and surface water
Results: Average LAS influent concentrations ranged from 4.2-5.7 mg/L among the various types of treatment plants. LAS removal rates averaged 99.3% for activated sludge (n = 15), 98.0-98.5% for lagoon/oxidation ditch (n = 14), 96.2% for rotating biological contact (n = 9) and 77.4% for trickling filters (n = 12). Concentrations of LAS below the mixing zone of wastewater treatment plants were generally below 50 μg/L, even though the samples

were collected under low flow (i.e., low dilution) conditions. The mean surface water concentrations ranged from <10 to 330 µg/L, with mean values of 42 to 46 µg/L. The highest concentration was observed in a low (less than 3-fold) dilution irrigation canal below a trickling filter plant. All other values were <180 µg/L, with more than 80% of the sites below 50 µg/L.

Remarks: Surface water samples were collected in rivers at 50 locations in 11 states below wastewater treatment plants. Alkyl chain lengths of LAS averaged 12.0 carbon units in most environmental compartments, with the exception of sludge solids and river sediments, in which an enrichment of longer chain lengths was observed. Since several of the wastewater treatment plants included in this study have dilution factors less than 3, these values include worst case estimates.

Reference: McAvoy, D.C., Eckhoff, W.S. and Rapaport, R.A. 1993. Fate of linear alkylbenzene sulfonate in the environment. Environ. Toxicol. Chem. 12:977-987.

Reliability: 2 Valid with restrictions

(d)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Rivers in U.S.A.**

Medium: sediment

Results: Below outfall of trickling filter treatment plant: 190 ± 95 mg/kg dry matter
< 5 miles downstream: 11.9 ± 9.5 mg/kg dry matter;
> 5 miles downstream: 5.3 ± 4.7 mg/kg dry matter

Remarks: Monitoring studies for LAS in river sediment in Rapid Creek, USA below the outfall of a trickling filter sewage treatment plant. Compiled by Procter & Gamble between 1973 and 1986.

Reference: Rapaport, R.A. and Eckhoff, W.S. 1990. Monitoring linear alkylbenzene sulfonate in the environment: 1973-1986. Environ. Toxicol. Chem. 9:1245-1257.

Reliability: 2 Valid with restrictions

(e)

Type of Measurement: Background **[X]**; At contaminated site **[ ]**; Other **[X]**

Medium: Sewage treatment influents & effluents; rivers and sediments.

Results: The removal from four activated sludge and five trickling filter wastewater treatment facilities averaged 99.5% & 82.9% for LAS and 99.1% and 97.3% for LAS intermediate, respectively, for the activated sludge and trickling filter facilities.

Remarks: LAS concentrations in receiving waters downstream of four activated sludge treatment plants ranged from 0.002 to 0.081 mg/L. LAS concentrations in receiving waters downstram of five trickling filter treatment plants ranged from 0.004 to 0.094 mg/L. Upstream LAS concentrations ranged from <0.001 to 0.110 mg/L and <0.001 to 0.005 mg/L for the activated sludge and trickling filter treatment plants, respectively.

Reference: Trehy, M.L., Gledhill, W.E., Mieure, J.P., Adamove, J.E., Nielsen, A.M., Perkins, H.O. and Eckhoff, W.S. 1996. Environmental monitoring for linear alkylbenzene sulfonates, dialkyltetralin sulfonates and their biodegradation intermediates. Environmental Toxicology and Chemistry 15:233-240.

Reliability: 2 Valid with restrictions

(f)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] concentrations in sludge from waste water treatment plants**

Medium: sludge

Results: (A) Conc. In sludge 0.7 and 0.4 g LAS/kg of dry matter (data from 2 plants)
(B) Conc. In sludge 0.5 and 0.1 g LAS/kg of dry matter (data from 2 plants)

(C) Conc. In sludge 30.2; 12.8; 11.4; 7.0 and 7.5 g LAS/kg of dry matter (from 5 plants)

Remarks: (A) Plants with aeration/settling system
(B) Plants with activated sludge & aerobic digestion of sludges system
(C) Plants with activated sludge & anaerobic digestion of sludges.
The concentrations in sludge correlate with water hardness. The higher the water hardness, the greater the amount of calcium-precipitated LAS in the sludge. For example, the water hardness that resulted in the 30.2 g/kg value was >500 mg/L as calcium carbonate. This level of hardness is very high and is 2-3 times higher than the more typical range of 200-300 mg/L as calcium carbonate. The amount of LAS physically removed to the sludge during primary settleing versus biodegradaded can be seen in the following table.

Treatment Plant (all from category C)	Physical Removal	LAS Biodegradation	Water Hardness (as mg/L $CaCO_3$)
Alicante	35%	68.2%	>500
Sevilla S.E.	30%	75.6%	220
Sevilla N.	27%	87%	315
La China (Madrid)	16%	91%	<100
Viveros (Madrid)	15%	91.2%	<100

Reference: Berna, J.L., de Ferrer, J., Moreno, A., Prats, D., Ruiz Bevia, F. 1989. The fate of LAS in the environment. Tenside Surfactants Detergents 26(2):101-107.

Reliability: 2 Valid with restrictions

(g)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] STP effluent in the UK**

Medium: Final effluent

Results: Final effluent concentration of LAS from four trickling filter STPs ranged from 40 to 430 µg/L (mean 80 to 300 µg/L).

Remarks: Removal from trickling filter STPs averaged 92.9%

Reference: Holt, M.S., Daniel, M., Buckland, H. and Fox, K.K. 2000. Monitoring studies in the UK designed for validation of the Geo-Referenced Exposure Assessment Tool for European Rivers (GREAT-ER), 5th World CESIO Congress. V.2:1358-1369, Firenze, Italy.

Reliability: 2 Valid with restrictions

(h)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Lambro River (Italy)**

Results: Mean background LAS concentration downstream from the STP was 28 µg/L.

Remarks: A two year water quality monitoring program was conducted in the river Lambro (northern Italy) during the period March 1997 to May 1998. Prior to 1998, 40% of the local waste water was discharged untreated directly into the river. The plants were undersized activated sludge plants. From April to September 1997, grab samples were collected approximately once a month from 19 stations along the main channel of the river, its two main tributaries, and at two STPs located within the monitoring area. From November 1997 to May 1998, the sampling protocol was modified and grab samples were replaced by 24-hour composite samples (one sample shot every 20 minutes) collected using automatic samplers, twice a month at four sites downstream of the Merone plant, at the STP overflow, and occasionally one site upstream of Merone. Additional studies were also performed in conjunction with the overall monitoring program.

Reference: Gandolfi, C., Facchi, A., Whelan, M.J., Cassarri, G., Tartari, G. and Marcomini, A. 2000. Validation of the GREAT-ER model in the River Lambro catchment. 5th World CESIO Congress. V.2:1370-1379.
Reliability: 2 Valid with restrictions

(i)
Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Tiber River**
Medium: Sewage treatment plant activated sludge and surface water
Results: The average LAS concentrations in the Roma Nord activated sludge sewage treatment plant were 4.6 mg/L (influent), 0.068 mg/L (effluent), and 6000 mg/kg dry matter (final sludge), which correspond to an overall 98.5% LAS removal rate in the plant. In the receiving waters of the Tiber River LAS was 9.7 μg/L in the aqueous phase and 1.8 mg/kg dry matter in the sediment. Total daily LAS entering the treatment plant amount to 1150 kg. About 1.5% (17 kg) leave the treatment plant through the final effluent and 234 kg (about 20% of the influent LAS) are removed by the digested sludge.
Remarks: Samples were collected over several days in June 1993. It is important to note that LAS environmental fingerprints in effluent and surface waters differ from the composition of the commercial material. The relative ratio of the various homologues detected in the aquatic environmental samples is as follows: C_{10}:C_{11}:C_{12}:C_{13} = 45:30:23:2 with an average carbon number of 10.8. That is due to the alkyl chain switch to shorter homologues in water as a consequence of both biodegradation in the water phase, which is faster for the higher homologues, and of adsorption into sediments, suspended solids, and the sludge, which is more pronounced for higher homologues. The LAS homologue distribution in sludge is approximately in the mole ratio C_{10}:C_{11}:C_{12}:C_{13} = 7:24:39:30 with an average carbon number of 11.9, as a consequence of a preferential adsorption of higher homologues.
Reference: DiCorcia, A., Samperi, R., Belloni, A., Marcomini, A., Zanette, M., Lemr, K. and Cavalli, L. 1994. LAS pilot study at the "Roma-Nord" sewage treatment plant and in the Tiber river. La Rivista Italiana Delle Sostanze Grasse. LXXI:467-475.
Reliability: 2 Valid with restrictions

(j)
Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Rivers in five European Countries**
Medium: Sewage treatment plant activated sludge, river surface water, sediment
Results: A very high average LAS total removal of 99.2% (98.5-99.9%) in sewage treatment was found. LAS concentrations in river water below activated sludge treatment plants in five European countries ranged from <2.1 to 47 μg/L.
Method: As part of a pilot study, LAS monitoring was conducted at five activated sludge sewage treatment plants located in Germany, the UK, the Netherlands, Spain and Italy. Samples were collected over 7-day monitoring periods. Daily flow-related composites of raw sewage and treated effluent were taken. On at least one day, samples were taken at 2 or 3 hour intervals to assess diurnal variations in LAS concentration. Sludge samples were also taken. Samples of river water and sediment were also collected from sites above and below the sewage effluent outfalls. Samples consisted of either grab or composite samples, as well as interval sampling to determine diurnal changes in LAS concentration. Sediment samples were collected from the top layer (0-5 cm) of the river bed in four of 5 pilot study locations. LAS determinations were made with validated trace enrichment-HPLC procedures employing a specific fluorescence detector.

Remarks: LAS concentrations in raw sewage ranged from 4.0 to 15.1 mg/L. Only low concentrations of LAS were discharged to the receiving waters. The range of mean effluent concentrations was 0.009-0.140 mg/L. The mean concentration of LAS in river sediments below effluent discharges ranged from 0.49-5.3 µg/g. Below treatment plants, LAS levels in sediments were very similar (and sometimes lower) than levels above treatment plants. Based on these observations, the authors suggest that LAS is bioeliminated in river sediments. LAS levels in digested sludge from Spain and Italy ranged from 6.0 to 9.4 g/kg dry weight. Differences in the main operating characteristics at the five sites (e.g., treatment type, plant size, sludge retention time, hydraulic retention time, temperature) were not found to greatly influence the removal of LAS.

Reference: Waters, J. and Feijtel, T.C.J. 1995. AIS/CESIO Environmental Surfactant monitoring programme: Outcome of five national pilot studies on linear alkylbenzene sulphonate (LAS). Chemosphere 30:1939-1956.

Reliability: 2 Valid with restrictions

(k)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Red Beck, a small Yorkshire stream**

Medium: Sewage treatment effluents

Results: The results show an LAS concentration, corrected for dilution, of 0.07 mg/L (uncorrected 0.033 mg/L) at Sunny Bank (the furthest downstream station, approximately 4.8 km from the out fall) after 6 hours of travel time. The calculated half-life was in the 2-3 h range, indicating kinetics faster than that of laboratory biodegradation studies in river waters.

Method: LAS and water quality parameters have been measured at seven sites downstream of the effluent discharge point of a trickling filter treatment plant (Shibden Head Sewage Treatment Works, Yorkshire, UK). This study was carried out specifically to measure in-stream removal kinetics of LAS. Time of travel was measured by detection of a fluorescent dye (Rhodamine WT) added to the effluent. Increase in flow as the river proceeds through the catchment was determined by flow measurements and boron dilution rate. Nine sampling stations were selected. The study began with the injection of Rhodamine WT dye to the final effluent. The concentration profile of the dye pulse was established from plots of fluorescence intensity versus time, which allowed the measurement of LAS concentration in the same stream volumes of water as the flow moved downstream. LAS concentrations were corrected for increased flow of the stream (and dilution of LAS) by inputs from side streams. Water samples were collected using automatic samples (time proportional or time proportional centroid composites) and/or grab samples and analyzed for water quality parameters and LAS. Boron was used as a reference substance for measuring the increasing stream flow as boron is highly soluble in water and non-degradable. LAS was analyzed as per the method of Holt et al. 1995. Briefly, LAS was extracted from the samples by solid phase extraction on C18 cartridges, eluted with methanol, evaporated under nitrogen to dryness, reconstituted in 1 mL methanol, and analyzed by reverse phase HPLC on a C18 column with fluorescence detection.

Remarks: The study indicates that an LAS removal half-life of 2-3 hours will be appropriate for small shallow streams, which have an LAS concentration between 50-250 µg/L, for use in the GREAT-ER model calibration exercise.

Reference: Fox, K., Holt, M., Daniel, M., Buckland, H., and Guymer, I. 2000. Removal of linear alkylbenzene sulfonate from a small Yorkshire stream. Contribution to GREAT-ER project #7. Sci. Total Environ. 251:265-275.

Reliability: 2 Valid with restrictions

(l)
Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Dutch surface water**
Medium: Surface water downstream of activated sludge STP outfalls just after the mixing zone.
Results: The mean LAS concentration in surface waters just downstream of the mixing zone was 14.2 µg/L, with a range mostly between <2 to 47 µg/L.
Remarks: Mean derived from a total of 23 records taken from the joint NVZ/VROM monitoring program of sewage treatment plants around the Netherlands. Samples were collected during three consecutive days from seven different sewage treatment plants.
Reference: 1) Feijtel, T.C.J. and van de Plassche, E.J. 1995. Environmental Risk Characterization of 4 Major Surfactants used in the Netherlands. RIVM Report No. 679101 025.
2) Matthijs, E., Holt, M.S., Kiewist, A.. and Rijs, G.B. 1999. Environmental monitoring for LAS, AE, AES, AS, and soap. Environ. Toxicol. Chem. 18:2634-2644.
Reliability: 2 Valid with restrictions

(m)
Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Rivers in Japan**
Medium: Surface water
Results: Measured LAS concentrations from March 1998 to September 2002 ranged from below the detection limit (< 4 µg/L) to 81µg/L. The 95th percentile values ranged from below detection (< 4 µg/L) to 48.7 µg/L. The following table shows the maximum, median and 95th percentile LAS concentrations along with the number of samples in which LAS was detected.

Site #	# Data Points	LAS Concentration (µg/L)		
		Maximum	Median	95th Percentile
1	18	7.0	<4.0	7.0
2	2	12.0	8.0	11.6
3	18	24.0	9.5	16.4
4	18	50.0	6.0	44.1
5	18	81.0	9.5	48.7
6	2	<4.0	<4.0	<4.0
7	14	17.0	5.0	13.8
All Sites	90	81.0	6.0	33.1

Methods: River water samples were collected from seven sites on four urban rivers in Japan (Tamagawa, Edogawa, Arakawa, and Yodogawa Rivers), as summarized in the following table.

Site #	River Name	Site Name	Water Area Category	Description	BOD in 1999 Median/75th% ile (mg/L)
1	Tamagawa	Hamura-seki	A	Upstream. Drinking water intake site.	0.5/0.5
2	Tamagawa	Harabashi	B	Midstream. Just below municipal wastewater treatment plant effluent discharge	2.1/2.3
3	Tamagawa	Denen-chofu-seki	B	Midstream	1.6/1.7
4	Edogawa	Kanamachi	A	Downstream. Drinking water intake site	1.4/1.7

5	Arakawa	Chisui-bashi	B	Midstream	4.6/5.5
6	Arakawa	Sasame-bashi	C	Downstream. Just below municipal wastewater treatment plant effluent discharge	2.5/3.1
7	Yodogawa	Hirakata-oohashi	B	Midstream. Drinking water intake site	1.6/1.9

Grab samples were collected four times a year (summer, autumn, winter, and spring) at each sampling location. River water was characterized at each sampling occasion for BOD, TOC, SS, pH, Cl, NH_4 and MBAS. LAS was complexed with MBAS, extracted, passed through a cation-exchange column, and the concentration of $C_{10\text{-}13}$ LAS measured using HPLC. Populations in the catchments of the four rivers are relatively dense and municipal wastewater treatment coverage rates are middle to high (i.e., from 60-70% to over 90% coverage). The seven sites cover upstream (Site 1), midstream (2, 3, 5, 7), and downstream (4, 6), and water area categories ranging from A to C. Two of the sites (2, 6) are just below municipal wastewater treatment plant effluent discharges. Three sites (1, 4, 7) are near drinking water intake sites.

Reference: Nishiyama, N., Yamamoto, A., and Takei, T. 2003. 37th Annual meeting of the Japan Society of Water Environment, Kumamoto, Japan.
Japan Soap and Detergent Association (JSDA). Annual reports of environmental issues (Years 1999, 2000, 2001, 2002).

Reliability: 2 Valid with restrictions

(n)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Europe STP sludge**

Medium: Anaerobic sludge

Results: Typical values are between 3.4 and 9.4 g/kg dry matter, with a mean of 5.6 g/kg.

Remarks: Mean based on a total of 16 records. The LAS homologue distribution in sludge is approximately in the mole ratio C_{10}:C_{11}:C_{12}:C_{13} = 7:24:39:30, with an average carbon number of 11.9, as a consequence of a preferential adsorption of higher homologues. The possible differences of LAS concentration is wet sludge, freshly produced at a STP from that of dry sludge, aged and dried before its use in agriculture, should be taken into account. It was found (Carlsen et al. 2002) that the LAS concentration in the bulk dry sludge could drop up to 74% compared to that of the wet sludge. Carlsen et al. (2002) also found that the average LAS concentration in soil core samples taken in a cultivated field spread with medium amounts of sludge was 1.12 mg/kg in the 0-10 cm depth. Lower LAS concentrations were recorded at depths from 10-50 cm.

Reference: 1) Carlsen, L., Metzon, M.B. and Kjelsmark, J. 2002. Linear alkylbenzene sulfonates (LAS) in the terrestrial environment. The Science of the Total Environment. 290:225-230.
2) Feijtel, T.C.J., Matthijs, E., Rottiers, A., Rijs, G.B.J., Kiewiet, A. and de Nijs, A. 1995. AIS/CESIO environmental surfactant monitoring program. Part 1: LAS monitoring study in “de Meer” STP and receiving river “Leidsche Rijn”. Chemosphere. 30:1053-1066.
3) Holt, M.S., Water, J., Comber, M.H.I., Armitage, R., Morris, G. and Nebery, C. 1995. AIS/CESIO environmental surfactant monitoring programme. SDIA sewage treatment pilot study on LAS. Wat. Res. 29:2063-2070.
4) Sanchez Leal, J., Garcia, M.T., Tomas, R., de Ferrer, J. and Bengoechea, C. 1994. Linear alkylbenzene sulfonate removal. Tenside Surf. Det. 31:253-256.

Reliability: 2 Valid with restrictions

(o)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] concentrations in sludge-amended agricultural soils**

Medium: soil

Method: An extensive monitoring study was performed on sludge-amended soils in the Thames Water Authority area, UK, by a Soap and Detergent Industry Association task force. A total of 51 fields from 24 farms were used, with sites representing a range of soil types, frequency and level of sludge applications, and agricultural uses. A total of 35 of the fields were pasture lands and 16 fields were arable land. The majority of fields were surface spread with primary and anaerobically digested sludge containing approximately 4.5% dry solids.

Results: Forty two farm sites that had received their most recent sludge application prior to 1987 (the study year) were monitored to establish the levels of LAS in sludge amended soils. Thirty five (83%) of the samples contained LAS levels below 1 mg/kg soil (mean = 0.7 mg/kg). The seven other sites contained LAS levels between 1.1 and 2.5 mg/kg soil. Nine sites received sludge applications in January to May 1987. Sampling was conducted in May 1987 and resulted in LAS concentrations ranging from <0.2 to 19.8 mg/kg. The highest LAS concentrations in soil (19.8, 10.6, 7.8, and 4.5 mg/kg) were recorded within days after the sludge application.

Remarks: Soil concentrations dropped significantly in less than two months (e.g., the 19.8 mg/kg value dropped to 2.1 mg/kg in 55 days). The average chain length of the LAS found in soil samples was $C_{11.7}$.

Reference: Waters, J., Holt, M.S., Matthijs, E. 1989. Fate of LAS in sludge amended soils. Tenside Surfactants Detergents 26(2):129-135.

Reliability: 2 Valid with restrictions

(p)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] concentrations in sludge-amended agricultural soils**

Medium: sludge and soil

Method: This paper collects the literature on the concentrations of LAS in sludge-amended soil resulting from the use of sewage sludge applications on agricultrual fields. Data were compiled from a variety of original reference sources.

Results: The concentrations of LAS in sludge are shown in the following table:

Sludge Description	Concentration (mg/kg dw)	Reference *
Anaerobic	2,900 - 11,900	McEvoy and Giger 1985
Anaerobic	4,660 - 1,540	Rapaport et al. 1987
Aerobic	182 - 432	Matthijs and De Henau 1987
Anaerobic	1,330 - 9,930	Matthijs and De Henau 1987
Anaerobic	5,500	Marcomini 1988
Aerobic	100 - 500	Berna et al. 1989
Anaerobic	7,000 - 30,200	Berna et al. 1989
Aerobic	152 ± 120	McAvoy et al. 1993
Anaerobic	10,460 ± 5,170	McAvoy et al. 1993
Anaerobic	11,500 - 14,000	Cavalli et al. 1993
Anaerobic	12,100 - 17,800	Prats et al. 1993
Anaerobic	6,000 ± 1,200	Di Corcia et al. 1994
Primary	3,400 - 5,930	Feijtel et al. 1995
Aerobic	205	Feijtel et al. 1995
Aerobic	11 - <500	VKI 1997

Anaerobic	1,000 - 16,100	VKI 1997

* See article for full citations.

The concentrations of LAS in sludge-amended soil are shown in the following table.

Initial Concentration (mg/kg dw)	Typical Concentration * (mg/kg dw)	Reference**
16, 27	--	Figge et al. 1989
45	5	Marcomini et al. 1989
16,53	0.3	Berna et al. 1989
Max. 66	0-20	Waters et al. 1989
Max. 145	0-8	Holt et al. 1992
Max. 250	1-7	Ward et al. 1989
22.4	0.7, 3.1	Prats et al. 1993

* Typical values after a test period

** See article for full citations

Remarks: The range of LAS concentrations in sludge rarely exceeds 30,000 mg/kg dw. The range of LAS concentrations in sludge-amended soil also is low.

Reference: Cavalli, L., and Valtorta, L. Surfactants in sludge-amended soil. Tenside Surfactants Detergents 36:22-28.

Reliability: 2 Valid with restrictions

(q)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Coastal waters and harbor sediments with municipal and industrial discharge**

Medium: marine sediments

Test Substance: The chemical standard was a commercial LAS with a low dialkyltetralinsulfonates content (<0.5%) in a single standard mixture with proportional composition of the homologues C_{10} 3.9%, C_{11} 37.4%, C_{12} 35.4% and C_{13} 23.1% (Petroquimica Espanola S.A.)

Method: Sediment samples were taken from 23 sites along the Mediterranean coast of Spain and from three sites on the Atlantic coast. Water samples were taken at 14 sites on the Mediterranean coast. Samples underwent standard sample preparation and were analyzed using HPLC/MS. Samples were analyzed for individual LAS homologues (C_{10}, C_{11}, C_{12}, C_{13}) and other nonionic surfactants and their degradation products.

Results: In seawater the concentrations of LAS across all the samples ranged from 2.4 to 92 µg/L and in marine sediment the concentrations of total LAS ranged from 0.1 to 238 mg/kg dry weight. Concentrations were higher in the sediments than in the water column, with the highest concentrations found in sediments collected in the proximity to the outflow of untreated urban wastewaters. The average carbon chain length of LAS ranged from 10.6 to 11.6 in water and 12.0 to 12.8 in sediment.

Remarks: High concentrations of nonionic surfactants and their degradation products have been shown to accumulate in sediments, which seem to act as a sink for LAS in studied areas. The relative concentrations of the lower homologues C_{10} and C_{11} LAS in water samples are higher than the typical laundry detergent, mainly due to the partial removal and/or enrichment of these species during transportation of the wastewater in the sewage system because of the higher degradation and adsorption tendency of the longer alkyl chain homologues. The longer chain lengths are preferentially sorbed to particulate matter because of their high lipophilicity, thus explaining the increase in relative concentration of C_{12} and C_{13} homologues in the sediment samples. When interpreting this study, it is important to note that hot spots such as

described are not representative of European coastal sediments. Little or no macrofauna lives in such sediment, probably due to multistressor pressure.

Reference: Petrovic, M., Fernandez-Alba, A.R., Borrull, F., Marce, R.M., Mazo, E.G., and Barcelo, D. 2002. Occurrence and distribution of nonionic surfactants, their degradation products, and linear alkylbenzene sulfonates in coastal waters and sediments in Spain. Environmental Toxicology and Chemistry 21:37-46.

Reliability: 2 Valid with restrictions

(r)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Coastal sediments in Bay of Cadiz, Spain**

Medium: Estuarine and marine sediments

Method: Sediment samples were collected from seven stations (5 in the Bay of Cadiz, 2 in the Barbate River), representing a range of low, moderate, and high levels of chemical contamination. Samples were collected using a $0.025m^2$ Van Veen grab sampler during winter and summer in the same year. LAS was measured using specific HPLC analytical techniques. Fourteen heavy metal contaminants were also measured. Concurrent sediment toxicity tests were also conducted in which the rate of burial for clams (Ruditipes philippinarum) was measured over 48 hours and the survival of amphipods (Microdeutopus gryllotalpa) was measured over 10 days of exposure to whole sediments.

Results: LAS concentrations in the sediment ranged from 1.2-26.7 mg/kg dw in the summer and 1.2-62.1 mg/kg dw in the winter. Five of the 7 stations had LAS concentrations < 2.6 mg/kg dw.

Remarks: No mortality was observed in the clam toxicity studies. Clam burial was fastest in the uncontaminated sites (e.g., ET_{50} = 0.01-0.76 hours in winter), intermediate in moderately polluted sites (e.g., ET_{50} = 0.92-1.29 hours in winter), and slowest in highly polluted sites (e.g., ET_{50} > 48 hours in winter).The highest survival in the amphipod studies was in the uncontaminated site (85% survival) and the lowest survival was in the highly polluted site (16% survival). LAS is the only organic component of untreated sewage discharges considered, and sediment contaminants also included high levels of Ag and Pb.

Reference: DelValls, T.A., Forja, J.M. and Gomez-Parra, A. 2002. Seasonality of contamination, toxicity, and quality values in sediments from littoral ecosystems in the Gulf of Cadiz (SW Spain). Chemosphere. 46:1033-1043.

Reliability: 2 Valid with restrictions

(s)

Type of Measurement: Background [ ]; At contaminated site [ ]; Other[X]; **Coastal sediments in Denmark**

Medium: marine sediments

Method: Two core samples of 1 meter length were taken in the Baltic Sea, one in the inner Stockholm archipelago, and one north of Gotland, in the autumn of 2000. Sediment samples were also taken from five locations in Haderslev Fiord on December 20, 2000. On April 3, 2001, samples were taken from five locations each in Vejle and Kolding Fiords. All samples were analyzed for total alkylbenzene sulfonates (LAS), and if possible, branched (branched dodecylbenzene sulfonates (BDS)) and linear alkylbenzene sulfonates separately. In addition, soap and volatile solids were analyzed separately.

Results: Danish marine sediments are not generally contaminated with LAS. The levels of health sediments are near or below detection limits. The concentration of LAS in soft sediments of the Baltic Sea along the Swedish coast is <0.5-1 mg/kg dry wt. Soap can be detected in high concentrations

(1,000-2,000 mg/kg dry wt.) in sediments, where LAS could not be detected (<0.05 mg/kg dry wt.). Sediments from a Danish shipping port (Haderslev Fiord), as previously reported by Danish EPA, were found to contain relatively high concentrations of LAS (2-20 mg/kg dry wt.) as well as extremely high soap concentrations (3,000-10,000 mg/kg dry wt.) and many other pollutants.

Remarks: The authors conclude that the environmental problem in Haderslev Fiord is not LAS or soap, but the fact that the whole sediment consists of stinking sludge formed by past discharges of untreated sewage and today's overflow of sewage from emergency spillways in the municipal sewage system. The presence of BDS in the sediments demonstrates that this a historical problem.

Reference: Folke, J., Cassani, G., de Ferrer, J., Lopez, I., Karlsson, M.O., and Willumsen, B. 2003. Linear alkylbenzene sulphonates, branched dodecylbenzene sulfonates and soap analyzed in marine sediments from the Baltic proper and Little Belt. Tenside Surf. Det. 40:17-24.

Reliability: 2 Valid with restrictions

(t)

Type of Measurement: Background **[ ]**; At contaminated site **[ ]**; Other **[X] Coastal sediments receiving untreated urban effluents**

Medium: marine sediments

Test Substance: LAS C_{10-14} (sum of all homologues)

Method: There were three objectives to the study: 1) determine LAS levels in coastal sediments in areas receiving discharges of untreated urban effluents; 2) determine LAS distribution between the solid phase and the interstitial water; and 3) determine the presence of SPCs in the sediment column at depths below the aerobic oxidation/reduction interface. The study was carried out in a salt marsh in the south part of the Bay of Cadiz in the southwest of Spain. Samples were taken at three stations in an area where LAS levels are very high due to untreated urban effluents. Ten cores of sediment were collected at each station, frozen, cut into 1 cm thick sections and analyzed using standard HPLC/FL preparation, analysis, and cleanup techniques. Analyses were conducted to determine both LAS concentrations and concentrations of long-chain sulfophenyl carboxylic acids (SPCs) resulting from LAS biodegradation.

Results: The vertical profile of LAS concentrations in the sediment and interstitial waters showed a sharp reduction with depth, whereas the long chain SPCs (6-13 carbon atoms) was greatest at 10-14 cm depth where the interstitial water becomes anoxic. Surface (0-8 cm) sediment concentrations (dry weight) for total LAS and SPCs are shown below.

Station	Location	Total LAS (mg/kg)	Total SPCs (µg/kg)
B	Close to discharge point	138.6	924.6
C	Distant, strong tidal current	16.4	224.2
A	Distant, weaker tidal current	0.8	70.6

The partition coefficients between the solid phase of the sediment versus the interstitial water are very different for LAS and for its degradation intermediates. For LAS, the organic carbon-based partition coefficient values were between 2.4×10^3 and 6.6×10^5 L/kg for the homologues C_{10} and C_{13}, respectively. For the longer chain SPCs, the partition coefficients are

	several orders of magnitude lower as a consequence as their lower hydrophobicity.
Remarks:	The LAS concentration in the upper sediment layer (0-8 cm) decreased with distance from the point of effluent discharge. The concentration of LAS in the sediment was up to 1000 times greater than that in the interstitial water. For SPC, the concentrations in the sediment and interstitial water were similar to each other.
Reference:	Leon, V.M., Gonzalez-Mazo, E., Pajares, J.M.F., and Gomez-Parra, A. 2001. Vertical distribution profiles of linear alkylbenzene sulfonates and their long-chain intermediate degradation products in coastal marine sediments. Environmental Toxicology and Chemistry 20:2171-2178.
Reliability:	2 Valid with restrictions

(u)

Type of Measurement:	Background **[ ]**; At contaminated site **[ ]**; Other **[X] Predicted marine water concentrations in the North Sea**
Medium:	Estuarine and marine surface water
Method:	LAS environmental concentrations were predicted from per capita LAS use (2.5 g LAS/cap/day in Western Europe), water treatment statistics, and population estimates for Western Europe.
Results:	The predicted LAS concentration range in the estuaries around the North Sea are 0.9-9 μg/L, which is in agreement with field monitoring data (1-9 μg/L) from the western Scheldt estuary.
Remarks:	A risk assessment of LAS in marine sediments was initiated in 2002 and is expected to be available in 2004.
Reference:	Temara, A., Carr, G., Webb, S., Versteeg, D. and Feijtel, T. 2001. Marine risk assessment: linear alkylbenzene sulfonate (LAS) in the North Sea. Marine Poll. Bulletin. 42:635-642.
Reliability:	2 Valid with restrictions

(v)

Type of Measurement:	Background **[ ]**; At contaminated site **[ ]**; Other **[X] Coastal waters and sediments in the Elbe estuary**
Medium:	Surface water and marine sediments
Test Substance:	LAS
Method:	Water samples (100-L) were collected from a depth of 5 m at several locations in the Elbe estuary of the German Bight of the North Sea. Sediment samples were collected at the same locations. All samples were extracted and analyzed for LAS and other compounds (e.g. nonylphenols) present in detergents.
Results:	The maximum concentration of LAS in surface waters was 0.03 μg/L and occurred in marinas in the Elbe estuary. Sediment LAS concentration ranged from 39-109 μg/kg dry weight.
Remarks:	The LAS found in marina sediment probably originated from the discharges of municipal wastewater treatment plants.
Reference:	Bester, K., Theobald, N., and Schroeder, H.Fr. 2001. Nonylphenols, nonylphenol-ethoxylates, linear alkylbenzenesulfonates (LAS) and bis (4-schlorophenyl)–sulfone in the German Bight of the North Sea. Chemosphere. 45:817-826.
Reliability:	2 Valid with restrictions

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION PATHWAYS

3.3.1 TRANSPORT

(a)

Type:	partition coefficient
Media:	sludge
Method:	Monitoring data were collected in a pilot-scale municipal activated sludge treatment plant. The plant consisted of a completely mixed aeration tank (490L) and a secondary settler (280L). The plant was operated at C_{12} LAS influent concentrations between 2 and 12 mg/L and at sludge retention times of 10 and 27 days. At least every other day 24-h samples of 2.5L influent and 2.5L effluent were collected in PE bottles and total (sum of adsorbed and dissolved) LAS concentrations were determined using an HPLC method adapted from Feijtel et al. 1995. At least once a day 200 mL grab samples were taken from the aeration tank and return sludge and transferred into PE centrifuge tubes for determination of dissolved and absorbed LAS. The sludge samples were immediately centrifuged for 15 min at 3500 rpm. The supernatant was transferred into PE bottles and preserved by 3% formalin and stored for a maximum of 10 days at 4°C until further analysis. Representative aliquots of pre-settled influent, final effluent, or supernatant of the centrifuged sludge samples were passed over 6 mL preconditioned C18 SPE columns at a rate not exceeding 10 mL/min. The SPE columns were washed with 2 mL methanol/water and eluted with 5 mL of methanol. The eluate was then passed through strong anion exchange (SAX) columns, washed, eluted and subsequently evaporated to dryness under a gentle flow of nitrogen gas. The dry residue was dissolved in 2-5 mL of HPLC mobile phase. The HPLC was operated according to specifications. Identification of the different LAS alkyl homologues and quantification were made against a commercial LAS mixture (Marlon A390). A sorption-isotherm and the kinetics of adsorption and desorption of LAS to activated sludge were determined in batch experiments. Three different biodegradation tests were also carried out (an OECD 301F ready biodegradation test; a batch activated sludge [BAS] test; and a "by-pass" test developed to mimic condition of the pilot scale activated sludge plant). Only the sorption results are presented here.
Results:	K_p (C_{12} LAS): 3210 L/kg (log K_p = 3.5) K_p (commercial $C_{11.6}$ LAS mixture): 2,500 L/kg (log K_p = 3.4)
Test Substance:	C_{12} LAS
Remarks:	Sorption equilibrium was achieved rapidly, within 5-10 minutes. Desorption was less pronounced, but still reached rapid equilibration. The sludge-water partition coefficient K_p of 3210 L/kg volatile suspended solids is reported. Applying the same QSAR for the commercial $C_{11.6}$ LAS mixture results in a value of log K_p = 3.4 (i.e., K_p = 2500 L/kg), consistent with Feijtel et al. 1999 (see section 3.3.1(b)). In the other experiments conducted in this study, only 2-8% was present as dissolved C_{12} LAS, with the remaining 92-98% adsorbed to the sludge. Despite this high degree of sorption, more than 99% of the LAS load was removed by biodegradation, showing that the adsorbed fraction as well as the soluble fraction of LAS is readily available for biodegradation.
Reference:	Temmink, H. and Klapwijk, B. 2004. Fate of LAS in activated sludge plants. Water Research 38:903-912.
Reliability:	2 Valid with restrictions

(b)

Type:	partition coefficient
Media:	sludge
Method:	QSAR analysis
Results:	K_p (C_{11} LAS): 1000 L/kg (log K_p = 3.0) K_p (C_{12} LAS): 3162 L/kg (log K_p = 3.5) K_p (commercial $C_{11.6}$ LAS mixture): 2,512 L/kg
Test Substance:	Pure C_{11} and C_{12} LAS; and commercial $C_{11.6}$ LAS
Remarks:	The K_p values for C_{11} and C_{12} LAS are reported in this study as experimentally determined by Games et al. (1982), although they actually appear to be as reported in Games (1982; see 3.3.1 (d) for summary). The K_p for the commercial $C_{11.6}$ LAS mixture is calculated by Feijtel et al. using the reported C_{11} and C_{12} values. Also cites as a model input the log K_{oc} from Traina et al. 1995 (see 3.3.1(b) for summary). These values are consistent with the experimental results of Temmink and Kapwijk (see 3.3.1(a).
Reference:	Feijtel, T.C.J., Struijs, J., and Matthijs, E. 1999. Exposure modelling of detergent surfactants – Prediction of 90th-percentile concentrations in The Netherlands. Environ. Toxicol. Chem. 18:2645-2652.
Reliability:	4 Not assignable (see 3.3.1(e) for Games 1982)

(c)

Type:	organic carbon partition coefficient
Media:	dissolved humic substances
Method:	The association of C_{10}, C_{12} and C_{14} LAS with natural and specimen-grade dissolved humic substances (DHS) was measured with fluorescence quenching and with ultracentrifugation techniques. Water-soluble organic carbon (Carlisle-WSOC) was obtained and extracted from 0-0.1 m depth of a Carlisle muck in northwest Ohio. The acid-soluble fraction (Carlisle-HA) was suspended, centrifuged, and dialyzed to remove Cl^- and to reduce the polyvalent cation content. The specimen-grade humic acid was purchased from Aldrich Chemical Company (Aldrich-HA). Suwanee River humic acid (SRHA) was obtained from the International Humic Substances Society. The fluorescence quenching followed the method of Guathier et al. (1986). Aliquots of the humic acid were placed in borosilicate bottles containing either NaCl, $CaCl_2$, or concentrated synthetic river water, capped and incubated at 25°C for 18-24 hours, after which an aliquot of C_{10}, C_{12} or C_{14} LAS was added and the solutions equilibrated at 25°C for 2 hours. All treatments were prepared in triplicate. After 2 hours, 3 mL of each sample solution was placed into cuvettes and the fluorescence of LAS measured with a Perkin Elmer LS 5B spectrofluorometer. Ultraviolet absorption measurements were made at 230 and 288 nm with a Beckman DU 6 UV-vis spectrophotometer. For the second independent analytical method, a batch ultracentrifugation method was developed. Aliquots of C12 LAS were added to polyallomer utltracentrifuge tubes containing the humic acid in a background electrolyte of either NaCl or $CaCl_2$ and allowed to equilibrate at 25°C. All treatments were prepared in triplicate. After 2 hours, the samples were centrifuged at 141,000 g for 6 hours at 25°C. The supernatants were decanted and saved for analysis. The walls of the centrifuge tubes were extracted with CH_3OH, which was saved for analysis. The concentration of C_{12} LAS in the supernatants and in the CH_3OH extracts was determined by exciting the solutions in cuvettes at 230 nm and the emission intensity recorded at 288 nm with a Perkin Elmer LS-5B spectrofluorometer. The quantity of C_{12} LAS associated with DHS was calculated from the difference in the initial and final solution concentrations, following the correction for the quantity of C_{12} LAS sorbed to the walls of the centrifuge tubes.

Results: The average Log Koc values over the four DHS materials (Aldrich-HA, Carlisle-WSOC, Carlisle-HA, and SRHA) for each LAS chain length tested are:
Log K_{oc} (C_{10} LAS): 4.02 L/kg
Log K_{oc} (C_{12} LAS): 4.83 L/kg
Log K_{oc} (C_{14} LAS): 5.49 L/kg
The data for Ca-saturated Aldrich-HA was linear over the entire concentration range of DHS, whereas some curvatura was present in the data from the Ca-saturated SRHA, and considerable deviation from linearity was apparent in many of the Na-saturated DHS solutions.

Test Substance: C_{10} LAS (98% purity), C_{12} LAS (93% purity), and C_{14} LAS (88% purity), each synthesized at Procter and Gamble. Uniformly ^{14}C-ring labeled C_{10}-, C_{12}- and C_{14}-LAS were obtained from New England Nuclear and were 93.8, 96.3 and 92.5% pure, with specific activities of 26.6, 68.2, and 34.3 µCi/mg, respectively.

Remarks: Good agreement was obtained with both of the analytical methods, indicating that both techniques can be used to quantify the effects of DHS on speciation of LAS in natural waters with certain limitations. LAS-DHS partition coefficients increased with increasing length of the alkyl chain in the LAS. These data indicate the significance of nonpolar forces in LAS-organic matter interactions. Good agreement was found between the partition coefficients obtained from the two analytical techniques and those calculated from the response of uptake and depuration studies conducted with fathead minnows.

Reference: Traina, S.J., McAvoy, D.C. and Versteeg, D.J. 1996. Association of LAS with dissolved humic substances and its effect on bioavailability. Env. Sci. Technol. 30:1300-1309.

Reliability: 2 Valid with restrictions

(d)

Type: Adsorption **[X]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**

Media: water - activated sludge

Method: estimation of K_d with Freundlich equation

Results: The K_d of commercial LAS was between 660 and 5200 L/kg (6 citations), dependant on organic carbon content and other characteristics of the solid phase.

Remarks: Concentration in liquid phase between 1 and 80 mg/L.

Reference: Painter, H.A. and Zabel, T.F. 1988. Review of the environmental safety of LAS. Wrc Medmendham, UK. Report No. CO 1659-M/1/EV 8658.

Reliability: 4 Not assignable

(e)

Type: Adsorption **[X]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**

Media: water - activated sludge and water - river sediment

Method: Comparison of K_d for LAS C_{10} to C_{14} - Year 1982

Results: Adsorption coefficients (L/kg) in activated sludge and river sediment, respectively, for LAS homologues:
C_{10}: 220 and 41
C_{11}: 1000 and 100
C_{12}: 3070 and 330
C_{13}: 9330 and 990
C_{14}: 2950 (for river sediment – not determined for activated sludge)

Remarks: K_d is highly dependent on the alkyl chain length of LAS with approximately a factor of 3 increase per carbon and on the position of the phenyl group on the alkyl chain. The organic carbon content is also an important factor, varying by a factor of 10 between activated sludge and river sediment.

Reference: 1) Games, L.M. 1982. Field validation of exposure analysis modelling systems (EXAMS) in a flowing stream. Ch. 18. In: Dickson, K.L., Maki, A.W. and Cairns, J. (ed.). 1981. Modelling and Fate of Chemicals in the Aquatic Environment. 4th Meeting. Sci. Ann Arbor Michigan Pp. 325-346.
2) Painter, H.A. and Zabel, T.F. 1988. Review of the environmental safety of LAS. Wrc Medmendham, UK. Report No. CO 1659-M/1/EV 8658.
Reliability: 4 Not assignable because no details of LAS concentration were provided.

(f)
Type: Adsorption **[X]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**
Media: water - river sediments
Method: estimation of K_d with Freundlich equation
Results: K_d between 6 and 300 L/kg (5 citations), dependent on organic carbon content and other characteristics of the solid phase.
Remarks: Concentration in liquid phase between 0.06 and 15 mg/L
Reference: Painter, H.A. and Zabel, T.F. 1988. Review of the environmental safety of LAS. Wrc Medmendham, UK. Report No. CO 1659-M/1/EV 8658.
Reliability: 4 Not assignable

(g)
Type: Adsorption **[X]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**
Media: water - soil
Method: estimation of K_d with Freundlich equation
Results: K_d between 2 and 20 L/kg (3 citations), dependent on organic carbon content and other characteristics of the solid phase.
Remarks: Concentration in liquid phase between 0.06 and 15 mg/L
Reference: Painter, H.A. and Zabel, T.F. 1988. Review of the environmental safety of LAS. Wrc Medmendham, UK. Report No. CO 1659-M/1/EV 8658.
Reliability: 4 Not assignable

(h)
Type: Adsorption **[X]**; Desorption **[ ]**; Volatility **[ ]**; Other **[ ]**
Media: water - soil
Method: compilation of K_F data from other sources. The Fruendlich isotherm is a general sorption isotherm which describes sorption behaviour and often is used in studies of surfactant sorption. K_F is the Fruendlich isotherm coefficient which expresses the affinity of a surfactant for a given solid sorbent. As shown in the equation and table below, the exponent n is a measure of isotherm non-linearity. For n approaching 1, the Freundlich model of sorption becomes equivalent to a linear sorption model.

$$C_s = K_F \times C_w^n$$

Results: Log K_F values for a selection of C_{12}-LAS types is shown in the table below:

Log K_F	n	Sorbent	Reference
1.7	1	EPA-B1	Hand and Williams (1987)
2.0	1	EPA-5	Hand and Williams (1987)
2.7	1	RC4	Hand and Williams (1987)
3.2	1	RC3	Hand and Williams (1987)
~0.1	1	different soils	Ou et al. (1996)
2.8	1.15	marine sediment	Rubio et al. (1996)
0.6	0.77	soil, clay loam(A)	Abe and Seno (1985)
1.4	1.20	soil, clay loam(B)	Abe and Seno (1985)
1.2	1.19	soil, sandy loam	Abe and Seno (1985)

Sorbent refers to the standard or natural soil or sediment used, as the affinity for sorption depends on both the chemical substance and the characteristics of the sorbent. All data were drawn from the original sources referenced in the table.

Remarks: The nonlinearity parameter implies that sorption affinity decreases with increasing LAS concentrations, which suggests that concentration dependency should be taken into account when assessing sorption of surfactants such as LAS.

Reference: Tolls, J. and Sijm, D.T.H.M. 2000. Estimating the properties of surface-active chemicals. In: Boethling, R.S. and Mackay, D. Handbook of Property Estimation Methods for Chemicals. Lewis Publishers.

Reliability: 4 Not assignable because the original articles were not directly reviewed.

3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)

(a)

Media: Air-biota **[ ]**; Air-biota-sediment-soil-water **[X]**; Soil-biota **[ ]**; Water-air **[ ]**; Water-biota **[ ]**; Water-soil **[ ]**

Method: Fugacity level I **[ ]**; Fugacity level II **[ ]**; Fugacity level III **[X]**; Fugacity level IV **[ ]**; Other (calculation) **[ ]**; Other (measurement)**[ ]**

Five stage Mackay-type modelling including evaluative, regional and local-scale models. The first two stages involve classifying the chemical and quantifying the emissions into each environmental compartment. In the third stage, the characteristics of the chemical are determined using a quantitative equilibrium criterion model (EQC), which is conducted in three steps using levels I, II, and III versions of the model that introduce increasing complexity and more realistic representations of the environment. The EQC uses a generic, evaluative environment, which is 100,000 km^2 in area. In the fourth stage, ChemCAN, which is a level III model for specific regions of Canada, was used to predict the chemical's fate in southern Ontario. The final stage was to apply local environmental models to predict environmental exposure concentrations. For LAS, the WW-TREAT, GRiDS, and ROUT models were used to predict the fate of LAS in a sewage treatment plant and riverine receiving waters. Estimated properties used as input parameters to the models are shown below for LAS (from various sources; average values; based on the best default environmental and physicochemical values available at the time of modeling):

Molecular mass	348
Air-water partition coefficient	0
Aerosol-water partition coefficient	100
Soil-water partitition coefficient (L/kg)	20
Sediment-water partitition coefficient (L/kg)	570
Fish-water partitition coefficient (L/kg)	250
Half-life in air (h)	--
Half-life in water (h)	24
Half-life in soil (h)	480
Half-life in sediment (h)	96

The level I calculation assumes a steady-state equilibrium partitioning of a fixed quantity of LAS (100,000 kg) with no reaction or advection processes. The level II calculation assumes a fixed input of 1000 kg/h, which is balanced by reaction and advection losses. Relative partitioning is identical to level I. For level III, the ChemCAN model assumes the following estimated input quantities for LAS:

Total discharge to the environment (kg/yr)	1,444,000
Discharge to the air	--
Discharge to water	144,000
Discharge to soil	1,296,000
Total input in the region (kg/year)	1,440,000
Total input in the region (kg/hour)	164.4

The authors base these input quantities for the ChemCAN model on a recent estimate of LAS annual production in North America, western Europe and Japan as approximately 1.4 million tons and an annual per capita consumption of LAS in the United States of 1.3 kg/year. LAS is disposed "down-the-drain" and approximately 98% is removed in sewage treatment. About 30% of the LAS is removed in treatment by adsorption onto primary and secondary sewage solids. Over 60% of the sludge was assumed to be disposed of in landfills or applied to agricultural soils, thus there is the potential for LAS to reach the soil environment. Therefore, the level III model assumes a substantial discharge (90%) of LAS to soil following sewage treatment. Inputs considered the specific nature of nonvolatile surfactants such as LAS. For example, the use of Kow as a descriptor for organic phase-water partitioning is inappropriate for LAS and there is no need for a vapor pressure or air-water partition coefficient. Because LAS is a mixture, average properties were used as inputs to the models. In the EQC model, LAS is treated using the equivalence approach as the equilibrium criterion.

Results: The level I and II models each resulted in LAS partitioning to air, water, soil, and sediment at percentages of 0%, 25.97%, 56.09%, and 17.76%, respectively. The overall residence time of LAS is 100 hours and removal is primarily by biodegradation in water (76%) and partitioning in sediment (13%). Thus, the impacts of LAS will be restricted to local receiving waters and their sediments and biota. In level III, when discharges are directly to water, the residence time is 33 hours and more than 99% remains in the water, though in shallower receiving waters more partitioning to sediments might be expected. When the discharge is to soil, as was assumed in the ChemCAN model, the residence time is 28 days because of the slower biodegradation rate and little transfers to other media. Based on these findings, the dominant fate processes are degradation rates in water and soil, and water-sediment transfer.

Using the ChemCAN 4 model, of the total amount of LAS released to the environment assuming the discharge rates above, the distribution and concentrations were predicted to be:

to air:	0%	(0 mg/m^3)
dissolved in water:	0.64%	(0.44 $\mu g/m^3$)
in soil:	99.35%	(7.06 $\mu g/kg$)
in sediment:	0.0036%	(0.00347 $\mu g/kg$)

Remarks: Based on an estimated total discharge to the environment of 1.44×10^6 kg/year (1.44×10^5 kg to water and 1.296×10^6 kg to soil). It should be noted that the discharge assumptions used by the authors are highly conservative and likely overpredict the amount of LAS entering various compartments, for example, the soil compartment. This study was conducted by the model developer and acknowledged expert on fugucity to demonstrate that the approach was appropriate for different types of chemicals.

Reference: Mackay, D., Di Guardo, A., Paterson, S., Kicsi, G., Cowan, C. and Kane, D. 1996. Assessment of chemical fate in the environment using evaluative, regional and local scale models: Illustrative application to chlorobenzene and linear alkylbenzene sulfonates. Environ. Toxicol. Chem. 15:1638-1648.

Reliability: 2 Valid with restrictions

(b)

Media: Air-biota **[ ]**; Air-biota-sediment-soil-water **[X]**; Soil-biota **[ ]**; Water-air **[ ]**; Water-biota **[ ]**; Water-soil **[ ]**

Method: Fugacity level I **[ ]**; Fugacity level II **[ ]**; Fugacity level III **[X]**; Fugacity level IV **[ ]**; Other (calculation) **[ ]**; Other (measurement)**[ ]** Multi-media model HAZCHEM derived from MacKay type level III model, including a water purification module (comparable to SIMPLETREAT model used by the Netherlands Authorities). Regional model for Europe. Includes probabilistic evaluation of natural variability and inaccuracy in determination of input parameters using Monte Carlo simulation. Input parameters held constant in the simulations for the LAS used in the model were based on the best available data at the time of modeling and are:

Molecular weight	347
Melting point (°C)	10
Vapor pressure (Pa)	1×10^{-10}
Solubility (mg/L)	350
Log Kow	2.5
Half-life life in air (h)	8
Half-life in water (h)	35
Half-life in soil (h)	339
Half-life in sediment (h)	17
Soil-water partitition coefficient (L/kg)	1000
Sediment-water partitition coefficient (L/kg)	1000
Suspended solids-water partitition coefficient (L/kg)	1000

Parameters that were varied using lognormal distributions for the Monte Carlo simulations included water surface and arable land fractions, depths of various compartments, fraction organic carbon in various compartments, advective residence times, temperature, and others.

Results: Predicted concentrations in the various compartments as defined by the model as shown in the table below. Degradation in the soil was not taken into account and the model was not calibrated. Measured concentrations in arable soil were generally below 1 ppm. Results are the 5th and 95th percentile values from the Monte Carlo analysis and the normal average.

	Average	**5 percentile**	**95 percentile**
air (ug/m^3)	3.23 E-12	--	--
biota (ppm)	5.99 E-2	7.11 E-3	1.95 E-1
sediment (ppm)	4.90 E-3	3.23 E-3	1.38 E-2
arable soil (ppm)	44.2	7.02	1.11 E+2
suspended. matter (ppm)	3.79	0.449	12.3
dissolved in water (mg/L)	3.79 E-3	4.49 E-4	1.23 E-2
suspended in water (mg/L)	7.81 E-5	1.54 E-5	2.16 E-4

Remarks: Input data were the best estimates from ECETOC Task Force members, including detergent industries. Note the predicted average value for arable soil was reported in ECETOC 1993 as 4.42E-4, which is not possible given

the 5th and 95th percentile values. Therefore, the recalculated value provided in the IUCLID HEDSET (Year 2000 data) was used above.

Reference: 1) ECETOC. 1993. Environmental hazard assessment of substances. Technical Report No. 51, European Centre for Ecotoxicology and Toxicology of Chemicals, Brussels.

2) BKH. 1993. The use of existing toxicity data for estimation of the Maximum Tolerable Environmental Concentration of Linear Alkyl Benzene Sulfonate, Part I: Main report; Part II: Data base. Study carried out for ECOSOL, BKH Consulting Engineers, Delft, NL.

Reliability: 4 Not assignable because of uncertainty related to the input parameters.

3.4 MODE OF DEGRADATION IN ACTUAL USE

Remarks: Refer to other sections.

3.5 BIODEGRADATION

(a)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]** Marl, East treatment plant (Germany)

Concentration: 10 mg/L

Medium: Semi-continuous activated sludge (SCAS)

Method: The Marl purification plant consists of a mechanical prepurifying area, two parallel trickling filters of 800 m^3 volume each, and a stimulation plant of 106 m^3 volume, as well as mechanical final clarification. Samples were collected at the inlet of the trickling filters and at the exit of the final clarifier. Three-hour composite samples were taken for each analysis. The MBAS procedure was used to quantify LAS concentrations. The specific method for analyzing the homologues is reported in Wickbold 1964.

Results: Results of the percent removal by activated sludge for different alkyl chain length homologues and phenyl positions are shown in the following table:

	Phenyl Position	% Degradation
C_{10}	5	52
	4	68
	3	88
	2	92
C_{11}	6	58
	5	72
	4	89
	3	93
	2	94
C_{12}	6	81
	5	92
	4	94
	3	95
	2	95
C_{13}	7,6[a]	92
	5	94
	4	95
	3	96
	2	96

[a] Not analytically separable

GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test Substance: C_{10} to C_{13} homologues of LAS with varying phenyl positions
Remarks: The results show that longer chain homologues are removed faster than the shorter chain homologues, indicating that primary biodegradation increases as the chain length increases. In addition, the greater the distance between the sulfonic group and the more distant terminal methyl group on the alkyl chain the faster the degradation (i.e., phenyl position 2 degrades faster than phenyl position 5 for the same homologue). For example, percent removal was 52, 68, 88 and 92% for the C_{10} LAS with phenyl positions 5, 4, 3, and 2, respectively.
Reference: 1) Bock, K.J. and Wickbold, R. 1966. Auswirkungen der Umstellung auf leicht abbaubare Waschrohstoffe in einer großtechnischen Kläranlage und im Vorfluter. Vom Wasser 33:242-253.
2) Wickbold, R. 1964. Zwischenprodukte beim Abbau eines geradkettigen Alkylbenzolsulfonates. Vortrage IV, Inern. Kongr. F. grenzflachenaktive Stoffe, Brussel. (not available for review)
Reliability: 2 Valid with restrictions

(b)
Type: aerobic **[X]**; anaerobic **[ ]**
Inoculum: adapted **[X]**; non-adapted **[X]**; activated sludge **[X]**
Concentration of the chemical: 10 mg/L related to COD **[ ]**; DOC **[X]** test substance
Medium: water **[ ]**; water-sediment **[X];** soil **[ ]**; sewage treatment **[ ]**
Degradation: 69.6% after 28 days (acclimated inoculum)
66.7% after 28 days (non-acclimated inoculum)
Results: readily biodeg. **[ ];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[X]**
Kinetics:

Days	% Biodegradation (Acclimated)	% Biodegradation (non-Acclimated)
5	14.3	9.2
8	32.4	24.5
12	49.5	43.6
19	63.9	60.8
28	69.6	66.7

Method: OECD 301 B, modified Sturm test, also reported as method C 5 in the Italian D.M. 109. The reference standard sodium benzoate was used at the same concentration of the tested surfactants (about 10 mg/L). The testing period was 28 days and during this time the testing solutions were kept in dark glass vessels. A supernatant solution from a sludge, which was aerated and left to settle, was used as an inoculum for each biodegradation test at an amount equal to 1% of the solution. Both the STP sludges and the laboratory assimilated sludges were analysed for the dry matter contents. Tests were conducted using acclimated or non-acclimated inocula to determine whether this affected ultimate biodegradation. Acclimation was achieved by running the laboratory activated sludge plant for seven days before testing with a synthetic influent containing LAS at a concentration of abourt 10 mg/L. Tests were conducted on LAS and three other surfactants.
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: $C_{10\text{-}13}$ LAS; average alkyl chain length = $C_{11.6}$
Remarks: LAS was biodegradable using both acclimated and non-acclimated inocula. Acclimated inocula did not significantly improve the total biodegradation, but did accelerate the attainment of the degradation plateau. The 10-day time-window criterion was missed slightly, so this study does not meet the

criteria for ready biodegradability. However, this is expected given biodegradation kinetic curve dynamics related to increasing dissolved organic carbon content because the CO_2 generated during the biodegradation process is not totally evolved and removed from the test medium.

Reference: Ruffo, C., Fedrigucci, M.G., Valtorta, L., and Cavalli, L. 1999. Biodegradation of anionic and non-ionic surfactants by CO_2 evolution. Acclimated and non-acclimated inoculum. Riv. It. Sostanze Grasse LXXVI: 277-283.

Reliability: 1 Valid without restriction

(c)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]**; domestic activated sludge from Enid, OK

Concentration: 10 mg/L

Medium: Semi-continuous activated sludge (SCAS)

Degradation: >98% in 20 days (primary biodegradation)
62% in 20 days (inherent biodegradation)

Results: readily biodeg. **[ ];** inherently biodeg. **[X]**; under test condition no biodegradation observed **[ ]**, other **[ ]**

Method: ^{14}C ring-labeled LAS and ^{14}C alkyl-labeled C_{12} LAS were introduced to a simulated secondary waste treatment system (SCAS) following the ASTM and SDA standard methods.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test Substance: 1) LAS with the following homologue composition: C_{11} 42%, C_{12} 38%, C_{13} 20%; average alkyl chain length $C_{11.8}$
2) C_{12} LAS

Remarks: In a secondary waste treatment environment, the alkyl and ring portions of LAS both biodegrade extensively, with the fate of the LAS alkyl and ring carbon nearly identical. Within the 20 day test period, 62% of the alkyl and ring carbon converted to carbon dioxide.

Reference: Nielsen, A.M. and Huddleston, R.L. 1981. Ultimate biodegradation of linear alkylbenzene sulfonate alkyl and ring carbon. Developments in Industrial Microbiology. 22:415-424.

Reliability: 2 Valid with restrictions

(d)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: Bacterial biomass obtained from the settled supernatant slurry solution of a fertile soil

Concentration: 10 mg/L

Medium: water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**

Degradation: See methods

Results: See remarks

Method: OECD 301E Ready Biodegradability test, with the following modifications: LAS was the sole source of carbon introduced (i.e., no activated sludge inoculum), along with an enriched level of bacterial biomass. Preliminary tests showed that more than 90% of the LAS disappeared within 4 days, so LAS was restored by adding about 10 mg/L of fresh substance every 4 days for 80 days. The test was stopped 4 days after the last LAS addition (i.e., at 84 days). Specific HPLC analysis was used to measure LAS and SPCs.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test Substance: Commercial HF-type LAS with a C_{10}-$_{13}$ alkyl chain and a linearity of about 93% (DATS <0.5%; iso-branching 5-6%). (CAS #68411-30-3); average alkyl chain length = $C_{11.6}$

Remarks: The final organic residue of this prolonged biodegradation test was characterized in detail and showed that no accumulation of iso-branching

structures had occurred. This indicates that iso-branched material of LAS is amenable to biodegradation as well as the linear components.

Reference: Cavalli, L., Cassani, G., Lazzarin, M., Maraschin, C., Nucci, G. and Valtorta, L. 1996b. Iso-branching of linear alkylbenzene sulphonate (LAS). Tenside Surf. Det. 33:393-398.

Reliability: 2 Valid with restrictions

(e)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]**; activated sludge, domestic

Concentration: 10.8 mg/L related to COD **[ ]**; DOC **[X]** test substance **[ ]**

Medium: water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**

Degradation: 93% after 28 days

Results: readily biodeg. **[X];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**

Kinetic: 7 day = 59%
14 day = 73%
21 day = 82%

Method: Directive 79/831/EEC, Appendix V, C.4-A 1990. DOC Die-Away Test. (OECD 301A Test). Samples were collected from an activated sludge basin with predominantly local municipal waste water. The final sludge concentration was 19.3 mg/L. Two replicates were used for the LAS test concentration (9.44 mg/L) with inoculum, one with inoculum without LAS, and two control replicates (sodium benzoate, 10.13 mg/L) with inoculum. A total of 900 mLs of the solutions were put into 2000 mL Erlenmeyer flasks at the beginning of the test. The loosely covered flasks were incubated at 21.5 to 22.6°C in the dark on a mechanical shaker for 28 days. Samples were collected on days 0, 7, 14, 21 and 28 for DOC analysis.

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: Marlon A 390 (CAS #68411-30-3) C_{10-13} LAS; average alkyl chain length = $C_{11.6}$

Remarks: LAS is readily biodegradable. The 10-day window criterion was fulfilled. The control substance (sodium benzoate) showed 99% degradation after 28 days. This is a key study for ready biodegradability (see SIAR Table 4).

Reference: Schoeberl, P. 1993b. Bestimmung der biologischen Abbaubarkeit von Marlon A 390 im DOC-DIE AWAY Test. Huels Final Report No. DDA-21.

Reliability: 1 Valid without restriction

(f)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]**; activated sludge

Concentration: 9.7 mg/L related to COD **[ ]**; DOC **[X]** test substance **[ ]**

Medium: water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**

Degradation: 94% after 28 days

Results: readily biodeg. **[X];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**

Kinetic: 3 day = 38%
7 day = 81%
14 day = 88%
21 day = 94%

Method: Directive 79/831/EEC, Appendix V, C.4-A - Year: 1990. DOC Die-Away Test. (OECD 301A Test). Samples were collected from an activated sludge basin with predominantly local municipal waste water. The final sludge concentration was 18.1 mg/L. Two replicates were used for the LAS test concentration (8.96 mg/L) with inoculum, one with inoculum without LAS, and two control replicates (sodium benzoate, 11.65 mg/L) with inoculum. A

total of 900 mLs of the solutions were put into 2000 mL Erlenmeyer flasks at the beginning of the test. The loosely covered flasks were incubated at 21.8 to 22.2°C in the dark on a mechanical shaker for 28 days. Samples were collected on days 0, 3, 7, 14, 21, 27 and 28 for DOC analysis.

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: Marlon A 390 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$

Remarks: LAS is readily biodegradable. The 10-day window criterion was fulfilled. The control substance (sodium benzoate) showed 96% degradation after 28 days. This is a key study for ready biodegradability (see SIAR Table 4).

Reference: Schoeberl, P. 1993c. Bestimmung der biologischen Abbaubarkeit von Marlon A 390 im DOC-DIE AWAY Test. Huels Report No. DDA-32.

Reliability: 1 Valid without restriction

(g)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]**; municipal sewage treatment plant effluent.

Concentration: 5 mg/L related to COD **[ ]**; DOC **[X]** test substance **[ ]**

Medium: water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**

Degradation: 76% after 28 day

Results: readily biodeg. **[X];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**

Method: Directive 84/449/EEC, C.3 Modified OECD screening test. (OECD 301E Test).

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Marlon A 350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$

Reference: European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).

Reliability: 4 Not assignable

(h)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]**; activated sludge

Concentration: 10 mg/L related to COD **[ ]**; DOC **[X]**; test substance **[ ]**

Medium: water **[X]**; water-sediment **[ ]**; soil **[ ]**; sewage treatment **[ ]**

Degradation: 91.6% based on DOC reduction

Results: readily biodeg. **[ ]**; inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[X]**

Method: OECD Guideline 303 A "Simulation Test - Aerobic Sewage Treatment: Coupled Unit Test" 1981. The studies were carried out in the OECD Confirmatory Test plant at different laboratories using synthetic wastewater as specified in the EC Guidelines 82/242 and 82/243. The amount of surfactant supplied was 10 mg/ of MBAS/L. The amount of MBAS in the wastewater feed corresponds approximately to that detected in the feed of municipal sewage plants, which corresponds to about 6 mg DOC/L. Test periods in the different laboratories ran from 33 to 139 days.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: C_{10-13} LAS, sodium salt (CAS #68411-30-3); average alkyl chain length = $C_{11.6}$

Remarks: The degradation rate of 91.6% is the mean of 10 studies conducted at 7 different laboratories, based on DOC reduction. Since numerous studies have shown that not only anionic surfactants are shown in the MBAS analysis, the degradation plant discharge was analyzed on days 22, 24, 29 and 30 using HPLC analysis. Results showed that the content of intact LAS was

< 20 µg/L, which is about 8% of the 250 µg/L MBAS content in the discharge. This means that the real LAS primary degradation reaches 99.8%.

Reference: Schoeberl, P. 1991. Coupling the OECD confirmatory test with continuous ecotoxicity tests. Tenside Surf. Det. 28:6-14.

Reliability: 2 Valid with restrictions

(i)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]**; municipal sewage treatment plant effluent

Concentration: 5 mg/L related to COD **[ ]**; DOC **[ ]**; test substance **[X]** MBAS

Medium: water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**

Degradation: 95% after 19 days

Results: readily biodeg. **[X];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**

Method: OECD Screening Test according to "Verordnung ueber die Abbaubarkeit anionischer und nichtionischer grenzflaechenaktiver Stoffe in Wasch- und Reinigungsmittel vom 30.1.1977". Bundesgesetzblatt Teil I, S. 244. 1977

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Marlon A 350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$

Reference: European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).

Reliability: 4 Not assignable

(j)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]**; synthetic sewage

Concentration: 19.2 mg/L related to COD **[ ]**; DOC **[ ]**; test substance **[X]**

Medium: water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**

Degradation: 92.3% based on DOC reduction

Results: readily biodeg. **[ ];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[X]**

Method: OECD-Guideline 303A coupled units test. The studies were carried out in the OECD Confirmatory Test plant at different laboratories using synthetic wastewater as specified in the EC Guidelines 82/242 and 82/243. In these studies, LAS was added to the test at 10 mg/L. Test periods in the different laboratories ran from 33 to 139 days. Test temperature ranged from 19.6-23.0°C.

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: Marlon A390 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = $C_{11.8}$

Remarks: The degradation rate of 92.3% is the mean of 10 studies conducted at 7 different laboratories, based on DOC reduction, with LAS added to the confirmatory test plant.

Reference: 1) Schoeberl, P. 1991. Coupling the OECD confirmatory test with continuous ecotoxicity tests. Tenside Surf. Det. 28:6-14.
2) European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).

Reliability: 2 Valid with restrictions

(k)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]**;

Concentration: 10 mg/L

Medium:	related to COD **[ ]**; DOC **[ ]**; test substance **[X]** as MBAS water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Degradation:	99.8% after 3 days (for sewage dose of 1.0 mg/L) 89.4% after 7 days (for sewage dose of 0.5 mg/L) 74.5% after 7 days (no sewage dose, but aerated) 40.7% after 7 days (no sewage, non aerated)
Results:	readily biodeg. **[ ];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[X]** primary biodegradation
Method:	Samples from test flasks were taken at 12 hour intervals and the detergent concentration expressed as methylene blue active substance was determined. The initial concentration of detergent was 10 mg/L. The degradation of LAS was evaluated in raw canal water and in canal water seeded with either 0.5 ml/L or 1.0 ml/L sewage from the Ismalia sewage treatment plant.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Commercial LAS detergent (provided by Merck, Darmstadt, Germany); likely average alkyl chain length = $C_{11.6}$
Remarks:	Medium was Ismailia Canal water (Cairo, Egypt). ABS and a 1:1 mixture of ABS:LAS were also examined. Degradation of LAS was rapid, whereas degradation of ABS and the 1:1 mixture of ABS/LAS was slower. In all cases, aeration and addition of sewage microflora enhanced degradation.
Reference:	Abdel-Shafy, H.I., Azzam, A.M. and El-Gamal, I.M. 1988. Studies on the degradation of synthetic detergents by sewage. Bull. Environ. Contam. Toxicol. 41:310-316.
Reliability:	2 Valid with restrictions

(l)

Type:	aerobic **[X]**; anaerobic **[ ]**
Inoculum:	adapted **[ ]**; non-adapted **[X]**;
Concentration:	15 mg/L related to COD **[ ]**; DOC **[ ]**; test substance **[X] HPLC**
Medium:	water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[X]**
Degradation:	95% after 28 days (LAS-A) 98% after 28 days (LAS-B)
Results:	readily biodeg. **[ ];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[X]**
Method:	OECD303A coupled units test modified by AIS/CESIO "ad hoc" working group.
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	Two $C_{10\text{-}13}$ LAS commercial products as described in the remarks.
Remarks:	LAS-A, produced by the HF process, was 93% linear with 0.5% tetralins and 6.5% iso-branching and the following homologue distribution of the alkyl chain: C_{10} 15%, C_{11} 34%, C_{12} 31%, C_{13} 20% (average alkyl chain length = $C_{11.56}$). LAS-B, produced by the $AlCl_3$ process, was 98% linear with 0.5% tetralins and 1.5% iso-branching and the following homologue distribution of the alkyl chain: C_{10} 15%, C_{11} 29%, C_{12} 32%, C_{13} 24%, average alkyl chain length = $C_{11.65}$. HPLC methods specific to LAS were used to directly measure the test substances (LAS as well as the biodegradable intermediates). The ultimate biodegradation rates determined by HPLC are >10% higher than those obtained using DOC determination. The studies were conducted according to high standards and should be considered reliable.
Reference:	Cavalli, L., Cassani, G. and Lazzarin, M. 1996a. Biodegradation of linear alkylbenzene sulphonate (LAS) and alcohol ethoxylate (AE). Tenside Surf. Det. 33:158-165.
Reliability:	2 Valid with restrictions

(m)

Type:	aerobic **[X]**; anaerobic **[ ]**
Inoculum:	adapted **[ ]**; non-adapted **[ ]**; None Stated
Concentration:	15 mg/L related to COD **[ ]**; DOC **[ ]**; test substance **[X] HPLC**
Medium:	water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**
Degradation:	95% after 6 days
Results:	readily biodeg. **[ ];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[X]**
Method:	LAS and water collected from a briny pond (salinity: 9.5 g/L) were tested in an aerated cylindrical reactor at 21°C. Samples were removed periodically and analyzed for parent compound and metabolites by HPLC.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	LAS (CAS #25155-30-0); activity: >99%; average alkyl chain length = $C_{11.6}$
Remarks:	The half-life of LAS was 1.5 days. The HPLC method employed accurately defines the metabolites formed by primary biodegradation. All metabolites were not persistent and rapidly underwent further biodegradation.
Reference:	Sarrazin, L., Arnoux, A., Rebouillon, P. and Monod, J.L. 1997. Biodegradation of linear alkylbenzenesulfonate (LAS) in briny water and identification of metabolites using HPLC analysis by direct injection of samples. Toxicological and Environmental Chemistry. 58:209-216.
Reliability:	2 Valid with restrictions

(n)

Type:	aerobic **[X]**; anaerobic **[ ]**
Inoculum:	adapted **[ ]**; non-adapted **[X]**; activated sludge
Concentration:	1 mg/L related to COD **[ ]**; DOC **[ ]**; test substance **[X]**
Medium:	Activated sludge
Degradation:	>96% after 6 hours
Results:	Primary and complete biodegradation were described by a first-order model, with rate constants of 0.96-1.10/h ($t_{½}$ = 0.63–0.72 h) for primary loss and 0.50-0.53/h ($t_{½}$ = 1.30–1.38 h) for complete degradation.
Method:	Radiolabeled LAS was dosed at an environmentally relevant concentration into biotic and abiotic activated sludge. Activated sludge mixed liquor was used from two STP (Polk Run and Sycamore) near Cincinnati. Standard methods were used and the test flasks (reactors) were maintained at 20+/-2°C.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test Substance:	^{14}C [uniform ring] C_{12} LAS
Reference:	Federle, T.W. and Itrich, N.R. 1997. Comprehensive approach for assessing the kinetics of primary and ultimate biodegradation of chemicals in activated sludge: Application to linear alkylbenzene sulfonate. Environ. Sci. Technol. 31:1178-1184.
Reliability:	2 Valid with restrictions

(o)

Type:	aerobic **[ ]**; anaerobic **[X]**
Methods:	Experiments were conducted in which enriched cultures of anaerobic bacteria were provided with 60 µmole/L LAS as the sole source of sulfur. Conditions were maintained anoxic in salts-medium containing several sources of carbon.
Results:	Strain RZ LAS, an anaerobic bacteria, was isolated from wastewater treatment plants in Germany. RZLAS was shown to degrade LAS, indicating that microorganisms able to metabolize LAS in anaerobic conditions exist in nature.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test Substance:	Commercial C_{10-13} LAS (CAS #68411-30-3; average alkyl chain length = $C_{11.6}$) and C_{12} LAS (pure homologue)

Reference: Denger, K. and Cook, A.M. 1999. Linear alkylbenzene sulphonate (LAS) bioavailable to anaerobic bacteria as a source of sulphur. Journal of Applied Microbiology. 86:165-168.
Reliability: 2 Valid with restrictions

(p)
Type: aerobic **[ ]**; anaerobic **[X]**
Inoculum: adapted **[ ]**; non-adapted **[X]**; granular sludge
Concentration: 9 concentrations ranging from 12.5 to 350 mg/bottle
Medium: Liquid
Degradation: 5-44% after 14 days
Method: Upflow Anaerobic Sludge Blanket (UASB) type reactors with a working volume of 315 mL in serum type glass bottles were used to measure degradation. The bottles were incubated at 30^{+}/-2°C for 14 days. The sludge concentration was 1.5 g/L. Methane production was measured daily using both the Head Space method and the Displacement method. LAS was specifically determined using HPLC.
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test Substance: LAS, sodium salt derived from commercial LAB with the homologue distribution: $<C_{10}$ 0.7%, C_{10} 8.4%, C_{11} 40.9%, C_{12} 32.5%, C_{13} 16.6%, and C_{14} 0.9%. Final molecular weight of 341.5. Average alkyl chain length = $C_{11.54}$
Remarks: The study determined an IC_{50} of 40 to 150 mg/L as inhibitory to anaerobic microbial populations. LAS concentrations are usually found in anaerobic digestors at 5-25 g/kg, which is about an order of magnitude lower than the observed IC_{50} values. The study demonstrates that LAS anaerobic biodegradation does occur under conditions that are not sulphur-limited, using anaerobic digestor sludge and specific HPLC methods to measure the loss of parent material.
Reference: Sanz, J.L., Rodriguez, M., Amils, R., Berna, J.L., de Ferrer, J. and Moreno, A. 1999. Anaerobic biodegradation of LAS (Linear Alkylbenzene Sulfonate): Inhibition of the methanogenic process. La Rivista Holiana Delle Sostanze Grasse. LXXVI:307-311.
Reliability: 2 Valid with restrictions

(q)
Type: aerobic **[ ]**; anaerobic **[X]**
Inoculum: Activated sludge
Medium: Sewage sludge
Degradation: 30-93% after 250 days; 50% in a second 90 day experiment
Results: LAS biodegrades under strict anaerobic conditions.
Method: The standard ECETOC-28 method, which measures the pressure of the biogas as an indicator of anaerobic degradation, was extended to 250 days and supplemented with specific HPLC analysis of LAS concentrations. Testing bottles were prepared in triplicate and monitored for the biodegradation of LAS already present in the sludge without extra LAS being added to the system. A second experiment was also based on the ECETOC-28 method, with several modifications used to further control the anaerobic test conditions.
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test Substance: LAS, as exists in sewage sludge
Remarks: Specific HPLC analysis (loss of LAS) confirms that LAS undergoes primary biodegradation anaerobically in the standard ECETOC-28, although increased gas production (mineralization) was not observed. A redisolution of precipitated adsorbed LAS seemed to occur in the digestion process. The product in liquid solution is probably the fraction being degraded.

Reference:	Prats, D., Rodriquez, M., Llamas, J.M., De La Muela, M.A., de Ferrer, J., Morena, A. and Berna, J.L. 2000. The use of specific analytical methods to assess the anaerobic biodegradation of LAS. 5th World CESIO Congress V2:1655-1658, Firenze, Italy.
Reliability:	2 Valid with restrictions

(r)

Type:	aerobic **[X]**; anaerobic **[ ]**
Inoculum:	Trickling filters
Medium:	Sewage sludge
Results:	ROC supported sulfur-limited growth of *P. putida*. Extensive desulfonation of ROC was observed.
Method:	Other studies have confirmed that LAS is completely biodegradable in trickling filters and by- products in commercial LAS (e.g., DATS, SPC) are subject to biotransformation to nondegraded compounds termed refractory organic carbon (ROC). The current study investigated the further desulfonation of ROC by a strain of *Pseudomonas putida*. ROC was generated from commercial LAS, which served as a carbon source, in a trickling filter and isolated by solid-phase extraction. The solution of ROC was then used as a potential sulfur source for the growth of *P. putida*. Experiments were conducted in triplicate at 30°C and cultures were aerated on an orbital shaker. Dissolved Organic Carbon was measured using a total organic carbon analyzer and HPLC.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test Substance:	Commercial LAS (Sirene 113)
Remarks:	Earlier work shows that the biodegradation and biotransformation of commercial LAS as a carbon source for growth leads to a residue of sulfonated aromatic compounds, termed refractory organic carbon (ROC), from the synthetic by-products. This study demonstrates that this ROC, after separation from sulfate ion, is utilized extensively as a sulfur source for bacterial growth. The products of desulfonation are expected to be biodegradable.
Reference:	Mampel, J., Hitzer, T., Ritter, A. and Cook, A.M. 1998. Desulfonation of biotransformation products from commercial linear alkylbenzene sulfonates. Environ. Toxicol. Chem. 17:1960-1963.
Reliability:	2 Valid with restrictions

(s)

Type:	aerobic **[ ]**; anaerobic **[X]**
Inoculum:	adapted **[ ]**; non-adapted **[ ]**; other **[X]**; lake sediments
Concentration:	20, 100, and 200 mg/L
Medium:	Water
Results:	Degradation occurred under anaerobic conditions when exposed to inoculum obtained from lake sediments. In addition, inocula that were found in aerobic environments such as compost and activated sludge from a wastewater treatment plant also showed capability of anaerobic degradation of LAS.
Method:	Tests were performed in batch serum vials under anaerobic conditions. The vials were filled with the appropriate pH 7 medium, autoclaved at 140°C for 30 minutes, and inoculated with 5 to 10% of the respective inocula. Inocula originated from several different natural environments and from anaerobic reactors. LAS was added at three different concentrations (20, 100, and 200 mg/L) plus three sets of controls, all in triplicate. Incubation time was 2 months.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test Substance:	Mixture of LAS with an alkyl chain length of 9 to 13 units; likely average alkyl chain length = $C_{11.6}$

Remarks:	This paper indicates qualitatively that LAS undergoes anaerobic degradation, but no quantitative results are presented.
Reference:	Angelidaki, I., Mogenen, A.S. and Ahring, B.K. 2000b. Degradation of organic contaminants found in organic waste. Biodegradation. 11:377-383.
Reliability:	2 Valid with restrictions

(t)

Type:	aerobic **[ ]**; anaerobic **[X]**
Inoculum:	Activated sludge
Concentration:	100 mg/L
Medium:	water **[ ];** water-sediment **[ ];** soil **[ ];** sewage treatment **[X]**
Degradation:	Transformation of C_{12} LAS occurred under anaerobic conditions. The degree of transformation varied between 14 to 25%.
Methods:	Two lab-scale continuous stirred tank reactors (CSTR) were set up with automatic, semi-continuous feeding and were run under mesophilic conditions (37^{o}C) with a hydraulic retention time of 15 days. The reactors were started with anaerobic stabilizer sewage sludge and operated for several months before the experiment started. The feed was diluted sludge at a total solids concentration of 20 g TS/L. The sludge was spiked with C_{12} LAS at a concentration of 100 mg/L and the two reactors were operated similarly for 36 days. After this period, the LAS concentration in reactor 1 was increased to 268 mg/L, while for reactor 2 the influent TS was decreased to 11.4 g TS/L, and both reactors continued to operate for a total of 90 days (including the original 36 days).
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test Substance:	C_{12} LAS (pure homologue)
Remarks:	A clear correlation was shown between degradation of organic matter contained in the sludge and anaerobic degradation of LAS, giving an increase in transformation with the higher the reduction of organic matter. Transformation was limited by bioavailability due to sorption of LAS (i.e., only the bioavailable fraction of LAS is transformed by anaerobic digestion). When the reduction degree of the organic matter increased from 22% to 28%, the transformation degree of C_{12} LAS increased from 14% to 20%. Decreasing the total solids concentration of the influent sludge or increasing the spiked concentration of C_{12} LAS did not significantly alter the degree of LAS transformation.
Reference:	Angelidaki, I., Haagensen, F. and Ahring, B.K. 2000a. Anaerobic transformation of LAS in continuous stirred tank reactors treating sewage sludge. 5th World CESIO Congress. V.2:1551-1557, Firenze, Italy.
Reliability:	2 Valid with restrictions

(u)

Type:	aerobic **[X]**; anaerobic **[ ]**
Medium	coastal sea water
Concentration:	5 mg/L related to test substance
Results:	LAS primary degradation half-lives ranged from 3.4 to 13.8 days, with 4-9 days being the most frequent values.
Method:	Coastal sea water from the Mediterranean Sea was collected from three areas in Spain (Barceloneta, Ebro delta, and Sant Feliu de Guixols, Girona). Samples of 1.5- L were placed in 3-L flasks and incubated in the dark at 20^{o}C with orbital shaking (100 rpm) for 30 days. Viable bacteria were determined by plate counts on marine agar media, while total bacteria were determined by flow cytometry after SYTO-13 staining. LAS degradation was monitored by HPLC. A reference substance was not used. LAS quantification was based on an external standard.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**

Test Substance: C_{10-14} LAS, activity 66.62%; average alkyl chain length = $C_{11.7}$
Remarks: In most cases, sea water samples showed a similar evolution of bacterioplankton over time, characterized by three phases: (a) a progressive increase in bacterial density; (b) a later decrease; and (c) a fluctuating stationary phase. Bacterioplankton degraded the LAS by growing to populations with a high percentage of viable bacteria. The bacteria were readily grazed by protozoa, preventing anomalous high bacterial growth and ensuring the later channeling of LAS carbon to upper trophic levels.
Reference: Vives-Rego, J., Lopez-Amoros, R., Guindulain, T., Garcia, M.T., Comas, J., and Sanchez-Leal, J. 2000. Microbial aspects of linear alkylbenzene sulfonate degradation in coastal water. Journal of Surfactants and Detergents. 3:303-308.
Reliability: 2 Valid with restrictions

(v)
Type: Respirometer
Method: Degradation of LAS in Ohio River water collected below the discharge of a municipal wastewater treatment plant (Muddy Creek, OH) was measured in an electrolytic respirometer. Background LAS concentrations were less than 0.5 mg/L. Oxygen consumption over time was determined at five LAS concentrations (5, 10, 20, 40, and 80 mg/L) plus a control until plateau values were reached. The maximum initial rates of oxygen uptake were calculated based on methods described in Larson and Perry (1981).
Results: LAS degradation was not affected in river water until the LAS concentration exceeded 10 mg/L. The degradation was partially affected at 20 mg/L but was not completely inhibited until 40 mg/L.
Substance: LAS; average chain length $C_{11.6}$.
Remarks: The level at which inhibition of degradation was complete (40 mg/L) is significantly higher than the levels observed in model ecosystem studies conducted by these researchers [see 4.7 (h) and (i)].
Reference: 1) Larson, R.J. and Maki, A.W. 1982. Effect of LAS on the structure and function of microbial communities in model ecosystems. Aquatic Toxicology and Hazard Assessment: Fifth Conference, ASTM STP 766, Pearson, J.G., Foster, R.B., and Bishop, W.E., Eds., American Society for Testing and Materials, pp. 120-136.
2) Maki, A.W. 1981. A laboratory model ecosystem approach to environmental fate and effects studies. Unpublished Internal Report, Environmental Safety Department Procter & Gamble Company, Cincinnati, Ohio.
3) Larson, R.J. and Perry, R.L. 1981. Water Research 15:697-702.
Reliability: 2 Valid with restrictions

(w)
Type: aerobic **[X]**; anaerobic **[ ]**
Substance: LAS
Remarks: The biodegradation of LAS has been thoroughly studied for its primary and total degradation and catabolism. It is mineralized biologically to form carbon dioxide, water and sulphate. Using UV spectroscopic analysis, Swisher (1987) and others showed the aromatic ring to be degradable up to 80%. Using the more reliable tracer technique with ^{14}C-ring labelled LAS, it was determined that degradation of the ring is predominantly between 50 and 80%. Further studies have shown that LAS degradation proceeds through oxidative conversion of the methyl groups of the alkyl chain into a carboxyl group (ω-oxidation), oxidative shortening of the alkyl chain by 2-carbon units (β-oxidation), oxidative ring splitting, then cleavage of the carbon-sulfur bond. This process forms sulfophenyl carboxylates (SPCs) as

biodegradation intermediates. The first detectable degradation product of LAS is ω-carboxylate. For example, Huddleston and Allred (1963) detected sulfophenyl decanoic acid as a catabolite of 2-benzenedecasulfonate. Oxidative degradation of the alkyl chain begins as soon as LAS has been converted into sulfophenyl carboxylic acid. The principal degradation pathway is β-oxidation. The rate of biodegradation is inversely related to the distance between the terminal alkyl-methyl group and the point of benzene ring attachment. Simple branching does not impair the oxidation of alkylbenzene, though more complex branching does decrease the rate.

Reference: 1) Swisher, R.D. 1987. Surfactant Biodegradation, second edition. Surfactant Science Series, Volume 18. Marcel Dekker, Inc. New York.
2) Schoeberl, P. 1989. Basic principles of LAS biodegradation. Tenside Surf. Detergents 26:86-94.
3) Huddleston, R.L. and Allred, R.C. 1963. Microbial oxidation of sulfonated alkylbenzenes. Dev. Ind. Microbiol. 4:24-38.

Reliability: 2 Valid with restrictions

(x)

Type: aerobic **[X]**; anaerobic **[ ]**

Method: Dialkyltetralin sulfonates (DATS) and LAS with single methyl branching on the alkyl chains (iso-LAS) are minor components in commercial LAS. In this study, DATS and iso-lAS were synthesized and exposed to simulated activated sludge, soil, and receiving water environments. In addition, the effluents coming from activated sludge treatment, which contained biodegradation intermediates, were exposed to simulated receiving water environments. Radiolabeled LAS, DATS and iso-LAS were used and all samples were analyzed using chemical-specific HPLC procedures. Surface soils were collected at three locations to represent "pristine" soil, sludge-amended soil, and gray water contaminated soil from the top of a percolation bed that receives surface applications of laundry water from a Laundromat. All samples were screened to remove vegetation, rocks and debris, and mixed with a mineral salts medium containing the test substance. Sediment samples were collected from the upper inch of a small stream that received effluent from a domestic wastewater treatment plant. Periphyton samples were collected as rocks coated with heavy growth from the same stream locations as the water and sediment samples. Each test system consisted of duplicate test flasks and a control flask. Tests lasted at least 30 days. For assessing biodegradation, the porous pot method was used in a simulated wastewater activated sludge modified from ASTM test method E1798-96. A 21-day acclimation phase was followed by a 15-day test phase in which radioactivities in C02, liquids and solids, and effluent total suspended solids and COD were determined each day. Radiochemical recoveries for the porous pot test were calculated. For the die-away tests with porous pot effluents, the combined effluents from individual units were tested for mineralization of radiolabeled parent and intermediate compounds. All tests were run at least 30 days and the radioactivities measured at the end of each test.

Results: Results indicate that radiolabeled DATS and iso-LAS is mineralized by indigenous microbial populations in laboratory simulations of aquatic and soil environments. Half-lives ranged from 2 to 20 days. In addition, upon exposure to laboratory activated sludge treatment, most iso-LAS compounds showed >98% parent compound removal, extensive mineralization (>50%), and 79-90% ultimate biodegradation. Activated sludge treatment of DATS resulted in >98% removal, 3-12% ultimate biodegradation, and apparent formation of carboxylated biodegradation intermediates that accounted for 88-97% of the original material. These intermediatel continued to mineralize

in simulated receiving water and soil environments at rates similar to that of sulfophenyl carboxylate (SPC) intermediates of a standard LAS.

Test Substances: ^{14}C-benzene ring labeled C_{12} LAS (97.5% radiochemical purity); ^{14}C-benzene ring labeled iso-LAS of the following types (IA, 97.8% purity; IB, 77.6% purity; IIA, 94.7% purity; IIB, 97.5% purity); ^{14}C-benzene ring labeled DATS (97.3% purity), plus the non-labeled versions of the same.

Reference: Nielsen, A.M., Britton, L.N., Beall, C.E., McCormick, T.P. and Russell, G.L. 1997. Biodegradation of coproducts of commercial linear alkylbenzene sulfonate. Environ. Sci. Technol. 31:3397-3404.

Reliability: 2 Valid with restrictions

(y)

Type: aerobic **[X]**; anaerobic **[ ]**

Method: OECD 301E. The study was designed to investigate the biodegradation of a relatively high iso-branched form of commercial LAS. The test was a prolonged batch-biodegradation experiment in which the material is kept "alive" for 80 days and in which the test compound present in a mineral salts medium is the sole carbon source. An enriched level of bacterial biomass, three times the amount recommended, was added at the test start using an inoculum obtained from the settled supernatant slurry solution of a fertile soil, without any previous exposure to the test compound. LAS was maintained by adding about 0 mg/L of fresh substance every four days for 80 days. After 80 days the test solution was sampled, centrifuged, sterilized with $HgCl_2$ solution and analyzed with a chemical specific HPLC method with fluorescence detection.

Results: Results indicate a residual LAS amount of 1.5 mg/L and SPC intermediate amount of 28.7 mg/L at the end of the 80 day study. Four distinct SPCs originating from the linear components of LAS were formed from the biodegradation experiment, and made up most of the organic residue. No evidence of structures related to the iso-branched material was found in the residue, therefore no accumulation of these materials is indicated. The iso-branched component of LAS and the corresponding SPCs mineralized at rates as fast as the linear components.

Test Substances: Commercial LAS (HF type) with a C_{10}-C_{13} alkyl chain and a linearity of about 93%, with a low DATS content (<0.5%) and a relatively high iso-LAS content (6.5%).

Reference: Cavalli, L., Cassani, G., Lazzarin, M., Maraschin, C., Nucci, G., and Valtorta, L. 1996. Iso-branching of linear alkylbenzene sulphonate (LAS). Tenside Surf. Det. 33:393-398.

Reliability: 2 Valid with restrictions

(z)

Type: aerobic **[X]**; anaerobic **[ ]**

Inoculum: adapted **[ ]**; non-adapted **[X]**; activated sludge

Concentration: 34.3 mg/L related to COD **[ ]**; DOC **[X]** test substance **[ ]**

Medium: water **[X];** water-sediment **[ ];** soil **[ ];** sewage treatment **[ ]**

Degradation: 85% after 29 days

Results: readily biodeg. **[X];** inherently biodeg. **[ ]**; under test condition no biodegradation observed **[ ]**, other **[ ]**

Kinetic:
0 day = -1%
2 day = -2%
5 day = 22%
9 day = 52%
12 day = 70%
14 day = 70%
21 day = 78%

28 day = 83%
29 day = 85%

Method: OECD Test Guideline 301B and EC Directive 92/69/EEC C.4-C. Modified Sturm Test.. The test substance was added to a defined liquid mineral medium which was inoclulated with an activated-sludge inoculum and aerated at 19.7-21.9°C (mean 21.1°C). The inoculum used was activated non-adapted sludge from the Marl-Ost municipal sewage treatment plant. The inoculum had a bacterial count of 81 x 10^4 CFU/mL as determined by the Koch pour-plate method. The CO_2 released was bound in the form of sodium carbonate in sodium hydroxide solution. Samples were collected and analyzed in duplicate for bound CO_2 by TIC analysis after 0, 2, 5, 9, 12, 14, 21, 28 and 29 days. Sodium benzoate was used as a suitable control substance to monitor the activity of the inoculum. On the 29th day, residual dissolved CO_2 was expelled by acidification.

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: Marlon A 365 WEL 6859 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; Activity: 65%

Remarks: LAS is readily biodegradable. The 10-day window criterion was fulfilled. The control substance (sodium benzoate) showed 89% degradation after 29 days. This is a key study for ready biodegradability (see SIAR Table 4).

Reference: Enste-Diefenbach, R.. 2002. Marlon A 365 WEL 6859: Determination of biodegradability in the modified Sturm test.. Infracor GmbH Analytical Tehcnical Services, Report ST-204/02.

Reliability: 1 Valid without restriction

3.6 BOD_5, COD OR RATIO BOD_5/COD

BOD_5

Method: DIN 38H03, Part 1. Bestimmung des biochemischen Sauerstoffbedarfs in 5 Tagen nach den Verduennungsprinzip.

Value: <10 mg O_2/g for both Marlon A 350 and Marlon A 375

GLP: Yes **[ ]** No **[ ]** ? **[X]**

COD

Method: DIN 38H03, Part 1

Values: 1151 and 1760 mg O_2/g for Marlon A 350 and Marlon A 375, respectively.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Ratio BOD_5/COD: < 0.005

Remarks: Marlon A 350 (C_{10-13} LAS, average chain length = 11.6, 50% a.i.)
Marlon A 375 (C_{10-13} LAS, average chain length = 11.6, 75% a.i.)
The extended term BOD determinations yield 60 to 70% of COD. The substance is degradable.

Reference: European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts (CAS #68411-30-3). Year 2000 CD-ROM edition, citing data by Huels AG Marl.

Reliability: 4 Not assignable

3.7 BIOACCUMULATION

(a)

Species: *Pimephales promelas* (fish, fresh water)

Exposure period: 48, 168, 192 hours

Temperature: Per Protocol

Concentration: 2.7 and 4.1 μM

BCF: Values of Steady-State Bioconcentration Factor (BCF_{ss}) and Average Length of Alkyl Chain ($n_{C,Av}$) are shown in the following table.

expt	comp*	BCF_{ss} L/kg	$n_{C,Av}$
A	C_{10}-2	1.7	10.8
	C_{11}-2	5.8	
	C_{12}-2	47.6	
	C_{13}-2	353.8	
B	C_{11}-5	6.1	11.7
	C_{12}-2	99.1	
	C_{12}-5	10.0	
	C_{13}-5	34.0	
C	C_{11}-5	9.8	11.4
	C_{12}-2	168.4	
	C_{12}-3	42.1	
	C_{12}-6	31.9	
D	C_{10}-2	6.0	10.6
	C_{11}-2	31.9	
	C_{12}-2	211.5	
	C_{13}-2	987.2	
	C_{10}-in	3.0	
	C_{11}-in	9.1	
	C_{12}-in	29.9	
	C_{13}-in	112.4	

*In the format C_n-m, n and m are the length of the alkyl chain and the position at which the sulfophenyl moiety is substituted to the alkyl chain, respectively.

Elimination: Yes **[X]** No **[ ]** ? **[ ]**

Method: OECD 305 E. The exposure phase in Experiment A was 48-hours. The exposure phase in Experiments B-D ranged from 168 to 192 hours. Due to the rapid equilibrium demonstrated in these studies, a longer exposure period was not needed. Fish were then transferred to untreated water for the depuration phase (duration not stated).

Type of test: calculated **[ ]**; measured **[X]**
static **[ ]**; semi-static **[ ]**; flow-through **[X]**

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: LAS (C_{10-13}), tested individually and as mixtures, activity: >97.4%

Remarks: As shown in the table, BCF values ranged between 2-1000 L/kg. Experiments A, B and D showed that BCFs increase with increasing alkyl chain length for a given isomer. In addition, the results of Experiments B and C demonstrate that the closer the p-sulfophenyl moiety is positioned to the terminal carbon of the alkyl chain, the higher the BCF. However, alkyl chain length has a much bigger effect than does the phenyl position. To address differences in composition of mixtures, bioconcentration potential was calculated for a mixture typical of LAS in European detergent formulations (C_{10} 12%, C_{11} 29%, C_{12} 34%, C_{13} 24%; average alkyl chain length = $C_{11.6}$) and a mixture typical of LAS in filtered Mississippi river water (C_{10} 45%, C_{11} 23%, C_{12} 23%, C_{13} 2%; average chain length = $C_{10.8}$), using BCF values for the individual components. This calculation of BCF for the typical mixtures was done using the following equation developed in the above testing:

$$(\Sigma C_{f,i}/\Sigma C_{w,i})_{rel} = \Sigma(\phi_{i,w} \cdot BCF_{i,rel})$$

The BCFs were 87 L/kg for a standard mixture typical of LAS in European detergent formulations (average alkyl chain length = $C_{11.6}$) and 22 L/kg for a representative environmental sample (filtered Mississippi river water, average alkyl chain length = $C_{10.8}$), indicating that the bioconcentration potential of LAS is low and is decreased by environmental processes such as biodegradation and absorption, which reduce aquatic concentrations.

Reference: Tolls, J., Haller, M., DeGraaf, I., Thijssenk, M.A.T.C. and Sijm, D.T.H.M. 1997. Bioconcentration of LAS: Experimental determination and extrapolation to environmental mixtures. Environ. Sci. Technol. 31:3426-3431.

Reliability: 2 Valid with restrictions

(b)

Species: *Lepomis macrochirus*
Exposure Period: 21 days
Temperature: 17^{+}/-1°C
Concentration: 0.5 mg/L
BCF: 104 (whole body); 36 (muscle)
Elimination: Yes
Method: Bluegill sunfish (avg wt. 4.0 g; avg length 68 mm) were placed in a 60 liter aquarium (375 fish total) and maintained for 21 days. A second aquarium held 100 control fish. Fish were fed daily with a dry pelleted trout chow ration of approximately 2% of body weight. Water samples were removed periodically for radiometric analysis of ^{14}C-labeled LAS. Four fish were removed on each of days 1, 2, 3, 5, 7, 9, 11 and 14 for radiometric analysis.
Type of test: calculated **[ ]**; measured **[ ];** static **[ ]**; semi-static **[ ]**; flow-through **[X]**
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: C_{10-13} LAS (CAS #68411-30-3) with the following alkyl chain length distribution: C_{11} 45%, C_{12} 36.5%, C_{13} 18.5%. Average chain length was 11.7 and molecular weight was 344.
Remarks: The site of greatest concentration was the gall bladder with a BCF of 5000, based on total radiolabeled materials. The BCFs for liver, gills and viscera, remaining carcass, and blood ranged from 64 to 283. Clearance of radiolabeled materials was rapid with half-lives of 2 to 5 days. However, no quantitative conclusions specific to LAS can be drawn from these data, as total radiolabeled materials were measured, and these likely include LAS metabolites.
Reference: Kimerle, R.A., Macek, K.J., Sleight, B.H. and Burrows, M.E. 1981. Bioconcentration of linear alkylbenzene sulfonate (LAS) in bluegill (*Lepomis macrochirus*). Wat. Res. 15:251-256.
Reliability: 2 Valid with restrictions

3.8 ADDITIONAL REMARKS

A. Sewage treatment

(a)

Results: LAS removal in sewers due to biodegradation can reach as high as 50% of the total LAS load when the sewer system is properly aerated.
Method: Integrated composite samples were collected in November and December 1988 from the sewer system of Estepona (Malaga), Spain. LAS was analyzed using a specific HPLC technique.

Remarks: This study demonstrates that significant biodegradation of LAS occurs prior to reaching wastewater treatment plants. Additional removal (up to >95%) occurs in the plants themselves.
Reference: Moreno, A., de Ferrer, J. and Berna, J.L. 1990. Biodegradability of LAS in a sewer system. Tenside Surf. Det. 27:312-315.
Reliability: 2 Valid with restrictions

(b)
Results: The average removal rate for LAS in activated sludge treatment was > 99%. A lower and more variable rate was observed in trickling filter treatment plants with an average removal of 82% for LAS.
Remarks: Samples were collected from six trickling filter and four activated sludge treatment plants located in the midwestern United States.
Reference: McAvoy, D.C., Dyer, S.D., Fendinger, N.J., Eckhoff, W.S., Lawrence, D.L. and Begley, W.M. 1998. Removal of alcohol ethoxylates, alkyl ethoxylate sulfates, and linear alkylbenzene sulfonates in wastewater treatment. Environ. Toxicol. Chem. 17:1705-1711.
Reliability: 2 Valid with restrictions

(c)
Results: The model predicted average removal of LAS from wastewater treatment plants is 99.2%. Predicted 90^{th}-percentile concentrations at 1,000 m downstream from the sewage outfall, based on actual measured raw sewage concentrations and actual measured effluent calculations, ranged from 3.7 to 9.2 µg/L for different predicted instream removal rates.
Method: Modeling was conducted to predict the 90^{th}-percentile environmental concentration (PEC) of LAS and other detergent substances in aquatic environments in the Netherlands. Inputs included emissions data, prediction of raw sewage concentration and initial material characterization. Model predictions included the removal of LAS in wastewater treatment plants, concentrations in surface waters, and prediction of the 90^{th}-percentile concentrations.
Remarks: The authors emphasize that to provide a fate assessment adequate for regulatory purposes, a need clearly exists for a fundamental interplay between monitoring, laboratory data, and these predictive models. This study is part of an extensive monitoring program executed jointly by the Dutch Soap Association (NVZ) and the Dutch Ministry of Housing, Spatial Planning and the Environment (VROM). Monitoring data from this program can be found in Matthijs et al. 1999.
Reference: Feijtel, T.C.J., Struijs, J., and Matthijs, E. 1999b. Exposure modeling of detergent surfactants – Prediction of 90^{th}-percentile concentrations in the Netherlands. Environmental Toxicology and Chemistry 18:2645-2652.
Reliability: 2 Valid with restrictions

(d)
Results: The average concentration of LAS in the treated sewage of the sum wastewater treatment plants was 39 µg/L. The average total removal of LAS was 99.2%.
Method: Twenty four hour flow proportional samples of raw, settled, and treated sewage were collected by automatic samples during three consecutive days at seven sewage treatment plants in the Netherlands. All samples were collected between April and July 1994 and analyzed for traditional sewage treatment plant water quality parameters. Samples for the analysis of LAS and other surfactants were taken every 15 minutes (hourly composites) using a time proportional automatic sampler. The LAS in these samples was analyzed using an HPLC method with fluorescence detection.

Remarks: This study is part of an extensive monitoring program executed jointly by the Dutch Soap Association (NVZ) and the Dutch Ministry of Housing, Spatial Planning and the Environment (VROM). The authors indicate that field studies suggest that in-sewer removal can play a significant role in reducing the concentrations of surfactants entering the sewage treatment plant.

Reference: Matthijs, E., Holt, M.S., Kiewiet, A., and Rijs, G.B.J. 1999. Environmental monitoring for linear alkylbenzene sulfonate, alcohol ethoxylate, alcohol ethoxy sulfate, alcohol sulfate, and soap. Environmental Toxicology and Chemistry 18:2634-2644.

Reliability: 2 Valid with restrictions

(e)

Methods: LAS was monitored seasonally for one year (winter, spring, summer) in a small river in Spain receiving untreated sewage from a non-industrial village (Caserras). Sampling was carried out during November 1994, May 1995 and July 1995. Grab samples were collected in the morning, afternoon and evening at five sampling sites representing the raw sewage discharge, a pre-discharge location on the river, and three downstream locations on the river (1.5, 3.0 and 4.8 km downstream of the discharge).

Results: Seasonal differences were observed in biodegradation, with total LAS removals (dissolved and adsorbed) at 4.8 km downstream of 31.8%, 95.5% and 98.3% for winter, spring and summer respectively.

Remarks: The seasonal differences in biodegradation are explained by hydraulic conditions. River flow rates are much greater in winter (75 m^3/min) versus spring (4.5 m^3/min) and summer (0.2 m^3/min), which results in a much reduced hydraulic retention time (and thus less contact time for biodegradation) in winter of 1.6 hrs compared to 26.6 hrs in spring and 25 days in summer. Overall, even in situations of direct discharge of untreated sewage, LAS biodegradation of >98% can be expected provided that the receiving water stream has adequate hydraulic conditions.

Reference: de Ferrer, J., Moreno, A., Vaquero, M.T. and Comellas, L. 1997. Monitoring of LAS in direct discharge situations. Tens. Surfactants Det. 34:278-283.

Reliability: 2 Valid with restrictions

(f)

Results: LAS removal of 98-99% and biodegradation of 80-84% was observed. Sulfophenyl carboxylates (SPC) were found only in water and not the absorbed phases (sludge).

Remarks: This study was conducted to specifically study LAS biodegradation in real WWTP conditions in Italy. LAS data was obtained by HPLC of influent, effluent, dissolved waters and sludges to reach a complete mass balance.

Reference: 1) Cavalli, L., Gellera, A., Lazzarin, A., Nucci, G.C., Romano, P., Ranzani, M. and Lorenzi, E. 1991. Linear alkylbenzene sulphonate removal and biodegradation in a metropolitan plant for water treatment. Riv. Ital. Sostanze Grasse 68:75-81.
2) Cavalli, L., Gellera, A. and Landone, A. 1993. LAS removal and biodegradation in a wastewater treatment plant. Environmental Toxicology and Chemistry 12:1777-1788.

Reliability: 2 Valid with restrictions

B. Other information

(a)

Remarks: A significant number of additional literature articles report data on the environmental fate of LAS. An additional bibliography of literature citations for LAS can be found in an Appendix to this dossier.

(b)
Type of Measurement: Background **[X]**; At contaminated site **[ ]**; Other **[ ]**
Medium: soil
Remarks: Where surfactant and hydrophobic organic compounds (HOCs) co-exist in soil-water systems there are a number of possible interactions which can occur simultaneously: 1) distribution of surfactant between monomeric, hemimicellar and miscellar forms, 2) competition for hydrophobic adsorption sites between the surfactant and HOC and 3) partitioning of HOC among soil hydrophobic adsorption sites, surfactant micelles and hemimicelles. The interaction of HOCs with surfactant monomers is usually very weak and insignificant. At concentrations where micelles and hemimicelles are present interactions can take place. Sorbed HOCs can be solubilised by free micelles, resulting in mobilisation. HOCs in solution are in equilibria between sorption onto hydrophobic adsorptive sites on the soil, partitioning into hemimicelles – both resulting in immobilisation, and partitioning into free micelles. Whether the HOCs are previously sorbed onto soil or are in solution, partitioning into micelles, hence mobilisation, is favoured by increasing surfactant concentration. A model has been put forward describing the effect of non-ionic surfactant on the distribution of HOC in a soil-water system. In simple terms the model illustrates that sorbed surfactant molecules tend to increase HOC sorption onto soil by increasing its fractional organic carbon content, and free surfactant tends to decrease sorption by increasing the apparent aqueous solubility of the HOC.

The biodegradation of HOCs in soil can be enhanced by surfactants due to enhanced solubility in the presence of micelles. In some cases however, biodegradation appears to be inhibited by micelles forming a barrier to the degrading organism. Any such inhibition is unlikely to be prolonged due to the biodegradable nature of most modern surfactants. In fact, it is very unlikely that micelles would be present in sludge-amended soils due to the low concentration of surfactants.

Although there is evidence that surfactants can effect the fate and behaviour of HOCs in soil, the potential for detergent ingredients to cause significant effects is limited due to the relatively low concentrations found compared with critical micelle concentrations (CMCs). In addition, the effective CMC in environments such as soil and sediments is generally much higher than in clean water systems. Typical soil concentrations of LAS, the most heavily used surfactant in domestic detergents, are significantly lower than those required to produce micelles in pore water. Therefore, it is unlikely that surfactants present in domestic detergents will contribute significantly to the mobilisation of HOCs in sludge-amended soil.

Reference: Haigh, S.D. 1996. A review of the interaction of surfactants with organic contaminants in soil. The Science of the Total Environment 185:161-170.

4. ECOTOXICITY

4.1 ACUTE/PROLONGED TOXICITY TO FISH

(a)

Type of Test:	static [ ]; semi-static [ ]; flow-through [X] Open-system [X]; closed-system [ ]
Species:	*Lepomis macrochirus* (Fish, fresh water)
Exposure Period:	96 hours
Results:	LC_{50} = 1.67 mg/L
Analytic Monitoring:	Yes [X]; No [ ]; ? [ ]
Method:	USEPA (1975) Stock solutions were made up in deionized water without the use of a solvent and metered into diluter chambers by peristaltic pump. Mortality was analyzed by four methods: (a) the toxic unit (TU) concept, (b) the additive index, (c) concentration addition, and (d) response addition.
GLP:	Yes [ ]; No [X]; ? [ ]
Test Substance:	$C_{11.8}$ LAS; Average molecular weight 345; 27.3% active; Alkyl chain Composition: C_{10} 9.5%, C_{11} 29.2%, C_{12} 37.7%, C_{13} 19.0%, C_{14} 4.9%
Remarks:	Average size of individual fish 1.1 g, mean standard length 4.2 cm; water hardness 137 mg/L Ca CO_3; temperature 20 ± 2°C; dissolved oxygen 8.4-9.6 mg/L; pH 7.3-8.1. Ten randomly selected fish were exposed to each of the five concentrations and the control. A 16:8 (light:dark) photoperiod was maintained. Fish were not fed during the study. Mortality was recorded at 1, 3, and 5 hours after test initiation and then daily until test termination. Samples were collected at the beginning and end of the study and analyzed for the test substance. Results reported are mean measured concentrations. The LC_{50} value reported represents the lowest value for this species. In addition to the studies conducted on LAS, the anionic LAS was also tested in binary and ternary equitoxic or equimolar mixtures with non-ionic C_{14-15} linear alkyl ethoxylate (AE) and cationic C_{12-14} MDAC. These mixture results are not reported in this robust summary. This is a key study for aquatic toxicity to fish (see SIAR Table 10).
Reference:	Lewis, M.A. and Perry, R.L. 1981. Acute toxicities of equimolar and equitoxic surfactant mixtures to *Daphnia magna* and *Lepomis macrochirus*. Aquatic Toxicology and Hazard Assessment: Fourth Conference, ASTM STP 737, D.R. Branson and K.L. Dickson, Eds., American Society for Testing and Materials, pp. 402-418.
Reliability:	2 Valid with restrictions. The studies are very well documented in this peer-reviewed publication.

(b)

Species:	*Lepomis macrochirus* and *Pimephales promelas*
Results:	LC_{50} values ranged from 1.67 to 7.7 mg/L for *L. macrochirus* (10 records) LC_{50} value for *P. promelas* = 4.1 mg/L (1 record) See study (q) below for robust summary
Test Substance:	C_{10-13} LAS (CAS #68411-30-3)
Remarks:	A total of 18 fish studies for these two species were reviewed by HERA in 2004. Seven of these studies were rejected because the test material was not commercial LAS, the study deviated significantly from standard protocols, or non-standard endpoints were measured. The remaining eleven studies were evaluated for reliability and the results reflect the range of acute LC_{50} values obtained for the most commonly tested fish species. These studies are tabulated and discussed further in the SIAR and SIAP in a weight-of-

evidence approach. A robust summary for the study with the lowest LC_{50} value was prepared (see Lewis and Perry 1981 above).

Reference: HERA-LAS team , May 2004; see SIAR, Annex 2.

Reliability: 4 Not assignable. This study is given a reliability score of 4 because it is a summary evaluation of a series of studies conducted by other researchers.

(c)

Species: *Lepomis macrochirus*

Results: LC_{50} = 3.0 mg/L (geometric mean of 88 records)

Test Substance: C_{10-14} LAS (all LAS in range, including data for individual homologues)

Remarks: Mean LC_{50} for bluegill sunfish was derived from a total of 88 records compiled from the BKH (1993) literature review.

Reference: van de Plassche, E.J., de Bruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J. and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: LAS, AE, AES, and soap, Environ. Toxicol. Chem. 18:2653-2663.

Reliability: 4 This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(d)

Species: *Pimephales promelas*

Results: LC_{50} = 3.2 mg/L (geometric mean of 35 records)

Test Substance: C_{10-14} LAS (all LAS in range, including data for individual homologues)

Remarks: Mean LC_{50} for fathead minnow was derived from a total of 35 records compiled from the BKH (1993) literature review. The range of LC_{50} values (0.40-100 mg/L) is very large due to the range of materials tested (including many materials not representative of commercial LAS) and the differences in test design (not necessarily following standard guidelines). It is unclear which values within the range refer to the commercial LAS products and the individual records are not available for validation.

Reference: van de Plassche, E.J., de Bruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J. and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: LAS, AE, AES, and soap, Environ. Toxicol. Chem. 18:2653-2663.

Reliability: 4 This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(e)

Species: *Leuciscus idus melanotus*

Results: LC_{50} = 2.9 mg/L (geometric mean of 11 records)

Test Substance: C_{10-14} LAS (all LAS in range, including data for individual homologues)

Remarks: Mean LC_{50} for golden orfe was derived from a total of 11 records compiled from the BKH (1993) literature review.

Reference: van de Plassche, E.J., de Bruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J. and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: LAS, AE, AES, and soap, Environ. Toxicol. Chem. 18:2653-2663.

Reliability: 4 This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(f)

Species: *Carassius auratus* (goldfish)

	Oncorhynchus mykiss (rainbow trout) *Oryzias latipes* (medaka) *Poecilia reticulata* (guppy)
Results:	LC_{50} (*C. auratus*) = 9.5 mg/L (46 records) LC_{50} (*O. mykiss*) = 3.0 mg/L (10 records) LC_{50} (*O. latipes*) = 13 mg/L (5 records) LC_{50} (*P. reticulata*) = 3.8 mg/L (9 records)
Test Substance:	C_{10-14} LAS (all LAS in range, including data for individual homologues)
Remarks:	Geometric mean LC_{50} values for the number of records listed for each species. The interspecies variation decreases considerably when the geometric mean value per species is calculated.
Reference:	van de Plassche, E.J., de Bruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J. and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: LAS, AE, AES, and soap. Environ. Toxicol. Chem. 18:2653-2663.
Reliability:	4 This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(g)

Species:	Fish species (all marine)
Results:	LC_{50} = 1.58 mg/L (6 records; SD = 0.16)
Test Substance:	LAS; average alkyl chain length $C_{11.7-12.0}$
Remarks:	LC_{50} is geometric mean of 6 records compiled from literature reviews. Geometric mean LC_{50} for all taxa (36 records; SD = 0.79) was 4.36 mg/L.
Reference:	Temara, A., Carr, G., Webb, S., Versteeg, D., and Feijtel, T.C.J. 2001. Marine risk assessment: Linear alkylbenzensulphonates (LAS) in the North Sea. Mar. Poll. Bulletin 42:635-642.
Reliability:	4 This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(h) **(Zebra fish)**

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other**[ ]** open-system **[X]**; closed-system **[ ]**
Species:	*Brachydanio rerio* (Fish, fresh water)
Exposure period:	96 hour
Results:	LC_{50} = 5.1 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{10-13} LAS (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. The submitter (Huels AG) judged the study quality to be good. Water hardness: 310 mg/L $CaCO_3$; tap water diluent; 25 ºC; adult fish tested.
Reference:	European Commission. 2000f. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, AT/FU/80/90.
Reliability:	4 Not assignable. The original study was not available for review.

(i)

Type of test:	static **[ ]**; semi-static **[X]**; flow-through **[ ]**; other **[ ]** open-system **[X]**; closed-system **[ ]**
Species:	*Brachydanio rerio* (Fish, fresh water)
Exposure period:	96 hour
Results:	LC_{50} = 7.8 mg/L

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**
Method: ISO 7346/1-3
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Marlon A 350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Concentration of test substance related to MBAS. LC_0 and LC_{100} = 5.6 and 11 mg/L, respectively
Reference: European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability: 4 Not assignable. The original study was not available for review.

(j)
Type of test: static **[ ]**; semi-static **[X]**; flow-through **[ ]**; other **[ ]**
open-system **[X]**; closed-system **[ ]**
Species: *Brachydanio rerio* (Fish, fresh water)
Exposure period: 14 day
Results: NOEC = 2 mg/L
LOEC = 8 mg/L
Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**
Method: OECD Guide-line 204 "Fish, Prolonged Toxicity Test: 14-day Study"
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Marlon A 350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Concentration of test substance related to MBAS.
Reference: European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability: 4 Not assignable. The original study was not available for review.

(k) **(Rainbow trout)**
Type of test: static **[ ]**; semi-static **[X]**; flow-through **[ ]**; other **[ ]**
open-system **[X]**; closed-system **[ ]**
Species: *Salmo gairdneri* (Fish, estuary, fresh water)
Exposure period: 96 hour
Results: LC_{50} = 5.8 mg/L
Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: C_{10-13} LAS (CAS # 68411-30-3)
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. The submitter (Huels AG) judged the study quality to be good. Analysis showed 92% of nominal concentration. Tap water diluent; water hardness = 96-120 mg/L $CaCO_3$; pH 6.8-7.3; daily renewal; 14.5-16ºC; 5 month old fish tested.
Reference: European Commission. 2000i. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, AT/17.
Reliability: 4 Not assignable. The original study was not available for review.

(l)
Type of test: static **[ ]**; semi-static **[X]**; flow-through **[ ]**; other **[ ]**
open-system **[X]**; closed-system **[ ]**
Species: *Salmo gairdneri* (Fish, estuary, fresh water)
Exposure period: 96 hour

Results:	LC_{50} = 3 mg/L
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	See remarks.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	DOBANIC ACID 102, C_{10-13} LAS (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Daily renewal of test solutions; 14-16 ºC; pH 7.6-8.4; water hardness = 210-240 mg/L $CaCO_3$; DO=10.0-10.4 mg/L. Fingerlings were tested, mean weight 5.2 g
Reference:	European Commission. 2000w. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Shell Research Ltd, SBGR.81.083, RR Stephenson.
Reliability:	4 Not assignable. The original study was not available for review.

(m) **(Bluegill sunfish)**

Type of test:	static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]** open-system **[X]**; closed-system **[ ]**
Species:	*Lepomis macrochirus* (Fish, fresh water)
Exposure period:	96 hour
Results:	LC_{50} = 5.0 mg/L (mean of 8 tests)
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	EPA-660/3-75-009
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{10-13} LAS, average chain length 11.8 (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. LC_{50} values for the 8 tests conducted ranged from 3.7 to 7.7 mg/L. Nominal concentration, (expected deviation <20%), reconstituted water, water hardness = 30-48 mg/L CaCO3; pH 7.3-7.8; 20-23ºC; fish size: 0.35-0.89 g
Reference:	European Commission. 2000q. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 22852, 23613, 23612, 23617, 23722, 22824, 28661, 27917.
Reliability:	4 Not assignable. The original studies were reviewed by HERA (2004) for Annex 2 and judged to be reliable.

(n)

Type of test:	static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]** open-system **[X]**; closed-system **[ ]**
Species:	*Lepomis macrochirus* (Fish, fresh water)
Exposure period:	96 hour
Results:	LC_{50} = 2.2 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	EPA-660/3-75-009
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{10-13} LAS, average chain length 11.8 (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Nominal concentrations, (expected deviation <20%). Reconstituted water with hardness = 44 mg/L $CaCO_3$; pH 7.58; 22ºC; fish size: 0.35 g, 40 mm; Note that this study was not included in the HERA LAS acute toxicity data summary tables in the SIAR because only a summary of the study, not the full report, is available.
Reference:	European Commission. 2000p. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 22581, 28361.
Reliability:	4 Not assignable. The original study was not available for review.

(o) **(Golden Orfe)**

Type of test:	static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]** open-system **[X]**; closed-system **[ ]**
Species:	*Leuciscus idus* (Fish, fresh water) (Golden orfe)
Exposure period:	48 hour
Results:	LC_{50} = 4.6 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	Determination of the effect of substance in water on fish, DIN 38412 part 15
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	C_{10-13} LAS, sodium salt (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3.
Reference:	European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Huels Study (unpublished).
Reliability:	4 Not assignable. The original study was not available for review.

(p) **(Fathead minnow)**

Type of test:	static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]** open-system **[X]**; closed-system **[ ]** not stated
Species:	*Pimephales promelas* (Fish, fresh water)
Exposure period:	96 hour
Results:	LC_{50} = 4.6 mg/L
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	Ten fathead minnows were exposed for 96 hours to LAS under the following conditions: hardness 35 mg/L as $CaCO_3$; pH 7.1; temperature 21°C. Fish were not fed during the exposure.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Low molecular weight LAS, sodium salt (CAS #68411-30-3); C_{10} 5%, C_{11} 27%, C_{12} 53%, C_{13} 13%, 2-phenyl 23%; average alkyl chain length = $C_{11.1}$.
Remarks:	The carboxylated intermediates formed in the biodegradation of LAS were also tested and found to be several orders of magnitude less toxic than LAS. These intermediates undergo further biodegradation, more rapidly in a natural river water than in a synthetic medium.
Reference:	Swisher, R.D., Gledhill, W.E., Kimerle, R.A. and Taulli, T.A. 1978. Carboxylated intermediates in the biodegradation of linear alkylbenzene sulfonates (LAS). VII International Congress on Surface Active Substance, Proceedings, Moscow, 1976 4:218-230.
Reliability:	2 Valid with restrictions

(q)

Type of test:	static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]** open-system **[X]**; closed-system **[ ]**
Species:	*Pimephales promelas* (Fish, fresh water)
Exposure period:	96 hour
Results:	LC_{50} = 4.1 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	USEPA methods for acute toxicity tests with fish, macroinvertebrates, and amphibians. Ecol. Res. Series. EPA-660/3-75-009.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	C_{10-13} LAS, average chain length 11.7 (CAS #68411-30-3) (C_{10} 7.3%; C_{11} 26.5%; C_{12} 56.7%; C_{13} 9.0%; C_{14} 0.5%); Mean phenyl position = 3.9; Mean molecular weight = 345.
Remarks:	Acute tests were conducted at EG&G Bionomics from 1971 to 1976 with 2-3 month old fathead minnows in 20-L glass vessels with soft reconstituted water (hardness = 40 mg/L as $CaCO_3$). Tests with LASs of average alkyl

chain length of 11.2 and 13.3 were conducted concurrently, with the resultant 96 hour LC_{50} values of 12.3 and 0.86 mg/L, respectively.

Reference: Holman, W.F. and Macek, K.J. 1980. An aquatic safety assessment of linear alkylbenzene sulphonate (LAS); chronic effects on fathead minnows. Trans. Am. Fish. Soc. 109(1):122-131.

Reliability: 2 Valid with restrictions

(r)

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[X]**; closed-system **[ ]**

Species: *Pimephales promelas* (Fish, fresh water)

Exposure period: 48 hour

Results: The following table shows the acute toxicity of the tested materials (LC_{50}, mg/L).

		Fathead minnow LC_{50} (mg/L)	
	Average chain length	**24 hour**	**48 hour**
High molecular weight LAS	13.3	1.9	1.7
Individual homologues LAS			
C_{10}	10	48.0	43.0
C_{11}	11	17.0	16.0
C_{12}	12	4.7	4.7
C_{13}	13	1.7	0.4
C_{14}	14	0.6	0.4
Nonlinear LAS components (DTIS)			
C_{10}	10	87.0 ± 7.5	86.1 ± 15.0
C_{12}	12	24.8 ± 5.8	21.5 ± 5.5
C_{14}	14	8.1 ± 5.1	5.3 ± 3.9
Model biodegradation intermediates			
C_4 (SØ Butyrate)	4	~10,000	~10,000
C_5 (SØ Valerate)	5	~10,000	~10,000
C_{11} (SØU)	11	85.9 ± 5.1*	76.6 ± 12.4*

*Subsequent repurification of this sample yielded a product with the same isomeric composition but with LC_{50} values over 1000 mg/L for fatheads.

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]** **MBAS**

Method: EPA-660/3-75-009 1975. Method for acute toxicity tests with fish, macroinvertebrates and amphibians.
Acute toxicity tests were conducted on high molecular weight LAS, individual pure homologues, non-linear LAS components (dialkyl tetralin or indane sulfonates, DTIS), and model biodegradation intermediates (sulfophenylundecane, SOU) in order to determine whether biodegradation decreases toxicity. Toxicity tests were conducted in 5 L of 100 mg/L hardness water using 5 fathead minnows per concentration.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: 1) High molecular weight LAS: Average chain length = 13.3; C_{11} 1%, C_{12} 8%, C_{13} 52%, C_{14} 39%
2) Individual LAS homologues of C_{10}, C_{11}, C_{12}, C_{13}, and C_{14}
3) Nonlinear LAS components (DTIS)
4) Model biodegradation intermediates

Remarks: The length of the alkyl chain is the most important factor influencing acute toxicity, which increases as the alkyl chain increases. These longer alkyl chain homologues are the first constituents of the LAS mixture to degrade. The nonlinear components (DTIS) showed 1/2 to 1/10 the toxicity of LAS with the same carbon chain length. Toxicity of biodegradation intermediates is significantly less than the parent LAS. Because of the shorter than normal study duration and smaller than standard number of fish per concentration, the reliability of the absolute values cannot be assessed. However, the study is considered reliable for the trends in the data because the homologues were tested under identical conditions.

Reference: Kimerle, R.A. and Swisher, R.D. 1977. Reduction of aquatic toxicity of linear alkylbenzene sulfonate (LAS) by biodegradation. Water Research 11:31-37.

Reliability: 2 Valid with restrictions

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

A. Daphnia

(a)

Type of Test: Static [X]; semi-static [ ]; flow-through
Open-system [X]; closed-system [ ]

Species: *Daphnia magna* (Crustacea)

Exposure Period: 48 hours

Effect Criteria: Immobility

Results: EC_{50} = 1.62 mg/L; The number of immobile animals at each concentration is shown in the following table:

Concentration of test substance (mg/L)								
Time (h)	**0**	**3.2**	**5.6**	**10**	**18**	**32**	**56**	**100**
0	0	0	0	0	0	0	0	0
24	0	0	0	0	0	0	12	20
48	0	0	0	1[a]	6[a]	12[a]	20	20

[a] Condition of mobile animals was impacted as compared to the controls in a dose-responsive manner.

Analytic Monitoring: Yes [X]; No [ ]; ? [ ]

Method: OECD Guideline 202. Seven concentrations (3.2, 5.6, 10, 18, 32, 56, and 100 mg/L) plus controls were tested. The dilution water was DSWL water, prepared from ground water. Four beakers containing five *Daphnia* each were used for each test or control solution. *Daphnia* were less than 24 hours old at test initiation. A fifth beaker with 100 mg/L solution and five *Daphnia* were added 24 hours after initiation. Test and control solutions were not renewed and the *Daphnia* were not fed. Dissolved oxygen and pH were measured at 0 and 48 hours in all concentrations, as well as at 24 hours in the 100 mg/L chambers 24 hours after initiation because of total immobility observed at that level. Dissolved oxygen ranged from 8.7 to 9.6 mg/L and pH ranged from 7.9 to 8.1. Water hardness was 215 mg/L as $CaCO_3$. Test temperature was maintained at 20 ± 1°C under a 16:8 (light:dark) cycle. The chambers were not aerated. Immobile animals were counted at 24 and 48 hours. Samples for analysis of each concentration were taken at 0, 24, and 48 hours. This is a key study for aquatic toxicity to invertebrates (see SIAR Table 10).

GLP: Yes [X]; No [ ]; ? [ ]

Test Substance: LAS; 87.85% activity

Remarks: A 24 hour EC_{50} of 3.58 mg/L and a 48 hour NOEC of 0.379 mg/L (both

based on immobility) were also calculated, as well as a 48 hour NOEC of 5.6 mg/L based on condition. Only nominal concentrations are reported. No further information on the test substance is reported.

Reference: Hooftman, R.N. and van Drongelen-Sevenhuijsen, D. 1990. The acute Toxicity of E-3473.01 (ETS 311) to *Daphnia magna*. TNO Netherlands Organization for Applied Research. TNO Report No. R 89/403.

Reliability: 1 Valid without restrictions.

(b)

Species: *Daphnia magna*

Results: EC_{50} values ranged from 1.62 to 9.3 mg/L

Test Substance: $C_{10\text{-}13}$ LAS (CAS #68411-30-3)

Remarks: A total of 20 daphnid studies were reviewed by HERA in 2004. Nine of these studies were rejected because the test material was not commercial LAS, the study deviated significantly from standard protocols, or non-standard endpoints were measured. The remaining 11 studies were evaluated for reliability and the results reflect the range of acute EC_{50} values obtained for *Daphnia magna*. These studies are tabulated and discussed further in the SIAR and SIAP in a weight-of-evidence approach. A robust summary for the study with the lowest acute EC_{50} value was prepared (see Hooftman and van Drongelen-Sevenhuijsen above).

Reference: HERA-LAS team, May 2004; see SIAR Annex 2.

Reliability: 4 Not assignable. This study has been given a reliability score of 4 because it is a summary evaluation of a series of studies conducted by other researchers.

(c)

Species: *Daphnia magna*

Results: EC_{50} = 4.7 mg/L (139 records)

Test Substance: C10-14 LAS (all LAS in range, including data for individual homologues)

Remarks: EC_{50} is geometric mean of 139 records compiled from a BKH (1993) literature review. Values range from 0.26 to 55 mg/L. This large range is caused by differences in the LAS tested with respect to alkyl chain and/or phenyl isomer distribution and differences in test design.

Reference: van de Plassche, E.J., de Bruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J. and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: LAS, AE, AES, and soap, Environ. Toxicol. Chem. 18:2653-2663.

Reliability: 4 This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(d)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[ ]**; closed-system **[ ]** not stated

Species: *Daphnia magna* (Crustacea)

Exposure period: 48 hour

Results: EC_{50} = 6.8 mg/L

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: Directive 84/449/EEC, C.2 "Acute toxicity for *Daphnia*" 1984

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: $C_{10\text{-}13}$ LAS, sodium salt (CAS #68411-30-3)

Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3.

Reference: European Commission. 2000a. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Huels Study (unpublished).

Reliability: 4 Not assignable. The original study was not available for review.

(e)

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**
Species: *Daphnia magna* (Crustacea)
Exposure period: 48 hour
Results: LC_{50} = 5.5 mg/L (mean of 3 valid tests)
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: EPA-660/3-75-009
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: C_{10-13} LAS, average chain length 11.8 (CAS #68411-30-3)
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Life-stage: <24 h. Effect: immobility. LC_{50} values for 4 tests ranged from 4.4 to 10.4 mg/L. Huels AG judged study quality to be good. Nominal concentrations (expected deviation <20%). Reconstituted water with hardness = 162-220 mg/L $CaCO_3$. Note that all four of these studies are included in Appendix 2, the HERA acute toxicity data review. Three of the studies, Reports 23618, 22853 and 23611 with respective values of 4.4, 4.9 and 7.1 mg/L, are considered reliable and are included in the table of acute toxicity values. The fourth study, Report 23276 with a value of 10.4 mg/L, is listed among the rejected studies because it was conducted as part of a QA program to qualify various labs and the result is not considered reliable. pH 7.86-8.53. 21-22ºC
Reference: European Commission. 2000r. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 23618, 22853, 23611, 23276.
Reliability: 2 Valid with restrictions for the three valid studies. The original studies were reviewed by HERA (2004) for Annex 2.

(f)

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**
Species: *Daphnia magna* (Crustacea)
Exposure period: 48 hour
Results: The following table shows the acute toxicity of original materials (LC_{50}, mg/L).

		Daphnia magna	
	Average chain length	**24 hour**	**48 hour**
High molecular weight LAS	13.3	2.6 ± 0.1	2.3 ± 0.1
Individual homologues LAS			
C_{10}	10	53.1 ± 0.4	12.3 ± 2.6
C_{11}	11	15.8 ± 3.0	5.7 ± 0.6
C_{12}	12	10.7 ± 1.6	3.5 ± 1.0
C_{13}	13	2.7 ± 0.4	2.0 ± 0.3
C_{14}	14	1.2 ± 0.2	0.7 ± 0.2
Nonlinear LAS components (DTIS)			
C_{10}	10	106.0 ± 27.0	98.0 ± 21.3
C_{12}	12	55.1 ± 9.1	34.1 ± 5.1
C_{14}	14	12.4 ± 1.4	10.0 ± 1.0
Model biodegradation intermediates			

		Daphnia magna	
	Average chain length	**24 hour**	**48 hour**
C_4 (SØ Butyrate)	4	~12,000	~6,000
C_5 (SØ Valerate)	5	~12,000	~5,000
C_{11} (SØU)	11	355 ± 150*	208 ± 85*

*Subsequent repurification of this sample yielded a product with the same isomeric composition but with LC_{50} values over 1000 mg/L for daphnids (Swisher et al., 1976).

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]** **MBAS**

Method: EPA-660/3-75-009 1975. Method for acute toxicity tests with fish, macroinvertebrates and amphibians.
Acute toxicity tests were conducted on high molecular weight LAS, individual pure homologues, non-linear LAS components (dialkyl tetralin or indane sulfonates (DTIS), and model biodegradation intermediates (sulfophenyl undecane, SØU) in order to determine whether biodegradation decreases toxicity. In 250 mL beakers with 200 mL of well water of approximately 250 mg/L hardness, ten *Daphnia*, less than 18 hours old, were placed in each of the three beakers. No food was added for the duration of the test.

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: 1) High molecular weight LAS: Average chain length = 13.3; C_{11} 1%, C_{12} 8%, C_{13} 52%, C_{14} 39%
2) Individual LAS homologues of C_{10}, C_{11}, C_{12}, C_{13}, and C_{14}
3) Nonlinear LAS components (DTIS)
4) Model biodegradation intermediates

Remarks: The length of the alkyl chain is the most important factor influencing acute toxicity, which increases as the alkyl chain increases. These longer alkyl chain homologues are the first constituents of the LAS mixture to degrade. The nonlinear components (DTIS) showed 1/2 to 1/10 the toxicity of LAS with the same carbon chain length. Toxicity of biodegradation intermediates is significantly less than the parent LAS. Daphnia acute toxicity tests on partially degraded LAS demonstrated that toxicity is significantly lessened as LAS biodegraded. Because of the shorter than normal study duration and smaller than standard number of *Daphnia* per concentration, the reliability of the absolute values cannot be assessed. However, the study is considered reliable for the trends in the data because the homologues were tested under identical conditions.

Reference: Kimerle, R.A. and Swisher, R.D. 1977. Reduction of aquatic toxicity of linear alkylbenzene sulfonate (LAS) by biodegradation. Water Research 11:31-37.

Reliability: 2 Valid with restrictions

B. Other aquatic invertebrates

(a)

Species: *Gammarus pulex* (amphipod)
Mysidopis bahia (mysid)
Panaeus duorarum (pink shrimp)

Results: EC_{50} (*G. pulex*) = 6.2 mg/L (25 records)
EC_{50} (*M. bahia*) = 1.7 mg/L (6 records)
EC_{50} (*P. duorarum*) = 49 mg/L (5 records)

Test Substance: C_{10-14} LAS (all LAS in range, including data for individual homologues)

Remarks: Geometric mean EC_{50} values for number of records listed for each species. The interspecies variation decreases considerably when the geometric mean value per species is calculated.

Reference:	van de Plassche, E.J., de Bruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J. and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: LAS, AE, AES, and soap, Environ. Toxicol. Chem. 18:2653-2663.
Reliability:	4 This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(b)

Species:	Crustacean species
Results:	LC_{50} = 17.0 mg/L (14 records; SD = 0.68)
Test Substance:	LAS; all in the alkyl chain length C_{10-14}
Remarks:	LC_{50} is geometric mean of 14 records compiled from literature reviews. Geometric mean LC_{50} for all taxa (36 records) was 4.36 mg/L.
Reference:	Temara, A., Carr, G., Webb, S., Versteeg, D., and Feijtel, T.C.J. 2001. Marine risk assessment: Linear alkylbenzensulphonates (LAS) in the North Sea. Mar. Poll. Bulletin 42:635-642.
Reliability:	4 This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(c)

Type of test:	static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**
Species:	*Chironomus riparius* (chironomid)
Exposure period:	96 hour
Results:	LC_{50} = 6.5 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	EPA
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{10-13} LAS, average chain length 12.3 (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Nominal concentrations (expected deviation <20%). Well water with hardness = 24-30 mg/L $CaCO_3$; pH 7.1; 21-22ºC
Reference:	European Commission. 2000v. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 34845.
Reliability:	4 Not assignable. The original study was not available for review.

(d)

Type of test:	static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**
Species:	*Limnodrilus hoffmeisteri* (aquatic worm)
Exposure period:	96 hour
Results:	LC_{50} = 1.8 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	EPA 660/3-75-009
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{10-13} LAS, average chain length 12.3 (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Additional LC_{50} values for extended exposure times: 144 h: 1.1 mg/L, 196 h: 0.96 mg/L. Huels AG judged study quality to be good. Nominal concentrations (expected deviation <20%). Well water with hardness = 24-30 mg/L $CaCO_3$; pH 7.1; 21-22ºC.

Reference: European Commission. 2000v. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 34845.
Reliability: 4 Not assignable. The original study was not available for review.

(e)
Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: *Planaria* sp. (aquatic worm)
Exposure period: 48 hour
Results: LC_{50} = 1.8 mg/L
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: EPA 660/3-75-009
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: C_{10-13} LAS, average chain length 12 (CAS #68411-30-3)
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Nominal concentrations (expected deviation <20%). Reconstituted water with hardness 165 mg/L $CaCo_3$. pH 8.1–8.4; 21-22^oC; size 3.4 cm.
Reference: European Commission. 2000u. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 31340.
Reliability: 4 Not assignable. The original study was not available for review.

(f)
Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**
Species: *Rhabditis* sp. (nematode)
Exposure period: 48 hour
Results: LC_{50} = 16 mg/L
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: EPA 660/3-75-009
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{12} LAS (CAS #25155-30-0) (average chain length 11.8)
Remarks: Nominal concentrations, (expected <20%), 3 replicates of 5 test concentrations plus a control. Reconstituted water with hardness = 65 mg/L $CaCO_3$; DO 5.3 mg/L; pH 8.1-8.4; 21-23ºC; size: 0.3 mm; 12 hr. photoperiod at 40-70 L/ft ^{2}. Five other species were also tested and had the following 48-hr LC_{50} values (all mg/L): Midge 23; *Gammarus* (amphipod) 3.3; *Asellus* (isopod) 270; *Dugesia* (flatworm) 1.8; and *Dero* (oligochaete) 1.7.
Reference: Lewis, M.A. and Surprenant, D. 1983. Comparative acute toxicities of surfactants to aquatic invertebrates. Ecotoxicol. Env. Saf. 7(3):313-322.
Reliability: 2 Valid with restrictions

4.3 TOXICITY TO AQUATIC PLANTS, e.g. algae

(a)
Type of Test: Static [X]; semi-static [ ]; flow-through [ ]
Open-system [X]; closed-system [ ]; not stated [ ]
Species: *Selenastrum capricornutum* (algae)
Endpoint: Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**
Exposure Period: 96 hours
Results: EC_{50} = 29.0 mg/L
NOEC = 0.5 mg/L

	LOEC = 1.0 mg/L
Analytic Monitoring:	Yes [ ]; No [ ]; ? [X]
Method:	ASTM. 1984. Standard Practice for Conducting Toxicity Tests with Microalgae, Draft #7, Philadelphia, PA. Algae were exposed to the test material for four days, after which cell counts were made. The EC_{50} value was calculated using the method of Larson and Schaefer. Assumed 1 x 10^4 cells/mL because ASTM protocol, but not reported.
GLP:	Yes [ ]; No [X]; ? [ ]
Test Substance:	$C_{11.8}$ LAS; MW = 345; technical grade LAS from P&G
	Remarks: The first significant effect concentrations were between 0.5 and 1.0 mg/L. Mean test temperature was 23.6 (21.2-25.6 °C). Total mean water hardness was 137 mg/L as $CaCO_3$. The pH range was 6.8 to 7.2. Mean dissolved oxygen was 9.1 mg/L. Results of the laboratory studies were compared with enclosure studies conducted with natural phytoplankton assemblages. Concentrations in the enclosures that first altered community structure were found to be between 27 and 108 mg/L. The EC_{50} value reported represents the lowest acute value for algal species for which a report or publication was available. This is a key study for aquatic toxicity to algae (see SIAR Tables 10 and 12).
Reference:	1) Lewis, M.A. 1986. Comparison of effects of surfactants on freshwater phytoplankton communities in experimental enclosures and on algal population growth in the laboratory. Environ. Toxicol. Chem. 5:319-332.
	2) Lewis, M.A. and Hamm, B.G. 1986. Environmental modification of the photosynthetic response of lake plankton to surfactants and significance to a laboratory-field comparison. Wat. Res. 20:1575-1582.
Reliability:	2 Valid with restrictions
(b)	
Species:	*Selenastrum capricornutum* and *Scenedesmus subspicatus*
Endpoint:	Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**
Results:	E_rC_{50} values ranged from 29 to 35.5 for *S. capricornutum* (two records)
	E_rC_{50} values ranged from 82 to 163 mg/L for *S. subspicatus* (three records)
Test Substance:	$C_{10\text{-}13}$ LAS (CAS #68411-30-3)
Remarks:	A total of 13 algae studies originally were reviewed by HERA in 2004. Eight of these studies were rejected because the test material was not commercial LAS, the study deviated significantly from standard protocols, or non-standard endpoints were measured. The remaining five studies were evaluated for reliability and the results reflect the range of acute E_rC_{50} values obtained for the two most commonly tested algal species. These studies are tabulated and discussed further in the SIAR and SIAP in a weight-of-evidence approach. A robust summary for the study with the lowest acute E_rC_{50} value was prepared (see Lewis 1986 above).
Reference:	HERA-LAS team, May 2004; see SIAR Annex 2.
Reliability:	4 Not assignable. This study is given a reliability score of 4 because it is a summary evaluation of a series of studies conducted by other researchers.
(c)	
Species:	*Chlamydomonas reinhardi, Chlorella kessleri, Microcystis sp., Plectonema boryanum, Scendesmus subspicatus, Selenastrum sp.* (algae)
Results:	NOEC (*C. reinhardi*) = 12 mg/L (1 record)
	NOEC (*C. kessleri*) = 3.5 mg/L (1 record)
	NOEC (*Microcystis sp.*) = 0.80 mg/L (4 records)
	NOEC (*P. boryanum*) = 15 mg/L (1 record)
	NOEC (*S. subspicatus*) = 7.7 mg/L (4 records)

NOEC (*Selenastrum sp.*) = 3.8 mg/L (9 records)
Test Substance: LAS normalized to $C_{11.6}$
Remarks: Geometric mean NOEC values for number of records listed for each species.
Reference: van de Plassche, E.J., de Bruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J. and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: LAS, AE, AES, and soap. Environ. Toxicol. Chem. 18:2653-2663.
Reliability: 4 This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(d) **(*Scenedesmus*)**
Species: *Scenedesmus subspicatus* (Algae)
Endpoint: Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**
Exposure period: 72 hour
Results: The 72-hr EC_{50} values were 240, 163, and 54.3 mg/L for the C_{11}, $C_{11.6}$, and C_{13} LAS, respectively. Other endpoints not determined.
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: OECD 201 Algal growth inhibition test. 1984. The test media recommended by AFNOR was used. All water quality parameters were maintained within acceptable ranges in compliance with the test protocol. Initial cell concentrations were 1 x 10^4 cells/mL. Final cell counts not reported.
open-system **[X]**; closed-system **[ ]**
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Three different alkyl chain lengths of LAS (C_{11}, $C_{11.6}$, C_{13}), with the following homologue distributions:

	Alkyl Chain Length Distributions (%)		
	LAS C_{11}	**LAS $C_{11.6}$**	**LAS C_{13}**
$<C_{10}$	1.5	0.4	--
C_{10}	29.0	8.9	1.0
C_{11}	39.0	33.7	3.5
C_{12}	28.5	31.0	17.8
C_{13}	1.8	24.0	37.0
C_{14}	0.2	2.0	40.4
$>C_{14}$	--	--	0.3
LAS MW (as Na-LAS)	334	343	363

Remarks: German strain of *S. subspicatus* from the University of Gottingen. Other endpoints were not reported.

Reference: Verge, C. and Moreno, A. 1996a. Toxicity of anionic surfactants to green microalgae *"Scenedesmus subspicatus"* and *"Selenastrum capricornutum."* Tenside Surf. Det. 33:166-168.

Reliability: 2 Valid with restrictions

(e)

Species: *Scenedesmus subspicatus* (Algae)
Endpoint: Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**
Exposure period: 72 hour

Results: The 72-hr EC_{50} values were 270, 111, 48, 30, and 18 mg/L for pure homologues C_{10}, C_{11}, C_{12}, C_{13}, and C_{14}, respectively. The corresponding NOEC values were 80, 40, 18, 12, and 7, respectively.
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: OECD 201 Algal growth inhibition test. 1984. The test media recommended by AFNOR was used. All water quality parameters were maintained within acceptable ranges in compliance with the test protocol. Initial cell concentrations were 1 x 10^4 cells/mL. Final cell counts not reported.
open-system **[X]**; closed-system **[ ]**
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Five pure homologue cuts were tested, with the following distribution.

	Alkyl Chain Length Distributions (%)				
	LAS C_{10}	**LAS C_{11}**	**LAS C_{12}**	**LAS C_{13}**	**LAS C_{14}**
<C_{10}	0.5	--	0.4	--	--
C_{10}	96.8	5.5	13.9	0.7	--
C_{11}	2.7	93.7	84.5	9.8	0.6
C_{12}	--	0.8	1.2	78.3	1.0
C_{13}	--	--	--	11.2	15.4
C_{14}	--	--	--	--	82.1
>C_{14}	--	--	--	--	0.9
LAS MW (as Na-LAS)	320.7	333.7	346.4	362.3	373.7

Remarks: French strain of *S. subspicatus* from the University of Metz. As NOEC (no observed effect concentration), the authors used the EC_5 because of the lack of noticeable variation in toxicity for the interval 0-5%. This is a key study for aquatic toxicity to algae (see SIAR Table 12).

Reference: Verge, C. and Moreno, A. 1996a. Toxicity of anionic surfactants to green microalgae *"Scenedesmus subspicatus"* and *"Selenastrum capricornutum."* Tenside Surf. Det. 33:166-168.

Reliability: 2 Valid with restrictions

(f)
Species: *Scenedesmus subspicatus* (Algae)
Endpoint: Biomass **[X]**; Growth rate **[X]**; Other **[ ]**
Exposure period: 72 hour
Results: E_rC_{50} (growth rate) = 127.9 mg/L; E_bC_{50} (biomass) = 43.2 mg/L
NOEC (growth rate) = 2.4 mg/L; NOEC (biomass) = 2.2 mg/L
LOEC (growth rate) = 10 mg/L

Inhibition of cell growth by concentration and duration is shown in the table below:

Cell number (x 10^4 cells/mL)				
	Time Period (hours)			
Test concentration (mg/L)	**0**	**24**	**48**	**72**
Control	2	8	29	95
0.6	2	8	30	89
2.4	2	9	28	85
10	2	9	27	75
40	2	8	20	48
160	2	7	9	8

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: open-system **[X]**; closed-system **[ ]**
Algal growth inhibition test (88/302/EWG) 1988.
Nominal test concentrations were control, 0.6, 2.4, 10, 40, and 160 mg/L. Algae were exposed to LAS in Erlenmeyer flasks in an environmental chamber on a light table at 8000 lux. Cell numbers were photometrically determined (8 subsets were taken for each concentration).
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Marlon A 390 (CAS #68411-30-3) $C_{10\text{-}13}$ LAS, average alkyl chain length = 11.6; 91.3% activity
Remarks: Initial cell concentrations were 20,000 cells/mL. Cell concentrations at 72 h were 95, 89, 85, 75, 48 and 8 (all x 10^4/mL) for the control, 0.6, 2.4, 10, 40 and 160 mg/L LAS concentrations, respectively. The pH ranged from 7.7 to 7.9 at the beginning of the study and 7.9 to 9.0 at the end of the study. Test temperature was maintained at 24 ± 2 °C. This is a key study for aquatic toxicity to algae (see SIAR Table 12).
Reference: Scholz, N. 1992. Bestimmung der Auswirkungen von Marlon A 390 auf das Wachstum von *Scenedesmus subspicatus* 86.81. SAG (Algenwachstumshemmtest nach Richtlinie 88/302/EWG) Huels Final Report No. AW-291.
Reliability: 1 Valid without restriction

(g)
Species: *Scenedesmus subspicatus* (Algae)
Endpoint: Biomass **[X]**; Growth rate **[X]**; Other **[ ]**
Exposure period: 72 hour
Results: E_rC_{50} (growth rate) = 82 mg/L; E_bC_{50} (biomass) = 20 mg/L
NOEC (growth rate) = 0.4 mg/L; NOEC (biomass) = 0.1 mg/L

Inhibition of cell growth by concentration and duration is shown in the table below:

Cell number (x 10^4 cells/mL)				
	Time Period (hours)			
Test concentration (mg/L)	**0**	**24**	**48**	**72**
Control	2	9	32	94
0.1	2	9	32	91
0.4	2	9	29	88
1.6	2	9	28	76
6.4	2	9	24	60
25	2	9	21	54
160	2	6	7	7

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**
Method: open-system **[X]**; closed-system **[ ]**
Algal growth inhibition test (92/69/EWG)
Nominal test concentrations were control, 0.1, 0.4, 1.6, 6.4, 25 and 160 mg/L. Test concentrations were measured at 0 and 72 h and found to confirm the nominal concentrations. Algae were exposed to LAS in Erlenmeyer flasks in an environmental chamber on a light table at 8000 lux. Cell numbers were photometrically determined (8 subsets were taken for each concentration).
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Marlon A 350 (CAS #68411-30-3) $C_{10\text{-}13}$ LAS, average alkyl chain length = 11.6; 52.1% activity

Remarks:	Initial cell concentrations were 20,000 cells/mL. Cell concentrations at 72 h 94, 91, 88, 76, 60, 54 and 7 (all x 10^4/mL) for the control, 0.1, 0.4, 1.6, 6.4, 25 and 160 mg/L LAS concentrations, respectively. The pH ranged from 8.2 to 8.3 at the beginning of the study and 8.0 to 9.4 at the end of the study. Test temperature was maintained at 24 ± 2 °C. This is a key study for aquatic toxicity to algae (see SIAR Table 12).
Reference:	Scholz, N. 1994. Bestimmung der Auswirkungen von Marlon A 350 auf das Wachstum von *Scenedesmus subspicatus* 86.81. SAG (Algenwachstumshemmtest nach Richtlinie 92/69/EWG) Huels Final Report No. AW-372.
Reliability:	1 Valid without restriction

(h)

Species:	*Scenedesmus subspicatus* (Algae)
Endpoint:	Biomass **[X]**; Growth rate **[ ]**; Other **[ ]**
Exposure period:	96 hour
Results:	EC_{50} = 5 mg/L
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[X]**
Method:	DIN 38412 Part 9
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Data refer to 100% active ingredient. Test method conforms with OECD-Guideline 201.
Reference:	European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability:	4 Not assignable. The original study was not available for review.

(i)

Species:	*Scenedesmus subspicatus* (Algae)
Endpoint:	Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**
Exposure period:	96 hour
Results:	EC_{50} = 9 mg/L
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[X]**
Method:	Directive 87/302/EEC, part C, p. 89 “Algal inhibition test”
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	C_{10-13} LAS, sodium salt; average chain length 11.6 (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good.
Reference:	European Commission. 2000c. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Huels AG, 1/90, N. Scholz, unpublished.
Reliability:	4 Not assignable. The original study was not available for review.

(j)

Species:	*Scenedesmus subspicatus* (Algae)
Endpoint:	Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**
Exposure period:	96 hour
Results:	EC_{50} = 30 mg/L
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	ISO 8692 “Water quality - Fresh water algal growth inhibition test with *Scenedesmus subspicatus* and *Selenastrum capricornutum*”
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{11-13} LAS

Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Nominal concentrations (deviation <3%); BBM medium; pH 6.4-6.7; 20-22ºC. Note that although this was cited in IUCLID as a Procter & Gamble report, Procter & Gamble indicates that it is unlikely that it is one of their reports.
Reference:	European Commission. 2000h. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, AL/12.
Reliability:	4 Not assignable. The original study was not available for review.

(k) **(*Selenastrum*)**

Species:	*Selenastrum capricornutum* (Algae)
Endpoint:	Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**
Exposure period:	96 hour
Results:	EC_{50} = 4.29-12.5 mg/L
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	OECD Guideline 201 "Algae, Growth Inhibition Test", 1984
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	LAS, average chain length 11.8 (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Water hardness = 150 mg/L as $NaHCO_3$. Reported results are EC_{50} values for 2 tests. Static mean EC_{50} = 7.3 mg/L.
Reference:	European Commission. 2000t. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 29101.
Reliability:	3 Invalid. Based on correspondence with Procter & Gamble, it appears that this study was mis-cited. The P&G report 29101 indicates 96-h EC_{50} values of 29 mg/L and greater than 10 mg/l, not the values reported above. In addition, the P&G study was not conducted under the OECD Guideline cited. Given these discrepancies, the values are uncertain and are considered invalid.

(l)

Species:	*Selenastrum capricornutum* (Algae)
Endpoint:	Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**
Exposure period:	72 hour
Results:	EC_{50} = 11 mg/L
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	ISO 8692 "Water quality - Fresh water algal growth inhibition test with *Scenedesmus subspicatus* and *Selenastrum capricornutum*"
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{11-13} LAS (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Nominal concentrations (deviation <13%); BBM medium; pH 6.5-6.6; static. Note that although this was cited in IUCLID as a Procter & Gamble report, Procter & Gamble indicates that it is unlikely that it is one of their reports.
Reference:	European Commission. 2000g. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, AL/10.
Reliability:	4 Not assignable. The original study was not available for review.

(m)

Species:	*Selenastrum capricornutum* (Algae)
Endpoint:	Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**

Exposure period: 96 hour
Results: EC_{50} = 12.2 mg/L
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**
Method: EPA, l987.
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: $C_{10\text{-}13}$ LAS, average chain length 12.3 (CAS #68411-30-3)
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. AAP medium; 24^{+}/-2ºC.
Reference: European Commission. 2000n. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, P2636.01.
Reliability: 4 Not assignable. The original study was not available for review.

(n)
Species: *Selenastrum capricornutum* (Algae)
Endpoint: Biomass **[ ]**; Growth rate **[X]**; Other **[ ]**
Exposure period: 48 hour
Results: EC_{50} ≈ 80 mg/L (Observation of graphical plot in paper indicates that the EC_{50} is between 50-100 mg/L)
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: Algal Assay Procedure Bottle Test, USEPA (1971).
Individual test flasks were spiked with a 1 mL algal suspension at 0.7 mg/L dry weight for each concentration. Test solutions were run in triplicate. Algae were maintained at 24 ± 2°Cat 4000 lux for 48 hours. Cell counts were accomplished with a Coulter Counter and the growth Rate calculated.
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: $C_{11.6}$ LAS; 23.4% activity
Remarks: Though generally valid, this study was not included in the HERA assessment because the exposure period was only 48 hours.
Reference: Yamane, A., Okada, M. and Sudo, R. 1984. The growth inhibition of planktonic algae due to surfactants used in washing agents. Water Res. 9:1101-1105.
Reliability: 2 Valid with restrictions. Duration of test considered too short for a chronic study, therefore not included in SIAR Table 12A.

(o) **(*Elodea*)**
Species: *Elodea canadensis* (aquatic plant)
Endpoint: Biomass **[ ]**; Growth rate **[ ]**; Other **[X]** inhibition of growth, productivity
Exposure period: 28 day
Results: NOEC > 4 mg/L
Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**
Method: The effect of LAS on the structure and function of microbial communities was studied in a flow-through model ecosystem containing several trophic levels. Duplicate 19-L glass aquaria containing model ecosystems at four nominal concentrations (0.5, 1.0, 2.0, 4.0 mg/L) contained water and 2.5 cm lake sediment (Winton Lake, Cincinnati, OH) and several trophic levels (bacteria, algae, macrophytes [*Elodea canadensis,Lemna minor*], macroinvertebrates [*Daphnia magna, Paratanytarsus parthenogenica*], and fish [*Lepomis macrochirus*]). Flow rate in the proportional diluter delivered approximately 8 replacement volumes per day. Additionally, at each cycle of the diluter, 1.5 mL of a Daphnia food suspension diluted with a culture of *Selenastrum* was added to each chamber. Following an initial 3 day acclimation period to analytically confirm test concentrations, 4 glass periphyton slides (5 x 5 cm), 8 vegetative shoots of *Elodea*, 10 early instar *Daphnia*, 25 midge eggs and 5 pre-weighed juvenile bluegills (2.5-5.0 cm

length) were added to each aquarium. Fish were screened from access to the macroinvertebrates by a 60 mesh stainless steel screen and were fed a daily supplement of frozen brine shrimp. Test duration was 28 days. Effects monitored included population and community effects. Nominal concentrations were confirmed with MBAS analysis. After 28 days the vegetative shoots of *Elodea* were removed, the total length measured, and the shoots were placed into aluminium dishes for determination of ash-free dry weights.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: LAS; C^{14}-LAS chain length C_{12} (91% purity) plus unlabeled LAS with average chain length $C_{11.6}$ (C_{10} 9.7%, C_{11} 27.9%, C_{12} 54.4%, C_{13} 8.0%; 95% purity) (tested together)

Remarks: Dissolved oxygen concentrations ranged between 7.0 and 9.0 mg/L. Temperature was maintained at 2°C and the mean pH was 8.1 ± 0.2. The growth and productivity of *Elodea* was not significantly inhibited at the highest concentration tested (4 mg/L) in Phase I. Growth throughout the 28-day exposure approximately doubled the initial biomass of the vegetative shoots from a mean of about 37 mg ash-free dry weight to a mean of about 72 mg for the treatment concentrations. Similarly, Phase II experiments resulted in an approximate doubling of the initial *Elodea* biomass in the controls and the 3.75% effluent concentration, though the heavy growth of attached bacteria and fungi (periphyton) that developed in the higher concentrations effectively covered the growing surface of the Elodea shoots resulting in progressively lower productivity in 7.5, 15 and 30% dilutions.

Reference: Maki, A.W. 1981. A Laboratory model ecosystem approach to environmental fate and effects studies. Unpublished Internal Report, Environmental Safety Department Procter and Gamble Company, Cincinnati, Ohio.

Reliability: 2 Valid with restrictions

(p) **(*Lemna*)**

Species: *Lemna minor* (aquatic plant)

Endpoint: Biomass **[ ]**; Growth rate **[ ]**; Other **[X]** frond count

Exposure period: 7 days

Results: EC_{50} = 2.7 mg/L

NOEC = 0.9 mg/L (calculated as $EC_{50}/3$); normalized to $C_{11.6}$ = 1.1 mg/L

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**

Method: A 7-day flow-through growth inhibition test was developed using duckweed (*Lemna minor*). Control water (carbon and reverse osmosis filtered well water) and five concentrations of test material were delivered from diluter mixing chambers to Pyrex glass exposure chambers at a rate of 1.5 L every 16 minutes (approximately 14 replacement volumes per day). At time 0, each chamber received seven 2-frond, root excised duckweed colonies (four replicates per treatment level). Plants were given continuous illumination at 3875 lux (360 foot candles) and temperature was maintained between 21 and 23°C. Total hardness was 120-130 mg/L $CaCO_3$ and pH was 7.2-7.6. The number of fronds was recorded once every 24 hours for 7 days. LAS concentrations were measured using the MBAS method.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: $C_{10\text{-}14}$ LAS, average alkyl chain length 11.8, MW = 345, 27.3% active

Remarks: Results based on frond count were found to provide the most useful information per unit of laboratory time. Other endpoints resulted in 7-day EC_{50} values of 3.6 mg/L (dry weight), 4.9 mg/L (root length), and 4.8 mg/L (growth rate/doubling time). Concurrent tests with bluegill sunfish (96-hr LC_{50} = 1.7 mg/L) and *D. magna* (48-hr LC_{50} = 4.4 mg/L) indicate that

protection criteria developed for these species should be adequate to protect the aquatic macrophyte community without the need for additional testing.

Reference: Bishop, W.E. and Perry, R.L. 1981. Development and Evaluation of a Flow-Through Growth Inhibition Test with Duckweed (*Lemna minor*). Aquatic ..... Toxicology and Hazard Assessment. ASTM STP 737. Branson, D.R. and Dickson, K.L. (ed.).

Reliability: 2 Valid with restrictions

(q)

Type of Test: Static [X]; semi-static [ ]; flow-through [ ]
Open-system [ ]; closed-system [ ]; not stated [X]

Species: *Chlamydomonas reinhardi* (algae)

Exposure Period: not stated

Effect Criteria: Growth inhibition

Results: NOEC = 15 mg/L
LOEC = 20 mg/L

Analytic Monitoring: Yes [ ]; No [ ]; ? [X]

Method: LAS concentrations of 1, 5, 10, 15, 20 and 30 mg/L were prepared in Deionized, sterilized double-distilled glass water. Algae were grown in Bold's medium. Cell counts were made using a spectrophotometer and dry weight observations.

GLP: Yes [ ]; No [X]; ? [ ]

Test Substance: $C_{11.2}$ LAS

Remarks: No morphological changes were observed. The growth rate was reduced at LAS concentrations of 20 mg/L. Protein analysis indicated that higher concentrations did affect protein synthesis. The NOEC normalized by van de Plassche et al. (1999) to $C_{11.6}$ LAS was 12 mg/L.

Reference: Dhaliwal, A.A., Campione, A., and Smaga, S. 1977. Effect of linear alkylbenzene sulfonate ($C_{11.2}$ LAS) on the morphology and physiology of *Plectonema boryanum* and *Chlamydomonas reinhardi*. J. Phycol. 13:18.

Reliability: 4 Not assignable. This study was given a reliability score of 4 because the document reviewed was an abstract.

(r)

Type of Test: Static [X]; semi-static [ ]; flow-through [ ]
Open-system [ ]; closed-system [ ]; not stated [X]

Species: *Chlorella kessleri* (algae)

Exposure Period: 15 days

Effect Criteria: Growth rate

Results: NOEC = 3.1 mg/L
LOEC = 10 mg/L

Analytic Monitoring: Yes [ ]; No [X]; ? [ ]

Method: EPA-600/9-78-018. Algal Assay Bottle Test. Determination of the Inhibitory effect of water constituents on green algae, by William E. Joseph C. Greene, and Tamotsu Shiroyama, Cornwallis Environmental Research Laboratory, Corvallis, Oregon.

GLP: Yes [ ]; No [X]; ? [ ]

Test Substance: Marlon A 350, Benzenesulfonic acid, C10-13-alkyl derives., sodium salts (CAS #68411-30-3); 25.7% activity.

Remarks: No morphological changes were observed. The growth rate was reduced at LAS concentrations of 20 mg/L. Protein analysis indicated that higher concentrations did affect protein synthesis. The NOEC normalized by van de Plassche et al. (1999) to $C_{11.6}$ LAS was 3.5 mg/L.

Reference: Henkel KGaA, Biological Research and Product Safety/Ecology, unpublished results of study conducted in 1984; test substance Fi 5829.

Reliability:	2 Valid with restrictions. Non-standard length of study, therefore not included in SIAR Table 12A.

(s)

Type of Test:	Static [X]; semi-static [ ]; flow-through [ ] Open-system [X]; closed-system [ ]; not stated [ ]
Species:	*Microcystis aeruginosa* (algae)
Exposure Period:	96 hours
Effect Criteria:	Growth rate
Results:	EC_{50} = 0.9 mg/L
Analytic Monitoring:	Yes [ ]; No [X]; ? [ ]
Method:	The test species was cultured following the procedures of USEPA 1971. Temperature was maintained at 24 ± 2°C. Water chemistry was determined at least once during each test according to Standard Methods (APHA 1985). EC50 values were calculated using the method of Larson and Schaeffer (1982) or graphical interpolation.
GLP:	Yes [ ]; No [X]; ? [ ]
Test Substance:	C_{12} LAS; average molecular weight = 345
Remarks:	Mean hardness was 137 mg/L as $CaCO_3$, pH range was 6.8-7.2, and the mean dissolved oxygen was 9.1 mg/L. Comparison was also made to *in situ* studies conducted in which lake water was bottled and suspended in Lake Acton (Ohio) for 3 hour periods. The mean 3-h EC_{50} (photosynthesis) for the *in situ* studies was 3.4 mg/L (0.5-8.0 mg/L). The NOEC normalized by van de Plassche et al. (1999) to $C_{11.6}$ LAS was 0.35 mg/L. Using the acute to chronic ratio calculation (documented in Annex 3 of the LAS SIAR), the EC_{50}/3 for *Microcystis* is 0.3 mg/L. This is a critical study for this SIDS endpoint.
Reference:	Lewis, M.A. and Hamm, B.G. 1986. Environmental modifications of the photosynthetic response of Lake Plankton to surfactants and significance to a laboratory-field comparison. Wat. Res. 20:1575-1582.
Reliability:	2 Valid with restrictions

(t)

Type of Test:	Static [ ]; semi-static [ ]; flow-through [ ] Open-system [ ]; closed-system [ ]; not stated [X]
Species:	*Plectonema boryanum* (algae); strain 597
Exposure Period:	not stated
Effect Criteria:	Growth rate
Results:	NOEC = 20 mg/L LOEC = 30 mg/L
Analytic Monitoring:	Yes [ ]; No [ ]; ? [X]
Method:	LAS concentrations of 1, 5, 10, 15, 20 and 30 mg/L were prepared in Deionized, sterilized double-distilled glass water. Algae were grown in Bold's medium.
GLP:	Yes [ ]; No [X]; ? [ ]
Test Substance:	$C_{11.2}$ LAS
Remarks:	Growth rate was reduced at 30 mg/L concentrations of LAS as indicated by spectrophotometer readings and dry weight. The NOEC normalized by van de Plassche et al. (1999) to $C_{11.6}$ LAS was 15 mg/L.
Reference:	Dhaliwal, A.S., Campione, A., and Smaga, S. 1977. Effect of linear alkylbenzene sulfonate ($C_{11.2}$ LAS) on the morphology and physiology of *Plectonema boryanum* and *Chlamydomonas reinhardi*. J. Phycol. 12:18.
Reliability:	4 Not assignable This study was given a reliability score of 4 because the document reviewed was an abstract. However, these data were considered reliable as part of a weight-of-evidence approach in the analysis conducted by van de Plaasche et al. (1999).

4.4 TOXICITY TO BACTERIA

(a)

Type: Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species: activated sludge
Exposure Period: 3 hour
Results: EC_{50} (Na LAS-C_{11}) = 760 mg/L
EC_{50} (Na LAS-$C_{11.6}$) = 550 mg/L
EC_{50} (Na LAS-C_{13}) = 650 mg/L
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: OECD 209 Activated Sludge Respiration Inhibition Test. 1984.
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Three different alkyl chain lengths of LAS (C_{11}, $C_{11.6}$, C_{13} sodium salts), with the following homologue distributions.

	Alkyl Chain Length Distributions **(%)**		
	LAS C_{11}	**LAS $C_{11.6}$**	**LAS C_{13}**
$<C_{10}$	1.5	0.4	--
C_{10}	29.0	8.9	1.0
C_{11}	39.0	33.7	3.5
C_{12}	28.5	31.0	17.8
C_{13}	1.8	24.0	37.0
C_{14}	0.2	2.0	40.4
$>C_{14}$	--	--	0.3
LAS MW (as Na-LAS)	334	343	363

Remarks: The purpose of the study was to determine the toxicity of three commercial LAS products to the activated sludge of a treatment plant basically operating on domestic sewage. A contact time of 3 hours instead of 15 minutes was chosen to better simulate the real residence time used in wastewater treatment plants (4-6 hours). The EC_{50} values are far above environmental concentrations and therefore provide a high margin of safety. The 3-hour EC_{50} range for the reference substance (3,5-dichlorophenol) ranged from 20-30 mg/L, within the valid range of 5-30 mg/L.
Reference: Verge C. and Moreno, A. 1996b. Toxicity of anionic surfactants to the bacterial population of a waste water treatment plant. Tenside Surf. Det. 33:323-327.
Reliability: 2 Valid with restrictions

(b)

Type: Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species: activated sludge
Exposure Period: 3 hour
Results: EC_{50} (Na LAS-C_{10}) = 1042-1200 mg/L
EC_{50} (Na LAS-C_{11}) = 740-782 mg/L
EC_{50} (Na LAS-C_{12}) = 500-723 mg/L
EC_{50} (Na LAS-C_{13}) = 700-795 mg/L
EC_{50} (Na LAS-C_{14}) = 900-1045 mg/L
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: OECD 209 Activated Sludge Respiration Inhibition Test. 1984.
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Five different pure homologues of LAS ($C_{10,}$ C_{11}, C_{12}, $C_{13,}$ C_{14} sodium salts), with the following homologue distributions.

	Pure Homologues (%)				
	LAS C_{10}	LAS C_{11}	LAS C_{12}	LAS C_{13}	LAS C_{14}
$<C_{10}$	0.5	--	0.4	--	--
C_{10}	96.8	5.5	13.9	0.7	--
C_{11}	2.7	93.7	84.5	9.8	0.6
C_{12}	--	0.8	1.2	78.3	1.0
C_{13}	--	--	--	11.2	15.4
C_{14}	--	--	--	--	82.1
$>C_{14}$	--	--	--	--	0.9
LAS MW (as Na-LAS)	320.7	333.7	346.4	362.3	373.7

Remarks: The purpose of the study was to determine the toxicity of five pure homologues of LAS to the activated sludge of a treatment plant basically operating on domestic sewage. A contact time of 3 hours instead of 15 minutes was chosen to better simulate the real residence time used in wastewater treatment plants (4-6 hours). The EC_{50} values are far above environmental concentrations and therefore provide a high margin of safety. The 3-hour EC_{50} range for the reference substance (3,5-dichlorophenol) ranged from 20-30 mg/L, within the valid range of 5-30 mg/L.

Reference: Verge C. and Moreno, A. 1996b. Toxicity of anionic surfactants to the bacterial population of a waste water treatment plant. Tenside Surf. Det. 33:323-327.

Reliability: 2 Valid with restrictions

(c)

Type: Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**

Species: activated sludge

Exposure Period: 15 minute

Results: EC_{50} = 107-152 mg/L

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: ESD-VIII-D-1, Issue II (9/8/80)

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: C_{10-13} LAS (CAS #68411-30-3)

Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Effect: inhibition of respiration. Nominal concentrations (expected deviation <20%). Mixed Liquor Suspended Solids 53.6-76.1 mg/g VSS/Sewage. Static, 25ºC. Activated sludge (2600 mg SS/L)

Reference: European Commission. 2000s. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, 27896, 27897, 27915.

Reliability: 4 Not assignable. The original study was not available for review. Summary included for competeness.

(d)

Type: Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**

Species: *Pseudomonas putida* (Bacteria)

Exposure Period: 18 hour

Results: EC_{50} = 60.9-63.5 mg/L
EC_{10} = 52.7-56.6 mg/L

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: Bacterial toxicity test according to DIN 38412 part 8. A total of 6 concentrations were tested (40-80 mg/L) under GLP conditions.

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance:	Marlon A 390 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = 11.6; activity 91.3%,
Remarks:	Results show EC_{50} and EC_{10} values for two tests.
Reference:	Scholz, N. 1993. Bestimmung der bacterientoxizitat von Marlon A 390 in Pseudomonas-zellvermehrungs-Hemmtest. Huels-Final Report No. PZ-93/10.
Reliability:	2 Valid with restrictions

(e)

Type:	Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species:	*Pseudomonas putida* (Bacteria)
Exposure Period:	30 minute
Results:	EC_{50} = 350 mg/L EC_0 = 250 mg/L
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[X]**
Method:	DIN 38412 Teil 27 (respiration inhibition test)
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Data refer to 100% active ingredient.
Reference:	European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability:	4 Not assignable

(f)

Type:	Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species:	*Pseudomonas putida* (Bacteria)
Exposure Period:	16 hour
Results:	EC_{50} = 150 mg/L EC_0 = 50 mg/L
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[X]**
Method:	DIN 38412 Teil 8 (cell multiplication inhibition test)
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Data refer to 100% active ingredient
Reference:	European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability:	4 Not assignable

(g)

Type:	Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species:	*Pseudomonas putida* (Bacteria)
Exposure Period:	30 minute
Results:	NOEC = 64 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	DIN 38412, Teil 27
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{10-13} LAS, average chain length 11.8 (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Synthetic water; static; pH 7.2^{+}/-0.2; 20ºC. Effect: Inhibition of oxygen consumption.

Reference: European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KgaA.
Reliability: 4 Not assignable

(h)
Type: Aquatic **[X]**; Field **[ ]**; Soil **[ ]**; Other **[ ]**
Species: *Pseudomonas putida* (Bacteria)
Exposure Period: 16 hour
Results: NOEC = 30 mg/L
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: DIN 38412, Teil 8
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: C_{10-13} LAS, average chain length 11.8 (CAS #68411-30-3)
Remarks: Synthetic medium; static; pH 7.4^{+}/-0.3; 21ºC. Effect: growth inhibition. Feitjel et al. reviews this study and also reports an NOEC = 35 mg/L for $C_{11.6}$ LAS.
Reference: Feijtel, T.C.J., Matthijs, E., Rottiers, A., Rijs, G.B.J., Kiewiet, A., and de Nijs, A. 1995. AIS/CESIO environmental surfactant monitoring programme. Part 1: LAS monitoring study in "de Meer" STP and receiving river "Leidsche Rijn" Chemosphere 30:1053-1066.
Reliability: 4 Not assignable

(i)
Results: Based on digester performance, even a high and atypical concentration of LAS (30 g/kg) did not inhibit microbial populations present in STP activated sludge digesters.
Remarks: The study was designed to monitor LAS during the different steps of 9 different standard sewage treatment plants operating mainly with domestic sewage. LAS-specific analytical methods were used. More details on the study can be found in the summary at 3.2(f).
Reference: Berna, J.L., de Ferrer, J., Moreno, A., Prats, D. and Ruiz Bevia, F. 1989. The fate of LAS in the environment. Tenside Surf. Det. 26:101-107.
Reliability: 4 Not assignable. Treatment plant operational records are not available for review.

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

4.5.1 CHRONIC TOXICITY TO FISH

(a)
Type of Test: Static [ ]; semi-static [X]; flow-through [ ]
Open-system [X]; closed-system [ ]; not stated [ ]
Species: *Brachydanio rerio* (Zebra Fish, fresh water)
Exposure Period: 14 days
Effect Criteria: Mortality, behavior
Results: NOEC = 2.0 mg/L
LOEC = 4.0 mg/L
Analytic Monitoring: Yes [ ]; No [X]; ? [ ]
Method: Based on UBA-Verfahrensvorschlag:Verlaengerter Toxizitaetstest beim Zebrabaerbling *Brachydanio rerio*, Bestimmung der Schwellenkonzentration der letalen und anderer Wirkungen, NOEC, mindestnes 14 Tage. This method conforms with OECD Guideline 204. Ten fish were exposed to each of seven concentrations (0.2, 0.4, 0.8, 1.6, 2.0, 4.0 and 8.0 mg/L) and the controls. Test chambers were 10-L basins containing 5-L of copper- and chlorine-free drinking water, maintained in a 16:8 light:dark illumination

	cycle. The NOEC normalized by van de Plassche et al. (1999) to $C_{11.6}$ LAS was 2.3 mg/L.
GLP:	Yes [ ]; No [X]; ? [ ]
Test Substance:	Marlon A 350 LAS (CAS #68411-30-3; Benzenesulfonic acid, C_{10-13}- alkyl derives., sodium salts, 25.7% activity)
Reference:	Henkel KGaA, Biological Research and Product Safety/Ecology: unpublished results (Test substance number Fi 5959).
Reliability:	2 Valid with restrictions. Duration of test considered too short for a chronic study, therefore not included in SIAR Table 12A.

(b)

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other **[ ]** open-system **[X]**; closed-system **[ ]**
Species:	*Pimephales promelas* (Fish, fresh water)
Exposure period:	30 day
Effect criteria:	Fry survival
Results:	NOEC = 1 mg/L LOEC = 2 mg/L
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ] HPLC**
Methods:	Two replicates of 100 egg-fry stage fathead minnows were exposed for 30 days to LAS under the following conditions: Hardness 41 mg/L as $CaCO_3$; pH 7.2; temperature 24°C. The exchange rate was 1 to 3 volume changes/day. Test chambers were 3500 mL volume. The studies were conducted at EG&G Bionomics (now Springborn Smithers Laboratory).
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	Commercial C_{10-13} LAS, sodium salt (CAS #68411-30-3); C_{10} 5%, C_{11} 27%, C_{12} 53%, C_{13} 13%; 2-phenyl 23%.
Remarks:	Carboxylated intermediates formed in the biodegradation of LAS exhibit toxicity several orders of magnitude less than LAS; LC_{50} values were >144 mg/L and >52 mg/L for sulfophenyl butarate and sulfophenyl undecanoate, respectively. NOEC based on fry survival. Egg hatchability and fry growth were less sensitive. This is a key study for chronic aquatic toxicity to fish (see SIAR Table 12).
Reference:	Swisher, R.D., Gledhill, W.E., Kimerle R.A. and Taulli, T.A. 1978. Carboxylated intermediates in the biodegradation of linear alkylbenzene sulfonates (LAS). VII International Congress on Surface Active Substance, Proceedings, Moscow, 1976 4:218-230.
Reliability:	2 Valid with restrictions

(c)

Type of Test:	Static [ ]; semi-static [X]; flow-through [ ] Open-system [X]; closed-system [ ]; not stated [ ]
Species:	*Poecilia reticulata* (Fish, Guppy, fresh water)
Exposure Period:	28 days
Effect Criteria:	Mortality, behavior, and growth
Results:	NOEC = 3.2 mg/L LOEC = 10 mg/L
Analytic Monitoring:	Yes [ ]; No [X]; ? [ ]
Method:	Fish were 3-4 weeks old at test initiation. Fifty fish were used per group. Temperature was maintained at 23 ± 2°C. The test volume (10-L per chamber) was renewed three times per week. Circadian lighting (16:8 light:dark) was used. Fish were fed a Tetramin/Tetraphyll mixture. Dissolved oxygen, water hardness and pH were measured during the study.
GLP:	Yes [ ]; No [ ]; ? [X]
Test Substance:	LAS, 42.4% activity (C_8 <1%, C_9 16.5%, C_{10} 23%, C_{11} 20%, C_{12} 18%, C_{13} 16%, C_{14} 6.5%); average = $C_{11.1}$

Remarks:	The only effect (98% mortality at 10 mg/L) occurred within 2 days of study initiation. The NOEC normalized by van de Plassche et al. (1999) to $C_{11.6}$ LAS was 3.2 mg/L.
Reference:	Canton, J.H. and Slooff, W. 1982. Substitutes for phosphate containing washing products: Their toxicity and biodegradability in the aquatic environment.
Reliability:	2 Valid with restrictions. Duration of test considered too short for a chronic study, therefore not included in SIAR Table 12A.

(d)

Type of Test:	Static [ ]; semi-static [ ]; flow-through [X] Open-system [X]; closed-system [ ]; not stated [ ]
Species:	*Oncorhynchus mykiss* (Fish, Rainbow Trout, fresh water)
Exposure Period:	14 days
Effect Criteria:	Mortality
Results:	14 day LC_{50} = 0.12 mg/L
Analytic Monitoring:	Yes [ ]; No [ ]; ? [X]
Method:	Rainbow trout at different developmental stages (egg [160-200 eggs per concentration], alevin with partially absorbed yolk sac [2-3 days old], alevin [60 days old], and adult [270-300 days old]) were exposed to LAS for 14 days. Temperature was maintained at about 15°C, dissolved oxygen at greater than 80% of saturation, pH at 7.3-7.4, and water hardness of 290-310 mg/L as $CaCO_3$.
GLP:	Yes [ ]; No [ ]; ? [X]
Test Substance:	C_{12} LAS, 45% activity
Remarks:	The egg was the most sensitive life stage in the 14 day tests, in contrast to the 24 hour tests, which showed the egg to be the least sensitive (alevins with partially absorbed yolk sac were the most sensitive in the 24 hour tests). Malformations were seen only in embryos treated with lethal concentrations. A NOEC value was not determined in the study and the data provided are inadequate to calculate an EC_{20} value.
Reference:	Vailati, G., Calamari, D. and Marchetti, R. 1975. Effetti dell'alchilbenzene sofonato (LAS) sugli staid di sviluppo del *Salmo gairdneri* Rich. Istituto di Ricerca sulle Acque (CNR) Sezione di Idrobiologia Applicata (Milano).
Reliability:	2 Valid with restrictions. Duration of test considered too short for a chronic study, therefore not included in SIAR Table 12A.

(e)

Type of Test:	Static [X]; semi-static [ ]; flow-through [ ] Open-system [X]; closed-system [ ]; not stated [ ]
Species:	*Tilapia mossambica* (Fish, Tilapia, fresh water)
Exposure Period:	90 days
Effect Criteria:	Feeding, growth rate, fecundity, yield
Results:	NOEC = 0.25 mg/L LOEC = 0.51 mg/L
Analytic Monitoring:	Yes [ ]; No [ ]; ? [X]
Method:	Tests generally followed the standard methods of APHA 1975, with the following specifics. Tests were conducted in outdoor earthen vats (62 cm diameter, 30 cm mean depth) containing 60-L of borehole water and 5 kg of uncontaminated soil. Borehole water is unchlorinated water with the following parameters: pH 7.1 ± 0.1, dissolved oxygen 10 mg/L, hardness 290 mg/L as CaCO3, and temperature 27.9 ± 0.14 °C. Fifteen fish purchased from local farms (35 mm, 0.786 g) and acclimated to the test conditions for 168 hours were added per vat. Test concentrations were 0.25, 0.38, 0.51, and 1.10 mg/L. Fish were exposed six times at 15 day intervals with the water renewals and were fed daily with a 1:1 mixture of rice bran and mustard oil

cake. Standard acute toxicity tests were also conducted in the laboratory. Statistical analysis was done using F and t tests and the significance of any change was measured at a 5% level of probability.

GLP: Yes [ ]; No [X]; ? [ ]

Test Substance: LAS (Parnol J Liquid), 20% activity; clear yellow liquid; pH in solution was 8 ± 1

Remarks: The feeding rates decreased significantly at 0.25, 0.38 and 1.10 mg/L. Fish showed erratic behaviour, irregular opercular movement, and at higher concentrations, blood exuded from the base of the pectoral and pelvic fins and head. No apparent difference in condition factor (K) was observed at any concentration. The maturity index (MI) of both male and female fish appeared to decrease at all concentrations, but the biological significance of this is questionable because historic control values for this parameter were not provided and the magnitude of the response did not increase with dose. Fecundity decreased at 0.51 mg/L but not at 1.10 mg/L. The gastrosomatic index (GSI) was significantly different at 0.51 and 1.10 mg/L. Based on the most reliable endpoints (GSI and fecundity), the NOEC would be 0.38 mg/L and the LOEC would be 0.51 mg/L. However, the study is incompletely documented, so details of the test substance composition and testing procedure are uncertain. True replicates were not used so statistics can not be validly conducted, though they are reported by the authors. In view of these limitations, and previous evaluations of the study which have reported a NOEC of 0.25 mg/L (van de Plassche et al., 1999), a conservative (protective) NOEC for this study is 0.25 mg/L. This is a critical study for this SIDS endpoint.

Reference: Chattopahyay, D.N. and Konar, S.K. 1985. Acute and chronic effects of linear alkyl benzene sulfonate on fish, plankton, and worm. Environment & Ecology, 3:258-262.

Reliability: 2 Valid with restrictions.

(f)

Type of test: Various types and durations of tests.

Results: The article compiles the no observed effect concentration (NOEC) values for many tests conducted on an assortment of species. The following table shows the geometric mean NOEC values for each fish species (n = number of studies included for each species).

Species	Geometric mean NOEC (mg/L)	*N*
Brachydanio rerio	2.3	1
Pimephales promelas	0.87	14
Poecilia reticulate	3.2	1
Oncorhynchus mykiss	0.34	7
Tilapia mossambica	0.25	1

Remarks: All data were from tests conducted on commercial LAS with $C_{10\text{-}13}$ alkyl chains and average carbon lengths close to $C_{11.6}$ and $C_{11.8}$. The NOEC values have been normalized using QSARs to the average structure of $C_{11.6}$ LAS.

Reference: van de Plassche, E.J., DeBruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J., and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: Linear alkyl benzene sulfonate, alcohol ethoxylates, alcohol ethoxylated sulfates, and soap. Environ. Toxicol. Chem. 18: 2653-2663.

Reliability: 4 Not assignable This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(g) **(Rainbow trout)**

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**
Species:	*Salmo gairdneri* (*Oncorhyncus mykiss,* fish, estuary, fresh water)
Endpoint:	Length of fish **[ ]**; Weight of fish **[ ]**; Reproduction rate **[ ]**; Other **[X]** Growth
Exposure period:	28 day
Results:	NOEC = 0.43-0.89 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	Crossland, N O.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{10-13} LAS (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Mean NOEC: 0.62 mg/1 (2 tests). Huels AG judged study quality to be good. Tap water with hardness 84-153 mg/L $CaCO_3$; pH 7.1-8.7; flow-through; 14-16ºC; age of fish at start of study: 6 months.
Reference:	European Commission. 2000k. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, CT/R153/01, CT/R153/06.
Reliability:	4 Not assignable. The original studies were not available for review.

(h)

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**
Species:	*Salmo gairdneri* (Fish, estuary, fresh water)
Endpoint:	Length of fish **[ ]**; Weight of fish **[ ]**; Reproduction rate **[ ]**; Other **[X]** Growth, Hatching, Survival
Exposure period:	70 day
Results:	NOEC = 0.23 mg/L
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	Unilever Research Protocol, Early Life Stage (ELS) test.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{10-13} LAS (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Huels AG judged study quality to be good. Tap water with hardness 70-133 mg/L $CaCO_3$; pH 7.3-7.8; flow-through; 8.5- 11.5ºC; life-stage: ELS.
Reference:	European Commission. 2000j. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, CT/R118/03.
Reliability:	4 Not assignable. The original study was not available for review.

(i)

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other **[ ]**; open-system **[X]**; closed-system **[ ]**
Species:	*Salmo gairdneri* (Fish, estuary, fresh water)
Endpoint:	Length of fish **[ ]**; Weight of fish **[ ]**; Reproduction rate **[ ]**; Other **[X]** Growth, Hatching, Survival
Exposure period:	70 day.
Results:	NOEC = 0.3-0.35 mg/L
Analytical monitoring:	Yes **[ ]** No **[X]** ? **[ ]**
Method:	Unilever Research Protocol.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	C_{10-13} LAS (CAS #68411-30-3)
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Mean NOEC: 0.32 mg/1 (2 tests). Huels AG judged study quality to be good.

Nominal concentrations (expected <20%). Tap water with hardness 64-159 mg/L $CaCO_3$; pH 6.6-8.0; flow-through; 7.5-15 ºC; life-stage: ELS

Reference: European Commission. 2000l. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Procter & Gamble, 1991, CT/R89/01, CT/R89/02.

Reliability: 4 Not assignable. The original studies were not available for review.

(j) **(Fathead Minnow)**

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other **[X]**; open-system **[X]**; closed-system **[ ]**

Species: *Pimephales promelas* (Fish, fresh water)

Endpoint: Length of fish **[ ]**; Weight of fish **[ ]**;
Reproduction rate **[ ]**; Other **[X]** Survival

Exposure period: 196 day

Results: NOEC = 0.63 mg/L; LOEC = 1.2 mg/L (based on effects on fry survival) Hatchability and growth were not significantly affected.

Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**

Method: Either a serial or proportional dilution unit was used to provide continuous exposures to fathead minnows. Each of the four test concentrations plus control received 12 randomly assigned fish obtained from ponds at the Newtown Fish Farm, Ohio Division of Wildlife. Pieces of half-tile were placed in each 10-gal aquarium for spawning sites. After spawning had been completed, the cluster of eggs was removed and counted. Four replicates of 100 eggs from each concentration were reared for 14 days and mortality of eggs and fry recorded daily. Mean dissolved oxygen, water hardness, and pH ranged from 5.84-6.42 mg/L, 194-214 mg/L $CaCO_3$, and 7.50-7.95, respectively. Test concentrations were 0.34, 0.63, 1.2 and 2.7 mg/L.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: LAS, activity: 60.8%; equivalent MW = 348

Reference: Pickering, Q.M. and Thatcher, T.O. 1970. The chronic toxicity of linear alkylate sulphonate (LAS) to *Pimephales promelas* Rafinesque. Water Pollut. Control Fed. 42:243-254.

Reliability: 2 Valid with restrictions

(k)

Type of test: static **[X]**; semi-static **[ ]**; flow-through **[ ]**; other **[ ]**
open-system **[X]**; closed-system **[ ]**

Species: *Pimephales promelas* (Fish, fresh water)

Exposure period: 28 day

Results: NOEC ($C_{11.8}$) = 0.9 mg/L
NOEC (C_{13}) = 0.15 mg/L

Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: C_{10-13} LAS (CAS #68411-30-3), average chain lengths 11.8 and 13

Remarks: Observations were made of the number of spawnings, total eggs produced, and number of eggs per female. Data were obtained from the literature.

Reference: Maki, A.W. 1979. Correlations between *Daphnia magna* and fathead minnow (*Pimephales promelas*), chronic toxicity values for several classes of test substances. J. Fish. Res. Bd Can. 36, 411-421.

Reliability: 4 Not assignable. This study was given a reliability score of 4 because the publication is a summary of previous tests and the original study reports were not available for review.

(l)

Type of Test: Static [ ]; semi-static [ ]; flow-through [ ]
Open-system [ ]; closed-system [ ]; not stated [X]

Species:	*Pimephales promelas* (Fish, Fathead Minnow, fresh water)
Exposure Period:	Up to 30 days post-hatch
Effect Criteria:	Embryolarval/fry survival
Results:	NOEC = 1.02 mg/L
Analytic Monitoring:	Yes [ ]; No [ ]; ? [X]
Method:	The publication summarizes the results of a series of critical life stage (embryolarval) tests, which are defined as exposure during the embryogenic period (incubation of the eggs), followed by exposure of fry for a period of 30-days after hatching for warm water fish with embryogenic periods ranging from 1 to 14 days.
GLP:	Yes [ ]; No [ ]; ? [X]
Test Substance:	$C_{11.7}$ LAS (commercial blend of C_{10} 8%, C_{11} 29%, C_{12} 34%, C_{13} 29%)
Remarks:	All of the original studies summarized in this publication were conducted at EG&G Bionomics (now Springborn Smithers Labs) using standard protocols. The minimum threshold concentration, defined as the lowest concentration causing significant effect on any parameter, was reported as >1.02 mg/L <2.05 mg/L. The NOEC normalized by van de Plassche et al. (1999) to $C_{11.6}$ LAS was 1.1 mg/L.
Reference:	Macek, K.J. and Sleight, B.H. III. 1977. Utility of toxicity tests with embryos and fry of fish in evaluating hazards associated with the chronic toxicity of chemicals to fishes. Aquatic Toxicology and Hazard Evaluation, ASTM STP 634. Mayer, F.L. and Hamelink, J.L, Eds. American Society for Testing and Materials, pp. 137-146.
Reliability:	4 Not assignable. This study is given a reliability of 4 because the publication is a summary of previous tests and the original study reports were not available for review.

(m)

Type of test:	static **[ ]**; semi-static **[ ]**; flow-through **[X]**; other **[ ]** open-system **[X]**; closed-system **[ ]**
Species:	*Lepomis macrochirus* (Fish, fresh water)
Exposure period:	28 day
Results:	NOEC = 1.0 mg/L for bluegill LOEC = 2.0 mg/L
Analytical monitoring:	Yes **[X]** No **[ ]** ? **[ ]**
Method:	The effect of LAS on the structure and function of microbial communities was studied in a flow-through model ecosystem containing several trophic levels. Duplicate 19-L glass aquaria containing model ecosystems at four nominal concentrations (0.5, 1.0, 2.0, 4.0 mg/L) contained water and 2.5 cm lake sediment (Winton Lake, Cincinnati, OH) and several trophic levels (bacteria, algae, macrophytes [*Elodea canadensis,Lemna minor*], macroinvertebrates [*Daphnia magna, Paratanytarsus parthenogenica*], and fish [*Lepomis macrochirus*]). Flow rate in the proportional diluter delivered approximately 8 replacement volumes per day. Additionally, at each cycle of the diluter, 1.5 mL of a Daphnia food suspension diluted with a culture of *Selenastrum* was added to each chamber. Following an initial 3 day acclimation period to analytically confirm test concentrations, 4 glass periphyton slides (5 x 5 cm), 8 vegetative shoots of *Elodea*, 10 early instar *Daphnia*, 25 midge eggs and 5 pre-weighed juvenile bluegills (2.5-5.0 cm length) were added to each aquarium. Fish were screened from access to the macroinvertebrates by a 60 mesh stainless steel screen and were fed a daily supplement of frozen brine shrimp. Test duration was 28 days. Effects monitored included population and community effects. Nominal concentrations were confirmed with MBAS analysis.
GLP:	Yes **[ ]** No **[ ]** ? **[X]**

Test substance:	LAS; C^{14}-LAS chain length C_{12} (91% purity) plus unlabeled LAS with average chain length $C_{11.6}$ (C_{10} 9.7%, C_{11} 27.9%, C_{12} 54.4%, C_{13} 8.0%; 95% purity) (tested together)
Remarks:	Dissolved oxygen concentrations ranged between 7.0 and 9.0 mg/L. Temperature was maintained at 2°C and the mean pH was 8.1 ± 0.2. Bluegill fish growth was reduced at the 2.0 and 4.0 mg/L concentrations but not at 0.5 or 1.0 mg/L. Results for the other species and community parameters tested are summarized in Section 4.7 (i). Juvenile growth was the most sensitive fish endpoint in this model ecosystem study and thus is appropriate to use for chronic toxicity. This is a key study for chronic aquatic toxicity to fish (see SIAR Table 12).
Reference:	Maki, A.W. 1981. A Laboratory model ecosystem approach to environmental fate and effects studies. Unpublished Internal Report, Environmental Safety Department Procter and Gamble Company, Cincinnati, Ohio.
Reliability:	2 Valid with restrictions

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Water-only Exposures

(a)

Type of test:	static [ ]; semi-static [ ]; flow-through [ ]; open-system [ ]; closed-system [ ]; not stated [X]
Species:	*Ceriodaphnia sp.* (Crustacea)
Endpoint:	Mortality [ ]; Reproduction [X]
Exposure period:	not stated
Results:	NOEC = 3 mg/L
Analytical monitoring:	Yes [ ] No [ ] ? [X]
Method:	Standard laboratory methods.
GLP:	Yes [ ] No [] ? [X]
Test substance:	$C_{11.7}$ LAS
Remarks:	Further information regarding study conditions was not provided in this peer-reviewed publication.
Reference:	Kimerle, R.A. 1989. Aquatic and terrestrial ecotoxicology of linear alkylbenzene sulfonate. Tenside Surfactants Detergents, 26:169-176.
Reliability:	4 Not assignable. Data table cites an unpublished report by Procter & Gamble.

(b)

Type of test:	static [ ]; semi-static [X]; flow-through [ ]; open-system [ ]; closed-system [X]; not stated [ ]
Species:	*Ceriodaphnia sp.* (Crustacea)
Endpoint:	Mortality [X]; Reproduction [X]
Exposure period:	7 day
Results:	NOEC = 0.7 mg/L (geometric mean of two tests); 0.84 mg/L (normalized for $C_{11.8}$ LAS) NOEC = 0.5 mg/L (trout chow/algae diet) EC_{10} = 0.99 mg/L (yeast diet); normalized EC_{10} = 1.18 mg/L
Analytical monitoring:	Yes [ ] No [X] ? [ ]
Method:	ASTM (Commotto 1982; Mount and Norberg 1983). *Ceriodaphnia* were cultured individually in 50 mL beakers containing 30 mL culture water. Two tests were conducted, representing animals fed with two different diets (troutchow and algae – *Selenastrum capricornutum* – or baker's yeast). They were acclimated to the test conditions and diet for two generations

before use in toxicity testing. Ten 50 mL beakers containing 30 mL of test solution were used for each test concentration. Nominal concentrations were 0.5, 1.0, 2.0, 3.5, 5.0 and 7.0 mg/L plus controls. Each beaker contained one *Ceriodaphnia* (for a total of 10 daphnids per concentration). Tests were begun with neonate animals (<24 hours old) and lasted seven days. The young were counted and removed from each beaker daily. All test chambers were cleaned and renewed with fresh test solution three times (on the second, fourth, and sixth day). Total water hardness (Ohio river water) was 110 ± 9 mg/L as $CaCO_3$, pH was 7.4 ± 0.2, dissolved oxygen was 9.7 ± 0.8 mg/L, and total suspended solids was 87 ± 106.

GLP: Yes [ ] No [X] ? [ ]

Test substance: $C_{11.8}$ LAS; activity 30.8%

Results: *Ceriodaphnia* fed trout chow/algae showed no dose-dependent response for any endpoint, so no EC_{20} could be calculated. The NOEC is considered to be 5.0 mg/L based on 100% mortality at 7.0 mg/L. Results of the test run with the trout chow/algae diet are shown in the following table:

LAS Concentration	Percent Mortality	Total Reproduction	1st Day of Reproduction	Reproduction per Individual	Broods	Brood Size
0	10	87	4.7	9.7	2.4	4.0
0.5	0	69	5.0	6.9	2.1	3.4
1.0	10	32	5.6*	3.6*	1.4*	2.4*
2.0	0	42	5.0	4.2*	1.8	2.2*
3.5	0	82	5.6*	8.2	2.0	4.2
5.0	0	105	4.7	11.6	2.3	4.9
7.0	100*	15	4.0	5.0*	--*	5.0

* Significantly different from the control ($p<0.05$)

Brood size and reproduction gave good dose-dependent responses for organisms fed yeast. Brood size was the most sensitive endpoint and resulted in an EC_{20} of 1.44 mg/L. Reproduction resulted in an EC_{20} of 2.70 mg/L. Results of the test run with the yeast diet are shown in the following table:

LAS Concentration	Percent Mortality	Total Reproduction	1st Day of Reproduction	Reproduction per Individual	Broods	Brood Size
0	0	229	4.0	22.9	2.9	8.0
0.5	0	208	3.9	20.8	2.9	7.3
1.0	0	178	4.0	17.8	2.9	6.1*
2.0	10	145	4.0	16.1*	3.0	5.4*
3.5	10	78	4.4	8.7*	2.4	3.4*
5.0	10	8	6.6*	0.9*	0.6*	1.8*
7.0	100*	0	--*	--*	--*	--*

* Significantly different from the control ($p<0.05$)

Remarks: Later experience with *Ceriodaphnia* has shown that a yeast diet is not optimum for this species. A geometric mean of 2.68 mg/L can be calculated for the two tests. This is a critical study for this SIDS endpoint.

Reference: 1) Procter & Gamble. 2004. *Ceriodaphnia* sp. Chronic toxicity test. Unpublished report, September 9, 2004.

2) Comotto, R.M. 1982. Proposed standard practice for conducting renewal life cycle toxicity tests with Daphnia magna. Draft 1, August 1982, ASTM committee E-47. American Society for Testing and Materials, Philadelphia, PA.

3) Mount, D.I. and Norberg, T.J. 1983. A seven-day life cycle cladoceran toxicity test. Pre-publication. USEPA (Duluth).
4) Snedecor, G.W. and Cochran, W.G. 1967. Statistical Methods. 6th Edition. Iowa State University Press, Ames, IA.
5) Versteeg, D.J., Belanger, S.E., and Carr, G.J. 1999. Understanding single-species and model ecosystem sensitivity: Data-based comparison. Environ. Toxicol. Chem. 18:1329-1346.

Reliability: 2 Valid with restrictions (actual exposure concentrations might have been less than nominal values; not GLP)

(c)

Type of test: static [ ]; semi-static [ ]; flow-through [X]; open-system [ ]; closed-system [X]; not stated [ ] diluter sytem based on Mount and Brungs 1967
Species: *Daphnia magna.* (Crustacea)
Endpoint: Mortality [ ]; Reproduction [X]
Exposure period: 21 day
Results: NOEC = 1.18 mg/L
LOEC = Not reported
Analytical monitoring: Yes [X] No [ ] ? [ ] MBAS method
Method: A modified 0.5-L proportional diluter was used to deliver four replicates to each of five test concentrations plus a control. No solvent was used. Five *Daphnia* (<12 hours old) were randomly assigned to each replicate. *Daphnia* were fed a suspension of ground trout chow and alfalfa daily. The dilution water was carbon and reverse osmosis filtered well water. Water quality parameters were measured at test initiation and at intervals of 3-5 days for the remainder of the test. Tests were run at 21 ± 1 °C, dilution water hardness 120 mg/L as $CaCO_3$, pH 7.4 ± 0.2, and dissolved oxygen 8.5 ± 0.5 mg/L. F_0 mortality was recorded at 24-h, 96-h, 7-d and daily thereafter. Total number of F_1 produced, mean brood size, and the percentage of days young were produced within each replicate was measured for all five concentrations and the controls. Mortality was evaluated using a computerized Probit procedure. The no effect concentration was determined as the highest measured concentration with no perceivable effects. This study was conducted in 1977.
GLP: Yes [ ] No [X] ? [ ]
Test substance: $C_{11.8}$ LAS; mean phenyl position 3.76; mean molecular weight = 345
Remarks: The most sensitive indicator of reproductive inhibition was the total number of young produced. This is a key study for chronic aquatic toxicity to invertebrates (see SIAR Table 12).
Reference: Maki, A.W. 1979. Correlations between *Daphnia magna* and fathead minnow (*Pimephales promelas*) chronic toxicity values for several classes of test substances. J. Fish. Res. Board Can. 36:411-421.
Reliability: 2 Valid with restrictions.

(d)

Species: *Daphnia magna*
Results: NOEC = 1.4 mg/L (12 records)
Test Substance: LAS normalized to $C_{11.6}$
Remarks: NOEC is geometric mean of 12 records compiled from literature reviews and normalized to $C_{11.6}$.
Reference: van de Plassche, E.J., de Bruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J. and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: LAS, AE, AES, and soap. Environ. Toxicol. Chem. 18:2653-2663.

Reliability: 4 Not assignable. This study was given a reliability score of 4 because all the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(e)

Type of test: static **[ ]**; semi-static **[X]**; flow-through **[ ];** open-system **[ ]**; closed-system **[ ]**
Species: *Daphnia magna* (Crustacea)
Endpoint: Mortality **[X]**; Reproduction rate **[X]**
Exposure period: 21days
Results: NOEC = 1.25-3.25 mg/L; LOEC = 2.25-3.75 mg/L
Geometric Mean NOEC = 1.99 mg/L (mean of studies using 5 different diets)
Analytical monitoring: Yes **[ ]** No **[ ]** ? **[X]**
Method: ASTM proposed standard practice for conducting renewal life cycle toxicity tests with *Daphnia magna*. Draft No. 1, August 1982. Ten 250 m/L beakers were used for each test concentration. Seven beakers contained one daphnid each and three beakers contained five daphnids each, for a total of 22 daphnids per concentration. All conditions were maintained as per protocol.
GLP: Yes **[ ]** No **[]** ? **[X]**
Test substance: Commercial $C_{10\text{-}13}$ LAS, average chain length $C_{11.8}$ (CAS #68411-30-3).
Remarks: NOEC and LOEC values represent the range of results from five tests using different diets. Diet had at most a three-fold effect on the results, which is within the variation expected within the tests themselves. Therefore, results of different diets can be considered roughly equivalent to five replications of the same diet. This is a key study for chronic aquatic toxicity to invertebrates (see SIAR Table 12).
Reference: Taylor, M.J. 1985. Effect of diet on the sensitivity of *Daphnia magna* to linear alkylbenzene sulfonate. In: Cardwell, R.D., Purdy, R. and Bahner, R.C. Aquatic Toxicology and Hazard Assessment. Seventh Symposium pp. 53-72. ASTM STP 854, America Society for Testing and Materials, Philadelphia.
Reliability: 2 Valid with restrictions

(f)

Type of test: static **[ ]**; semi-static **[** X **]**; flow-through **[ ]**; open-system **[X]**; closed-system **[ ]**
Species: *Daphnia magna* (Crustacea)
Endpoint: Mortality **[ ]**; Reproduction rate **[X]**; Other **[ ]**
Exposure period: 21 day
Results: NOEC = 0.3 mg/L
Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**
Method: OECD Guide-line 202, part 2 "*Daphnia* sp., Reproduction Test
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: $C_{10\text{-}13}$ LAS, with average chain length of $C_{11.8}$ (CAS #68411-30-3)
Remarks: Information as cited in IUCLID Data Sheet for CAS #68411-30-3. Natural water 3x weekly renewal pH 6.0-8.5; 20^{+}/-2 ºC; life-stage: 6-24 h.
Reference: European Commission. 2000a. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA.
Reliability: 4 Not assignable. The original study was not available for review.

(g)

Type of test: static **[ ]**; semi-static **[X]**; flow-through **[ ]**; other **[ ]**; open-system **[ ]**; closed-system **[ ]**
Species: *Daphnia magna* (Crustacea)
Endpoint: Mortality **[ ]**; Reproduction rate **[X]**; Other **[ ]**

Exposure period:	21 day
Results:	NOEC = 0.3 mg/L
Analytical monitoring:	Yes **[ ]** No **[ ]** ? **[X]**
Method:	UBA – draft protocol
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	C_{10-13}, avg.: $C_{11.6}$
Remarks:	Huels AG judged study quality to be good. Semistatic; pH 8.0; life-stage: adult.
Reference:	European Commission. 2000d. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Huels AG, 2/87, N. Scholz, unpublished.
Reliability:	4 Not assignable. The original study was not available for review.

(h)

Type of test:	static [ ]; semi-static [ ]; flow-through [X]; open-system [ ]; closed-system [X]; not stated [ ]
Species:	*Paratanytarsus parthenogenica* (Insecta, Midge)
Endpoint:	Reproduction and survival
Exposure period:	28 days
Results:	NOEC = 3.4 mg/L (from previous study) NOEC = >2.0-<4.0 mg/L (from model ecosystem community study) LOEC = 4.0 mg/L
Analytical monitoring:	Yes [X] No [ ] ? [ ]
Method:	Initial experiments (Phase I) were designed to determine the effects of LAS on the structure and function of model ecosystem communities. Each test concentration consisted of duplicate 19-L glass aquaria containing 2.5 cm of natural lake sediment and several trophic levels (bacteria, algae, macrophytes, macroinvertebrates, and bluegill sunfish). Dilution water was carbon and reverse-osmosis filtered well water of 120 mg/L as $CaCO_3$ hardness. Four nominal concentrations of 0.5, 1.0, 2.0, and 4.0 mg/L were delivered to duplicate chambers by a modified Mount and Brungs proportional diluter. Fish were screened from access to invertebrates with a stainless steel screen. In Phase II, conditions were similar except that the model ecosystem aquaria were treated with LAS in sewage effluent (supplied from a CAS unit) to more closely simulate actual receiving water conditions.
GLP:	Yes [ ] No [X] ? [ ]
Test substance:	C_{12} LAS
Remarks:	Dissolved oxygen concentrations ranged between 7.0 to 9.0 mg/L with a mean of 7.8 mg/L during the Phase I studies. In Phase II, dissolved oxygen ranged between 3.1 and 7.3 mg/L (mean 5.4 mg/L), with the lowest values occurring in the chambers receiving the highest sewage effluent concentrations. Tempertures were maintained at 21 ± 2°C in both phases. The pH values were 8.1 ± 0.2 and 7.5 ± 0.3 for Phases I and II, respectively. No significant differences in the development and growth of midge populations was observed in Phase I. Apparent inhibition of total population size was observed at the highest concentration (4.0 mg/L), where total individuals were 4100 as compared to 6300 in the controls. The results indicate that the effect concentrations after 28 days were found to be between 2.0 and 4.0 mg/L. This agrees with a previous 28-day study (Maki 1978) that resulted in a NOEC of 3.4 mg/L.
Reference:	1) Maki, A.W. 1981. A laboratory model ecosystem approach to environmental fate and effects studies. Procter & Gamble Company. 2) Maki, A.W. 1978. Development of a chronic toxicity test wit the dipteran midge, *Paratanytarsus parthenogenica*. Presented at the Annual Meeting of the Entomological Society of America, Washington, DC, December.

Reliability: 2 Valid with restrictions.

(i)
Type of test: static [X]; semi-static [ ]; flow-through [ ]; open-system [X]; closed-system [ ]; not stated [ ]
Species: *Brachionus calyciflorus* (rotifer)
Endpoint: Reproduction and survival
Exposure period: 2 days
Results: EC_{10} = 1.18 mg/L
EC_{20} = 1.4 mg/L (95% confidence intervals 0.882-2.27 mg/L)
EC_{50} = 2.0 mg/L (95% confidence intervals 1.70-2.33 mg/L)
Analytical monitoring: Yes [X] No [ ] ? [ ]
Method: Chronic toxicity tests were performed by placing six newly hatched (less than 3 h old), swimming rotifers in 10 mL of test water containing an equal mixture of green algae (a mixture of *Selenastrum capricornutum* and *Chlorella vulgaris*) at 1.0 x 10^6 cells/mL as food. Three replicates were used for each concentration and control, with additional replicates used for analytical verification of the test compound as needed. Tests consisted of four to six concentrations and appropriate controls. Concentrations up to the limit of solubility were tested. All test vessels were placed on a rotator (1/5 rpm) in a 16/8 h light:dark cycle under low light conditions at 25±2 °C. Dilution water was a 50/50 blend of locally obtained well water and deionized water and had mean water quality properties of pH 8.6, dissolved oxygen 8.5 mg/L, hardness 152 mg/L as $CaCO_3$, and conductivity 450 µmhos. Rotifers were counted after 48 h in all control and test concentration replicates. Since rotifers produce multiple broods in 48 hours, the endpoint for this study is effects on reproduction. The 48 h EC_{20} and EC_{50} values with associated 95% confidence intervals were estimated by an iterative nonlinear regression technique using SAS, version 6.0.
GLP: Yes [ ] No [X] ? [ ]
Test substance: $C_{12.1}$ LAS, sodium salt; 92.3% purity
Remarks: LAS was one of about 20 surfactants tested in separate tests as part of this study. While test concentrations were measured, they were not reported in the publication. The authors do note that concentrations decreased by 20 to 90% over the two-day test (depending on which surfactant was tested) and time-weighted averages exposure concentrations were used. NOEC or LOEC values were not reported.
Reference: Versteeg, D.J., Stanton, D.T., Pence, M.A., and Cowan, C. 1997. Effects of surfactants on the rotifer, *Brachionus calyciflorus*, in a chronic toxicity test and the development of QSARs. Environ. Toxicol. Chem. 16:1051-1058.
Reliability: 2 Valid with restrictions. Duration of test may be too short for a chronic study, therefore not included in SIAR Table 12A.

(j)
Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[X]**; open-system **[X]**; closed-system **[ ]**
Species: *Campeloma decisum* (freshwater mollusc; operculate snail)
Endpoint: Mortality **[X]**; Reproduction rate **[ ]**; Other **[X]** mobility and feeding responses
Exposure period: 6 weeks
Results: NOEC = 0.4 mg/L
LOEC = 1.0 mg/L
Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**
Method: Two 6-week chronic studies were performed in which an amphipod, a pulmonate snail, and an operculate snail were tested together. A serial diluter was used to provide continuous flow conditions into duplicate 4-

gallon glass aquaria for each of five concentrations plus controls. Ten snails were placed in each of two replicate chambers per concentration. The frequency of snails crawling on the test chamber walls was recorded throughout the tests. Mean measured LAS concentrations were 0.2, 0.4, 1.0, 1.9, and 4.4 mg/L.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Commercial LAS formulation containing 14% LAS, 2.3% alcohol ethoxylate oxide condensate, 2.5% sodium soap, 48% sodium tripolyphosphate, 9.7% sodium silicate, 15.4% sodium sulphate, and 8.1% moisture and miscellaneous.

Remarks: Survival of *C. decisum* was affected only in the highest test concentration (4.4 mg/L). Mobility and feeding responses were altered in LAS concentrations of 1.9 and 1.0 mg/L, respectively.

Reference: Arthur, J.W. 1970. Chronic effects on linear alkylbenzene sulfonate detergent on *Gammarus pseudolimnaeus*, *Campeloma decisum* and *Physa integra*. Water Res. 4:251-257.

Reliability: 4 Not assignable. Test substance is a formulation containing a mixture of materials, of which only 14% is LAS. The contribution of each component cannot be separately assigned.

(k)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[X]**; open-system **[X]**; closed-system **[ ]**

Species: *Physa integra* (freshwater mollusc; pulmonate snail)

Endpoint: Mortality **[X]**; Reproduction rate **[ ]**; Other **[X]** mobility and feeding response

Exposure period: 6 weeks

Results: NOEC = 4.4 mg/L
LOEC = >4.4 mg/L

Analytical monitoring: Yes **[ ]** No **[X]** ? **[ ]**

Method: Two 6-week chronic studies were performed in which an amphipod, a pulmonate snail, and an operculate snail were tested together. A serial diluter was used to provide continuous flow conditions into duplicate 4-gallon glass aquaria for each of five concentrations plus controls. The frequency of snails crawling on the test chamber walls was recorded throughout the tests. Mean measured LAS concentrations were 0.2, 0.4, 1.0, 1.9, and 4.4 mg/L.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: Commercial LAS formulation containing 14% LAS, 2.3% alcohol ethoxylate oxide condensate, 2.5% sodium soap, 48% sodium tripolyphosphate, 9.7% sodium silicate, 15.4% sodium sulphate, and 8.1% moisture and miscellaneous.

Remarks: No significant effects on survival, mobility, or feeding responses was observed in P. integra at any LAS concentration tested.

Reference: Arthur, J.W. 1970. Chronic effects on linear alkylbenzene sulfonate detergent on *Gammarus pseudolimnaeus*, *Campeloma decisum* and *Physa integra*. Water Res. 4:251-257.

Reliability: 4 Not assignable. Test substance is a formulation containing a mixture of materials, of which only 14% is LAS. The contribution of each component cannot be separately assigned.

(l)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[X]**; open-system **[X]**; closed-system **[ ]**

Species: *Gammarus pseudolimnaeus* (freshwater amphipod)

Endpoint: Mortality **[X]**; Reproduction rate **[ ]**; Other **[X]** mobility and feeding responses

Exposure period: 6 weeks

Results: For adult survival: NOEC = 0.2 mg/L, LOEC = 0.4 mg/L
For reproduction: NOEC < 0.2 mg/L, LOEC = 0.2 mg/L

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**

Method: Two 6-week chronic studies were performed in which an amphipod, a pulmonate snail, and an operculate snail were tested together. A serial diluter was used to provide continuous flow conditions into duplicate 4-gallon glass aquaria for each of five concentrations plus controls. Ten snails were placed in each of two replicate chambers per concentration. Complete immobilization was taken as a sign of death for the amphipods. Mean measured LAS concentrations were 0.2, 0.4, 1.0, 1.9, and 4.4 mg/L. Only adult amphipods were started in each 6-week test. Following the termination of the second 6-week test, however, the newly hatched *Gammarus* were counted and allowed to remain in each respective test chamber for 15 weeks of additional exposure.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Commercial LAS formulation containing 14% LAS, 2.3% alcohol ethoxylate oxide condensate, 2.5% sodium soap, 48% sodium tripolyphosphate, 9.7% sodium silicate, 15.4% sodium sulphate, and 8.1% moisture and miscellaneous.

Remarks: Adult survival was affected at all concentrations after 6-weeks in a somewhat dose-responsive manner, as shown in the following table. Based on adult survival, the NOEC is 0.2 mg/L and the LOEC is 0.4 mg/L.

Mean LAS Concentration (mg/L)	Duplicate Chambers	Trial 1	Trial 2
4.4	A	0	0
	B	0	0
1.9	A	10	0
	B	10	0
1.0	A	40	20
	B	30	30
0.4	A	30	20
	B	40	40
0.2	A	70	50
	B	40	50
Control	A	80	60
	B	70	40

Newly hatched amphipods were not produced in the highest concentration (4.4 mg/L). The results on survival of F_1 *Gammarus* from the second 6-week study, and the final numbers of gravid F_1 females and F_2 young produced after 15 weeks of exposure are shown below. Control F_1 females were the first to release F_2 young, and this occurred after 9 weeks. Females began liberation of F_2 young at 13 and 13.5 weeks for the 0.2 and 0.4 mg/L chambers, respectively. Based on variability and apparent reproductive effects at the lowest concetration, no NOEC value could be determined. The LOEC is 0.2 mg/L.

Mean LAS concentration (mg/L)	Duplicate Chambers	F_1 Initial young numbers	Final F_1 numbers		F_1 Females		Number of births	Number F_2 produced
			Males	Females	% Survival	Final number gravid		
4.4	A	0	0	0	0	0	0	0
	B	0	0	0	0	0	0	0
1.9	A	4	3	0	75	0	0	0
	B	9	3	3	66	0	0	0
1.0	A	32	3	4	22	1	0	0
	B	37	10	16	70	3	0	0
0.4	A	29	8	7	52	2	0	0
	B	59	25	24	83	4	1	32
0.2	A	52	11	9	38	8	2	45
	B	58	11	16	47	11	3	48
Control	A	77	26	22	62	5	6	109
	B	91	19	31	55	17	5	74

Reference: Arthur, J.W. 1970. Chronic effects on linear alkylbenzene sulfonate detergent on *Gammarus pseudolimnaeus*, *Campeloma decisum* and *Physa integra*. Water Res. 4:251-257.

Reliability: 4 Not assignable. Test substance is a formulation containing a mixture of materials, of which only 14% is LAS. The contribution of each component cannot be separately assigned.

(m)

Species: *Mysidopsis bahia* (marine mysid)

Results: NOEC = 0.12 mg/L (2 records)

Test Substance: LAS normalized to $C_{11.6}$

Remarks: NOEC is geometric mean of 2 records

Reference: van de Plassche, E.J., de Bruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J. and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: LAS, AE, AES, and soap, Environ. Toxicol. Chem. 18:2653-2663.

Reliability: 4 This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(n)

Type of test: static **[ ];** semi-static **[ ];** flow-through **[X]; other [ ];** open-system **[X];** closed-system **[ ]**

Species: *Gammarus pulex* (amphipod)

Endpoint: Mortality **[X];** Reproduction rate **[X];** Other **[ ]**

Exposure period: Adults = 8 weeks; Juveniles = 15 weeks

Results: LC_{50} (adults; 56 days) > 354 µg/L
LC_{50} (juveniles; 107 days) > 375 µg/L
NOEC (number of offspring) = 97 µg/L

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**

Method: Two separate groups of field-collected adults in the pre-copulatory amplexus and early juveniles were exposed to five concentration of LAS (nominally 30, 60, 120, 240, 480 µg/L) and control under flow-through conditions. The exposure vessel consisted of a plastic trough that was 40 cm by 10 cm. The water depth was approximately 3 cm with standpipe to drain and a 2 µm stainless steel piece of mesh was placed approximately 5 cm from the end of the vessel to prevent the loss of *Gammarus*. The solution was made up of a 1:1 mixture of pond water and carbon-filtered tap water. Mean measured

concentrations for adult exposure were <1, 19, 35, 83, 176, 354 µg/L and for juvenile exposure were <1, 22, 36, 97, 141 and 375 µg/L. Survival and reproduction were recorded over an 8 week exposure for adults and a 15 weeks of exposure for juveniles. Offspring produced during the exposure were counted weekly but not removed from the test areas.

GLP: Yes **[X]** No [ ] ? [ ]

Test substance: Commercial LAS, C_{10-14} Sodium alkyl benzene sulfonate (CAS# 85117-50-6); Alkyl chain distribution: C_{10} 10.3%, C_{11} 34.6%, C_{12} 32.7%, C_{13} 21.6%, C_{14} 0.9%; Average chain length 11.7.

Remarks: This study is considered invalid due to high control mortality, which was 23% and 37% for adult and juvenile exposures, respectively. Mortality of adults and juveniles exposed to test materials was in the same range, indicating that survival was not affected by exposure to LAS. Although the reproductive output at the highest two concentrations was lower than that in the lowest concentrations, it was not possible to conclude that this was due to LAS because the control reproduction was also lower. There was no significant difference in cumulative number of juvenile produced between the control and the highest concentration tested (354 µg/L). For the juveniles, the time of formation of pre-copular pairs was slower at the highest concentration tested, 375 µg/L. By day 86, the number of offspring produced at 141 and 375 µg/L was significantly lower than produced at the other LAS concentrations and control. The NOEC remained at 97 µg/L until the end of the study (day 107).

Reference: ERASM. 2000. Long-term toxicity of LAS on *Gammarus pulex*. Internal Report AISE/CESIO, Brussels.

Reliability: 3 Not valid due to excessive control mortality.

(o)

Type of test: static [ ]; semi-static [ ]; flow-through [X]; open-system [ ]; closed-system [X]; not stated [ ]

Species: *Chironomus riparius* (Insecta, Midge)

Endpoint: Survival and emergence

Exposure period: Approximately 24 day

Results: NOEC = 2.4 mg/L in water w/o sediment
LOEC = 3.72 mg/L in water w/o sediment

Analytical monitoring: Yes [X] No [ ] ? [ ]

Method: Tests were conducted as an aqueous fraction in the absence of sediment. A flow-through diluter system delivered test material in water to glass containers with 120-140 cm^2 bottom surface area each. Intact egg masses were incubated in Petri dishes containing 20-30 mL of dilution water at 22 °C until hatching commenced. Newly hatched larvae were allowed to mature 72 hours before testing. Twenty larvae were randomly distributed to each duplicate test chamber for each of five test concentrations plus the controls. Larvae were fed daily until emergence of the first adult in each chamber. Tests were continued until each midge emerged as an adult or larvae were determined to be dead. The number of winged adults was recorded daily. The average test duration was 24 days. Total hardness, pH, dissolved oxygen, and temperature were monitored frequently during the test.

GLP: Yes [ ] No [] ? [X]

Test substance: $C_{11.8}$ LAS; 30.4% activity; mean molecular weight = 346

Remarks: Adults typically emerged 12-14 days after hatching. Control values for adult emergence were similar to or exceeded the historical average observed in their laboratory (>90%). For comparison, additional flow-through studies were conducted with sediment from a naturally unspiked stream and using spiked sediments (see 4.5.2 (v)). The study with spiked sediments resulted in

a NOEC of 319.0 ppm (LOEC = 993 ppm). This indicates that sorption onto sediment significantly mitigates LAS bioavailability. Thus, the water-only values above should be considered conservative. This is a critical study for this SIDS endpoint.

Reference: Pittinger, C.A., Woltering, D.M., and Masters, J.A. 1989. Bioavailability of sediment-sorbed and aqueous surfactants to *Chironomus riparius* (midge). Environ. Toxicol. Chem. 8:1023-1033.

Reliability: 2 Valid with restrictions.

Water and Sediment Exposures

(p)

Type of Test: Semi-static
Species: *Anodonta cygnea* (fresh water bivalve mollusc)
Endpoint: Mortality **[X]**; Reproduction rate **[ ]**; Other **[ ]** growth, reproduction
Exposure period: 80 days
Results: NOEC ≥ 200 mg/kg dw
Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**
Method: Sediments were collected from a pond and LAS was sorbed to sediment by repeated additions for 80 days. Glass tanks containing a 4 cm thick layer of spiked sediment and eight liters of dechlorinated tap water were used. A continuous water exchange allowed for a whole water mass change every 24 hours. Ten bivalves (10^{+}/-1 cm or larger diameter) were introduced into each tank. The LAS sorbed to sediment was 750 mg/kg dw at the beginning of the experiment and 200 mg/kg dw at the end of the experiment.
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test Substance: Commercial LAS (unspecified)
Remarks: All animals survived the 80 day exposures and were actively filter-feeding without differences from the controls.
Reference: Bressan, M., Brunetti, R., Casellato, S., Fava, G.C., Giro, P., Marin, M., Negrisolo, P., Tallandini, L., Thomann, S., Tosoni, L., Turchetto, M. and Campesan, G.C. 1989. Effects of linear alkylbenzene sulfonate (LAS) on benthic organisms. Tenside Surf. Det. 26:148-158.
Reliability: 2 Valid with restrictions (no GLP, statistical methods not described)

(q)

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[X] Natural sediment**
Species: *Branchiura sowerbyi* (tubificid worm)
Endpoint: Mortality **[ ]**; Weight **[ ]**; Other **[X] Reproductive Cycle**
Exposure period: 220 days
Results: NOEC ≥ 7.18 mg/kg.
Mean measured LAS concentrations in the sediment were 26, 9.8, and 7.18 mg/kg at 0, 45, and 220 days of exposure. No significant differences were observed between treated and control sediments for any parameter (survival, timing and percentage of cocoons, percent of hatching worms, number of eggs per cocoon, and mean embryonic development time). Total number of cocoons was slightly higher in treated worms than cocoons.
Method: Twenty specimens in duplicate were used for both the control and treated sediments for testing the possible effects of a long exposure to LAS adsorbed on sediment to oligochaetes. Worms with a well known reproductive cycle were collected and maintained in the dark at 15ºC in a glass container with natural sediment for at least two weeks before the experiment. The sediment for the experiments was gently washed with deionized water and dried at 70ºC. It was organized by grain size, carbonate and organic carbon contents.

It was then treated in order to obtain the irreversibly adsorbed concentration of LAS.
The test substance and sediment mixture were equilibrated for 6 hours on a rotary shaker and then allowed to settle for 48 hours. Twenty eight washes were made with deionized water to ensure the sediment did not release any methylene blue material to the overlaying water. The residual concentration was checked after every wash in the overlaying water of desorbed LAS using the MBAS method. When an ~0 was observed, it was considered that the irreversibly adsorbed quantity of LAS in sediment was attained. This sediment was used in the experiment. The concentration of LAS in sediment was measured by HPLC at 0, 45, and 220 days. Endpoints measured included the number of cocoons, number of oocytes per cocoon, total number of oocytes, period of embryonic development, percent of degenerated cocoons, and percent of hatching worms.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: LAS solution (1000 mg/kg) mixed with 200 g dried sediment (from EniChem Augusta Industriale S.A.)

Remarks: The LAS concentration in sediment used did not produce any effect on *B. sowerbyi* during the 220 days of exposure. The authors conclude that LAS absorbed on sediment has a much lower influence on the examined worms than LAS dissolved in water. The intitial concentration of LAS in treated sediments was 25.87 mg/kg (3.99 mg/kg in control). After 45 days, a reduction of 62-63% of the nominal concentration was measured. After 220 days, the reduction reached 72%.

Reference: Casellato, S., Aiello, R., Negrisolo, P.A., and Seno, M. 1992. Long-term experiment on *Branchiura sowerbyi* Beddard (Oligochaeta, Tubificidae) using sediment treated with LAS (Linear Alkylbenzene Sulphonate). Hydrobiologia 232:169-173.

Reliability: 4 Not assignable. Documentation is incomplete, including identification of the structure, description of methods, lack of statistics, etc.

(r)

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[X] Spiked Sediment**

Species: *Lumbriculus variegatus* (Oligochaete)

Endpoint: Mortality **[ ]**; Weight **[ ]**; Other **[X] Survival, Reproduction, and Growth**

Exposure period: 28 days

Results: $LC_{50\ (28\ d)} \geq 105$ mg/kg soil dry weight (see table)
NOEC = 81 mg/kg soil dry weight

Method: A 28 day chronic study was conducted using sediment spiked with radio-labelled material. The test species, *Lumbriculus variegatus*, is a true sediment feeder (i.e., subsurface ingestion of sediment particles). The nominal concentrations were 50, 75, 100, 150, 300, 600 mg/kg/dry weight and controls. The test sediment contained 44% sand, 48% silt, and 8% clay. Twenty grams (wet weight) of the prepared sediment was added to clean 60 mL glass vessels followed by 30 mL of groundwater drawn from an aquifer. After 24 hours of equilibration, 10 mature *Lumbriculus* (ca. 15 mm in length, 8 mg dry weight) were added to each vessel. Vessels were aerated for 5 minutes every day and the overlying water replenished with distilled water every two days. Each test concentration was replicated 6 times. LAS concentrations were measured at 0 and 28 days. After 28 days the sediment was removed and all live worms counted, blotted dry, and wet weighed prior to air drying for 48 hours to a constant dry weight. Toxicity endpoints included survival, reproduction and biomass. The mode of reproduction (architomy) necessitates the treatment of survival and reproduction as a single endpoint, i.e., number of organisms at test

termination. Sediment concentrations were monitored using LSC and verified with HPLC.

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: LAS (Procter & Gamble), average alkyl chain length $C_{11.4}$. The radio-labelled LAS was 3-dodecylbenzene sulfonate (DOBS; 95% purity)

Results: There was a loss of between 15 and 78% of the LAS radioactivity over the duration of the test, which was attributed to mineralization of LAS by the worms and microorganisms present in the sediment (biodegradation). Results are therefore based on the average of day 0 and day 28 measured sediment concentrations. All results are shown in the following table.

	Sediment Concentration (mg/kg dw)			
Survival Endpoint	**NOEC**	**LOEC**	**EC_{20}**	**EC_{50}**
Based on nominal values	100	150	90	136
Based on measured day 0 values	136	170	131	164
Based on mean of days 0 & 28 values	81	110	73	105
Biomass Endpoint				
Based on nominal values	100	150	108	144
Based on measured day 0 values	136	170	146	166
Based on mean of days 0 & 28 values	82	110	102	109

Remarks: LAS half-life in aerobic sediment was approximately 20 days. This is shorter than studies conducted in the same sediment without worms (half-life of 38 days), most likely due to increased bioturbation due to worm activity. No specific endpoint was particularly sensitive to LAS.

Reference: Comber, S.D.W., Conrad, A.U., Hurst, K., Hoss, S., Webb, S., and Marshall, S. 2004. Chronic toxicity of sediment-associated linear alkylbenzene sulphonates (LAS) to freshwater benthic organisms. Manuscript in preparation.

Reliability: 2 Valid with restrictions

(s)

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[X] Spiked Sediment**

Species: *Caenorhabditis elegans* (Nematode)

Endpoint: Mortality **[ ]**; Weight **[ ]**; Other **[X] Survival, Fertility, Egg Production**

Exposure period: 3 days

Results: LC_{50} (3 d) > 100 mg/kg soil dry weight
NOEC = 100 mg/kg soil dry weight (egg production)

Method: A 3 day chronic study was conducted using sediment spiked with cold-material LAS. Nominal concentrations were in the range of 10 to 1,000 mg/kg/dw. The test species is an infaunal bacterial feeder with a short life cycle, so 72 hours (3 days) is considered a chronic test. The nominal concentrations were 50, 75, 100, 150, 300, 600 mg/kg/dry weight and controls. The test sediment contained 44% sand, 48% silt, and 8% clay, with 2% organic matter. At the start of the test, ten juvenile worms of the first stage (270 ± 16 µm body length) were transferred to each test vial containing 0.75 g wet weight of spiked sediment mixed with 0.25 mL of a bacterial suspension. Five replicates were set up for each treatment, and the samples were incubated on a shaker at 20°C. After 72 hours the test was stopped by heat-killing the worms at approximately 50°C. The samples were mixed with an aqueous solution of rose Bengal to stain the worms for easier recovery. Sublethal toxicity endpoints were determined for growth based on the body length of the organisms, and fecundity by counting the number of eggs in the body of the test organism (egg production). The test was regarded as valid as the fertility of the test organisms in the control was ≥ 80%.

GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test substance: LAS (Procter and Gamble), average alkyl chain length $C_{11.4}$.
Results: Results are shown in the following table.

	Nominal Sediment Concentration (mg/kg dw)			
Test Parameter	**NOEC**	**LOEC**	**EC_{10}**	**EC_{30}**
Growth	200	300	275	
Fertility	200	300		258
Egg Production	100	200		125

Remarks: For growth, with a low variability, an EC_{10} was chosen, whereas it was more appropriate to use an EC_{30} for the more variable parameters fertility and egg production. Egg production was the most sensitive endpoint. Toxicity values might be underestimated slightly, as threshold values were calculated using nominal concentrations (chemical analysis was only performed for selected test concentrations). The chemical analysis at the end of the test showed values 73 to 80% of the initial, nominal concentrations, which equates to mean exposure concentrations of 87 to 90% for the nematodes during the test.
Reference: Comber, S.D.W., Conrad, A.U., Hurst, K., Hoss, S., Webb, S., and Marshall, S. 2004. Chronic toxicity of sediment-associated linear alkylbenzene sulphonates (LAS) to freshwater benthic organisms. Manuscript in preparation.
Reliability: 2 Valid with restrictions

(t)
Type of test: Various types and durations of tests
Results: The two articles compile the no observed effect concentration (NOEC) values for many tests conducted on an assortment of marine species. The following table shows the geometric mean NOEC values for each species for marine invertebrates, as well as one fish and two algae species.

Genus (and species)	**Geometric mean NOEC (mg/L)**
Limanda (*yokohamae*)	0.05
Arbacia	0.45
Chaetopterus	0.45
Asterias	0.35
Mysidopsis (*bahia*)	0.12
Mysidopsis	0.20
Crassostrea (*virginica*)	0.025
Crassostrea	0.04
Mytilus (*edulis*)	0.025
Mytilus	0.04
Arcatia	0.30
Botrylloides	1.94
Molgula	0.90
Spisula	0.80
Botryllus	0.75
Laminaria	5.00
Dunaliella	0.11

Remarks:	All data were from tests conducted on commercial LAS with C_{10-13} alkyl chains and average carbon lengths of $C_{11.6}$ and $C_{11.8}$. The NOEC values have been normalized using QSARs to the average structure of $C_{11.6}$ LAS.
Reference:	1) Temara, A., Carr, G., Webb, S., Versteeg, D. and Feijtel, T. 2001. Marine risk assessment: Linear alkylbenzenesulphonates (LAS) in the North Sea. Marine Pollution Bulletin 42:635-642. 2) van de Plassche, E.J., DeBruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J., and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: Linear alkyl benzene sulfonate, alcohol ethoxylates, alcohol ethoxylated sulfates, and soap. Environ. Toxicol. Chem. 18: 2653-2663.
Reliability:	4 Not assignable. This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(u)

Type:	static **[ ];** semi-static **[X];** flow-through **[ ]; other [ ];** open-system **[ ];** closed-system **[ ]**
Species:	*Mytilus galloprovincialis* (marine mussel)
Endpoints:	Other. filtration rate, oxygen uptake, nitrogen excretion
Exposure period:	7 days
Results:	NOEC = 32.19 mg/kg dry weight (geometric mean of initial [132 mg/L] and final [7.85 mg/L] LAS concentration)
Analytical Monitoring:	Yes
Method:	Thirty mussels (5.8 cm average main axis length) collected from a mussel cultivation area of the Lagoon of Venice, Italy were divided into groups of 10 and placed in net tubes in a 60-L tank for 7 days in contact with 50 mg/L continuously suspended LAS-spiked sediments. Mussels were fed an algal suspension and water, food, and sediment were renewed daily. Filtration rate was determined twice a day (immediately before and after water changes) as defined by the volume of water cleared of algal particles/animal/hour. Faeces were collected daily and pooled for analysis of LAS concentrations by HPLC. Oxygen consumption and ammonia excretion rates were determined at the end of each treatment.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Commercial LAS; likely average alkyl chain length = $C_{11.6}$
Remarks:	No significant differences in survival or physiological responses between treatments and controls were observed. The LAS concentration in treated sediments decreased by about 90% over the duration of the study (mean 132 mg/kg at initiation to mean 7.85 mg/kg at completion).
Reference:	Marin, M.G., Pivotti, L., Campesan, G., Turchetto, M. and Tallandini, L. 1994. Effects and fate of sediment-sorbed linear alkylbenzene sulphonate (LAS) on the bivalve mollusk *Mytilus galloprovincialis* Lmk. Wat. Res. 28:85-90.
Reliability:	2 Valid with restrictions

(v)

Type of test:	static [ ]; semi-static [ ]; flow-through [X]; open-system [ ]; closed-system [X]; not stated [ ]
Species:	*Chironomus riparius* (Insecta, Midge)
Endpoint:	Emergence
Exposure period:	Approximately 24 day
Results:	NOEC = 319 ppm in sediment LOEC = 993 ppm in sediment
Analytical monitoring:	Yes [X] No [ ] ? [ ]

Method: Tests were conducted as an aqueous fraction in the presence of sediment. Natural stream sediments (71% clay, 19% fine silt, 4% medium sand, 6% fine sand) were collected from a pristine site in Rapid Creek, SD. Before testing, wet sediment was autoclaved for 40-60 minutes to reduce microbial populations and minimize initial rates of surfactant biodegradation. LAS was added to a sediment slurry at a nominal concentration and stirred overnight, then 350 g was poured into each test chamber and allowed to settle. The organic carbon content of the test sediment was 4.2% prior to testing. A flow-through diluter system delivered test material in water to glass containers with 120-140 cm^2 bottom surface area each. Test concentrations were control, 8, 42, 146, 319, and 993 ppm. Intact egg masses were incubated in Petri dishes containing 20-30 mL of dilution water at 22 °C until hatching commenced. Newly hatched larvae were allowed to mature 72 hours before testing. Twenty larvae were randomly distributed to each duplicate test chamber for each of five test concentrations plus the controls. Larvae were fed daily until emergence of the first adult in each chamber. Tests were continued until each midge emerged as an adult or larvae were determined to be dead. The number of winged adults was recorded daily. The average test duration was 24 days. Total hardness, pH, dissolved oxygen, and temperature were monitored frequently during the test.

GLP: Yes [ ] No [] ? [X]

Test substance: $C_{11.8}$ LAS; 30.4% activity; mean molecular weight = 346

Remarks: Adults typically emerged 12-14 days after hatching. Control values for adult emergence were similar to or exceeded the historical average observed in their laboratory (>90%). Percent emergence was 98, 95, 90, 90, 90, and 73 for the control, 8, 42, 146, 319, and 993 ppm concentrations, respectively. For comparison, additional flow-through studies were conducted without sediment (see 4.5.2 (o)). Results indicate that sorption onto sediment significantly mitigates LAS bioavailability.

Reference: Pittinger, C.A., Woltering, D.M., and Masters, J.A. 1989. Bioavailability of sediment-sorbed and aqueous surfactants to *Chironomus riparius* (midge). Environ. Toxicol. Chem. 8:1023-1033.

Reliability: 2 Valid with restrictions.

4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

(a)

Species/Endpoints: See table

Results: The following table shows the available NOEC, EC_{10} and EC_{50} values for eleven soil dwelling invertebrate species (in mg/kg dry weight).

Species	Endpoint	NOEC	EC_{10}	EC_{50}
Eisenia foetida	Reproduction		383	558
Lumbricus terrestris	Weight	667		
Aporrectodea caliginosa	Reproduction		14	129
Aporrectodea longa	Reproduction		27	137
Folsomia fimetaria	Reproduction		96	442
Folsomia candida	Reproduction		18	91
Hypoaspis aculeifer	Reproduction		81.7	236
Enchytraeus albidus	Reproduction		6.2	40.5
Platynothrus peltifer	Reproduction	320		467
Isotoma viridis	Growth		41	

Species	Endpoint	NOEC	EC_{10}	EC_{50}
Hypogastrura assimilis	Reproduction		99.8	421

Test Substance: LAS (unspecified)
Remarks: Values were extracted from a variety of original references and compiled for this article.
Reference: Jensen, J., Lokke, H., Holmstrup, M., Krogh, P.H. and Elsgaard, L. 2001. Effects and risk assessment of linear alkylbenzene sulfonates in agriculture soil. 5. Probabilistic risk assessment of linear alkylbenzene sulfonates in sludge-amended soils. Environ. Toxicol. Chem. 20:1690-1697.
Reliability: 4 This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(b)
Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[X] Sandy, agricultural soil**
Species: *Enchytraeus albidus*, *Aporrectodea caliginosa*, *Aporrectodea longa*, *Folsomia fimetaria*, *Hypogastrura assimilis*, and *Hypoaspis aculeifer*
Endpoint: Mortality **[X]**; Weight **[X]**; Other **[X] Reproduction**
Exposure period: 21 days (28 days for *A. caliginosa* and *A. longa* growth tests)
Results: The following table shows the results of all tests. All values are nominal LAS concentrations in mg/kg dry weight.

Species	Parameter	NOEC	LOEC	LC_{10} or EC_{10}	LC_{50} or EC_{50}	Reliability Rating	Rationale for Reliability Rating
Enchytraeus albidus	Survival, adults Reproduction	198 20	397 40	194 6	430 41	1 1	Draft ISO/WD 16387 protocol
Aporrectodea caliginosa	Survival, adults Cocoon production Survival, juveniles Growth, juveniles	278 >793 >397 278	793 >793 >397 397	329 14 >397 105	535 129 >397 354	2 3 2 2	Comparable to ISO 11268-2 Deviations; limited cocoons Comparable to ISO 11268-2, but with only weight measurement
Aporrectodea longa	Survival, adults Cocoon production Survival, juveniles Growth, juveniles	278 >793 397 79	793 >793 793 278	329 27 296 84	535 137 517 349	2 3 2 2	Comparable to ISO 11268-2 Deviations; limited cocoons Comparable to ISO 11268-2, but with only weight measurement
Folsomia fimetaria	Survival, adults Reproduction	>793 278	>793 278	>793 85	>793 424	1 1	Comparable to ISO 11267
Hypogastrura assimilis	Reproduction	79	278	99	421	1	Comparable to ISO 11267
Hypoaspis aculeifer	Survival, adults Reproduction	>793 278	>793 793	>793 82	>793 236	2 2	No guideline available

Method: The effect of LAS on six species of soil invertebrates was determined using the following methods.
Earthworm tests:
No internationally accepted guideline is available for *A. caliginosa* and *A. longa*. For the reproduction tests, 1 kg dry weight of soil was carefully mixed with 160 mL of LAS solution using an electric mixer and filled into plastic pots. The six treatments consisted of one control and five concentrations of LAS and these treatments were randomly assigned to the experimental units. After 24-hour equilibration of the test soil, 3 (rather than

10) earthworms were added to closed containers with perforated lids for ventilation. Approximately 5 g per worm were added after the test animals had been introduced. The containers were then incubated for 21 days in darkness and the contents were later wet sieved through a 1-mm mesh. Water content was adjusted after 14 days.

For the growth test with juvenile *A. caliginosa* (2-3 weeks old), 60 g dry weight of soil were mixed with 9.6 mL of LAS solution with a spatula and filled into 160-mL polyethylene beakers with perforated lids for ventilation. The six treatments consisted of one control and five concentrations of LAS and these treatments were randomly assigned to the experimental units. After 24-hour equilibration of the test soil, one earthworm was added to each container. The beakers were incubated for 28 days in darkness and then the earthworms were recovered and their guts were cleared. The surviving animals were dried for 24 hours and their dry weight was recorded to the nearest 0.1 mg. The examination of the effects on growth of *A. longa* used the same method except the test period was 42 days.

Enchytraeid test:

The enchytraeid reproduction test followed a previously described protocol (draft ISO/WD 16387) using the potworm (*Enchytraeus albidus*). Forty grams dry weight of soil were mixed with 6.4 mL of LAS solution and filled into 160-mL beakers with perforated lids for ventilation. After 24-hour equilibration of the test soil, 10 adult *E. albidus* were added to each container and incubated in darkness for 21 days. After incubation, the surviving adult animals were removed from the soil. Now only containing cocoons, the soil was incubated in the beakers for another 21 days to allow development and hatching of the juveniles. After this period, the soil containing juveniles was stained with Bengal red, and water was added to facilitate counting of the juveniles. The test concentrations were not provided but can be estimated from Figure 5 to be 0, 20, 40, 80, 200 and 400 mg/kg with the numbers of adults surviving per replicate to be approximately 10, 10, 10, 10, 9, and 6, and the numbers of juveniles per replicate (reproduction) to be approximately 77, 50, 37, 21, 0, and 0, respectively.

Springtail tests:

No internationally accepted guideline is available for springtail reproduction. Effects of reproduction of *F. fimetaria* were determined using a method described by Wiles and Krogh. Twenty-seven grams dry weight of soil were mixed with 3 mL of LAS solution and filled into cylindrical test containers with lids. The bottom of the cylinder consisting of a 1-mm mesh to allow later extraction of the test animals. The mesh was covered with a layer of plastic film to prevent escape of the test animals. Adult, rather than juvenile, springtails were used. Ten male and ten female *F. fimetaria* (23-26 days old) were added to the test containers after 24-hour equilibration of the test soil. The containers were incubated for 21 days with 12:12 photoperiod (h). after incubation, the animals were extracted using MacFadyen high-gradient extraction and the number of offspring counted. The same procedure was used for the springtail species *H. assimilis* Krausbauer, using ten male and ten female adults (16-19 days old). The test concentrations were not listed but can be estimated from Figure 6 to be 0, 10, 25, 75, 275, and 800, with the numbers of adult surviving per replicate to be approximately 145, 155, 115, 110, 165, and 165 and the numbers of juveniles per replicate (reproduction) to be approximately 285, 275, 190, 145, 205, and 10.

Predacious mite test:

No internationally accepted guideline is available for mite reproduction. Effects on reproduction on the predacious mite (*H. aculeifer*) were examined according to a method described by Krogh and Axelsen. A total of 54 g dry weight of soil was mixed with 6 mL of LAS solution and filled into test

containers (as described for springtails). Ten female and five male *H. aculeifer* (16-19 days old) were added to each test container together with 100 *F. fimetaria* (16-19 days old) serving as prey for the mites. Incubation and extraction of mite offspring followed the same procedure as described for springtails.
A natural sandy, agricultural soil was used for all tests, rather than synthetic test soil. Nominal concentrations of LAS for some tests were verified by chemical analysis using HPLC.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: $C_{10\text{-}13}$ LAS was obtained as an aqueous sodium salt solution with an active matter concentration of 16.1% (w/w), average molecular weight = 342 g/mol, distribution of the linear alkyl chains: C_{10} 14%, C_{11} 34%, C_{12} 31%, and C_{13} 21%; average alkyl chain length = $C_{11.6}$

Remarks: Toxic effects on reproduction and growth were revealed when the concentration in soil exceeded 40 to 60 mg/kg dry weight. Reproduction was approximately fourfold more sensitive in earthworms and enchytraeids than in springtails and mites. It is argued that this difference in sensitivity is related to the dependency of soil pore water, which is high in the annelids but comparatively low in the arthropods. It should be noted that these studies report worst case exposures due to the use of a sandy test soil and the fact that LAS was added as an aqueous solution to the soil. In addition, too few replicates were used for the ECx approach (e.g., <5 controls) and several key deviations from draft protocols limited the reliability of endpoints for some studies (e.g., *A. caliginosa* and *A. longa* cocoon production). Nominal concentrations were derived from tables and figures since actual values were not found in the text.

Reference: Holmstrup, M. and Krogh, P.H. 2001. Effects and risk assessment of linear alkylbenzene sulfonates in agricultural soil. 3. Sublethal effects on soil invertebrates. Environmental Toxicology and Chemistry 20:1673-1679.

Reliability: See table for reliability of individual endpoints by species.

(c)

Type : Artificial soil **[X]**; Filter paper **[ ]**; Other **[ ]**

Species: *Eisenia foetida* (Worm (Annelida), soil dwelling).

Endpoint: Mortality **[X]**; Weight **[X]**; Other **[ ]**

Exposure period: 14 day

Results: LC_{50} >1000 mg/kg
NOEC = 250 mg/kg soil dw

Method: OECD Guideline 207, 1984. Ten adult worms (mean wt. 0.66 g/animal) were placed into each of four glass jars per concentration with soil comprised of 70% 5010 grade silica sand, 20% kaolinite clay, and 10% finely ground sphagnum peat. Nominal test concentrations in the soil were 1000, 500, 250, 125, 63 and 0 mg/kg dry weight. Temperature was maintained at 20^{+}/-2ºC with 24-hour continuous lighting at 600 lux. Earthworms were assessed for mortality, general health, body weight, and behavior after 7 and 14 days.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: LAS (commercial blend) with average alkyl chain length $C_{11.6}$ (typical of LAS chain lengths found in the environment).

Remarks: No significant mortality was observed at the highest nominal concentration of 1000 mg/kg. A 33% and 23% reduction in body weight was observed at 100 and 500 mg/kg vs. a 14% reduction for the controls. Based on statistical analysis of the weight data, the no effect concentration was the nominal 250 mg/kg dose, which was confirmed by HPLC to be 235 mg/kg.

Reference: Mieure, J.P., Waters, J., Holt, M. and Matthijs, E. 1990. Terrestrial safety assessment of LAS. Chemosphere 21:251-262.

Reliability: 2 Valid with restrictions

(d)

Type : Artificial soil **[X]**; Filter paper **[ ]**; Other **[ ]**

Species: *Lumbricus terrestris* (soil dwelling worm)

Endpoint: Mortality **[X]**; Weight **[X]**; Other **[ ]**

Exposure period: 14 day

Results: LC_{50} >1333 mg/kg soil dw
NOEC = 667 mg/kg soil dw

Method: U.S.FDA Environmental Assessment Technical Guide No. 412, 1987. Ten adult earthworms (mean wt. 3.2 g/animal) were placed in each of four replicate one-gallon glass jars for each test concentration. Nominal test concentrations in the soil were 1333, 667, 333, 167, 84, and 0 mg/kg dry weight. Soil was comprised of 70% silica sand, 20% kaolinite clay, and 10% sphagnum peat. Rabbit faeces was added as food at 50 g/kg. Temperature was maintained at 13^{+}/-2^{o}C with 24 hour continuous lighting at 700-750 lux. Worms were assessed for mortality, general health, body weight, and behavior after 7 and 14 days.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: LAS (commercial blend) with average alkyl chain length $C_{11.6}$ (typical of LAS chain lengths found in the environment).

Remarks: No statistically significant mortality was observed at the highest nominal concentration of 1333 mg/kg. Based on weight and burrowing behavior, the no effect concentration was the nominal 667 mg/kg dose, which was confirmed by HPLC to be 613 mg/kg. It should be noted that the continuous lighting prevented normal feeding, which normally occurs at night on the surface, and thus the test conditions and results should be considered highly conservative.

Reference: Mieure, J.P., Waters, J., Holt, M., and Matthijs, E. 1990. Terrestrial safety assessment of LAS. Chemosphere 21:251-262.

Reliability: 2 Valid with restrictions

(e)

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[X] Natural soil**

Species: *Folsomia fimetaria* (Collembola; springtails)

Endpoint: Mortality **[X]**; Weight **[X]**; Other **[X] molting rate, reproduction**

Exposure period: 21 days

Results: Results are shown in the following table. All results are in mg/kg dry weight of soil.

Endpoint	NOEC	LOEC	LC_{10} or EC_{10}	LC_{50} or EC_{50}
Adult survival	>1000	>1000	>1000	>1000
Juvenile survival	500	700	196	570
Reproductive output	500	1000	147	737
Juvenile growth	<200	200	163	896
Molting frequency	<300	300	185	923

Method: No internationally accepted guideline was available. Adult and juvenile collembola were exposed to LAS mixed with 30 g of a natural, commonly available moist soil. Concentration levels for survival and reproduction of adults were control, 100, 150, 300, 500, 700 and 1000 mg/kg dry weight. Concentrations for survival and growth of juveniles were control, 200, 3000, 500, 700, and 1000 mg/kg dry weight. Concentrations for molting of juveniles were control, 300 and 600 mg/kg dry weight. In all cases, four replicates per concentration were used. For measurement of molting frequency, juveniles were held singly on a compressed surface of soil in multidishes with 24 circular holes. The multidishes were assessed every

second day and exuviae were recorded and removed for a period of 20 days. Deviations from the subsequently developed ISO 11267 protocol included use of adults, use of 20 individuals instead of 10 per test chamber, and an exposure of 21 days instead of 28 days.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Marlon A350 (CAS #68411-30-3) C_{10-13} LAS; 50% active substance; mean chain length of $C_{11.53}$; mean molecular weight 344

Remarks: The most sensitive endpoint was reproduction (EC_{10} = 147 mg/kg dry weight). Nominal concentrations are derived from tables and figures since values were not listed directly in the text. While there were some deviations from the subsequently developed ISO 11267 protocol, the procedures are considered reliable.

Reference: Holmstrup, M. and Krogh, P.H. 1996. Effects of an anionic surfactant, linear alkylbenzene sulfonate, on survival, reproduction and growth of the soil-living collembolan, *Folsomia fimetaria*. Environ. Toxicol. Chem. 15:1745-1748.

Reliability: 2 Valid with restrictions. Well documented publication, no GLP, EC_x calculation not fully detailed.

(f)

Type : Artificial soil **[ ]**; Filter paper **[ ]**; Other **[X] Natural soil**

Species: *Folsomia candida* (Collembola; springtails) and *Enchytraeus albidus* (potworm)

Endpoint: Mortality **[X]**; Weight **[ ]**; Other **[X] reproduction**

Exposure period: 4 to 6 weeks

Results: The resulting EC_{50} values were very similar for the two species, as shown in the following table. All values are mg/kg dry weight.

Species	Endpoint	NOEC	LOEC	LC_{10} or EC_{10}	LC_{50} or EC_{50}
F. candida	Adult survival	1000	2500	750	1338
	Reproduction	500	1000	480	1437
E. albidus	Adult survival	<750	750	511	1400
	Reproduction	750	1500	447	1143

The EC_{50} values for nitrification and CH_4 production were 431 and 277 mg/kg, respectively, for LAS. Aerobic respiration and dentrification were not inhibited at the test concentrations.

Method: LAS may enter the soil environment during sludge application. The toxic effects of LAS and nonylphenol (NP) to two soil invertebrates (*Folsomia candida* and *Enchytraeus albidus*) and five microbial processes (aerobic respiration, nitrification, dentrification, anaerobic CH_4 production, and anaerobic CO_2 production) were assessed in sludge-soil mixtures.

A coarse sandy soil collected from the upper 20 cm of an agricultural field in Jyndevad, Denmark was used for the laboratory experiments and mineralization controls. The Jyndevad soil consisted of 76.8% coarse sand, 12.2% fine sand, 4.1% silt, 3.9% clay, 3.0% organic matter and a pH of 6.0. A similar soil was collected in Lundgaard for use in the microbiological tests was 63.1% coarse sand, 26.6% fine sand, 3.8 silt, 4.3% clay, 2.2% organic matter and pH of 6.1. Dewatered activated sludge collected from a WWTP in Lundtofte was used in all experiments. LAS was applied to the sludge in a demineralized water solution and allowed to sorb for 24 hours at 4ºC in at N_2 atmosphere before mixing the sludge with soil. The soil insects were exposed to a sludge:soil ratio of 1:20 on a dry weight basis. In the microbiological tests, 0.5 mL aliquot solutions of LAS in methanol were added to 1 g of sand, the methanol allowed to evaporate, and sorbed for 24 hours at 4ºC under an N_2 atmosphere to minimize biodegradation during the

sorption period. The sand was then mixed with sludge (0.3 g dry weight) and finally soil was mixed in with the sludge and sand. A sludge:soil ratio of 1:100 (dry weight basis) was used to avoid depletion of oxygen.

Folsomia candida
The springtail reproduction test was initiated with 10- to 12-day old juveniles and lasted 4 weeks. The resulting nominal LAS concentrations were 125, 250, 500, 1000, 2500, and 4000 mg/kg sludge-soil mixture. Ten juvenile *F. candida* were added to each of the 4 replicate vials per concentration containing 30 g (wet weight) of the sludge-soil mixture. The numbers of surviving adults and offspring were counted after 4 weeks.

Enchytraeus albidus
The enchytraeid worm reproduction test was initiated by introducing 10 worms with visible clitellum to each of 4 replicate vials per concentration. Nominal LAS concentrations were 750, 1500, 2250, and 3000 mg/kg sludge-soil mixture (dry weight). Test duration was six weeks. After 3 weeks, the adult worms were removed and counted. At 6 weeks, the number of offspring hatched from cocoons were counted.

Microbiological tests
The toxicity of LAS to microbiological processes was evaluated using one aerobic system (simultaneous determination of aerobic respiration and nitrification) and two anaerobic systems (denitrification and methanogenesis). Nominal LAS concentrations were 0, 125, 250, 500, 1000, and 2500 mg/kg mixture (dry weight) for both the aerobic and methanogenic systems, and 0, 250, 500, 1500, 300, and 5000 mg/kg (dry weight) in the dentrifying system.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test Substance: The test substance for soil invertebrates consisted of an aqueous sodium salt solution containing 14% (w/w) of ^{14}C-labeled C_{10-13} LAS (EniChem Augusta Industriale; purity 95%). The average alkyl chain length of C_{10-13} LAS was 11.6 and the distribution was C_{10} 14%, C_{11} 34%, C_{12} 32% and C_{13} 20%. A pure C_{12} LAS, 4-(2-dodecyl)benzene sulfonate sodium salt, was used in the microbiological tests.

Remarks: Reproduction of *E. albidus* was the most sensitive endpoint (EC_{10} = 447 mg/kg dry weight). Danish laws stipulate a maximum cut-off value of 1300 mg/kg for LAS in sludge for agricultural use.

Reference: Gejlsbjerg, B., Klinge, C., Samsoe-Petersen, L., and Madsen, T. 2001. Toxicity of linear alkylbenzene sulfonates and nonylphenol in sludge-amended soil. Environmental Toxicology and Chemistry 20:2709-2716.

Reliability: 2 Valid with restrictions. Well documented publication, comparable to ISO.

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

(a)

Species/Endpoints: See table

Results: The following table shows the available NOEC, EC_{10} and EC_{50} values for twelve terrestrial plant species (in mg/kg dry weight).

Species	Endpoint	EC_{10}	EC_{50}
Brassica rapa	Growth		134
Brassica rapa	Growth	90	200
Malvia pusila	Growth		204
Solanum nigrum	Growth		169

Species	Endpoint	EC_{10}	EC_{50}
Chenopodium album	Growth		164
Amaranthus retroflexus	Growth		142
Nigella arvensis	Growth		132
Galinsoga parviflora	Growth		90
Sorghum bicolour	Growth		137
Helianthus annuus	Growth		289
Phaseolus aureus	Growth		316
Avena sativa	Growth	50	300
Sinapis alba	Growth	200	300

Test Substance: LAS (unspecified)
Remarks: Values are extracted from a variety of original references and compiled for this article. NOEC values were extrapolated by applying an assessment factor of 10 to the EC_{50}. This is considered an unreliable assumption as measured acute-to-chronic ratios for LAS in plants vary between 2 and 6.
Reference: Jensen, J., Lokke, H., Holmstrup, M., Krogh, P.H. and Elsgaard, L. 2001. Effects and risk assessment of linear alkylbenzene sulfonates in agricultural soil. 5. Probabilistic risk assessment of linear alkylbenzene sulfonates in sludge-amended soils. Environmental Toxicology and Chemistry 20:1690-1697.
Reliability: 4 This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary.

(b)
Species: Grass, beans, radishes, potatoes
Radiolabel: Yes
Results: No adverse effects on plant biomass were observed at the concentrations tested [initial concentrations in soil = 27.2 mg/kg (grass, beans, radishes); = 16.2 mg/kg (potatoes)]
Temperature: Room temperature
Method: Soil cores taken from two ecosystems were collected and placed in a climate controlled "plant metabolism box". Ecosystem Section I consisted of a heavy, clay-like soil. Radiolabeled LAS (a defined mixture) absorbed to digested sludge was incorporated into the soils, after which the soils were planted with either grass, bush beans and radishes (Section I) or potatoes (Section II). The test systems were maintained under a defined standard climate (i.e., an average day in June in Northern Germany) for the vegetative period (76 and 106 days, respectively for Sections I and II). At the end of the growing season samples were collected from plants and soil and subjected to radioanalysis.
GLP: Yes **[ ]** No **[ ]** ? **[X]**
Test Substance: LAS. The authors state that they tested a defined mixture of LAS, but do not report the composition in this paper.
Reference: Figge, K. and Schoberl, P. 1989. LAS and the application of sewage sludge in agriculture. Tenside Surf. Det. 26:122-128.
Reliability: 2 Valid with restrictions

(c)
Species: radish, tomato, oats
Endpoint: Emergence **[ ]**; Growth **[X]**; Other **[ ]**
Exposure period: 14 day
Results: EC_{50} >77.1 mg/kg soil dw
NOEC = 25.7 mg/kg soil dw
Method: OECD Guide-line 208 "Terrestrial Plants, Growth Test".

GLP:	Yes **[ ]** No **[ ]** ? **[X]**
Test substance:	Commercial LAS with an average carbon chain length of $C_{11.8}$.
Remarks:	Information as cited in IUCLID Data Sheet for CAS #68411-30-3. The substance was tested in the range of 2.57 to 257 mg MBAS/kg Nominal concentrations, synthetic soil, static, pH 5.0-7.5, temperature 20-25 ºC. Results are expressed as mg MBAS per kg soil. First Observed Effect Concentration (FOEC) is 77.1 mg MBAS/kg, EC50 is about 77.1 but below 257 mg MBAS/kg.
Reference:	European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished data (Registry No. 5929).
Reliability:	4 Not assignable

(d)

Species:	*Brassica rapa* (Dicotyledon)
Endpoint:	Emergence **[ ]**; Growth **[ ]**; Other **[X]** emergence of seedlings
Exposure period:	21 day
Results:	NOEC = 50 mg/kg soil dw FOEC = 150 mg/kg soil dw
Method:	EEC Directive 79/831, Annex V; EEC Ring Test C (L1) 3: Higher Plant, 1986.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks:	Data refer to 100% active ingredient
Reference:	European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability:	4 Not assignable

(e)

Species:	*Lycopersicum esculentum* (tomato)
Endpoint:	Emergence **[ ]**; Growth **[ ]**; Other **[X]** emergence of seedlings
Exposure period:	21 day
Results:	NOEC = 50 mg/kg soil dw FOEC = 150 mg/kg soil dw
Method:	EEC Directive 79/831, Annex V; EEC Ring Test C (L1) 3: Higher Plant, 1986.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks:	Data refer to 100% active ingredient
Reference:	European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability:	4 Not assignable

(f)

Species:	*Avena sativa* (Monocotyledon)
Endpoint:	Emergence **[ ]**; Growth **[ ]**; Other **[X]** emergence of seedlings
Exposure period:	21 day
Results:	NOEC = 50 mg/kg soil dw FOEC = 150 mg/kg soil dw
Method:	EEC Directive 79/831, Annex V; EEC Ring Test C (L1) 3: Higher Plant, 1986.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**

Test substance:	Marlon A 350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = 11.6
Remarks:	Data refer to 100% active ingredient
Reference:	European Commission. 2000b. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing Henkel KGaA, unpublished results (Registry No. 5929).
Reliability:	4 Not assignable

(g)

Species:	*Sorghum bicolour* (crop sorghum), *Helianthus annuus* (sunflower), *Phaseolus aureus* (mung bean)
Endpoint:	Emergence **[ ]**; Growth **[X]**; Other **[ ]**
Exposure period:	Emergence: 7 days; Growth: 21 days
Results:	NOEC = 100 mg/kg soil dw (all three species) EC_{50} = 167, 289, and 316 mg/kg dw (for listed above listed species, respectively)
Method:	A laboratory standard operating procedure based on OECD Guideline 208 (OECD 1984) was used. The test was conducted in an artificial soil consisting of commercially available potting compost (WC-B) and washed, sieved (1 mm mesh), dried (temperature and time not reported) silver sand (1:9 potting soil:washed sand). Concentrations tested were control, 1, 10, 100 and 1000 mg/kg dw. Deviations from the guideline included: % particles less than 20 µg not given; 4.1% instead of maximum 3% organic carbon in the test soil; sand was sieved with 1 mm mesh instead of 0.5 mm mesh; weight and variability of seeds not reported. The EC_{50} values were calculated with probit analysis according to Finney (1971).
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	C_{11} LAS (57.3% activity; average MW = 343)
Remarks:	The NOEC is for the most sensitive endpoint, which was growth (shoot fresh weight). Nominal concentrations not measured.
Reference:	Windeat, A.J. 1987. Effects on the growth of *Sorghum bicolour*, *Helianthus annuus*, *Phaseolus aureus*. Unilever study report BL/B/3078 (R118). Unilever Research Port Sunlight Laboratory, Sunlight, UK.
Reliability:	2 Valid with restrictions.

(h)

Species:	*Araucaria heterophylla*
Endpoint:	Foliar penetration of NaCl
Exposure period:	4 weeks
Methods:	The influence of surfactants on foliar NaCl uptake was examined in Norfolk Island Pines (*Araucaria heterophylla*). Plants were exposed to seawater with different concentrations of LAS by spraying with a handheld sprayer three times a week for four weeks. Plants were sprayed until the foliage was wetted sufficiently for the spray to run off.
Results:	At 10 mg/L of LAS, which corresponds with a reduced surface tension of 32 mN/m, the Na^+ content in the foliage increased almost tenfold to a level of approximately 500 µmol/g dw and damage symptoms were recorded.
Remarks:	The potential for LAS and other surfactants to influence defoliation in coastal trees was reviewed in a literature review sponsored by ERASM in 2002. In laboratory studies in which young trees are exposed to artificial sea spray, it has been demonstrated that the presence of surfactants at a concentration that causes a dynamic surface tension < 30 mN/m lead to an increased foliar penetration of NaCl via the stomata. It was found that a low surface tension increases the contact angle with the leave and makes it possible for an aqueous solution to enter the stomata. This is a hypothesized mechanism of defoliation.

Reference: 1) Grieve, A.M. and Pitman, M.G. 1978. Salinity damage to Norfolk Island pines caused by surfactants. III. Evidence for stomatal penetration as the pathway of salt entry to leaves. Aust. J. Plant. Physiol. 5:397-413.
2) Hamwijk, C. 2002. Literature study: Exposure and possible indirect effects of aerosol borne surfactants on coastal vegetation. TNO Chemistry report, Study number 02-4077/01. Prepared for CEFIC ERASM.

Reliability: 4 Not assignable. Original studies were not directly reviewed.

(i)

Species: *Pinus halepensis* (pine tree)
Endpoint: Accumulation of LAS in plant tissues
Exposure period: 2 minutes
Method: The concentration of LAS tested was 1.7 x 10^{-4} mol/kg, which is equivalent to 58 mg/L based on a $C_{11.6}$ LAS with a molecular weight of 342. Three batches of ten 2-year old pine trees were immersed for 2 minutes in distilled water alone (batch 1), in LAS-distilled water (batch 2), or LAS-synthetic sea water (batch 3). The objective was to simulate the exposure to severe storms on the seashore. Only the aerial parts of the plants were immersed in a large volume container (50 x 50 x 8 cm) containing 1 L of the respective solutions. The root system was isolated with a plastic bag enclosure and not exposed directly to the solutions. Controls were run on ten plants. Trees were removed from the solutions and gently shaken to eliminate liquid droplets. Radiolabeled and control trees were kept in a greenhouse for 48 hours under a 16:8 day:night photoperiod, temperatures of 22° C (day):16° C (night), and a constant relative humidity. Before analysis, the trees were washed twice in distilled water for 1 minute while shaking to simulate rainfall. Trees were cut back at the soil surface and the aerial part divided into several parts for analysis (epicuticular wax from needles, dewaxed needles, and remaining plant material consisting of branches without needles and tree stem). Respective samples were extracted, prepared, and the radioactivity measured in each fraction using a liquid scintillation cocktail and spectrometer. For scanning electron microscopy, 48 hours after the exposure period ten needles from each of the five replicates of treated and control plants were cut into small segments and air dried, fixed on aluminium stubs with conductive glue and carbon coated. Axial surfaces were examined with a Stereoscan 90B electron microscope with 15 kV acceleration voltage.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Stated by authors as LAS with an alkyl chain length of 12 carbons, with no further information. For our review, we have assumed this to be the typical European $C_{11.6}$ LAS (average MW = 342). LAS was radiolabeled with ^{35}S in the sulphonate group attached to the phenyl ring and had a specific radioactivity of 8712 µCi/mol.
Results: The amount of LAS (as a percent of total in solution; mean ± SD) found in each analyzed fraction of the trees and the wash water is shown below:

Fraction	Distilled water only (Batch 1)	LAS-distilled water (Batch 2)	LAS-seawater (Batch 3)
Epicuticular waxes	~ 0	0.18 ± 10	1.48 ± 1.03
Dewaxed needles	~ 0	~ 0	0.09 ± 0.16
Remaining plant material	~ 0	~ 0	~ 0
Distilled water wash	~ 0	0.17 ± 0.06	1.41 ± 0.57

The amount of uptake and percent of the total radioactivity incorporated in each fraction for the LAS-seawater and LAS-distilled water treatments are shown below:

	LAS-seawater treatment	LAS-distilled water treatment
^{35}S LAS uptake µg/mg dw		
Epicuticular waxes	9.96 ± 3.10	4.90 ± 1.10
Dewaxed needles	0.007 ± 0.001	~ 0
Remaining plant material	0.006 ± 0.001	~ 0
% of total radioactivity		
Epicuticular waxes	89.70 ± 6.02	96.90 ± 2.34
Dewaxed needles	9.90 ± 5.95	~ 0
Remaining plant material	0.37 ± 0.23	3.10 ± 0.02

After LAS exposure in seawater or distilled water, alterations of the epicuticular wax fine structure were observed by SEM.

Remarks: Forty-eight hours after exposure, half of the radioactivity detected was in the epicuticular waxes, with nearly all the rest in the washing solution. LAS was absorbed to a much greater extent in the seawater treatment (surface tension = 29 mN/m) than in the distilled water treatment (surface tension = 45 mN/m). LAS accumulated mainly in the epicuticular wax of the needles. Very little accumulated in the dewaxed needles or remaining plant material. More dramatic changes in epicuticular wax fine structure were observed following LAS treatment in seawater than in distilled water. These observations are in agreement with the studies reported by Hamwijk (2002) and Grieve and Pitman (1978), who demonstrated that low surface tension (<30 mN/m) could increase foliar penetration of salts from sea spray (dossier section 4.6.2h).

Reference: Richard, B., Grieu, P., Badot, P.M., and Garrec, J.P. 1996. Influence of marine salts on the localization and accumulation of surfactant in the needles of *Pinus halepensis* Mill. Ann. Sci. For. 53:921-930.

Reliability: 2 Valid with restrictions

4.6.3 TOXICITY TO OTHER NON MAMMALIAN TERRESTRIAL SPECIES (INCLUDING AVIAN)

Species: Chicken (Leghorn hens)

Endpoint: Mortality **[X]**; Reproduction rate **[ ]**; Weight **[ ]**; Other **[X]** egg quality

Exposure period: 45 day

Results: NOEC = 200 mg/kg diet

Method: Ten month old Leghorn chicken hens were given a dosage of 200 mg/kg in drinking water for 45 days. Four groups of six hens were used in the treatment group, with an additional six hens used as a control group.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Commercial LAS

Remarks: No mortality or adverse effects on egg quality occurred at 200 mg/kg. While this is a non-standard study, it does indicate that up to 200 mg/kg in the drinking water does not adversely affect hens or egg laying.

Reference: Lopez-Zavalla, A., de Aluja, A.S., Elias, B.L., Manjarrez, L., Buchmann, A., Mercado, L., and Caltenco, S. 1975. The effects of ABS, LAS and AOS detergents on fish, domestic animals and plants. Prog. Water Technol. 7:73-82.

Reliability: 2 Valid with restrictions

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

(a)

Type of test: static **[ ]**; semi-static **[ ]**; flow-through **[ ]**; other **[X]** outdoor experimental streams
open-system **[X]**; closed-system **[ ]**

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**

Method and Results: An integrated model stream ecosystem fate and effects study of a C_{12}LAS homologue, with a high content (35.7%) of its most hydrophobic and toxic 2-phenyl isomer, was performed in the summer and fall of 1996 in Procter and Gamble's Experimental Stream facility. The study addressed responses of periphytic microbes, immature benthic fauna including abundance and drift, and emergence of adult insects in a 56-day exposure. Exposures ranged from 126 to 2978 µg/L and were continuously presented in a single-pass, flow through test system. Microbial heterotrophs acclimated to C_{12}LAS exposure quickly (14 days) and biodegraded C_{12}LAS at all concentrations. Blue-green algae responded by increasing in abundance with increasing C_{12}LAS concentration. Invertebrates responded by increased drift and reduced benthic abundances at concentrations exceeding 293 µg/L. Emergence at 927 µg/L also declined relative to the control. Adverse responses for mayflies and chironomids were indicated using univariant statistical techniques. Multivariant techniques indicated these taxa plus molluscs, aquatic worms, caddisflies, and stoneflies were impaired at some concentrations. Bioavailability of C_{12}LAS was investigated in streams as a function of the total suspended solids load in the water column driven by local weather and watershed patterns. A continuous bioavailability model indicated exposure was reduced by an average of 8.5 ± 8.9%. A model ecosystem NOEC (no-observed-effect-concentration) was concluded to be 293 µg/L based on measured water column exposure and adjusted to 268 µg/L by the bioavailability model. A summary of selected population and community responses at 8 weeks from the current study is shown in the following table:

Community/Measure	Dose Response	Temporal	NOEC (µg/L)
Heterotrophic microbial			
Biomass (total lipid phosphate/mm^2)	NS		
Amino acid uptake (^{3}H dpm/mm^2/min)	NS		
Phospholipid fatty acid (PLFA) distr.		Shift at >293 µg/L	
Surfactant mineralization (% CO_2)		Acclimation at all conc.	
Autotrophic microbial			
Bicarbonate uptake (^{14}C dpm/mm^2/min)	+	+	
Algal density (cells/mm^2)	NS		
Algal biovolume (µm^3/mm^2)	NS		
Blue-green algal density (cells/mm^2)	++	++	
Green algal density (cells/mm^2)	NS		
Diatom algal density (cells/mm^2)	NS		
Algal richness	-	-	927
Dominant taxa (cells/mm^2)			
Cocconeis placentula	-	-	927
Melosira varians	NS		
Chrococcus sp.	+	+	
Nitzschia dissipata	NS		
Navicula salinarum v. *intermedia*	NS		
Pleurosira (= Biddulphia) laevis	NS		
Nitzschia inconspicua	++	++	
Nitzschia palea	+	+	
Diatoma vulgare	--	--	927

Gyrosigma acuminatum	-	-	927
Invertebrates			
Richness	NS		
Diversity (Shannon-Weaver)	NS		
Total abundance (No./m^2)	--	--	293
Insect abundance (No./m^2)	NS		
EPT abundance (No./m^2)	-	-	927
Mayfly abundance (No./m^2)	NS		
Caddisfly abundance (No./m^2)	NS		
True fly abundance (No./m^2)	NS		
Chironomid abundance (No./m^2)	NS		
Mollusk abundance (No./m^2)	NS		
Oligochaete abundance (No./m^2)	--	--	293
Dominant populations (No./m^2)			
Baetis sp. (mayfly)	[b]		
Isonychia sp. (mayfly)	---	---	927
Stenonema sp. (mayfly)	NS		
Thienemannimyla sp. (chironomid)	---	---	293
Tanytarsus sp. (chironomid)	++	++	
Cricotopus sp. (chironomid)	+	+	
Polypedilum sp. (chironomid)	+	+	
Reotanytarsus sp. (chironomid)	NS		
Naididae (aquatic worm)	NS		

[a] Plus (+) and minus (-) signs indicate whether the response significantly increased or decreased from the control condition ($\alpha = 0.05$). The strength to the response was graded as slight (+/-), moderate (++/--), or great (+++/---) based on statistical analyses. NS indicates not significant. [b] Taxon too low in abundance, emerged.

A literature review of 13 available model ecosystem studies was conducted and NOEC conclusions were adjusted by a structure-activity-relationship to dodecyl chain length (sulfophenyl position and distribution being ignored due to lack of information in the reviewed studies). Lentic studies (n = 7) were found to have higher NOECs than lotic studies (n = 6) and were more variable. Mean NOEC ± standard deviations for all studies, lentic studies only, and lotic studies only were 3320 ± 6040, 5720 ± 7640, and 530 ± 430 µg/L, respectively. Interpretation of results for anomalies from specific studies suggest the importance of experimental design, use of laboratory versus natural surface water, biological complexity of the test system, and physical test system design as relevant factors for consideration.

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: Dodecyl linear alkylbenzene sulfonate (C_{12}LAS) (CAS# 25155-30-0)

Remarks: The mesocosm studies indicate that the lower limits of field studies can be considered between 0.12 to 0.5 mg/L. It should be noted that the lowest NOEC value (0.12 mg/L) was observed in an artificial stream study (Tattersfield et al. 1995, 1996) in which river water was seeded from field collections and a hydrocyclone used to prevent colonization of biota throughout the study. Drift therefore comprised only emigration and not immigration. Thus, the Tattersfield et al. study is an ecologically restrictive study design that ignores the importance of recovery vectors present in natural systems. The current study (Belanger et al. 2002) did not have these design limitations. The current critical review of all field studies, including the Tattersfield et al. study, concluded that a NOEC = 0.27 mg/L for a C_{12}LAS homologue (0.37 mg/L if normalised to $C_{11.6}$ LAS) is the most reliable, robust and defendable value for the aquatic freshwater ecosystem. This is a key study for aquatic toxicity in model ecosystems (see SIAR Table 15).

Reference: Belanger, S.E., Bowling, J.W., Lee, D.M., LeBlanc, E.M., Kerr, K.M., McAvoy, D.C., Christman, S.C., and Davidson, D.H. 2002. Integration of aquatic fate and ecological responses to linear alkyl benzene sulfonate (LAS) in model stream ecosystems. Ecotoxicology and Environmental Safety. 52:150-171.

Reliability: 1 Valid without restriction

(b)

Results: Time averaged mean measured concentrations over the 28 day exposure period were 0.03, 0.06, 0.12, 0.32, 0.52, 1.0 and 3.0 mg/L in the artificial streams and 0.24, 0.81, and 2.0 mg/L in the downstream pools.

Problems were experienced with dosing LAS into the streams after day 45 due to extreme weather conditions causing freezing of stock solutions of LAS in the delivery tubes. Results should therefore be treated with caution as exposure data is extrapolated from 45 to 56 days. Time averaged mean measured concentrations over the first 45 days of the 56 day study period were 0.03, 0.06, 0.12, 0.32, 0.52, 1.0 and 3.0 mg/L in the artificial streams and 0.22, 0.69, and 1.6 mg/L in the downstream pools.

A total of 65 taxa were identified in the artificial streams and downstream pools. Effects data were generated for 24 endpoints, which included ten invertebrate taxa, two fish species and algae. The inclusion of downstream pool sections increased the range of taxa investigated. The downstream pool community appeared generally less sensitive to the LAS than the stream channel community. Individual taxa were found to differ in susceptibility to LAS depending on their location in the stream channels. The same taxa were generally more susceptible when in the riffle section than in the pool sections. This may have been the result of differences in exposure or physiological state of the organism.

Results from the first 28 days of the study concluded that there were no NOECs below 0.12 mg/L. Extending the study to 56 days resulted in no change in NOECs for the majority of endpoints. NOECs determined in the artificial streams were in the range of 0.03 to >3.0 mg/L although the most reliable NOECs were in the range 0.12 to 3.0 mg/L. In the downstream pools the NOECs ranged from 0.69 to >1.6 mg/L. Only two NOECs were below 0.12 mg/L; the population density of *Gammarus pulex* in the riffle and population density of *Baetis sp*. Some uncertainty is associated with the extended 56 day study due to three main factors. First, lack of exposure data between days 45 and 56. Further uncertainty is associated with the low NOECs for some end points, particularly for *G. pulex* in the riffle section of the artificial streams. Second, the uncertainty in the lower NOEC is due to the times dependent effects (increased susceptibility at 56 compared to 28 days) only being observed for individuals of *G. pulex* in the riffle but not the pool section of the artificial streams. Reduction in NOEC from 28 to 56 days for *G. pulex* in the riffle was not evident in the pool section of the artificial streams where the 28 and 56 day NOEC was 0.52 mg/L. The exact cause of the difference between riffle and pool is unknown. Third, uncertainty was due to variability of the G. *pulex* data and sensitivity to statistical transformation.

Conclusion: The lowest NOEC value observed in this artificial stream study was 0.12 mg/L. However, the river water was seeded from field collections and a hydrocyclone used to prevent colonization of biota throughout the study. Drift therefore comprised only emigration and not immigration. This is an ecologically restrictive study design that ignores the importance of recovery vectors present in natural systems.

Method: Communities of freshwater organisms were established in eight artificial streams and four downstream pools over a 10 day period, five weeks prior to the onset of dosing. Seven nominal LAS exposure concentrations (0.02, 0.05, 0.1, 0.3, 0.5, 1.0 and 3.0 mg/L) and an untreated control were randomly allocated to the eight artificial streams to yield a regression model experiment design. Four of the streams (Control, 0.3, 1.0 and 3.0 mg/L) were connected to downstream pools. Effects measurements were taken after 28 and 56 days. The streams were operated as once-through systems with a residence time of three minutes. Each individual stream was divided approximately equally into a slow flowing pool section (0.20 m water depth, ~3 cm/s flow velocity) and a faster flowing riffle section (0-0.02 m water depth, ~30 cm/s flow velocity). The total volume of water in each stream system was 240 litres. The downstream pools consisted of plastic cylindrical tanks (1.04 m diameter and 510L capacity) with a residence time of approximately 2 days.

The water used in the study was from a local chalk stream with a hardness of 194 to 392 and 280 to 378 mg/L $CaCO_3$ in the streams and downstream pools, respectively. The water temperature was relatively low ranging from 3.0 to 13.2ºC and 3.2 to 13.1ºC in the streams and downstream pools, respectively. Concentrations of suspended solids and total organic carbon (TOC) in the artificial streams were low (suspended solids 1.8 to 3.0 and 0.4 to 6.6 mg/L and TOC 1.5 to 5.2 and 1.9 to 7.9 mg/L in the steams and downstream pools, respectively). The low concentrations of suspended solids and TOC would have tended to maximise the availability of LAS in the system. Also Goyer et al. showed that toxicity of surfactants to daphnia correlated with water hardness. Given the above conditions, effects data generated in this system should be judged to be at the most sensitive end of the distribution.

Remarks: Effects measurements were taken after 28 and 56 days. The streams were operated as once-through systems with a residence time of three minutes. Each individual stream was divided approximately equally into a slow flowing pool section and a fast flowing riffle section.

There is uncertainty connected to the extended 56 day study having to do with the lack of exposure data between days 45 and 56. Uncertainty is also linked with the low NOEC values for some of the end points. This is related to time dependant effects (increased susceptibility at 56 compared to 28 days) being observed only for individuals of *G. pulex* in the riffle but not the pool section of the artificial streams and variability of the *G. pulex* data and sensitivity to statistical transformation. The NOEC values of ≥0.12 mg/L determined after 28 days of exposure are considered estimates of no effect for LAS. For the previously mentioned reasons, the indications of NOECs below 0.12 mg/L from the extended 56 day study appear to be outliers and are not considered reliable for assessment purposes (i.e., would be Klimish 3).

Also, it should be noted that a hydrocyclone was used to prevent colonization of biota throughout the study. Thus, drift comprised only emigration and not immigration. Therefore, the study design is ecologically restrictive in that it ignores the importance of recovery vectors present in natural systems. In a review of 13 model ecosystem studies, including this one, Belanger et al. (2002) concluded that a NOEC of 0.27 mg/L for a C_{12}LAS homologue is the most reliable, robust and defendable vaule for aquatic freshwater ecosystems.

Test Substance: $C_{10\text{-}13}$ LAS, 38.3% active matter, average carbon chain length = 11.52

Reference: 1) Tattersfield, L.J., Holt, M., Girling, A.G., Mitchell, G.C., Pearson, N., and Ham, L. 1995. The fate and effects of linear alkylbenzene sulfonate (LAS) in outdoor artificial streams and pools. External report. Shell Research Limited, Sittingbourne Research Centre. Document No. SBER.95.009.

2) Tattersfield, L.J, Mitchell, C.G., Holt, M., Girling, A.G., Pearson, N., and Ham, L. 1996. Linear alkylbenzene (LAS): Fate and effects in outdoor artificial streams and pools – An extended study. Internal report. Shell Research and Technology Centre, Thornton. Document No. TNER.96.005.

Reliability: 4 Not assignable due to restrictive test design and inconsistencies in the data

(c)

Type: Aquatic [ ]; Field [ ]; Soil [X]; Other [ ]

Results: LAS had no effect on heterotrophic respiration in the sludge compartment but stimulated activity and metabolic quotient (microbial activity per unit of biomass) in the surrounding soil. Basil respiration (BR) was significantly stimulated up to 60 days in the 0-10 mm compartment, but only after 60 and 82 days in the 10-30 mm compartment. No significant stimulation in BR was observed at 30-60 mm. Substrate-induced respiration stimulation was variable and restricted only to soil in the 0-10 mm compartment. Autotrophic ammonia oxidation was initially inhibited in the LAS-spiked sludge, which led to dramatic but transient increases of NH_4^+ availability in the sludge and surrounding soil, subsequently stimulating soil ammonia oxidizers. As judged from a bioluminescence toxicity assay, however, LAS or other sludge components never accumulated to toxic levels in the soil and the LAS tolerance of the indigenous microbes further remained unchanged following LAS exposure. Bioluminescence was slightly, but not significantly, reduced in the 0-10 mm compartment at the first sampling, but not thereafter and not in the 10-30 or 30-60 mm compartments. LAS effects on the microbial populations largely occurred during the first two months and were confined to soil closer than 30 mm from LAS-spiked sludge.

Test Substance: $C_{10\text{-}13}$ LAS, sodium salt; average alkyl chain length $C_{11.6}$

Method: Well-defined bands of sewage sludge spiked with 0 (control), 7.1, or 31.3 g LAS/kg dry weight were applied to loamy sand soil in an agricultural field in Lundgaard, Denmark using a random block design. To each block, three sludge bands (one per LAS treatment) were carefully applied such that the bands were eventually applied at a specific soil depth of approximately 6 to 10 cm and covered by soil. All treatments were replicated five times. A few days after sludge application, the entire experimental site was sown with oats in order to make experimental conditions as realistic as possible. Sampling for microbial parameters was done on a weekly to monthly basis for the first 100 days, with the last samples being taken approximately one year after the start of the experiment. A rectangular corer providing a 40 mm wide cross section of the sludge bands and the surrounding soil was sectioned into four compartments representing various distances (0-10, 10-30, 30-60 mm) from the sludge. At each sampling date, two replicate cores from each sludge band were sampled and the corresponding samples from the two cores were pooled. Microbial parameters measured included basal respiration (BR), substrate-induced respiration (SIR), potential ammonia oxidation (PAO), and pollution-induced community tolerance. Bioluminescence toxicity tests were also conducted and correlated with ammonia oxidation activity as a measure of the physiological state of the cells. Two-way analysis of variance statistics were used for each sampling date, followed by Dunnett's test. Data were transformed if necessary.

Remarks: Measured LAS concentrations were 0.069 (control), 7.1 and 31.3 g/kg dw sludge. Results strongly suggest that disposed of LAS-contaminated sludge will not produce a significant adverse effect on the function of the soil microbial community under field conditions. Measured effects generally lasted two months or less and were confined to soil closer than 30 mm from the LAS-spiked sludge. No signs of long-term selection due to toxicity were noted. According to the authors, the study should be considered a worst-case

due to the application of high LAS concentrations only occasionally encountered in sewage sludge, the use of LAS-spiked sludge possible overestimating the actual bioavailability relative to aged surfactants in natural sludge, the application of relatively large (4 x 4 cm) two dimensional sludge bands possible retarding oxygen intrusion and consequently LAS degradation in the sludge relative to smaller spherical sludge clumps present under more realistic field conditions, and the use of a coarse, sandy soil with relatively low organic matter content. While NOEC, LOEC, EC50, etc. were not calculated, significant differences from the control sludge were detected in the high (31.3. g/kg dw sludge) and in the low (7.1 g/kg dw sludge) treatments. Therefore, the NOEC should be <7.1 g/kg dw sludge.

Reference: Brandt, K.K., Krogh, P.H., and Sorensen, J. 2003. Activity and population dynamics of heterotrophic and ammonia-oxidizing microorganisms in soil surrounding sludge bands spiked with linear alkylbenzene sulfonate: a field study. Environ. Toxicol. Chem. 22:821-829.

Reliability: 2 Valid with restriction. Well documented publication, no GLP, concentrations only measured at start of experiment

(d)

Type: Aquatic **[ ]**; Field **[ ]**; Soil **[X]**; Other **[ ]**

Results: No short-term or long-term (4 years) adverse effects on 9 different microbial functions/processes or the abundance or diversity of microarthropods and earthworms were observed after sludge application of up to 21 t dw/ha dry weight, corresponding to a LAS dose of approximately 35 kg/ha, or approximately 15 mg/kg dry weight.

Method: This study was conducted by the Danish EPA to assess the effects of using sewage sludge applications on soil fauna and microbial processes in winter-wheat and barley undersown with clover grass. Three levels of sludge and cow dung (3.5, 7, and 21 t dw/ha) were tested along with control fields. Concentrations of LAS in sludges from the two waste water treatment plants were 1,100 and 1,700 mg/kg.

Test Substance: LAS (unspecified)

Reference: 1) Jensen, J., Lokke, H., Holmstrup, M., Krogh, P.H. and Elsgaard, L. 2001. Effects and risk assessment of linear alkylbenzene sulfonates in agriculture soil. 5. Probabilistic risk assessment of linear alkylbenzene sulfonates in sludge-amended soils. Environ. Toxicol. Chem. 20:1690-1697.

2) Jensen, J. and Krogh, P.H. 1999. Ecological assessment of sewage sludge application. Proceedings, Nordiska Jordbruks forskares Forening, Seminar 292. Jokionen, Finland, November 23-25, 1998, pp. 98-100.

3) Krogh, P.H., Holmstrup, M., Jensen, J., and Peterssen, S.O. 1997. Ecotoxicological assessment of sewage sludge in agricultural soil. Working Report No. 69. Ministry of Environment and Energy, Danish Environmental Protection Agency.

Reliability: 2 Valid with restrictions

(e)

Type: Aquatic **[ ]**; Field **[ ]**; Soil **[X]**; Other **[ ]**

Species: cellulolytic bacteria, fungi and actinomycetes and microbial parameters

Exposure Period: up to 8 weeks

Results: EC_{50} = 17 to 128 mg/kg dry weight for all parameters other than as indicated.
EC_{10} = < 8 to 22 mg/kg dry weight for all parameters other than as indicated.
Except for β-glucosidase activity, basal respiration, and total PLFA content, all soil parameters were sensitive to LAS, with EC_{10} values in the range of less than 8 to 22 mg/kg dry weight. The authors indicate that this probably reflected a similar mode of LAS toxicity, ascribed to cell membrane interactions, and showed than sensitivity to LAS was common for various

soil microorganisms. The extracellular β-glucosidase activity was rather insensitive to LAS (EC_{10}, 47 mg/kg dry weight), whereas the basal soil respiration was not inhibited even at 793 mg/kg dry weight. This was interpreted as a combined response of inhibited and stimulated compartments of the microbial community. The PLFA content showed no decrease even at 488 mg/kg.

Analytical monitoring: Yes **[X]** No **[ ]** ? **[ ]**

Method: The short-term effects of aqueous LAS on microbial parameters was tested in a sandy agricultural soil that was incubated for up to 11 days. The assays included 10 microbial soil parameters: ethylene degradation; potential ammonium degradation; potential dehydrogenase activity; β-glucosidase activity; iron reduction; populations of cellulolytic bacteria, fungi and actinomycetes; the basal soil respiration; and the phospholipid fatty acid (PLFA) content. Soil from the plough layer was sampled at an agricultural field at Lundgaard, Denmark. The soil consisted of coarse sand (67%), fine sand (16%), silt (8.6%), clay (6.2%), humus (2.7%) and had a total carbon content of 1.5%. The soil had not been treated with sewage sludge and had not been sprayed with pesticides in the last two years. For the experiments with aqueous LAS, triplicate soil incubations were amended with the appropriate LAS solutions to produce the LAS contents. The soils were carefully mixed and incubated in the dark and duplicate soil samples for LAS analyses were frozen at the beginning of the incubation period. EC_{10} and EC_{50} values were calculated by a linear-interpolation analysis (IC_p), which was based on bootstrapping. The NOECs and LOECs were determined by Dunnett's test using a SAS analysis-of-variance procedure. Nominal concentrations were control, 8, 22, 62, 174 and 488 mg/kg dw soil, except for BR (control, 0.8, 8, 79 and 793 mg/kg dw soil). On average, 84 to 95% of the nominal concentrations were initially recovered by the chemical analysis. Nominal levels were used for the calculation of effect concentrations.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: $C_{10\text{-}13}$ LAS obtained as an aqueous sodium salt solution with a LAS content of 16.1% (w/w), Na-LAS average molecular weight = 342 g/mol, distribution: C_{10} 14%, C_{11} 34%, C_{12} 31%, and C_{13} 21%

Remarks: The study demonstrated that LAS inhibited specific compartments of the soil microbial community. The lowest EC_{10} values for microbial soil parameters were slightly higher than the predicted no-effect concentrations recently derived for plants and soil fauna (~5 mg/kg dry weight). A subsequent study (Elsgaard et al. 2001, Part 2) further indicated that the short-term effects observed for aqueous LAS on soil microbiology were modified by the dosage of LAS with sewage sludge and by a prolonged incubation time. The data suggest that a terrestrial risk assessment based on short-term affects of aqueous LAS fully encompasses the risk that may occur when LAS is applied to agricultural soil by means of sewage sludge.

Reference: 1) Elsgaard, L., Petersen, S.O., and Debosz, K. 2001a. Effects and risk assessment of linear alkylbenzene sulfonates in agricultural soil. 1. Short-term effects on soil microbiology. Environmental Toxicology and Chemistry 20:1656-1663.

2) Elsgaard, L., Petersen, S.O., and Debosz, K. 2001b. Effects and risk assessment of linear alkylbenzene sulfonates in agricultural soil. 2. Effects on soil microbiology as influenced by sewage sludge and incubation time. Environmental Toxicology and Chemistry 20:1664-1672.

Reliability: 2 Valid with restrictions. Well documented publication, no GLP, EC_x calculation not fully detailed.

(f)

Type: Outdoor experimental stream

Methods: Species or ecosystem studied. Taxonomic groups tested were periphyton, detritus, invertebrates, snails, amphipods, and fish. One concentration was tested in triplicate. The substance was dosed eight times at seven day intervals. Test duration 45 days.
Effects monitored: Population and community effects.

Results: The best estimated NOEC is >0.36 mg/L.
For fish (caged larval fathead minnows) no effects on mortality occurred at the only concentration tested. However growth was significantly decreased in the dosed systems. The authors state that this is caused by the better food and light conditions in the controls.
Growth of periphyton, the degradation rate of detritus, population and community growth of invertebrates and the population density of snails were not inhibited at the only concentration tested.
For Amphipods no NOEC could be determined. Mortality was highest (45%) at a control location.
Chemical analysis: Concentrations were measured.

Test Substance: LAS; average chain length $C_{11.9}$ (representative of homologues found in typical sewage effluents in the U.S.).

Reference: Fairchild, J.F., Dwyer, F.J., La Point, T.W., Burch, S.A., and Ingersoll, C.G. 1993. Evaluation of a laboratory-generated NOEC for linear alkylbenzene sulfonate in outdoor experimental streams. Environ. Toxicol. Chem. 12:1763-1775.

Reliability: 2 Valid with restrictions

(g)

Type: Outdoor ponds.

Methods: Species or ecosystem studied: Outdoor ponds were used with three compartments (700 L each) with sediment. Taxonomic groups tested were phytoplankton, plants, cyclopedia, and cladocerans. Two concentrations were tested with no duplicates. Test duration 56 days and one year.
Effects monitored: Population and community effects.
Chemical analysis: The substance was dosed according to need.

Results: For phytoplankton slight inhibition of photosynthesis and chlorophyll occurred at 5.0 mg/L. The best estimated NOEC was determined at slightly below 5 mg/L.
For plants reduction of species number and composition and for cladocerans inhibition of development occurred at the highest concentration tested. The best estimated NOEC for these groups was 5.0 mg/L. The best estimated LOEC was 10 mg/L.
For cyclopedia egg production was reduced at 5 mg/L. The best estimated NOEC was determined at 3.5 mg/L. The best estimated LOEC was 5 mg/L.
For midge no NOEC could be determined. Survival was strongly reduced due to low oxygen concentrations and a high level of suspended solids.

Substance: LAS; chain length is probably C_{12}.

Remarks: A concentration-effect relationship was found. Concentrations were measured. Data as reported by BKH, Huls, and Henkel in IUCLID dataset for CAS #90194-45-9 dated 19 February 2000.

Reference: Huber, W., Zieris, F.J., Feind, D., and Neugebaur, K. 1987. Ecotoxicological evaluation of environmental chemicals by means of aquatic model ecosystems (Translation). Bundesministerium fuer Forschung und Technologie, Research Report (03-7314-0).

Reliability: 4 Not assignable. Original report not available for review.

(h)

Type: Laboratory aquaria

Methods: The effect of LAS on the structure and function of microbial communities was studied in a flow-through model ecosystem containing several trophic levels. The LAS was applied to 19-L glass aquaria in either well water (Phase I) or sewage effluent (Phase II). In Phase I, duplicate chambers contained water and 2.5 cm lake sediment (Winton Lake, Cincinnati, OH) and several trophic levels (bacteria, algae, macrophytes [*Elodea canadensis,Lemna minor*], macroinvertebrates [*Daphnia magna, Paratanytarsus parthenogenica*], and fish [*Lepomis macrochirus*]). Chambers were allowed to equilibrate for about four weeks and then were exposed to 0.5 and 5.0 mg/L LAS. Flow rate in the proportional diluter delivered 6 to 10 replacement volumes per day. In Phase II, the aquaria were supplied with LAS in sewage effluent to simulate more closely the situation in an actual receiving stream. Sewage effluent was generated in a continuous activated sludge (CAS) unit and was adjusted to maintain 50 percent LAS degradation. Effluent from the CAS unit was then supplied to the test chambers at sewage dilutions of 3 and 30 percent to achieve nominal undegraded LAS concentrations of 0.5 and 5.0 mg/L, respectively. Test duration was 28 days. Microbial structure was estimated by measurements of total viable bacterial biomass as CFU/mL. Microbial function was estimated in Phase I by measuring the rates of oxygen consumption during the degradation of glucose and LAS. In Phase II, microbial function was assayed by radiochemical methods.

Results: In Phase I, the structure of microbial communities was not affected, and no significant differences were reported in mean biomass or number of colony-forming units between the microorganisms exposed at the two levels. The mean total biomass calculated for all tanks and across all sampling points was about 3×10^5 CFU/mL. The function of the microbial communities was reduced only at 5.0 mg/L. In Phase II, no effect was seen on the structure of the microbial community, with mean CFU/mL in the low and high dose aquaria (0.9×10^5 and 1.4×10^5, respectively) similar to the control aquaria (1.4×10^5). Also, no effects were observed microbial function in Phase II, which was measured only as the degradation of LAS. Therefore, the NOEC based on the most sensitive endpoint (microbial community function) is 0.5 mg/L.

Substance: LAS; radiolabeled C^{14}-LAS with chain length C_{12} (91% purity) plus unlabeled LAS with average chain length $C_{11.6}$ (C_{10} 9.7%, C_{11} 27.9%, C_{12} 54.4%, C_{13} 8.0%; 95% purity)

Remarks: Function assays in Phase II were based on LAS degradation only, since the Phase I results indicated that LAS degradation was the most sensitive indicator of toxic effect levels.

Reference: Larson, R.J. and Maki, A.W. 1982. Effect of linear alkylbenzene sulfonate on the structure and function of microbial communities in model ecosystems. Aquatic Toxicology and Hazard Assessment: Fifth Conference, ASTM STP 766, Pearson, J.G., Foster, R.B., and Bishop, W.E., Eds., American Society for Testing and Materials, pp. 120-136.

Reliability: 2 Valid with restrictions

(i)

Type: Laboratory aquaria

Methods: Two exposures were conducted. Phase I was designed to develop basic toxicological information. Phase II introduced partially degraded LAS contained within the effluent of a continuous activated sludge unit and was designed to to simulate real-world fate and effects for LAS. In Phase I, duplicate 19-L glass aquaria containing model ecosystems at four nominal concentrations (0.5, 1.0, 2.0, 4.0 mg/L) contained water and 2.5 cm lake sediment (Winton Lake, Cincinnati, OH) and several trophic levels (bacteria,

algae, macrophytes [*Elodea canadensis,Lemna minor*], macroinvertebrates [*Daphnia magna, Paratanytarsus parthenogenica*], and fish [*Lepomis macrochirus*]). Flow rate in the proportional diluter delivered approximately 8 replacement volumes per day. Additionally, at each cycle of the diluter, 1.5 mL of a Daphnia food suspension diluted with a culture of *Selenastrum* was added to each chamber. Following an initial 3 day acclimation period to analytically confirm test concentrations, 4 glass periphyton slides (5 x 5 cm), 8 vegetative shoots of *Elodea*, 10 early instar *Daphnia*, 25 midge eggs and 5 pre-weighred juvenile bluegills (2.5-5.0 cm length) were added to each aquarium. Fish were screened from access to the macroinvertebrates by a 60 mesh stainless steel screen and were fed a daily supplement of frozen brine shrimp. In Phase II, the aquaria were supplied with LAS in sewage effluent to simulate more closely the situation in an actual receiving stream. Sewage effluent was generated in a continuous activated sludge (CAS) unit and was adjusted to maintain 50 percent LAS degradation. Effluent from the CAS unit was then supplied to the test chambers at continuous dilutions of 3.75, 7.5, 15, and 30 percent sewage concentrations to simulate sewage dilutions existing in natural receiving waters. Test duration was 28 days. Effects monitored included population and community effects. Nominal concentrations were confirmed with MBAS analysis.

Results: Dissolved oxygen concentrations ranged between 7.0 and 9.0 mg/L during Phase I. Dissolved oxygen concentrations in Phase II ranged between 3.1 and 7.3 mg/L, with the lowest readings consistently observed in the aquaria receiving the 30% sewage concentrations, as would be expected. Temperature was maintained at 2°C, mean pH was 8.1 ± 0.2 in Phase I and 7.5 ± 0.3 in Phase II. MBAS analysis confirmed the nominal concentrations. No significant effects on microbial community structure occurred in Phase I, with biomass levels in the high dose (4.0 mg/L) comparable to or greater than the biomass levels in the controls. Similarly, no significant effects on microbial community structure were observed in Phase II. The function of microbial communities in Phase I was affected at the high dose (4.0 mg/L), as evidenced by significant depression in the rates of both glucose and LAS degradation. No effects on microbial function were observed in Phase II. No dose response correlation in overall productivity was evident for the periphyton (aufwuchs) community in Phase I. In Phase II, the introduction of the sewage effluent produced a generally higher turbidity level and the higher organic concentrations were conducive to the growth of thick sheets of bacterial and fungal communities. Very little direct periphytic plant growth was observed. The stimulatory effect of the increasingly higher sewage concentration is evident in the progressively higher aufwuchs production observed between 3.75 and 30% effluent. No effects on *Elodea* production were observed in Phase I. However, in Phase II, *Elodea* and *Lemna* plant growth was inhibited at all concentrations except 3.75% by the increased bacterial and fungal periphyton growth as periphytic sheaths tended to cover the leaves and vegetative tips of the macrophytes. Evaluation of the *Daphnia magna* data from Phase I is confounded by unexpected poor control survival, although productivity appeared to be lower in the 1.0, 2.0 and 4.0 mg/L concentrations than at 0.5 mg/L. In Phase II, all *Daphnia* died in the 30% sewage concentration but production reached much greater numbers in the other concentrations than they did in Phase I. The midge species had an apparent reduction in numbers at 4.0 mg/L compared to the controls in Phase I. In Phase II, erratic growth in the controls and all exposures led to no meaningful midge survival at the end of Phase II. Bluegill fish growth at the end of Phase I was reduced at the 2.0 and 4.0 mg/L concentrations but not at 0.5 or 1.0 mg/L. In Phase II, fish in all wastewater dilution concentrations from 3.75 to 30% grew less than the controls. The following table

summarizes the NOEC values (mg/L) for Phase I and Phase II, as determined from the data described above.

Species	Phase I	Phase II
Bacterial Structure	4.0	30%
Bacterial Function	1.41[a]	30%
Periphyton/Algae	4.0	3.75%
Elodea	4.0	3.75%
Duckweed (*Lemna minor*)	Not Reported	3.75%
Daphnia magna	--[b]	--[c]
Midge (*Paratanytarsus parthenogenica*)	2.0	--[c]
Bluegill (*Lepomis macrochirus*)	1.0	<3.75%

[a] Data available only for the low and high concentrations (0.5-4.0 mg/L). Value is geometric mean.
[b] Poor control survival precludes calculation of a NOEC.
[c] Data not interpretable

Therefore, the NOEC based on the most sensitive endpoint (bluegill growth) is 1.0 mg/L.

Substance: LAS; C^{14}-LAS chain length C_{12} (91% purity) plus unlabeled LAS with average chain length $C_{11.6}$ (C_{10} 9.7%, C_{11} 27.9%, C_{12} 54.4%, C_{13} 8.0%; 95% purity)

Reference: Maki, A.W. 1981. A laboratory model ecosystem approach to environmental fate and effects studies. Unpublished Internal Report, Environmental Safety Department Procter & Gamble Company, Cincinnati, Ohio.

Reliability: 2 Valid with restrictions

(j)

Type: *In situ* river exposures

Methods: Species or ecosystem studied: Test system was rectangular plexiglass plates (108 cm^2) suspended in river water. Plates were colonized with periphyton for four weeks before testing at locations above and below the Xenia sewage treatment plant outfall in the Little Miami River (Ohio). Studies below the outfall assessed the toxicity of LAS in the presence of 2030% treated municipal effluent. Colonized plates were then placed in five submerged plexiglass tubes (1 cm thick, 1 m long), which were then attached to an aluminium frame supported by rubber floats. LAS stock solutions were stored in 80-L polypropylene containers on the river bank and solutions were pumped daily at a delivery rate adjusted based on river flow to maintain four concentrations (0.2, 1.1, 9.8 and 28.1 mg/L) and a control. Duplicate set ups were used as replicates. Identical set ups were used above and below the outfall.
Test duration 21 days.
Effects monitored: Phytoplankton inhibition of photosynthesis and reduction of the number of taxa was determined.
Chemical analysis: Concentrations were measured.

Results: For inhibition of photosynthesis the best estimated NOEC and LOEC were 9.8 and 28.1 mg/L respectively. At the highest concentration tested the number of taxa was not reduced. For this effect parameter the best estimated NOEC was >28.1 mg/L.

Substance: Dodecyl LAS (CAS #25155-30-3); average chain length $C_{11.9}$; average molecular weight 346; C_{10} 9%, C_{11} 30%, C_{12} 34%, C_{13} 19%, C_{14} 9%

Remarks: A concentration-effect relationship was found. Suspended solids were measured.

Reference: Lewis, M.A., Pittinger, C.A., Davidson, D.H., and Ritchie, C.J. 1993. *In situ* response of natural epiphyton to an anionic surfactant and an environmental safety assessment for phytotoxic effects. Environ. Toxicol. Chem. 12:1803-1812.
Reliability: 2 Valid with restrictions

(k)
Type: Laboratory bottles/lake exposures
Methods: Species or ecosystem studied: Bottles (300 ml) filled with lake water were used as the test systems. Nine concentrations were tested in triplicate.
Once a month the bottles were suspended in a lake at 1 m depth for three hours. The experiment was repeated for six months.
Effects monitored: photosynthetic response of phytoplankton was determined.
Chemical analysis: Concentrations were measured.
Results: Mean EC_{50} values were 3.4 and 1.9 mg/L for C_{12} and C_{13}, respectively. The ranges of EC_{50} values for the different tests were 0.5-8.0 and 0.2-8.1 mg/L for C_{12} and C_{13}, respectively.
Substance: Dodecyl LAS; average chain length $C_{11.8}$ (CAS #25155-30-3); and Tridecyl LAS, average chain length $C_{13.3}$ (CAS #26248-24-8).
Remarks: A concentration-effect relationship was found. Suspended solids were not measured. The wide range of EC_{50} values is in part due to seasonal differences in temperature and community dynamics.
Reference: Lewis, M.A. and Hamm, B.G. 1986. Environmental modification of the photosynthetic response of lake plankton to surfactants and significance to a laboratory-field comparison. Water. Res. 20:1575-1582.
Reliability: 2 Valid with restrictions

4.8 BIOTRANSFORMATION AND KINETICS

(a)
Type: Animal **[ ]**; Aquatic **[X]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Methods: In a flow-through system a 21 day uptake and 14 day elimination experiment was conducted with *Lepomis macrochirus*. The LSC-measured exposure concentration was 0.5 mg/L (1.45 uM). Flow-through; water renewal rate: 20 renewals per day; hardness as $CaCO_3$ 35 mg/L; pH 7.1; water/fish ratio: 0.04 L/g.
Results: k_1/k_2 concentration factors were for muscle 36, liver 171, blood 237, carcass 64, gall bladder 5224, gill and viscera 282 (on wet weight basis).
k_2 values are almost the same (0.24-0.28 d-L) in all tissues but the liver. The value for the liver is double (0.48 d-L) of the other tissues. This indicates biotransformation in the liver. The value of k_1 in the gall bladder (1461 L/kg/d) is at least 16 times higher than those in the other tissues (9-82 L/kg/d).
t95 in the different tissues range between 150 and 300.
No information on metabolism was given.
Test Substance: Na-alkylbenzenesulfonate average chain length: $C_{11.7}$ (C_{11} 45%, C_{12} 36.5%, C_{13} 18.5%) radiolabeled material (^{14}C uniformly labelled benzene ring) is spiked with unlabelled LAS (identical homologue composition), spiking ratio 4:1 (unlabeled:^{14}C labeled).
Remarks: Whole body concentration factors are reliable. Steady state attained within 24 h.
Reference: Kimerle, R.A., Macek, K.J., Sleight, B.H., and Burrows, M.E. 1981. Bioconcentration of linear alkylbenzene sulfonates (LAS) in bluegill (*Lepomis macrochirus*). Water. Res. 15:251-256.

Reliability: 2 Valid with restrictions

(b)
Type: Animal **[ ]**; Aquatic **[X]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Methods: Fathead minnows (*Pimephales promelas*) were exposed to LAS in a flow-through system according to OECD guideline 305E.
Results: Steady state uptake was achieved by 96-h of exposure. Uptake constants (k_1) range from 4.3 to 642.2 L/kg/day with C_{11} and C_{13} having the lowest and highest, respectively. The elimination rate constants (k_2) range from 0.5 and 1.5 days. k_1 was dependent on hydrophobicity and alkyl chain length. k_2 did not vary with hydrophobicity.
Reference: Tolls, J., Haller, M., De Graaf, I., Thijssen, M.A.T.C., and Sijm, D.T.H.M. 1997. Bioconcentration of LAS: Experimental determination and extrapolation to environmental mixtures. 31:3426-3431.
Reliability: 2 Valid with restrictions

(c)
Type: Animal **[ ]**; Aquatic **[X]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Method: In a flow-through system a 14 day uptake experiment was conducted with fish (*Pimephales promelas*). Two concentrations of 0.100 and 0.135 mg/L (0.3 and 0.4 uM) were tested resulting in concentration factors. Tissue extracts of the fish exposed to LAS were analysed by desulfonation-GC. Flow-through; water renewal rate: 3-4 renewals per day; no feeding; hardness 250 mg/L; well water. Chemical analyses by LSC.
Results: On the basis of the concentration in fish tissues (wet weight) and the two concentrations in water concentration factors in muscle were 4 and 3, and in the gall bladder 13,700 and 7,500. It remains unclear whether the observed variation of the concentration factors indicates a concentration dependence of bioaccumulation. The results indicate metabolic transformation, since the parent compound radioactivity could not account for all the radioactivity in the fish. Percentages of radioactivity accounted for by parent LAS in muscle 50-70%, other organs 50-80%, gall bladder <1%. The authors report clearance of "substantially all ^{14}C activity" within 3 days.
Test Substance: Linear LAS, chain length C_{12}; uniformly ^{14}C-labelled benzene ring, 2-phenyl-isomer-content: 17%.
Remarks: Steady state attained within 144 h.
Reference: Kimerle, R.A., Swisher, R.D., and Schroeder-Comotto, R.M. 1975. Surfactant structure and aquatic toxicity. Proc. IJC Symposium of Structure Activity Correlations in studies on toxicity and bioconcentration with aquatic organisms, pp. 22-35.
Reliability: 2 Valid with restrictions

(d)
Type: Animal **[X]**; Aquatic **[ ]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Methods: Fish (*Ictalurus punctatus* 250-450 g) were dosed with LAS via liquid gavage, gavage of food impregnated with LAS, and by intraperitoneal injection. Amount dosed: 425 ug (1.22 umole). Metabolism and elimination pathways were investigated. No aqueous exposure; metabolism chamber operated in a static mode; water was exchanged twice per day; 1 g of food, no feeding of the fish dosed by liquid gavage. Chemical analysis via LSC.
Results: Percentage eliminated from the different tissues 48 h after the end of the 24 exposure period:

	Percent Eliminated:		
	i.p. injection	**Gavage**	
		Food	**Fluid**

Total	42	68	71
Gills	4	49	33
Urine	26	7	11
Faeces+ Skin	12	12	27
$C0_2$	<1	<1	<1

Test substance: Linear LAS, chain length C_{12}; uniformly isomer distribution not specified.
Remarks: Elimination pathways for the three modes of dosing differed. As a considerable fraction of radiolabel administered via gavage is excreted via the gills it can be concluded that:
a) LAS is resorbed readily in the GI-tract.
b) The compounds excreted via the gills (LAS or its metabolites) are able to pass the gill membrane.
Reference: Schmidt, E.J. and Kimerle, R.A. 1981. New design and use of a fish metabolism chamber. In: Branson, D.R. and Dickson, K.L. (eds.). Aquatic Toxicology and Hazard Assessment: Fourth Conference, ASTM STP 737, 436-448.
Reliability: 2 Valid with restrictions

(e)
Type: Animal **[ ]**; Aquatic **[X]**; Plant **[ ]**; Terrestrial **[ ]**; Other **[ ]**
Method: Fish (*Cyprinus carpio* 34.6 g) were exposed to combinations of LAS, polyoxyethylene and sorbitan monooleate to assess the influence of these substances on the uptake of LAS. Exposure period was 3 h. Exposure concentration was 1 x 10^{-5} M LAS. LSC was used for tissue specific analysis, HPLC was used for measurement of gill adsorption. Dechlorinated tap water, filtered over active carbon; hardness 63 mg/L CaCO3; water/fish ratio: 0.14 g/L; no feeding during experiment.
Results: Concentration factors for specific tissues (measured by LSC) were for blood 4.2, hepatopancreas 4.0, spleen 1.0, kidney 3.3, heart 1.7, brain 0.6, muscles 0.2, gill 11, gall bladder 21. Adsorption of LAS to gills (Cgill/Cwater), measured by HPLC, isomer specific: 2-phenyl 16; 3-phenyl 5.4; 4-phenyl, 2.6; 5- and 6-phenyl 1.9.
C_{12}-LAS associated radiolabel is taken up by gills rapidly. It reaches the highest body level in the gall bladder after only three hours. The adsorption to the gills is related to the phenyl-substitution of the alkane.
The closer the benzenesulfonate-group is attached to the terminal carbon atom of the alkyl chain, the higher the adsorption to the gills. As the gills are an important organ in the uptake of xenobiotic compounds, it seems reasonable to expect that those isomers which sorb strongly to the gills will also be taken up preferentially.
Test substance: Labelled linear LAS, isomer distribution not specified. (CAS #25155-30-3)
Remarks: No whole body concentration factors.
Reference: Toshima, S., Moriya, T., and Yoshimura, K. 1992. Effects of polyoxyethylene (20) sorbitan monooleate on the acute toxicity of linear alkylbenzenesulfonate (C_{12}-LAS) to fish. Ecotox. Environ. Saf. 24:26-36.
Reliability: 2 Valid with restrictions

4.9 ADDITIONAL REMARKS

(a)
Remarks: Pre-1993 published data and company owned aquatic toxicity test data are collected in a common data base (BKH, 1993). Statistical analysis showed:
-After removal of outliners, the dataset contains 586 records covering 93 species. Algae, crustaceans and fish together make 68% of the 93 species.

Dominating species (genera) are: *Scenedesmus, Selenastrum, Daphnia, Gammarus, Lepomis, Pimephales and Carassius* (71% of the 586 records). 34 of the 93 species are marine species.
-LAS does not have a specific mode of action for different species. The variability in the sensitivity between species is comparable to the variability within a species.
-The acute to chronic ratio is approximately a factor 5.
-The mean LC_{50} of all species is 5.5 mg/L.
-The mean NOEC (chronic) of all species is 0.8 mg/L.
-A quantitative structure activity relationship for chain length was determined for fish and crustaceans, longer chain lengths corresponding to higher toxicity. The bioavailability of adsorbed LAS molecules for aquatic organisms as midge larvae, daphnids and fish is assumed to be low, because observed toxicity thresholds in the presence of adsorbing material correspond to the calculated concentration of the fraction LAS dissolved and the toxicity data for the completely dissolved substance (Pittinger et al., 1989).

Reference: 1) BKH. 1993. The use of existing toxicity data for estimation of the Maximum Tolerable Environmental Concentration of Linear Alkyl Benzene Sulfonate, Part I: Main report; Part II: Data base. Study carried out for ECOSOL, BKH Consulting Engineers, Delft, NL.
2) Hand, V.C., Rapaport, R.A., Pittinger, C.A. 1990. First validation of a model for the adsorption of linear alkylbenzene sulfonate to sediment and comparison to chronic effects data. Chemosphere 21(6):741-750.
3) Pittinger, C.A., Woltering, D.M., and Masters, J.A. 1989. Bioavailability of sediment sorbed and aqueous surfactants to Chironomus riparius (midge). Environm. Toxicol. Chem. 8:1023-1033.

Reliability: 4 Not assignable

(b)

Results: Neither LAS nor its sulfophenylcarboxylate degradation products displayed any estrogenic effects.

Remarks: A recombinant yeast estrogen screen using *Saccharomycea cerevisiae* was employed to determine the potential estrogenic activity of LAS and its degradation products.

Reference: Routledge, E.J. and Sumpter, J.P. 1996. Estrogenic activity of surfactants and some of their degradation products assessed using a recombinant yeast screen. Environ. Toxicol. Chem. 15:241-248.

Reliability: 2 Valid with restrictions

(c)

Type: Endocrine Disruption

Results: In the yeast screen, no statistical differences in absorbance were induced in any concentration of either of the three substances. In the hepatocyte assay, no increase in the concentration of Vg over the concentration of the controls was observed for LAS or any other three test substances. Results of both assays indicate that no estrogenic effects occurred after exposure to LAS or two of its biodegradation intermediates (SPC5 and SPC11).

Method: LAS, SPC5, or SPC11 were prepared in sterile distilled water and added to the culture media. Two *in vitro* screening assays for measurement of estrogenic activity were used: 1) the ER assay, with the recombinant yeast screen, and 2) the vitellogenin assay, with hepatocytes. ER was used as the positive control. Serial dilutions of the test compounds were used, with the maximum concentrations used in the hepatocytes assay were 150 μM (50 mg/L) for LAS, 25 μM (7.4 mg/L) for SPC5, and 200 μM (72.8 mg/L) for SPC11.

Test Substance: 1) LAS-C_{11}, 47% a.i., supplied by Petroquimica Espanola S.A.

2) Sulfophenylcarboxylic acids (SPC5 and SPC11) (formed from successive oxidation of terminal methyl groups on the alkyl chain)

Reference: Navas, J.M., Gonzalez-Mazo, E., Wenzel, A., Gomez-Parra, A., and Segner, H. 1999. Linear alkylbenzene sulfonates and intermediate products from their degradation are not estrogenic. Marine Pollution Bulletin 38:880-884.

Reliability: 2 Valid with restrictions

(d)

Results: The final predicted no-effect concentration (PNEC) for $C_{11.6}$ LAS was 250 µg/L based on a single species PNEC of 320 µg/L and the range of field NOECs of 250-500 µg/L. All data values are expressed as dissolved concentrations.

Method: Predicted no-effect concentrations (PNECs) were derived for LAS and three other surfactants using three stages in an aquatic effects assessment. In the Initial stage, assessment factors are applied to available short-term toxicity data. In the Refined stage, statistical extrapolation based on long-term (i.e., chronic) toxicity data are employed. In the Comprehensive stage of effects assessment, a wide variety of laboratory and field model ecosystem studies are incorporated into the analysis. To determine the PNEC for LAS, all data types were compiled and evaluated. Since toxicity is related to carbon chain length, all data were normalized to LAS with a mean carbon chain length of 11.6, the structure typically present in the environment based on the monitoring study described by Matthijs et al. 1999.

Remarks: For LAS, the predicted environmental concentrations (PECs) in the environment are about 50 to 100 times lower than the PNECs. This PNEC determination is part of an extensive monitoring program executed jointly by the Dutch Soap Association (NVZ) and the Dutch Ministry of Housing, Spatial Planning and the Environment (VROM).

Reference: van de Plassche, E.J., de Bruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J., and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: Linear alkylbenzene sulfonate, alcohol ethoxylates, alcohol ethoxylated sulfates, and soap. Environmental Toxicology and Chemistry 18:2653-2663.

Reliability: 2 Valid with restrictions

(e)

Results: A realistic worst-case estimation of the LAS concentration in sludge-amended soil is predicted to be 7 mg/kg dry weight, which is compared to the PNEC of 4.6 mg/kg. The LAS concentration will drop to a level below the PNEC within 6 to 24 days after sludge application, depending on the degradation rate of LAS.

Methods: LAS can be found in high concentrations in sewage sludge and may enter the soil compartment as a result of sludge application. To evaluate the effects and risk to soil organisms, a probabilistic (log-normal) distribution model was used to predict a no effect concentration (PNEC) for soil fauna, flora, and a combination of these. By extrapolation, the method determines a lower statistical tolerance limit. The preferred inputs to the current model are EC_{10} data from laboratory studies. By use of the log-normal distribution, a concentration (K_p) is found, for which the EC_{10} or NOEC values for 95% of all species in the community are greater. The value of K_p is used as the estimate of the PNEC. The soil concentration after sludge application was predicted by a number of scenarios and used as the predicted environmental concentration (PEC) in the risk characterization and calculation of risk quotients (RQ = PEC/PNEC). A LAS concentration of 4.6 mg/kg was used as the current best estimate of PNEC in all RQ calculations. The exposure scenarios included three levels of LAS contamination (530, 2,600 and 16,100

	mg/kg), three half-lives (10, 25 and 40 days) and five different sludge loads (2, 4, 6, 8 and 10 t/ha).
Remarks:	Even in the most extreme scenarios, the level of LAS is expected to be far below the estimated PNEC one year after application.
Test Substance:	LAS (various, based on each study used)
Reference:	Jensen, J., Lokke, H., Holmstrup, M., Krogh, P.H., and Elsgaard, L. 2001. Effects and risk assessment of linear alkylbenzene sulfonates in agricultural soil. 5. Probabilistic risk assessment of linear alkylbenzene sulfonates in sludge-amended soils. Environmental Toxicology and Chemistry 20:1690-1697.
Reliability:	2 Valid with restrictions

5. TOXICITY

5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

(a) **(Rat)**

Type:	LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	rat
Value:	1080 mg/kg bw
Method:	OECD Guide-line 401 "Acute Oral Toxicity" 1981. Five male and five female rats were given LAS doses of 1075, 1220, 1360, 1710 or a control by gavage. Body weight and other signs were measured on days 7 and 14. Temperature was maintained at $20^{+}/-1^{o}C$ with a 12 hr light-dark cycle. Animals were observed for 14 days after dosing.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 386 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; Activity: 86%
Remarks:	Symptoms beginning about 30 minutes past application included diarrhea, squatting attitude, breathing difficulties, nose bleeding, ataxia, and lethargy. These symptoms had disappeared in surviving animals by 120 hours. Virtually all animals died in doses of 1220 mg/kg and above. Note that all doses are corrected for 86% activity. The original doses were 1250, 1415, 1580 and 1990 mg/kg.
Reference:	Murmann, P. 1984a. Akute orale Toxizitat von Marlon A 386 fur Ratten. Huels Report No. 0191.
Reliability:	2 Valid with restrictions

(b)

Type:	LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	rat
Value:	1630 mg/kg bw
Method:	OECD Guide-line 401 "Acute Oral Toxicity" 1981. Five male and five female rats were given LAS doses of 1260, 1580, 1785, and 1990 or a control by gavage. Body weight and other signs were measured on days 7 and 14. Temperature was maintained at $20^{+}/-1^{o}C$ with a 12 hr light-dark cycle. Animals were observed for 14 days after dosing.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; Activity: 50%
Remarks:	Symptoms beginning about 1-4 hours past application included diarrhea, squatting attitude, breathing difficulties, nose bleeding, ataxia, and lethargy. The symptoms in the lower doses disappeared with 24 to 48 hours. Symptoms disappeared in the 1785 mg/kg dose and higher within 8 days. Virtually all animals died in doses of 1785 mg/kg and above. Note that all doses are corrected for 50% activity. The original doses were 2510, 3160, 3570 and 3980 mg/kg.
Reference:	Murmann, P. 1984c. Akute orale Toxizitat von Marlon A 350 fur Ratten. Huels Report No. 209.
Reliability:	2 Valid with restrictions

(c)

Type:	LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain:	rat
Value:	1410 mg/kg bw

Method: OECD Guide-line 401 "Acute Oral Toxicity" 1981. Five male and five female rats were given LAS doses of 1190, 1500 and 1890 or a control by gavage. Body weight and other signs were measured on days 7 and 14. Temperature was maintained at 20^{+}/-1^{o}C with a 12 hr light-dark cycle. Animals were observed for 14 days after dosing.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Marlon A 330 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; Activity: 30%.
Remarks: Symptoms beginning about 90 minutes past application included diarrhea, squatting attitude, breathing difficulties, nose bleeding, ataxia, and lethargy. These symptoms had disappeared in surviving animals by 72 hours. Virtually all animals died in doses of 1500 mg/kg and above. Note that all doses are corrected for 30% activity. The original doses were 3980, 5010 and 6310 mg/kg.
Reference: Murmann, P. 1984a. Akute orale Toxizitat von Marlon A 330 fur Ratten. Huels Report No. 0186.
Reliability: 2 Valid with restrictions

(d)
Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: rat
Value: LD_{50} for male animals: 1460 mg/kg
LD_{50} for female animals: 1470 mg/kg
Method: Male and female rats were given a single dose of LAS by gavage and observed for mortality.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{10-13} LAS, sodium salt (CAS #68411-30-3)
$<C_{10}$ 0.1%, C_{10} 10.1%, C_{11} 33.7%, C_{12} 31%, C_{13} 25.1%.; average alkyl chain length = $C_{11.7}$; activity: 99.5%
Remarks: Information as reported in IPCS document.
Reference: Ito, R., Kawamura, H., Chang, H.S., Kudo, K., Kajiwara, S., Toida, S., Seki, Y., Hashimoto, M., and Fukushima, A. 1978. Acute, subacute and chronic toxicity of magnesium linear alkylbenzene sulfonate (LAS-Mg). J. Med. Soc. Toho, Japan. 25 (5-6):850-875 (in Japanese). Referenced in IPCS, Environmental Health Criteria 169. Linear Alkylbenzene Sulfonates and Related Compounds, WHO.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document, therefore it is considered to be reliable.

(e)
Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: Rat, CFY (Sprague-Dawley origin); male and female
Value: 1980 mg/kg bw
Method: OECD Guideline 401. Five male and five female rats were given single doses by gavage at 1500, 2350 and 3760 mg/kg bw. Rats were housed in cages grouped by sex and given standard laboratory diet and water *ad libitum*. Mean daily temperature was maintained at 21-22^{o}C at a mean relative humidity of 56%. Lighting was on a 12 hrs dark and 12 hrs light photoperiod. Animals were observed for 14 days after dosing.
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Alkylbenzene sulfonate, sodium salt (designated as P-500 N-Na). Activity 47%. Average alkyl chain length = $C_{11.2}$ Clear yellow liquid.
Remarks: Four rats from each of the two lowest concentrations and all rats from the highest concentration died. All deaths occurred between 6 and 23 hours after

dosing. Signs of reaction to treatment included pilo-erection, hunched posture, abnormal gait (waddling), lethargy, decreased respiratory rate, ptosis, pallor of the extremities, and diarrhea. All surviving animals appeared to recover completely by day 4. Autopsy of rats that died revealed isolated cases of pallor of the kidneys or spleen. Terminal necropsy findings for survivors were normal. Note that all doses are corrected for 47% activity. The original doses were 3200, 5000, and 8000 mg/kg.

Reference: Kynoch, S.R. 1986a. Acute oral toxicity to rats: P-500 N-Na. Huntingdon Research Cener Report. No. 86546D/PEQ 7/AC.

Reliability: 1 Valid without restriction

(f)

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**

Species/strain: Sprague-Dawley strain albino male and female rats

Value: 1320 mg/kg (lower limit: 1220 mg/kg; upper limit: 1430 mg/kg)

Method: Acute Oral Minimal Lethal Dose Test

The test substance was applied as a 20% aqueous solution by stomach tube to Sprague-Dawley strain albino male and female rats. After the approximate LD_{50} was determined, groups of male and female rats were fed in increasing doses at increments of 0.1 fractional log intervals at three levels (1000, 1260 and 1580 mg/kg) designed to blanket the toxicity range thereby supplying data for calculation of the LD_{50} which was performed according to the method of E.J. de Beer. Observations of toxic signs were recorded and the viscera of the test animals were examined macroscopically.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Sodium sulfonate of linear alkylbenzene (Alkylate-225); C_9 1%; C_{10} 7%, C_{11} 25%, C_{12} 48%, C_{13} 19%, C_{14} 1%; average alkyl chain length = $C_{11.9}$.

Remarks: The compound was classified as mildly toxic by oral ingestion in male and female rats. All rats at 1000 mg/kg and 4 of 5 rats at 1260 mg/kg survived. Survival time was one to two days for rats that died at 1580 mg/kg. The toxic signs included reduced appetite and activity (one to two days in survivors), diarrhoea, increasing weakness, collapse, and death. The autopsy revealed hemorrhagic lungs, liver discoloration, and acute gastrointestinal inflammation. Surviving animals were sacrificed seven days after dosing. In these animals the vircera appeared normal by macroscopic examination.

Reference: Monsanto Company. 1971. Linear alkylbenzene sodium sulfonate – Alkylate 225 Lot CC 6450 – Acute toxicity screen. Project No. Y-71-119. Unpublished report.

Reliability: 2 Valid with restrictions

(g)

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**

Species/strain: Sprague-Dawley strain albino male and female rats

Value: 1430 mg/kg (lower limit: 1300 mg/kg; upper limit: 1570 mg/kg)

Method: Acute Oral Minimal Lethal Dose Test

The test substance was applied as a 10% aqueous solution by stomach tube to Sprague-Dawley strain albino male and female rats. After the approximate LD_{50} was determined, groups of male and female rats were fed in increasing doses at increments of 0.1 fractional log intervals at four levels (1000, 1260, 1580 and 2000 mg/kg) designed to blanket the toxicity range thereby supplying data for calculation of the LD_{50} which was performed according to the method of E.J. de Beer. Observations of toxic signs were recorded and the viscera of the test animals were examined macroscopically.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Sodium sulfonate of linear alkylbenzene (Alkylate-215); C_9 1%, C_{10} 16%, C_{11} 43%, C_{12} 40%, C_{13} 1%, C_{14} <1%; average alkyl chain length = $C_{11.35}$.

Remarks: The compound was classified as mildly toxic by oral ingestion in male and female rats. All rats survived at 1000 mg/kg. Three of 5 and 2 of 5 survived 1260 and 1580, respectively. Survival time was sixteen hours to two days in the rats that died. The toxic signs included reduced appetite and activity (two to three days in survivors), increasing weakness, slight tremors, collapse, and death. The autopsy revealed lung and liver hyperaemia and gastrointestinal inflammation. Surviving animals were sacrificed seven days after dosing. In these animals the vircera appeared normal by macroscopic examination.

Reference: Monsanto Company. 1972a. Linear alkylbenzene sodium sulfonate – Alkylate 215 Lot CC 6772S – Acute toxicity screen. Project No. Y-72-274. Unpublished report.

Reliability: 2 Valid with restrictions

(h)

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**

Species/strain: Sprague-Dawley strain albino male and female rats

Value: 1360 mg/kg (lower limit: 1240 mg/kg; upper limit: 1500 mg/kg)

Method: Acute Oral Minimal Lethal Dose Test
The test substance was applied as a 10% aqueous solution by stomach tube to Sprague-Dawley strain albino male and female rats. After the approximate LD_{50} was determined, groups of male and female rats were fed in increasing doses at increments of 0.1 fractional log intervals at four levels (1000, 1260, 1580 and 2000 mg/kg) designed to blanket the toxicity range thereby supplying data for calculation of the LD_{50} which was performed according to the method of E.J. de Beer. Observations of toxic signs were recorded and the viscera of the test animals were examined macroscopically.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Sodium sulfonate of linear alkylbenzene (Alkylate-222L); average alkyl chain length = $C_{11.5}$

Remarks: The compound was classified as slightly toxic by oral ingestion in male and female rats. Survival time was sixteen hours to three days in the rats that died. The toxic signs included reduced appetite and activity (one to three days in survivors), increasing weakness, collapse, and death. The autopsy revealed lung and liver hyperaemia and gastrointestinal inflammation. Surviving animals were sacrificed seven days after dosing. In these animals the vircera appeared normal by macroscopic examination.

Reference: Monsanto Company. 1972b. Linear alkylbenzene sodium sulfonate – Alkylate 222L Lot CC 6773S – Acute toxicity screen. Project No. Y-72-275. Unpublished report.

Reliability: 2 Valid with restrictions

(i) **(Mouse)**

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**

Species/strain: mouse

Value: LD_{50} male animals: 2160 mg/kg
LD_{50} female animals: 2250 mg/kg

Method: Male and female mice were given a single dose of LAS and observed for mortality.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: $C_{10\text{-}13}$ LAS, sodium salt (CAS #68411-30-3).
$<C_{10}$ 0.1%, C_{10} 10.1%, C_{11} 33.7 %, C_{12} 31%, C_{13} 25.1%; average alkyl chain length = $C_{11.7}$; activity: 99.5%

Remarks: Information as cited in IPCS document.

Reference: Ito, R., Kawamura, H., Chang, H.S., Kudo, K., Kajiwara, S., Toida, S., Seki, Y., Hashimoto, M., and Fukushima, A. 1978. Acute, subacute and chronic toxicity of magnesium linear alkylbenzene sulfonate (LAS-Mg). J.

Med. Soc. Toho, Japan. 25 (5-6):850-875 (in Japanese). Referenced in IPCS, Environmental Health Criteria 169. Linear Alkylbenzene Sulfonates and Related Compounds, WHO.

Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

5.1.2 ACUTE INHALATION TOXICITY

Type: LC_0 **[ ]**; LC_{100} **[ ]**; LC_{50} **[ ]**; LCL_0 **[ ]**; Other **[X]** Approximate lethal concentration (ALC)

Species/strain: Rat/Male Crl: CD (SD) BR

Exposure time: single 4-hour period

Value: 310 mg/m^3 of particulate

Method: Groups of six male 8-week old rats were restrained in perforated, stainless steel cylinders with conical nose pieces. Exposure was nose-only to an aerosol atmosphere for 4 hours. After exposure, rats were returned to their cages and observed for clinical signs for 14 days. Mean measured concentrations in the test chambers were 65, 120, 260, and 310 mg/m^3. Chamber temperature ranged between 25-26°C.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: LAS (CAS #25155-30-0); activity 98%

Remarks: The ALC is defined as the lowest atmospheric concentration generated that caused death in 1 or more rats either on the day of exposure or within 14 days post exposure. No mortality occurred at concentrations up to 260 mg/m^3. At 310 mg/m^3, one rat died during exposure and 2 rats died one day post exposure. The test material is considered moderately toxic by inhalation. However, it is important to note that this laboratory exposure is not representative of the possible LAS exposure during actual use. In this study, animals were given high exposures to respirable-sized particles (MMAD at 310 mg/m^3 = 2.5 microns). Spray products containing LAS are designed to produce large particle sizes. These large particles are needed for efficient delivery of the spray to the surface being cleaned. This results in particle sizes that are much larger than the respirable particle sizes used in testing and therefore would not be able to reach far into the lungs where effects could occur. Given this lack of relevance to real-world exposure potential, the use of this study for risk assessment purposes is limited.

Reference: Kinney, L.A. 1985. Approximate lethal concentrations (ALCs) by inhalation of sodium lauryl sulfate & sodium dodecylbenzene sulfonate. Dupont Haskell Laboratory Report No. 474-84.

Reliability: 2 Valid with restrictions

5.1.3 ACUTE DERMAL TOXICITY

(a)

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**

Species: Rat, CFY (Sprague-Dawley origin); male and female

Value: >2000 mg/kg bw

Method: OECD Guideline 402. Five male and five female rats were exposed to 2000 mg/kg in a limit test. The test substance was applied to clipped intact skin in the dorso-lumbar region and covered with gauze held in place with an impermeable dressing. The dressing was removed after 24 hours and the treated area of the skin washed with warm water and blotted dry. Observations for dermal irritation were made daily for 14 days.

GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Alkylbenzene sulfonate, sodium salt (designated as P-500 N-Na). activity 47%. Average alkyl chain length = $C_{11.2}$. Yellow, viscous liquid.
Remarks: There were no deaths or signs of a systemic reaction following a single dermal application at 2000 mg/kg bw. Well defined or slight erythema and slight oedema were observed at all test sites after removal of the occlusive dressing on Day 2. All test sites were entirely covered by scab formation from Day 7. Sloughing from the scabbed skin began at various times between Day 7 and Day 12 and was completed before termination. Low bodyweight gains or loss of body weight were recorded for one male and three females in Day 8. Two of the same females and a third female also showed low bodyweight gain between Days 8 and 15.
Reference: Kynoch, S.R. 1986b. Acute dermal toxicity to rats of P-500 N-Na. Huntingdon Research Center. Report No. 86718D/PEQ 8/AC.
Reliability: 1 Valid without restriction

(b)
Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: New Zealand white rabbit
Value: > 200 mg/kg and < 316 mg/kg
Method: Acute Skin Absorption Minimal Lethal Dose Test
The test substance was applied as a 30% aqueous solution and the doses of the solution administered were 126, 200, 316, 501, 794, 1260, 2000, 3160 and 5010 mg/kg. The doses were administered to a closely clipped area of intact skin of male and female rabbits (1 animal/dose). The treated areas were covered with plastic strips and the animals were placed in wooden stocks for up to twenty-four hours. After the twenty-four hours the animals were assigned to individual cages. Observations of toxic signs were recorded daily and the viscera of the test animals were examined macroscopically.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Sodium sulfonate of linear alkylbenzene (Alkylate-225; C_9 1%; C_{10} 7%, C_{11} 25%, C_{12} 48%, C_{13} 19%, C_{14} 1%; average alkyl chain length = $C_{11.9}$)
Remarks: The test substance was classified as moderately toxic. Animals exposed dermally to 126 and 200 mg/kg survived for the 14 day study duration. Survival time for animals receiving all other doses ranged from two to eight days. The toxic signs included reduced appetite and activity, increasing weakness, collapse and death. The autopsy revealed hemorrhagic lungs, liver discoloration, enlarged gall bladder, and gastrointestinal inflammation. The animals that survived were sacrificed fourteen days after dosing. In these animals the viscera appeared normal by macroscopic examination.
Reference: Monsanto Company. 1971. Linear alkylbenzene sodium sulfonate – Alkylate 225 Lot CC 6450 – Acute toxicity screen. Project No. Y-71-119. Unpublished report.
Reliability: 4 (insufficient animals per dose of mixed sex, etc.)

(c)
Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: New Zealand white rabbit
Value: > 631 mg/kg and < 1000 mg/kg
Method: Acute Skin Absorption Minimal Lethal Dose Test
The test substance was applied as a 20% aqueous solution and the doses of the solution administered were 200, 316, 631, 1000, 1260, 2000 and 3160 mg/kg. The doses were administered to a closely clipped area of intact skin of male and female rabbits (1 animal/dose). The treated areas were covered with plastic strips and the animals were placed in wooden stocks for up to twenty-four hours. After the twenty-four hours the animals were assigned to

individual cages. Observations of toxic signs were recorded daily and the viscera of the test animals were examined macroscopically.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Sodium sulfonate of linear alkylbenzene (Alkylate-215; C_9 1%, C_{10} 16%, C_{11} 43%, C_{12} 40%, C_{13} 1%, C_{14} <1%; average alkyl chain length = $C_{11.35}$)

Remarks: The test substance was classified as moderately toxic. Survival time ranged from one to two days. The toxic signs included reduced appetite and activity, increasing weakness, collapse and death. The autopsy revealed lung hyperemia, areas of liver discoloration and gastrointestinal inflammation. The animals that survived were sacrificed fourteen days after dosing. In these animals the viscera appeared normal by macroscopic examination.

Reference: Monsanto Company. 1972a. Linear alkylbenzene sodium sulfonate – Alkylate 215 Lot CC 6772S – Acute toxicity screen. Project No. Y-72-274. Unpublished report.

Reliability: 4 (insufficient animals per dose of mixed sex, etc.)

(d)

Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**

Species/strain: New Zealand white rabbit

Value: > 631 mg/kg and < 1000 mg/kg

Method: Acute Skin Absorption Minimal Lethal Dose Test
The test substance was applied as a 20% aqueous solution and the doses of the solution administered were 200, 398, 631, 1000, 1260, 2000 and 3160 mg/kg. The doses were administered to a closely clipped area of intact skin of male and female rabbits (1 animal/dose). The treated areas were covered with plastic strips and the animals were placed in wooden stocks for up to twenty-four hours. After the twenty-four hours the animals were assigned to individual cages. Observations of toxic signs were recorded daily and the viscera of the test animals were examined macroscopically.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Sodium sulfonate of linear alkylbenzene (Alkylate-222L; average alkyl chain length = $C_{11.5}$)

Remarks: The test substance was classified as moderately toxic. Survival time was two days. The toxic signs were reduced appetite and activity, increasing weakness, collapse and death. The autopsy revealed lung hyperemia, areas of liver discoloration and gastrointestinal inflammation. The animals that survived were sacrificed fourteen days after dosing. In these animals the viscera appeared normal by macroscopic examination.

Reference: Monsanto Company. 1972b. Linear alkylbenzene sodium sulfonate – Alkylate 222L Lot CC 6773S – Acute toxicity screen. Project No. Y-72-275. Unpublished report.

Reliability: 4 (insufficient animals per dose of mixed sex, etc.)

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION

(a)

Type: LD_0 **[ ]**; LD100 **[ ]**; LD50 **[X]**; LDL_0 **[ ]**; Other **[ ]**

Species/strain: rat

Administration: i.m. **[ ]**; i.p. **[ ]**; i.v. **[ ]**; infusion **[ ]**; s.c. **[X]**; other **[ ]**

Value: Females = 810 mg/kg; males = 840 mg/kg bw

Method: Rats were given subcutaneous injections of LAS

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: C_{10-13} LAS, sodium salt (CAS #68411-30-3)
<C_{10} 0.1%, C_{10} 10.1%, C_{11} 33.7 %, C_{12} 31%, C_{13} 25.1%; average alkyl chain length = $C_{11.7}$; activity: 99.5%

Remarks: Information as cited in IPCS document.
Reference: Ito, R., Kawamura, H., Chang, H.S., Kudo, K., Kajiwara, S., Toida, S., Seki, Y., Hashimoto, M., and Fukushima, A. 1978. Acute, subacute and chronic toxicity of magnesium linear alkylbenzene sulfonate (LAS-Mg). J. Med. Soc. Toho, Japan. 25 (5-6):850-875 (in Japanese). Referenced in IPCS, Environmental Health Criteria 169. Linear Alkylbenzene Sulfonates and Related Compounds.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(b)
Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: mouse
Administration: i.m. **[ ]**; i.p. **[ ]**; i.v. **[ ]**; infusion **[ ]**; s.c. **[X]**; other **[ ]**
Value: Females = 1400 mg/kg; males = 1250 mg/kg bw
Method: Mice were given subcutaneous injections of LAS.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: $C_{10\text{-}13}$ LAS, sodium salt (CAS #68411-30-3)
$<C_{10}$ 0.1%, C_{10} 10.1%, C_{11} 33.7 %, C_{12} 31%, C_{13} 25.1%; average alkyl chain length = $C_{11.7}$; activity: 99.5%
Remarks: Information as cited in IPCS document.
Reference: Ito, R., Kawamura, H., Chang, H.S., Kudo, K., Kajiwara, S., Toida, S., Seki, Y., Hashimoto, M., and Fukushima, A. 1978. Acute, subacute and chronic toxicity of magnesium linear alkylbenzene sulfonate (LAS-Mg). J. Med. Soc. Toho, Japan. 25 (5-6):850-875 (in Japanese). Referenced in IPCS, Environmental Health Criteria 169. Linear Alkylbenzene Sulfonates and Related Compounds.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(c)
Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: rat
Administration: i.m. **[ ]**; i.p. **[ ]**; i.v. **[X]**; infusion **[ ]**; s.c. **[ ]**; other **[ ]**
Value: Females = 126 mg/kg; males = 119 mg/kg bw
Method: Rats were given intravenous injections of LAS.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: $C_{10\text{-}13}$ LAS, sodium salt (CAS #68411-30-3)
$<C_{10}$ 0.1%, C_{10} 10.1%, C_{11} 33.7 %, C_{12} 31%, C_{13} 25.1%; average alkyl chain length = $C_{11.7}$; activity: 99.5%
Remarks: Information as cited in IPCS document.
Reference: Ito, R., Kawamura, H., Chang, H.S., Kudo, K., Kajiwara, S., Toida, S., Seki, Y., Hashimoto, M., and Fukushima, A. 1978. Acute, subacute and chronic toxicity of magnesium linear alkylbenzene sulfonate (LAS-Mg). J. Med. Soc. Toho, Japan. 25 (5-6):850-875 (in Japanese). Referenced in IPCS, Environmental Health Criteria 169. Linear Alkylbenzene Sulfonates and Related Compounds.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(d)
Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: mouse

Administration: i.m. **[ ]**; i.p. **[ ]**; i.v. **[X]**; infusion **[ ]**; s.c. **[ ]**; other **[ ]**
Value: Females = 298 mg/kg; males = 207 mg/kg bw
Method: Mice were given intravenous injections of LAS.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{10-13} LAS, sodium salt (CAS #68411-30-3)
<C_{10} 0.1%, C_{10} 10.1%, C_{11} 33.7 %, C_{12} 31%, C_{13} 25.1%; average alkyl chain length = $C_{11.7}$; activity: 99.5%
Remarks: Information as cited in IPCS document.
Reference: Ito, R., Kawamura, H., Chang, H.S., Kudo, K., Kajiwara, S., Toida, S., Seki, Y., Hashimoto, M., and Fukushima, A. 1978. Acute, subacute and chronic toxicity of magnesium linear alkylbenzene sulfonate (LAS-Mg). J. Med. Soc. Toho, Japan. 25 (5-6):850-875 (in Japanese). Referenced in IPCS, Environmental Health Criteria 169. Linear Alkylbenzene Sulfonates and Related Compounds.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(e)
Type: LD_0 **[ ]**; LD_{100} **[ ]**; LD_{50} **[X]**; LDL_0 **[ ]**; Other **[ ]**
Species/strain: mouse, albino, Harlan strain
Administration: i.m. **[ ]**; i.p. **[ ]**; i.v. **[X]**; infusion **[ ]**; s.c. **[ ]**; other **[ ]**
Exposure time: 24 hours
Value: 105 mg/kg bw (C_{12} LAS); 115 mg/kg bw (C_{10} LAS)
Method: Mice in groups of 10 were given intravenous injections of C_{10} or C_{12} LAS.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{12} LAS homologue; C_{10} LAS homologue
Remarks: Varying doses were given with an increasing increment between doses of 20% or less.
Reference: Hopper, S.S., Hulpieu, H.R. and Cole, V.V. 1949. Some toxicological properties of surface active agents. J. Am. Pharmacol. Assoc. 38:428-432.
Reliability: 2 Valid with restrictions

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION

(a)
Species: New Zealand albino rabbits
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**; Moderate to severe irritating **[X]**
Method: OECD Guideline 404. A 0.5 ml aliquot of P-500 N-Na was applied under a 2.5 cm^2 gauze pad to an approximate 10 cm^2 area of clipped intact skin of 3 rabbits. Each treatment site was occluded with an elastic adhesive dressing for four hours, after which the dressing was removed and the area washed with distilled water. Examination of the treated skin was made approximately 30 minutes after removal of the patch and daily through 14 days. Grading and scoring of the dermal reactions was performed using the standard numerical scoring system.
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Alkylbenzene sulfonate, sodium salt (designated as P-500 N-Na). Activity 47%. Average alkyl chain length = $C_{11.2}$. Clear yellow liquid.
Remarks: Well defined to moderate skin reactions were observed in all three animals following removal of the bandages. Desquamation of the stratum corneum

was observed in all three animals. The reaction in all three animals gradually ameliorated from Days 5, 10 and 11, respectively, and had all resolved completely in one animal by Day 12.

Reference: Liggett, M.P. and Parcell, B.I. 1986a. Irritant effects on rabbit skin of P-500 N-Na. Huntingdon Research Center. Report No. 86400D/PEQ 9/SE.

Reliability: 1 Valid without restriction

(b)

Species/strain: New Zealand albino rabbits

Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ]**

Method: OECD Guideline 404. A single dose of 0.5 g was applied to the clipped intact skin of six rabbits and secured with a gauze pad covered by an impermeable covering. The patch was removed after a 4 hour exposure and the site washed with water. Animals were examined for signs of erythema and oedema and the responses scored at 60 minutes, 24, 48 and 72 hr, and daily as needed up to 7 days. Skin irritation was scored using the standard rating system and averaged.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: LAS activity 50%; average alkyl chain length = $C_{11.6}$

Remarks: Average score after 72 hours were 2.4 and 2.83 for erythema and oedema, respectively.

Reference: Biolab SGS. 1989a. Primary skin irritation. Report No. T00428/4.

Reliability: 2 Valid with restrictions

(c)

Species/strain: rabbit

Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ]**

Classification: Highly corrosive (causes severe burns) **[ ]**; Corrosive (causes burns) **[ ]**; Irritating **[X]**; Not irritating **[ ]**

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion" 1984

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: C_{10} LAS (CAS #1322-98-1) and C_{12} LAS (CAS #25155-30-0).

Remarks: Reference reports the results of many experiments conducted on LAS and other surfactants.

Reference: Kaestner, W. 1997. Local tolerance (animal tests): mucous membranes and skin. In: Anionic Surfactants: Biochemistry, Toxicology, Dermatology. 2nd Edition.

Reliability: 4 Not assignable

(d)

Species/strain: rabbit

Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ]**

Classification: Highly corrosive (causes severe burns) **[ ]**; Corrosive (causes burns) **[ ]**; Irritating **[X]**; Not irritating **[ ]**

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion" 1981. Three male and female rabbits received 0.5 ml of 50% active material to the shaved intact skin.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Marlon A 350 (CAS # 68411-30-3) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; activity: 50%.

Remarks: Mean irritation index: 5.1 out of 8. Individual scores: edema: 2.28, erythema: 3.0
Reference: Murmann, P. 1983a. Prufung der akuten Hautreizwirkung von Marlon A 350. Huels Report No. 0171.
Reliability: 2 Valid with restrictions

(e)
Species/strain: New Zealand albino rabbits
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderately irritating **[X]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Method: OECD Guideline 404. A single dose of 0.5 g was applied to the clipped intact skin of six rabbits and secured with a gauze pad covered by an impermeable covering. The patch is removed after a 4 hour exposure and the site washed with water. A second site with the skin abraded received the same treatment. Animals are examined for signs of erythema and oedema and the responses scored at 60 minutes, 24, 48 and 72 hr, and daily as needed up to 7 days. Skin irritation is scored using the standard rating system and averaged.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS (made from Sirene LAB); activity 5%; average alkyl chain length = $C_{11.6}$
Remarks: Average scores after 72 hours were 1.67 and 2.17 for erythema and oedema, respectively. The primary irritation index was calculated to be 3.82, which classifies 5% LAS as a moderate skin irritant. No differences were observed between intact and abraded skin.
Reference: Biolab SGS. 1989b. Primary skin irritation. Report No. T343.
Reliability: 2 Valid with restrictions

(f)
Species/strain: New Zealand albino rabbits
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[X]**
Method: OECD Guideline 404. A single dose of 0.5 g was applied to the clipped intact skin of six rabbits and secured with a gauze pad covered by an impermeable covering. The patch is removed after a 4 hour exposure and the site washed with water. A second site with the skin abraded received the same treatment. Animals are examined for signs of erythema and oedema and the responses scored at 60 minutes, 24, 48 and 72 hr, and daily as needed up to 7 days. Skin irritation is scored using the standard rating system and averaged.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS (made from Sirene LAB); activity 2.5%; average alkyl chain length = $C_{11.6}$
Remarks: No signs of irritation were observed during the study.
Reference: Biolab SGS. 1989c. Primary skin irritation. Report No. T00430/2.
Reliability: 2 Valid with restrictions

(g)
Species/strain: New Zealand albino rabbits
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[X]**
Method: OECD Guideline 404. A single dose of 0.5 g was applied to the clipped intact skin of six rabbits and secured with a gauze pad covered by an

impermeable covering. The patch is removed after a 4 hour exposure and the site washed with water. A second site with the skin abraded received the same treatment. Animals are examined for signs of erythema and oedema and the responses scored at 60 minutes, 24, 48 and 72 hr, and daily as needed up to 7 days. Skin irritation is scored using the standard rating system and averaged.

GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS (made from Sirene LAB); activity 1%; average alkyl chain length = $C_{11.6}$
Remarks: No signs of irritation were observed during the study.
Reference: Biolab SGS. 1983. Primary skin irritation. Report No. T116/2.
Reliability: 2 Valid with restrictions

(h)
Species/strain: albino male and female rabbits
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[X]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification: Highly corrosive (causes severe burns) **[ ]**;
Corrosive (causes burns) **[ ]**; Irritating **[X]**; Not irritating **[ ]**
Method: The clipped, intact and abraded skin of six albino male and female rabbits was exposed to 0.5 g of finely ground sample moistened with water under a one inch by one inch square patch, two single layers thick. The patches were positioned in place with adhesive tape. The trunk of each animal was wrapped with plastic strips to avoid contamination and retard evaporation for the 24 hour exposure period. Observations were made over a period of seven days for irritation. The data was scored according to the method of Draize, et al.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Sodium sulfonate of linear alkylbenzene (Alkylate-225); C_9 1%, C_{10} 7%, C_{11} 25%, C_{12} 48%, C_{13} 19%, C_{14} 1%; average alkyl chain length = $C_{11.9}$
Remarks: Primary Irritation Score: 6.2
Intact Skin: 6.8/8
Abraded Skin: 6.8/8
Slight to moderate erythema and edema were present after 24 hours. These symptoms persisted through 120 hours. The compound was classed as a primary skin irritant under the grading system as outlined in the Federal Hazardous Substance Act. The sample had a defatting effect on the skin causing the skin to slough off in ten to fourteen days. There was no injury in depth.
Reference: Monsanto Company. 1971. Linear alkylbenzene sodium sulfonate – Alkylate 225 Lot CC 6450 – Acute toxicity screen. Project No. Y-71-119. Unpublished report.
Reliability: 2 Valid with restrictions

(i)
Species/strain: New Zealand white male and female rabbits
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[X]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification: Highly corrosive (causes severe burns) **[ ]**;
Corrosive (causes burns) **[ ]**; Irritating **[X]**; Not irritating **[ ]**
Method: The clipped, intact and abraded skin of three New Zealand white male and female rabbits was applied with 0.5 g of finely ground sample moistened with water under a one inch by one inch square patch, two single layers thick. The patches were positioned in place with adhesive tape. The trunk of

each animal was wrapped with plastic strips to avoid contamination and retard evaporation for the 24 hour exposure period. Observations were made over a period of seven days for irritation. The data was scored according to the method of Draize, Woodard and Calvery (Journal of Pharm. and Exp. Therapeutics, Volume 82, December 1944).

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Sodium sulfonate of linear alkylbenzene (Alkylate-215); C_9 1%, C_{10} 16%, C_{11} 43%, C_{12} 40%, C_{13} 1%, C_{14} <1%; average alkyl chain length = $C_{11.35}$

Remarks: Moderate to severe erythema and edema were present after 24 hours. These symptoms persisted through 120 hours. The average maximum score was 7.3 out of a possible 8 at 24 hours. The compound was classed as a severe skin irritant. The sample had a defatting effect on the skin causing the skin to slough off in ten to fourteen days. There was no injury in depth.

Reference: Monsanto Company. 1972a. Linear alkylbenzene sodium sulfonate – Alkylate 215 Lot CC 6772S – Acute toxicity screen. Project No. Y-72-274. Unpublished report.

Reliability: 2 Valid with restrictions

(j)

Species/strain: New Zealand white male and female rabbits

Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[X]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**

Classification: Highly corrosive (causes severe burns) **[ ]**;
Corrosive (causes burns) **[ ]**; Irritating **[X]**; Not irritating **[ ]**

Method: The clipped, intact and abraded skin of three New Zealand white male and female rabbits was applied with 0.5 g of finely ground sample moistened with water under a one inch by one inch square patch, two single layers thick. The patches were positioned in place with adhesive tape. The trunk of each animal was wrapped with plastic strips to avoid contamination and retard evaporation for the 24 hour exposure period. Observations were made over a period of seven days for irritation. The data was scored according to the method of Draize, Woodard and Calvery (Journal of Pharm. and Exp. Therapeutics, Volume 82, December 1944).

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Sodium sulfonate of linear alkylbenzene (Alkylate-222L); average alkyl chain length = $C_{11.5}$

Remarks: Moderate to severe erythema and edema were present after 24 hours. These symptoms persisted through 120 hours. The average maximum score was 7.0 out of a possible 8 at 24 hours. The compound was classed as a severe skin irritant. The sample had a defatting effect on the skin causing the skin to slough off in ten to fourteen days. There was no injury in depth.

Reference: Monsanto Company. 1972b. Linear alkylbenzene sodium sulfonate – Alkylate 222L Lot CC 6773S – Acute toxicity screen. Project No. Y-72-275. Unpublished report.

Reliability: 2 Valid with restrictions

5.2.2 EYE IRRITATION/CORROSION

(a)

Species/strain: New Zealand albino rabbits

Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**

Method: OECD Guideline 405. Nine rabbits received a 0.1 mL aliquot of P-500 N-Na placed into the lower everted lid of one eye per animal. For three rabbits the eyelids were then gently held together for one second before releasing. For three other rabbits the eyes were irrigated with water for 5 minutes following a 4-second exposure. For the remaining three rabbits the eyes were irrigated for 5 minutes following a 30-second exposure. Eyes were examined after 1 hour and 1, 2, 3, 4, 7, 14 and 21 days after exposure. Grading was performed using the standard scoring system.

GLP: Yes **[X]** No **[ ]** ? **[ ]**

Test substance: Alkylbenzene sulfonate, sodium salt (designated as P-500 N-Na). Activity 47%. Average alkyl chain length = $C_{11.2}$. Clear yellow liquid.

Remarks: The following results were noted:

1) Three animals without any rinsing: averaged irritation scores (24, 48, 72 hours) for each animal: cornea 2.3, 1.7, 2; iris: 1.3, 0, 0; conjunctivae redness: 3, 1.7, 2; conjunctivae chemosis: 3, 2, 2. In the first animal the effects were persistent at day 14.

2) Three animals with rinsing for five minutes following a 30 second exposure: averaged scores: cornea 0.7, 1, 1.3; iris: 0, 0.7, 0.3; conjunctivae redness: 1.7, 2, 1.3; conjunctivae chemosis: 2, 1.3, 2. The eyes were normal 7 or 14 days after instillation.

3) Three animals with rinsing for five minutes following a 4 second exposure: averaged scores: cornea 0.7, 2.3, 0.7; iris: 0, 0, 0; conjunctivae redness: 1.7, 1.7, 1; conjunctivae chemosis: 1.3, 2, 1. The eyes were normal 7 days after instillation.

Findings lead to a definition of irritating for LAS at 47% applied without rinsing, irritating (even if with lower effects, mainly as cornea opacity and conjunctivae redness) with rinsing after 30 second of exposure, and not irritating with rinsing after 4 second of exposure.

Overall, instillation of P-500 N-Na into the eyes of rabbits elicited positive responses in all animals. Irrigation of the eyes only slightly reduced the irritation potential.

Reference: Liggett, M.P. and Parcell, B.I. 1986b. Irritant effects on the rabbit eye of P-500 N-Na. Huntingdon Research Ctr Report No. 86570D/PEQ 10/SE.

Reliability: 1 Valid without restriction

(b)

Species/strain: New Zealand albino rabbits

Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**;
Not irritating **[ ]**

Method: OECD Guideline 405. Six rabbits were exposed to 0.1 ml of 50% LAS, which was placed into the conjunctival sac of one eye per animal. The eyelids were gently held together for one second and then released. No irrigation step was performed The eyes were examined at 1, 24, 48 and 72 hours and at 7 days and scored for irritation using the standard system.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: LAS (made from Sirene LAB); activity 50%; average alkyl chain length = $C_{11.6}$

Remarks: Average irritation scores were 1.3, 1.0, 2.6, and 2.7 for the cornea, iris, conjunctival redness, and conjunctival chemosis, respectively. Effects were persistent to Day 6. This classifies LAS at 50% as irritating.

Reference: Biolab SGS. 1989d. Acute eye irritation. Report No. 00428/13.

Reliability: 2 Valid with restrictions

(c)

Species/strain: rabbit

Results:	Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ]**
Classification:	Irritating **[X]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion" 1981
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; activity: 50%.
Remarks:	The mean irritation index was 26.5 out of 110. Individual scores: 1.0; iris: 0; conjunctivae chemosis: 1.11, conjunctivae redness: 2.39
Reference:	Murmann, P. 1983b. Prufung der akuten Augen-und Schleimhautreiz Wirkung von Marlon A 350. Huels Report No. 0172.
Reliability:	2 Valid with restrictions

(d)

Species/strain:	rabbit
Results:	Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ]**
Classification:	Irritating **[X]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion" 1984
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	LAS
Remarks:	Possibility of persistent effects on the eye.
Reference:	Kaestner, W., Henkel KGaA, unpublished data, Report No. 870553 (1987).
Reliability:	4 Not assignable

(e)

Species/strain:	rabbit
Results:	Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ]**
Classification:	Irritating **[X]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method:	0.1 mL solutions of LAS at 5 different concentrations ranging from 0.01 to 1.0 % were instilled in the eyes of rabbits (13 per group). The rabbits were observed for 24 hours after LAS application.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	C_{10-13} LAS, (CAS #68411-30-3). Molecular weight 346.5; average alkyl chain length = $C_{11.9}$
Remarks:	Information as cited in IPCS document. The 0.01 % group showed no abnormalities, but the 0.05 % group showed slight congestion. The groups of 0.5 % and higher concentrations showed marked reactions such as severe congestion and oedema, increased secretion, turbidity of the cornea, and disappearance of corneal reflex.
Reference:	Oba, K., Mori, A. and Tomiyama, S. 1968. Biochemical studies of n-alpha-olefin sulfonates (II) Acute toxicity, skin and eye irritation, and some other physical properties. Journ. Jap. Oil Chem. Soc. 17:628-634. (In Japanese) cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability:	4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(f)

Species/strain:	rabbit

Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[X]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[ ]**

Classification: Irritating **[X]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**

Method: LAS solutions at 6 different concentrations ranging from 0.01% to 5.0% were instilled in the eyes of rabbits (3 per group). The rabbits were observed for 168 hours after LAS application.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: LAS (chain length distribution C_{10-14}; 80.9% of C_{11-13}) (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = $C_{11.7}$

Remarks: Information as cited in IPCS document. The 0.01% group showed no reaction. Within 2 hours, the 0.05% group showed slight congestion and the 0.1% group showed considerable congestion or oedema, which disappeared at 24 hours. In the group of 0.5% and higher, marked reactions such as severe congestion an oedema, increased secretion, turbidity of the cornea, and disappearance of the corneal reflex were observed for 24 hours. The effects disappeared completely at 120 hours.

Reference: Iimori, M., Ogata, T. and Kudo, K. 1972. Eye irritation testing of surface active agents in experimental animals. Jour. Jap. Oil Chem. Soc. 22:807-813 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(g)

Species/strain: New Zealand albino rabbits

Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[ ]**; Not irritating **[X]**

Method: OECD Guideline 405. Six rabbits were exposed to 0.1 ml of 1% LAS, which was placed into the conjunctival sac of one eye per animal. The eyelids were gently held together for one second and then released. No irrigation step was performed The eyes were examined at 1, 24, 48 and 72 hours and at 7 days and scored for irritation using the standard system.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: LAS (made from Sirene LAB); activity 1%; average alkyl chain length = $C_{11.6}$

Remarks: Average irritation scores were 0, 0, 0.1, and 0.1 for the cornea, iris, conjunctival redness, and conjunctival chemosis, respectively. This classifies LAS at 1% as not irritating.

Reference: Biolab SGS. 1984. Acute eye irritation. Report No. T3R/27.

Reliability: 2 Valid with restrictions

(h)

Species/strain: New Zealand albino rabbits

Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[ ]**; Moderate irritating **[X]**; Slightly irritating **[ ]**; Not irritating **[ ]**

Methods: OECD Guideline 405. Six rabbits were exposed to 0.1 ml of 5% LAS, which was placed into the conjunctival sac of one eye per animal. The eyelids were gently held together for one second and then released. No irrigation step was performed The eyes were examined at 1, 24, 48 and 72 hours and at 7 days and scored for irritation using the standard system.

GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS (made from Sirene LAB); activity 5%; average alkyl chain length = $C_{11.6}$
Remarks: Average irritation scores were 0, 0, 1.83, and 1.16 for the cornea, iris, conjunctival redness, and conjunctival chemosis, respectively. This classifies LAS at 5% as moderately irritating.
Reference: Biolab SGS. 1988. Acute eye irritation. Report No. T343.
Reliability: 2 Valid with restrictions

(i)
Species/strain: albino male and female rabbits
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[X]**; Slightly irritating **[ ]**;
Not irritating **[ ]**
Classification: Irritating **[X]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method: A total of 100 mg of finely ground sample was administered in the conjunctival sac of the right eye of each of six albino male and female rabbits. Observations for inflammation were made over seven days. The treated eyes were washed with sodium chloride solution USP after the 24 hour reading. The left eye served as a control. The data was scored according to the method of Draize, et al. Tests were conducted in accordance with the Federal Hazardous Substance Act.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Sodium sulfonate of linear alkylbenzene (Alkylate-225) C_9 1%, C_{10} 7%, C_{11} 25%, C_{12} 48%, C_{13} 19%, C_{14} 1%; average alkyl chain length = $C_{11.9}$
Remarks: The compound is classified as an eye irritant under the grading system as outlined in the Federal Hazardous Substances Act. Slight to moderate erythema was present after 10 minutes and persisted through 72 hours. Edema was present after 1 hour and persisted through 24 hours. The average maximum irritation score was 19.3 out of a possible 110.
Reference: Monsanto Company. 1971. Linear alkylbenzene sodium sulfonate – Alkylate 225 Lot CC 6450 – Acute toxicity screen. Project No. Y-71-119. Unpublished report.
Reliability: 2 Valid with restrictions

(j)
Species/strain: albino male and female rabbits
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**;
Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[X]**;
Not irritating **[ ]**
Classification: Irritating **[X]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method: A total of 100 mg of finely ground sample was administered in the conjunctival sac of the right eye of each of three albino male and female rabbits. Observations for inflammation were made over seven days. The treated eyes were washed with isotonic saline solution after the 24 hour reading. The left eye served as a control. The data was scored according to the method of Draize, et al. Tests were conducted in accordance with the Federal Hazardous Substance Act.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Sodium sulfonate of linear alkylbenzene (Alkylate-215) C_9 1%, C_{10} 16%, C_{11} 43%, C_{12} 40%, C_{13} 1%, C_{14} <1%; average alkyl chain length = $C_{11.35}$
Remarks: Slight erythema and a copious discharge were present 10 minutes after application. A slight erythema persisted for 72 hours after which the eyes returned to normal. The average maximum score was 10 out of a possible 110 after 24 hours. This compound is classified as a slight eye irritant.

Reference: Monsanto Company. 1972a. Linear alkylbenzene sodium sulfonate – Alkylate 215 Lot CC 6772S – Acute toxicity screen. Project No. Y-72-274. Unpublished report.
Reliability: 2 Valid with restrictions

(k)
Species/strain: albino male and female rabbits
Results: Highly corrosive **[ ]**; Corrosive **[ ]**; Highly irritating **[ ]**; Irritating **[ ]**; Moderate irritating **[ ]**; Slightly irritating **[X]**; Not irritating **[ ]**
Classification: Irritating **[X]**; Not irritating **[ ]**; Risk of serious damage to eyes **[ ]**
Method: A total of 100 mg of finely ground sample was administered in the conjunctival sac of the right eye of each of three albino male and female rabbits. Observations for inflammation were made over seven days. The treated eyes were washed with isotonic saline solution after the 24 hour reading. The left eye served as a control. The data was scored according to the method of Draize, et al. Tests were conducted in accordance with the Federal Hazardous Substance Act.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Sodium sulfonate of linear alkylbenzene (Alkylate-222L; average alkyl chain length = $C_{11.5}$)
Remarks: Moderate erythema and slight edema and a copious discharge were present 10 minutes after application. A slight erythema persisted for 72 hours after which the eyes returned to normal. The average maximum score was 18 out of a possible 110 after 24 hours. This compound is classified as a mild eye irritant.
Reference: Monsanto Company. 1972b. Linear alkylbenzene sodium sulfonate – Alkylate 222L Lot CC 6773S – Acute toxicity screen. Project No. Y-72-275. Unpublished report.
Reliability: 2 Valid with restrictions

5.3 SKIN SENSITIZATION

(a)
Type: Sensitisation test
Species/strain: Guinea pig (males & females, albino)
Results: Sensitising **[ ]**; Not sensitising **[X]**; Ambiguous **[ ]**
Classification: Sensitising **[ ]**; Not sensitising **[X]**
Method: Buehler Test; OECD Guideline 406 "Skin Sensitization" 1981; Directive 84/449, EEC B.6. "Acute Toxicity - Skin Sensitization".
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test Substance: LAS; activity: 6.7%; average alkyl chain length = $C_{11.6}$
Remarks: The purpose of this study was to assess the allergenic potential of LAS when administered to the skin. 10 animals (5M/5F) remained untreated and were used as controls to be treated at first challenge. 10 animals (5M/5F) remained untreated and were used as additional controls to be treated at second challenge; 20 animals (10M/10F) were treated with LAS. Induction concentration was 1.0% in water; first and second challenge concentrations were 0.8% in water. 0/20 animals responded in the treated group; 0/10 animals responded in the control group.
Reference: European Commission. 2000o. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition, citing The Procter & Gamble Company, unpublished data, Reports No. RCC-2315547.
Reliability: 4 Not assignable

(b)

Type:	Guinea pig maximisation test
Species/strain:	guinea pig, females
Results:	Sensitising **[ ]**; Not sensitising **[X]**; Ambiguous **[ ]**
Classification:	Sensitising **[ ]**; Not sensitising **[X]**
Method:	OECD Guide-line 406 "Skin Sensitisation" 1981
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	Marlon A 350 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; activity: 50%.
Remarks:	0.1% intracutaneous and 3% epidermal doses. No sensitizing effects were observed.
Reference:	Murmann, P. 1988. Prufung auf hautsensibilisierende Wirkung am Meerschweinchen von Marlon A 350. Huels Report No. 1387.
Reliability:	2 Valid with restrictions

(c)

Type:	Maximization test
Species/strain:	Guinea pig, Hartley
Results:	Sensitising **[ ]**; Not sensitising **[X]**; Ambiguous **[ ]**
Classification:	Sensitising **[ ]**; Not sensitising **[X]**
Method:	OECD Guideline 406, 1981; Directive 179/831 Annex, Part B.
GLP:	Yes **[X]** No **[ ]** ? **[ ]**
Test substance:	LAS, activity: 50%; average alkyl chain length = $C_{11.6}$
Remarks:	Solutions of LAS were applied intracutaneously and epicutaneously to 10 male and 10 female animals. Induction concentration was 25% in water; the challenge concentration was 12.5%. No positive responses were observed.
Reference:	RBM. 1985. Test di sensibilizzazione cutanea nella cavia. RBM Exp. No. 2076.
Reliability:	1 Valid without restriction

5.4 REPEATED DOSE TOXICITY

(a)

Species/strain:	Rat (FDRL)
Sex:	Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Administration:	Oral feed
Exposure period:	12 weeks
Dose:	50 or 250 mg/kg bw d
Control group:	Yes **[X]**; No **[ ]**; No data **[ ]**; Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL:	50 mg/kg bw d
LOAEL:	250 mg/kg bw d
Results:	No behavioural abnormalities were noted during the test period. Growth responses were equal in all groups. There were no differences in food intake or in efficiency of food utilization. The clinical data showed no abnormal variations in any of the dose groups. The relative organ weights and the histopathological evaluation did not show significant differences among the dose groups except a liver weight increase in female animals of the high dose group.
Method:	Based on Fitzhugh and Schouboe (1959) Subacute toxicity in: Assoc. Food Drug Offices of the U.S., Austin, Texas, p. 26-35. Weanling rats were distributed into 5 groups of 15 male and 15 female animals per dose group. All rats were given standard diet daily. Doses were 0, 50 and 250 mg/kg bw d in the diet. Daily observations of behavior and signs of toxicity were made. Food consumption and blood and urine chemistries were also measured

periodically. Organ weights and gross pathological findings were measured at the end of the study in the liver, kidneys, spleen, heart, adrenals, pituitary, and cecum.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: C_{10-13} LAS, sodium salt, activity: 39.5%; average molecular weight 346; average alkyl chain length = 11.9

Reference: Oser, B.L. and Morgareidge, K. 1965. Toxicological studies with branched and linear alkyl benzene sulfonates in rats. Toxicol. Appl. Pharmacol. 7:819-825.

Reliability: 2 Valid with restrictions

(b)

Species/strain: rat (Sprague-Dawley)

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**

Administration: oral feed

Exposure period: 90 days

Frequency of treatment: *Ad libitum*

Dose: 0.02/0.1/0.5% (corresponding to 8.8, 44 and 220 mg/kg bw d)

Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOAEL: 0.5% (220 mg/kg bw d)

Results: No adverse effects were found upon the following parameters: growth, food efficiency, survival, haematologic values, and urinary analytical values. In addition, no treatment-related adverse effects were observed in absolute and relative organ weights, nor were gross histopathological changes observed in any of the organs examined.

Method: Groups of 10 male and 10 female weanling rats were fed levels of 0.02, 0.1 or 0.5% LAS in a commercial chow for 90 days. Body weights, food consumption, mortality, and several blood parameters were measured periodically during the study and at termination. Autopsy and microscopic examination of the organs was performed at test termination. Organ weights and gross pathological findings were recorded for the liver, kidneys, spleen, gonads, heart, and brain.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: C_{10-14} LAS, sodium salt (CAS #69669-44-9), activity: 87.9%; C_{10} 1.8%, C_{11} 43.2%, C_{12} 32.2%, C_{13} 16.0%, C_{14} 5.3%, C_{15} 1.5%; average alkyl chain length = $C_{11.8}$; mean molecular weight 346.

Remarks: Two male rats at the 0.2% level died in the early stages of the study. These deaths were attributed to respiratory illness and were not considered to be treatment related.

Reference: Kay, J.H., Kohn, F.E. and Calandra, J.C. 1965. Subacute oral toxicity of a biodegradable linear alkylbenzene sulfonate. Toxicol. Appl. Pharmacol. 7:812-818.

Reliability: 2 Valid with restrictions

(c)

Species/strain: Rat/Sprague-Dawley

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**

Administration: gavage

Exposure period: one month

Frequency of treatment: daily

Dose: 125, 250, 500 mg/kg bw d.

Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOAEL: 125 mg/kg bw d

LOAEL: 250 mg/kg bw d

Results: Diarrhea was observed in the 500 mg/kg group and soft stools were observed in the other 2 groups. Body weight gain was suppressed in all the male groups and in the female 500 mg/kg group. Haematological examinations revealed no abnormalities. Serum-biochemical examinations revealed several differences among the mid and high dose group compared to the control group. The weight of the spleen and the heart significantly decreased in the male high dose group. In the female high dose group, the weight of the liver increased while the weight of the heart and thymus decreased. Histological findings of the liver revealed no abnormalities.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Remarks: Information as cited in IPCS document. 12 animals per dose group.

Test substance: C_{10-13} LAS, sodium salt (CAS #68411-30-3)
$<C_{10}$ 0.1%, C_{10} 10.1%, C_{11} 33.7%, C_{12} 31.0%, C_{13} 25.1%; average alkyl chain length = $C_{11.7}$; activity: 99.5%

Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Ito, R., Kawamura, H., Chang, H.S., Kudo, K., Kajiwara, S., Toida, S., Seki, Y., Hashimoto, M. and Fukushima, A. 1978. J. Med. Soc. Toho, Japan, 25:850-875 (in Japanese). cited in IPCS. 1996. Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates and Related Compounds. World Health Organization, Geneva, Switzerland.

Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(d)

Species/strain: Rat (Wistar)

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**

Administration: oral feed

Exposure period: 9 months

Frequency of treatment: Daily in feed

Dose: 0.6% and 1.8% (260 and 780 mg/kg bw d)

Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**

LOAEL: = 0.6% (260 mg/kg bw d)

Results: In the 1.8% dose group, the body weight gain was suppressed and haematological and serum-biochemical adverse effects were observed in both treatment groups of both sexes. The weight of the cecum of the male rats and the weight of the liver and cecum of the females in the high dose groups were significantly increased. Enzymatic examinations of the liver and kidneys revealed changes in different enzyme activities in the 1.8% groups. The intake of LAS was 230 mg/kg bw d in the male 0.6% group and 290 mg/kg bw d in the female 0.6% group.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: C_{10-14} LAS, sodium salt (CAS #69669-44-9) C_{10} 10.6%, C_{11} 34.1%, C_{12} 27.7%, C_{13} 19.0%, C_{14} 8.7%; average alkyl chain length = $C_{11.8}$; mean molecular weight: 345.8.

Remarks: Information as cited in IPCS document. 8 rats were used per dose group.

Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Yoneyama, M., Mabuchi, Y., Ikawa, M., Kobayaski, H. and Ichikawa, H. 1976. Subacute toxicity of linear alkyl benzene sulfonate. Ann. Rep. Tokyo Metr. Res. Lab. P.H. 27(2): 105-112 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(e)
Species/strain: Rat (Wistar)
Sex: Female **[ ]**; Male **[X]**; Male/Female **[ ]**; No data **[ ]**
Administration: oral feed
Exposure period: 2, 4, 12 weeks
Frequency of treatment: Daily in feed
Dose: 1.5% (750 mg/kg bw d)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
LOAEL: 1.5% (750 mg/kg bw d)
Results: LAS suppressed body weight gain, and the relative liver weight was increased from 2 weeks of LAS administration. Serum biochemical examinations revealed significant increases in ALP and GTP at each observation period and significant decreases in cholesterol and protein in 4 weeks. Enzymatic examinations of the liver revealed decreases in G6Pase and G6PDH and an increase in isocitrate dehydrogenase (IDH) at each observation period. Enzymatic examinations of the renal cortex revealed decreases in G6Pase and 5'-nucleotidase at each observation period, an increase in LDH at 12 weeks, and an increase in IDH at 2 and 4 weeks. Enzymatic examinations in the renal medulla revealed a decrease in NA,K-ATPase, an increase in LDH at 12 weeks, a decrease in IDH at 2 weeks, and an increase in IDH at 12 weeks.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS (unspecified)
Remarks: Information as cited in IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Ikawa, M., Yoneyama, M., Nakao, T. and Hiraga, K. 1978. Uptake of organic acid and organic base by renal cortical slices of rats treated with LAS and ABS. Ann. Rep. Tokyo Metr. Res. Lab. P.H. 29:51-54 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(f)
Species/strain: Rat (Wistar)
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Administration: oral feed
Exposure period: 6 months
Frequency of treatment: Daily in feed
Dose: 0.07, 0.2, 0.6, 1.8% (40, 115, 340, 1030 mg/kg bw d)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL: = 40 mg/kg bw d
LOEL: = 115 mg/kg bw d
Results: The 1.8% group showed diarrhoea, markedly suppressed growth, increased weight of the cecum, and remarkable degeneration of the renal tubes. The 0.6% group showed slightly suppressed growth, increased weight of the cecum, increased activity of serum alkaline phosphatase (ALP), a decrease in

serum protein and degeneration of the renal tubes. The 0.2% group showed increased weight of the cecum and slight degeneration of the renal tubes, the 0.07% group showed no adverse effects related to the administration of LAS. The intake of LAS in the 0.07% group was about 40 mg/kg bw d.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: C_{10-14} LAS, sodium salt (CAS #69669-44-9). C_{10} 10.6%, C_{11} 34.1%, C_{12} 27.7%, C_{13} 19.0%, C_{14} 8.7%; average alkyl chain length = $C_{11.8}$; mean molecular weight: 345.8.

Remarks: Information as cited in IPCS document. This is a key study for repeated dose toxicity because it represents the lowest LOAEL (see SIAR Table 6).

Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.

2) Yoneyama, M. Fujii, T., Ikawa, M., Shiba, H., Sakamoto, Y., Yano, N., Kobayashi, H., Ichikawa, H. and Hiraga, K. 1972. Studies on the toxicity of synthetic detergents. (II) Subacute toxicity of linear and branched alkyl benzene sulfonates in rats. Ann. Rep. Tokyo Metrap. Res. Lab. Public Health. 24:409-440. (In Japanese). cited in IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(g)

Species/strain: Rat

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**

Administration: gavage

Exposure period: 10 weeks

Doses: 50, 100 or 250 mg/kg bw d

Control: Yes **[X]**; No **[ ]**; No data **[ ]**;Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**

LOEL: 50 mg/kg bw d

Results: Histopathology was evaluated in the females only. At the highest dose level, the kidneys showed mild degeneration and desquamation of the tubular epithelium and there was a moderate degree of fatty change in the liver as well as proteinaceous degeneration. Sections of the intestine did not exhibit any significant histologic variation. Adenosine triphosphatase activity was inhibited with increasing dose in both sexes while alkaline phosphatase and acid phosphatase activities were increased with increasing dose. The activity of lactate dehydrogenase was significantly inhibited at all dose levels in females but was not measured in males. SGOT and SGPT were significantly decreased in females at 100 and 250 mg/kg/day and SGPT was inhibited in males at 250 mg/kg/day.

Method: Twenty four male (50+/-5g) and 36 female (40+/-5g) rats were given daily oral (cannula) doses of LAS detergent solution (0, 50, 100 and 250 mg/kg) by gavage for 10 weeks. Animals were maintained on standard pellet diets and drinking water *ad libitum*. After 10 weeks, animals were fasted for 24 hours and sacrificed. Liver, kidney, heart, and intestine were removed immediately, weighed, and parts sectioned for histological examinational. The remaining parts of the liver and kidney homogenized in ice cold 0.25 M sucrose solution using Potter-Elvehjem type homogenizer and 10% w/v homogenates were prepared for histopathology and enzyme analysis. The activities of adenosine triphoshatase (ATPase), acid phosphatase (ACP), alkaline phosphatase (ALP), glutamic oxaloacetic transaminase (GOT), and glutamic pyruvic transaminase (GPT) were determined in the homogenates.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Remarks: All of the effects observed are related to energy metabolism, so given the lack of morphological and structural changes, the reduced food intake and body weight gain may have compromised energy dynamics and affected the enzyme levels. The reliability and use of this study for risk assessment purposes is limited and the 50 mg/kg/day level should be considered a LOEL rather than a LOAEL.
Test Substance: Commercial LAS synthetic detergent solution
Reference: 1) Gupta, B.N., Mathur, A.K., Agarwal, C., and Singh, A. 1986. Effect of synthetic detergent on certain enzymes in liver and kidney in male rats. Arogya-J. Health Sci. 12:50-54.
2) Mathur, A.K., Gupta, B.N., Singh, A., and Shanker, R. 1986. Toxicological evaluation of a synthetic detergent after repeated oral ingestion in rats. Biol. Mem. 12:187-191.
Reliability: 2 Valid with restrictions

(h)
Species/strain: Rat (Wistar)
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Administration: drinking water
Exposure period: 9 months
Frequency of treatment: Daily in drinking water.
Dose: 0.07, 0.2%, 0.6% (85, 145, 430 mg/kg bw d; average of male and female)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL: 0.07% (85 mg/kg bw d)
LOAEL: 0.2% (145 mg/kg bw d)
Results: Body weight gain was suppressed in the male 0.6% group. Hematological examination revealed no significant change in any of the experimental groups, but a dose-related decrease in cholesterol level was seen in males. Significant decreases in the activities of glutamate-oxalate transaminase and lactate dehydrogenase were seen in males at 0.2% and a dose-related increase in the activity of glutamate-oxalate transaminase in females. A significant decrease in renal Na,K-ATPase was seen in the group given 0.2%. No organ weight changes were observed. The intake of LAS was 50 mg/kg bw d in the male 0.07% group and 120 mg/kg bw d in the female group. The values for the 0.2% group were 120 and 170 mg/kg bw d for males and females, respectively.
Method: Groups of 8-9 male and 8-9 female rats were given LAS for 9 months.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Remarks: Information as cited in IPCS document. This is a key study for repeated dose toxicity because it represents the highest NOAEL below the lowest LOAEL (see SIAR Table 6).
Test substance: $C_{10\text{-}14}$ LAS (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = $C_{11.7}$
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Yoneyama, M., Mabuchi, Y., Ikawa, M., Kobayashi, H. and Ichikawa, H. 1976. Subacute toxicity of linear alkylbenzene sulfonate. Ann. Rep. Tokyo Metr. Res. Lab. Public Health 27:105-112 (in Japanese); cited in: IPCS (1996); Environmental Heath Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(i)

Species/strain: mouse (DDY)
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[ ]**; No data **[X]**
Administration: drinking water
Exposure period: 6 months
Frequency of treatment: Daily
Observation period: 2 months post exposure
Dose: 100 ppm in the drinking water (20 mg/kg bw d)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
Results: Atrophy of the golgi apparatus, degeneration of the mitochondria, and increased appearance of lysosomes were observed. The severity of these adverse effects were dependent on the length of the administration. After six months, some cells showed degenerative cytoplasm and indications of cell necrosis. Effects on the rough endoplasmatic reticulum were observed. Some animals still showed cellular effects after the two months post administration period while other animals showed full recovery. Given the unknown significance of the effects for the health of the animals and the reversibility of the effects, as well as the consistent lack of adverse effects in other studies at similar or higher doses, the dose tested in this study is considered a LOEL rather than a LOAEL.
Method: LAS was administered up to 6 months. The animals were sacrificed at 1, 2, 3, and 6 months. Some animals were observed an additional 2 months without test substance administration. Liver slices were investigated using electron microscopy.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Remarks: The reliability and usefulness of this study for risk assessment purposes is limited. The study employed only a single dose (i.e., no dose response information). In addition, there is the likelihood of dehydration of the animals. Because of these study deficiencies, it was determined that it is inappropriate to derive a LOAEL from this study.
Test substance: LAS (unspecified)
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Watari, N., Torizawa, K., Kanai, M. and Suzuki, Y. 1977. Ultrastructural observations of the protective effect of glycyrrhizin for mouse liver injury caused by oral administration of detergent ingredient (LAS) J. Clin. Electron. Microscopy 10:121-139 (in Japanese) cited in IPCS. 1996. Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates and Related Compounds. World Health Organization, Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. While the study was evaluated by IPCS prior to inclusion in their criteria document, the deficiencies noted above make its usefulness in risk assessment questionable.

(j)
Species/strain: mouse (ICR)
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Administration: Oral feed or water
Exposure period: 9 months
Frequency of treatment: Daily
Dose: Diet: 0.6 and 1.8% (corresponding to 500 and 1000 mg/kg bw d).
Diet: Drinking water: 0.07, 0.2, and 0.6% (100, 250, and 600 mg/kg bw d for males and 100, 250, and 900 mg/kg bw d for females)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL: 250 mg/kg bw d in drinking water

LOAEL:	500 mg/kg bw d in diet
Results:	In the mice given 0.6% in their diet, body weight gain was not suppressed, but the weight of the liver increased in male and female mice. Enzymatic examinations revealed significant decreases in LDH of the liver and in acid phosphatase of the kidneys in the male mice. For mice given LAS in drinking water, body weight was depressed at the highest dose for males and females. This dose also elicited an increase in liver weight in females and significant decreases in renal Na and K-ATPase.
Method:	Groups of 8 or 9 mice were given diets containing LAS at concentrations of 0.6 and 1.8% or drinking water containing LAS at concentrations of 0.07, 0.2, and 0.6% for 9 months.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	LAS
Reference:	1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition. 2) Yoneyama, M., Mabuchi, Y., Ikawa, M., Kobayashi, H. and Ichikawa, H. 1976. Subacute toxicity of linear alkylbenzene sulfonate. Ann. Rep. Tokyo Metr. Res. Lab. P.H. 27(2):105-112 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland. 3) HERA. 2002. HERA-LAS Human and Environmental Risk Assessment: Linear Alkylbenzene Sulphonates, LAS. CAS No. 68411-30-3, Draft #6, May 2002.
Reliability:	4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(k)

Species/strain:	Rat: Charles River
Sex:	Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Administration:	oral feed
Exposure period:	2 years
Frequency of treatment:	continuous in feed
Doses:	0.02, 0.1, 0.5% (10, 50, 250 mg/kg bw d)
Control group:	Yes **[X]**; No **[ ]**; No data **[ ]**; Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[X]**
Results:	Gross examination of all animals for pathology did not reveal any abnormalities. No consistent dietary induced changes that could be considered a toxic response were observed. Animals that showed significant loss of weight, development of tumors, or other evidence of abnormalities were sacrificed and tissues examined. The incidence of tumors and the common incidental diseases were similar in all dieting groups. No treatment-related adverse histological effects were observed in any of the tissue sections examined.
Method:	Four groups of Charles River weanling rats, divided by sex, were given 0.5, 0.1, and 0.02% LAS in their food for 2 years. Following completion of those studies, five male and five female rats from each of the parental groups (F_{1b} and F_{2b}) and all survivors were selected for necropsy. Livers and kidneys were removed and weighed. Body weight and organ to body weight ratios were recorded, and routine hematology and histology were performed. Sections for histological examination were taken from the liver, kidney, thyroid, trachea, esophagus, lung, heart, spleen, pancreas, adrenals, stomach, small intestine, urinary bladder, gonads and mesenteric lymph nodes. Weanling animals for the F_{3a} generation were similarly treated.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**

Test substance: C_{10-14} LAS, sodium salt; activity: 98.1% on an anhydrous basis (41.9% active)
Reference: Buehler, E.V., Newmann, E.A., and King, W.R. 1971. Two year feeding and reproduction study in rats with linear alkylbenzene sulfonate (LAS). Toxicol. Appl. Pharmacol. 18:83-91.
Reliability: 2 Valid with restrictions

(l)
Species/strain: Rat/Wistar
Sex: Female **[ ]**; Male **[X]**; Male/Female **[ ]**; No data **[ ]**
Administration: Drinking water
Exposure period: 2 years
Frequency of treatment: Daily
Doses: 0.01%, 0.05%, 0.1% (20,100, 200 mg/kg bw d)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
Results: There were no changes due to the administration of LAS in regard to growth, mortality, the weight of major organs, or histopathological findings. The intake of LAS was about 200 mg/kg bw d in the 0.1% group.
Method: Groups of 20 male Wistar rats were given LAS in drinking water daily for 2 years.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS, activity: 34.55%
Remarks: Information as cited in the IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Tiba, S. 1972. Studies on the acute and chronic toxicity of linear alkylbenzene sulfonate. J. Food Hyg. Soc. Jpn. 16:66-71 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(m)
Species/strain: Rhesus monkey (*Macaca mulatta*)
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Administration: Simultaneous oral and subcutaneous
Exposure period: 28 days
Frequency of treatment: daily
Dose: 30, 150, 300 mg/kg/day oral via gavage given simultaneously with 0.1, 0.5, 1.0 mg/kg/day subcutaneous administration
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL: 150 mg/kg/day (oral) with 0.5 mg/kg/day (sc)
Results: At 300 (oral) and 1.0 (sc) mg/kg/day, the monkeys vomited frequently and usually within 3 hours of administration. An increased frequency of loose or liquid faeces was recorded for animals receiving 150 (oral) and 0.5 (sc) mg/kg. These effects are probably related to the inherent irritative effects of LAS rather than its systemic toxicity. Fibrosis of the injection sites was found among all the test group, the incidence and severity being dose related. Ophthalmoscopy, laboratory examination of blood and urine, organ weight analysis and histopathological investigation did not detect any further treatment-related responses.
Method: Three male and 3 female monkeys were given simultaneous oral and subcutaneous administration doses daily for 28 days. Animals were observed

for physical and behavioral signs of toxicity. Analysis of blood, biochemistry and urine were conducted. Monkeys were held in individual wall-mounted cages at a room temperature of 22^{+}/-1°C and normal daylight. Food consisted of 300 g dry diet and bread daily, and fresh fruit on alternate days. Tap water for drinking was freely available.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: C_{10-13} LAS, activity: 20.5%

Remarks: The SDA/NOTOX report sets a systemic NOAEL of 30 mg/kg/day (oral) with 0.1 mg/kg/day (sc). However, based on the information provided in the article and reiterated above, the actual systemic NOAEL is considered to be 150 mg/kg/day (oral) with 0.5 mg/kg/day (sc). According to the authors, the three combined doses correspond to 100, 500 and 1000 times the estimated maximum human daily intake.

Reference: Heywood, R., James, R.W., and Sortwell, R.J. 1978. Toxicology studies of linear alkylbenzene sulphonate (LAS) in rhesus monkeys. I. Simultaneous oral and subcutaneous administration for 28 days. Toxicology 11:245-250.

Reliability: 2 Valid with restrictions

(n)

Species/strain: Rat (Wistar)

Sex: Female **[ ]**; Male **[X]**; Male/Female **[ ]**; No data **[ ]**

Administration: Dermal

Exposure period: 15 days

Frequency of treatment: daily

Dose: 0.5 g applied 20 and 30% LAS solutions (about 286 and 427 mg/kg bw d)

Control group: Yes **[ ]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**

LOAEL: 20% (286 mg/kg bw d) (lowest dose tested)

Results: Body weight gain was suppressed in the 20% group and the body weight was decreased in the 30% group. An infiltrating, yellowish-reddish brown crust was observed 2-3 days in the 20% group, and at 1-2 days in the 30% group. At 4-6 days the crust was abraded and erosion occurred at the abraded site. Histological examinations of the application site revealed severe necrosis of the region from the epidermis cuticle to the upper layer of the dermis, severe infiltration of leukocytes in the necrotic site, diffuse inflammatory cell infiltration of all layers of the corium. No changes were observed in the tongue, but the oral mucosa revealed atrophy and slight degeneration of the epithelium. No systemic effects were observed.

Method: LAS was applied to the backs of the rats. On the 16th day of the experiment, skin at the application site and the tissues of the tongue and oral mucosa (to examine the effects of licking) of the rats that received 30% were examined histologically.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: LAS, activity: 99.9%

Remarks: Information as cited in the IPCS document. Because of necrosis at the application site, it is not possible to know exactly how much LAS was absorbed. Effects were probably due to local effects, so the results are best described as a local LOAEL.

Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Sadai, M. and Mizuno, N. 1972. Effect of long term topical application of some anionic surfactants on the skin, oral mucous membrane, and tongue. Jpn Journal Dermatol. 82:207-221. (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

(a)
Type: Ames test
System of testing: *Salmonella typhimurium* TA 1535, TA 1537, TA 1538, TA 98, TA 100
Concentration: 8 -5000 ug/plate
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation: > 5000 μg/plate
Without metabolic activation: > 5000 μg/plate
Genotoxic effects: + ? -
With metabolic activation: **[ ] [ ] [X]**
Without metabolic activation: **[ ] [ ] [X]**
Method: Directive 84/449/EEC, B.14 Mutagenicity (*Salmonella typhimurium* - reverse mutation assay)" 1984
GLP: Yes **[X]** No **[ ]** ? **[ ]**
Test substance: Marlon A 390 (CAS #68411-30-3) C_{10-13} LAS, average alkyl chain length = $C_{11.6}$; activity 91.3%
Remarks: Negative and positive controls used.
Reference: Schoeberl, P. 1993a. Bestimmung der Mutagenitat von Marlon A 390 im Salmonella/Sauger-Mikrosomen-Mutagenitatstest nach Ames. Huels Final Report No. AM-93/12.
Reliability: 1 Valid without restriction

(b)
Type: Ames test
System of testing: *Salmonella typhimurium* TA 100, TA 98
Concentration: 10, 25, 50, 100 and 200 ug/plate
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation: > 200 μg/plate
Without metabolic activation: > 200 μg/plate
Genotoxic effects: + ? -
With metabolic activation: **[ ] [ ] [X]**
Without metabolic activation: **[ ] [ ] [X]**
Method: Ames test
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{10-14} LAS, sodium salts (CAS#69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = $C_{11.7}$; activity: 22.2%
Remarks: Not mutagenic
Reference: Inoue, K., Sunakawa, T. and Takayama, S. 1980. Studies of *in vitro* cell transformation and mutagenicity by surfactants and other compounds. Fd. Cosmet. Toxicol. 18:289-296.
Reliability: 2 Valid with restrictions

(c)
Type: Ames test
System of testing: *Salmonella typhimurium* TA 98, TA 100
Concentration: up to 500 ug/plate

Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation: > 500 μg/plate
Without metabolic activation: > 500 μg/plate
Genotoxic effects: + ? -
With metabolic activation: **[ ] [ ] [X]**
Without metabolic activation: **[ ] [ ] [X]**
Method: Ames test
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{10-14} LAS, sodium salts (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = $C_{11.7}$; activity: 20.5%
Remarks: Information as cited in IPCS documents. Not mutagenic
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Sunakawa, T., Inoue, K. and Okamoto, K. 1981. Studies on the mutagenicity of surfactants, mutagenicity of surfactants following activation with various liver homogenates (S-9) and mutagenicity in the presence of norharman. Hyg. Chem. 27:204-211. (In Japanese); Cited in IPCS. 1996. Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates and Related Compounds. World Health Organization, Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(d)
Type: *Bacillus subtilis* recombination assay
System of testing: H17 (rec+) and M45 (rec-)
Concentration: Up to 50 μg/plate
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:
Cytotoxicity conc: With metabolic activation: > 50 μg/plate
Without metabolic activation: > 50 μg/plate
Genotoxic effects: + ? -
With metabolic activation: **[ ] [ ] [X]**
Without metabolic activation: **[ ] [ ] [X]**
Method: *Bacillus* recombination assay
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{10-14} LAS, sodium salts (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = $C_{11.7}$; activity: 99.5%
Remarks: Information as cited in IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Inoue, IK. and Sunakawa, T. 1979. Mutagenicity tests of surfactants. Jpn Fragrance J. 38:67-75 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: for Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(e)
Type: *Escherichia coli* reverse mutation assay.
System of testing: WP23 uvr A
Concentration: Not specified
Metabolic activation: With **[ ]**; Without **[ ]**; With and Without **[X]**; No data **[ ]**
Results:

Cytotoxicity conc:	With metabolic activation:	Not specified
	Without metabolic activation:	Not specified
Genotoxic effects:		+ ? -
	With metabolic activation:	**[ ] [ ] [X]**
	Without metabolic activation:	**[ ] [ ] [X]**

Method: *E. coli* assay
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{10-14} LAS, sodium salt; activity: 99.5%
Remarks: Information as cited in IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Inoue, I.K. and Sunakawa, T. 1979. Mutagenicity tests of surfactants. Jpn Fragrance J. 38(7)(5):67-75 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

B. NON-BACTERIAL IN VITRO TEST

Type: Transformation test with SHE-cells
System of testing: Syrian hamster embryo (SHE) cells
Concentration: up to 50 ug/mL
Metabolic activation: With **[ ]**; Without **[X]**; With and Without **[ ]**; No data **[ ]**
Results:

Cytotoxicity conc:	Without metabolic activation: 50 μg/mL	
Genotoxic effects:		
		+ ? -
	Without metabolic activation:	**[ ] [ ] [X]**

Method: Cell cultures were prepared and plated in 75 cm^2 flasks containing 20 mL of culture medium. On day 5, target cells were trypsinized and a suspension of target cells was added to the solution plated on complete medium. Plates were dosed on day 6. Nine dishes were used for each dose level. On day 14, the cultures were fixed, stained, and examined to count normal and transformed colonies.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{10-14} LAS, sodium salts (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = $C_{11.7}$; activity: 22.2%
Remarks: LAS did not produce transformation at any of the doses tested.
Reference: Inoue, K., Sunakawa, T., and Takayama, S. 1980. Studies of *in vitro* cell transformation and mutagenicity by surfactants and other compounds. Fd. Cosmet. Toxicol. 18:289-296.
Reliability: 2 Valid with restrictions

5.6 GENETIC TOXICITY IN VIVO

(a)
Type: Mammalian bone marrow cytogenetic assay
Species/strain: mouse: ICR: JCL
Sex: Female **[ ]**; Male **[X]**; Male/Female **[ ]**; No data **[ ]**
Administration: gavage
Exposure period: 5 days and 1 day
Doses: 200, 400, 800 mg/kg bw d

Results:	There was no significant difference in the incidence of chromosomal aberrations between any of the groups given LAS and the negative control group.
Control Group:	Concurrent no treatment, positive and historical controls were used.
Method:	Chromosomal aberrations were examined 6, 24, 48 hours after administration. Mytomycin C was used as a positive control and appropriately induced severe chromosomal aberrations.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	C_{10-14} LAS, sodium salt (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = 11.7
Remarks:	Besides the pure LAS, commercial preparation containing 19% LAS and another containing 17.1% LAS were given to mice as single doses only by gavage at 800, 1600 or 3200 mg/kg bw d and 1000, 2000 or 4000 mg/kg bw d, respectively. The highest doses were 50% of the respective LD_{50} values. No significant differences in the incidence of chromosomal aberrations were observed in any LAS treatment relative to the controls. Information as cited in the IPCS document.
Reference:	1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition. 2) Inoue, K., Shibata, T., Hamano, Y., Oda, Y., Kuwano, A., Yamamoto, H., Mitsuda, B. and Kunita, N. 1977. *In vivo* cytogenetic tests of some synthetic detergents in mice. Ann Res. Osaka Prefect Inst. Public Health. 8:17-24 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability:	4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document

(b)

Type:	Mammalian bone marrow cytogenetic assay
Species/strain:	rat (Wistar, SD); mouse (ICR)
Sex:	Female **[ ]**; Male **[X]**; Male/Female **[ ]**; No data **[ ]**
Administration:	oral feed
Exposure period:	9 months
Doses:	0.9% (450 mg/kg bw d in rats; 1170 mg/kg bw d in mice)
Results:	There were no significant differences in the incidences of chromosomal aberrations between the experimental and control groups.
Method:	Groups of 5 male Wistar rats, Sprague-Dawley rats, and ICR mice were given a diet containing 0.9% LAS for 9 months after which the chromosomes of the bone marrow cells were examined.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	LAS
Remarks:	Information as cited in the IPCS document.
Reference:	1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition. 2) Masabuchi, M., Takahashi, A., Takahashi, O. and Hiraga, K. 1976. Cytogenetic studies and dominant lethal tests with long term administration of butylated hydroxytoluene (BHT) and linear alkylbenzene sulfonate (LAS) in mice and rats. Ann. Rep. Tokyo Metrop. Res. Lab. Public Health. 27:100-104 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability:	4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(c)

Type:	Dominant lethal assay
Species/strain:	mouse (ICR: JCL)
Sex:	Female **[ ]**; Male **[X]**; Male/Female **[ ]**; No data **[ ]**
Administration:	oral feed
Exposure period:	9 months
Doses:	0.6% (300 mg/kg bw d)
Results:	There were no significant differences in fertility, the mortality of ova and embryos, the number of surviving fetuses, or the index of dominant lethal induction between the experimental groups and the control group.
Method:	Seven male mice received LAS in the diet for 9 months. Each of the male mice was then mated with 2 female mice that had not been given LAS. The pregnant mice were laparotomized on day 13 of gestation to determine the numbers of luteal bodies, implantations, surviving fetuses, and dead fetuses.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	LAS
Remarks:	Information as cited in the IPCS document.
Reference:	1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition. 2) Masabuchi, M., Takahashi, A., Takahashi, O. and Hiraga, K. 1976. Cytogenetic studies and dominant lethal tests with long term administration of butylated hydroxytoluene (BHT) and linear alkylbenzene sulfonate (LAS) in mice and rats. Ann. Rep. Tokyo Metrop. Res. Lab. Public Health. 27:100-104 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability:	4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(d)

Type:	Micronucleus assay
Species/strain:	mouse: (ddy)
Sex:	Female **[ ]**; Male **[X]**; Male/Female **[ ]**; No data **[ ]**
Administration:	Intraperitoneal injection
Exposure period:	single dose
Doses:	100 mg/kg bw
Results:	There were no differences in the incidences of polychromatic erythrocytes with micronuclei in the bone marrow cells between the treated group and the control group.
Method:	Three male ddy mice were each given a single i.p. injection of 100 mg/kg bw LAS.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	LAS
Remarks:	Information as cited in the IPCS document.
Reference:	1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition. 2) Kishi, M., Satoh, S., Horiguchi, Y. and Ito, K. 1984. Effects of surfactants on bone marrow cells. Bull. Kanagaw Public Health Lab. 14:57-58. (In Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

5.7 CARCINOGENICITY

(a)
Species/strain: Rat: Charles River
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Administration: oral feed
Exposure period: 2 years
Frequency of treatment: continuous in feed
Doses: 0.02, 0.1, 0.5% (10, 50, 250 mg/kg bw d)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[X]**
Results: Gross examination of all animals for pathology did not reveal any abnormalities. No consistent dietary induced changes that could be considered a toxic response were observed. Animals that showed significant loss of weight, development of tumors, or other evidence of abnormalities were sacrificed and tissues examined. The incidence of tumors and the common incidental diseases were similar in all dieting groups.
Method: Four groups of Charles River weanling rats, divided by sex, were given 0.5, 0.1, and 0.02% LAS in their food for 2 years. Following completion of those studies, five male and five female rats from each of the parental groups (F_{1b} and F_{2b}) and all survivors were selected for necropsy. Body weight and organ to body weight ratios were recorded, and routine hematology and histology were performed. Weanling animals for the F_{3a} generation were similarly treated.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{10-14} LAS; activity: 98.1% on an anhydrous basis (41.9% active)
Reference: Buehler, E.V., Newmann, E.A., and King, W.R. 1971. Two year feeding and reproduction study in rats with linear alkylbenzene sulfonate (LAS). Toxicol. Appl. Pharmacol. 18:83-91.
Reliability: 2 Valid with restrictions

(b)
Species/strain: Rat/Wistar
Sex: Female **[ ]**; Male **[X]**; Male/Female **[ ]**; No data **[ ]**
Administration: Drinking water
Exposure period: 2 years
Frequency of treatment: Daily
Doses: 0.01%, 0.05%, 0.1% (20,100, 200 mg/kg bw d)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
Results: There were no changes due to the administration of LAS in regard to growth, mortality, the weight of major organs, or histopathological findings. The intake of LAS was about 200 mg/kg bw d in the 0.1% group. There is no description of tumors.
Method: Groups of 20 male Wistar rats were given LAS in drinking water daily for 2 years.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS, activity: 34.55%
Remarks: Information as cited in the IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.

2) Tiba, S. 1972. Studies on the acute and chronic toxicity of linear alkylbenzene sulfonate. J. Food Hyg. Soc. Jpn. 16:66-71 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document

(c)
Species/strain: Rat/Wistar
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Administration: drinking water
Exposure period: up to 26 months
Frequency of treatment: Daily
Doses: 0.1% (140 mg/kg bw d)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
Results: The administration of LAS had no effect on the intake of water, mortality, body weight gain, or general condition. In pathological examination, looseness, atrophy, and fatty change of the hepatic cells in the liver were found in the experimental group at 6 months. The experimental group showed significant increases in GOT, GTP and bilirubin at 6 months and thereafter. In haematological examinations no effects due to LAS were observed.
Method: A group of 62 male and 62 female rats were given drinking water treated with LAS and a control group of 37 male and 37 female rats were given pure water. Five to 12 of the rats in the experimental group and 3 to 12 rats in the control group at 3, 6, 12, and 18 months, respectively, and all surviving rats between 24 and 26 months, were sacrificed for pathological, biochemical, and haematological examinations.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS; mean molecular weight 348; average alkyl chain length = $C_{12.0}$; activity: 38.74%
Remarks: Information as cited in the IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Endo, T., Furuido, Y., Namie, K., Yamamoto, N., Hasunuma, H. and Ueda, K. 1980. Studies of the chronic toxicity and teratogenicity of synthetic surfactants. Ann. Rep. Tokyo Metrop. Res. Inst. Environ. Prot. 236-246 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(d)
Species/strain: Rat/Wistar
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Administration: oral feed
Exposure period: 1, 3, 6, 24, or more months
Frequency of treatment: Daily
Doses: 0.04, 0.16, 0.6% (20, 80, 300 mg/kg bw d)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**

Results:	The 0.6% group showed slight increases in the weight of liver and cecum, and increased activity of GPT and ALP in serum. LAS administration had no adverse effects upon the intake of food, body weight gain, general condition, mortality or mean survival. At one month, proliferation of hepatic cells in the liver and slight swellings of the renal tubes and narrowing of the tubular lumen in the kidneys were found in the 0.16% and 0.6% groups. These findings later disappeared, and are considered to be adaptation phenomena to the administration of LAS. There were no histopathological lesions attributable to LAS administration in any of the organs in rats fed for 24 months or more. Various types of tumors were observed in various organs, but findings suggestive of tumorigenicity of LAS were not present. Therefore, the authors concluded that the diet containing LAS at a concentration of 0.6% (300 mg/kg bw d) did not have any adverse effects on rats.
Method:	Groups of 50 male and 50 female rats were given diets containing LAS at 0.04, 0.16 and 0.6%. In each group, 5 rats of each sex were fed for 1, 3, 6, and 12 months, respectively, and groups of 15 rats of each sex were fed for 24 months or more. Detailed histopathological examinations were made on the rats.
GLP:	Yes **[ ]** No **[X]** ? **[ ]**
Test substance:	C_{10-14} LAS; C_{10} 10.6%, C_{11} 34.1%, C_{12} 27.7%, C_{13} 19.0%, C_{14} 8.7%; average alkyl chain length = $C_{11.8}$; mean molecular weight 345.8
Reference:	1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition. 2) Fujii, T., Sakamoto, Y., Abe, Y., Mikurita, H., Yuzawa, K. and Hiraga, K. 1977. Pathological examination of rats fed with linear alkylbenzene sulfonate for their lifespan. Ann. Rep. Tokyo Metrop. Res. Lab. Public Health. 28:85-108 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland. 3) Yoneyama, M., Masubuchi, M., Oishi, S., Takahashi, O., Ikawa, M., Yoshida, S., Oishi, H., Mikuriya, H., Yuzawa, K. and Hiraga, K. 1977. Subacute toxicity of linear alkylbenzene sulfonate. Ann. Rep. Tokyo Metrop. Res. Lab. Public Health. 28:73-84 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability:	4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

5.8 TOXICITY TO REPRODUCTION

(a)

Type:	Fertility **[ ]**; One-generation study **[ ]**; Two-generation study **[ ]**; Other **[X] :** 3-generation reproduction study
Species/strain:	Rat: Charles River
Sex:	Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Administration:	oral feed
Exposure period:	2 years
Frequency of treatment:	continuous in feed
Premating exposure period:	male: 84 days, female: 84 days
Duration of the test:	3 generations
Doses:	0.02, 0.1, 0.5% (14, 70, 350 mg/kg bw d)
Control group:	Yes **[X]**; No **[ ]**; No data **[ ]**;

Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[X]**
NOAEL Parental: = 0.5%. (350 mg/kg bw d)
NOAEL F1 Offspring: = 0.5% (350 mg/kg bw d)
NOAEL F2 Offspring: = 0.5% (350 mg/kg bw d)
Results: General reproduction including fertility gestation, parturition, neonatal viability, lactation, and post-weaning growth was normal for all test groups and did not deviate from the controls in each generation. No gross abnormalities were noted. No definitive adverse effects due to the test material were noted in the haematology and pathology.
Method: Na-LAS (chain length distribution C_{10-14}) was fed for 84 days to 4 groups of weanling rats (3 dose levels, plus control), each dose consisting of 50 animals each of both sexes (P_O-generation). When the P_0 generation was 107-112 days old, 20 females from each dose group were mated with 20 males from the same group and maintained together for 17 days. The first litters of each generation (F_{1a}- and F_{2a}-generation) were sacrificed at 21 days of age. Ten days after the final litter was sacrificed, all females were remated with different males from the same group to obtain the F_{1b} generation. From the F_{1b}-generation, 20 males and females of each group were selected at weaning to continue their respective diets and to be used for further reproduction studies. Reproduction studies on the F_{1b} and F_{2b} generations were started when the rats were 80 to 85 days old, and were continued until the F_{3b} generation was weaned.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Sodium salt LAS (C_{10-14}), activity: 98.1% on an anhydrous basis (41.9% active)
Reference: Buehler, E.V., Newmann, E.A., and King, W.R. 1971. Two year feeding and reproduction study in rats with linear alkylbenzene sulfonate (LAS). Toxicol. Appl. Pharmacol. 18:83-91.
Reliability: 2 Valid with restrictions

(b)
Type: Fertility **[ ]**; One-generation study **[ ]**; Two-generation study **[ ]**;
Other **[X] Three generation study**
Species/strain: Charles River CD strain rats
Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**
Administration: diet
Exposure period: up to > 1 year
Frequency of treatment: continuous in diet
Premating exposure period: male: 60 days, female: 60 days
Duration of the test: 3 generations
Doses: 0.08, 0.4, and 2.0% continuously administered throughout the three generations (40, 200 and 1000 mg/kg bw d CLD [6.8, 3.4 and 170 mg/kg bw d LAS]
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL Parental: 170 mg/kg bw d LAS (1000 mg/kg bw d CLD)
NOAEL F1 Offspring: 170 mg/kg bw d LAS (1000 mg/kg bw d CLD)
NOAEL F2 Offspring: 170 mg/kg bw d LAS (1000 mg/kg bw d CLD)
Results: General parental toxicity: There were no signs of malreaction to treatment among parents and the incidence of sporadic deaths and total litter losses were unrelated to dosage. Pregnancy rate and the duration of gestation were unaffected. Food consumption and bodyweight changes showed no consistent relationship to dosage over the three generations.
Toxicity to offspring: Examining litter parameters, statistically significant differences were occasionally observed but they showed no consistent dosage

related trends over the three generations and were considered to be unrelated to treatment. The incidence of malformations was unaffected by treatment. Additional organ weight analysis, histopathology and skeletal staining of representative young from the F_{3b} generation revealed no changes that could be conclusively related to treatment.

Method: CLD was administered in the diet of the rats and new batches of diet were prepared each week. Males and females of each generation (F_o, F_{1b}, and F_{2b}) were kept on their respective diets for 60 days. The mating period for the first litter lasted 19 days. After the weaning of the first litters, approximately 10 days, the animals were re-mated and a second litter was produced. From the second litters of the initial (F_o) and second (F_{1b}) generations, 10 males and 20 females were selected from each group at weaning in order to form the second and third (F_{2b}) generations, respectively.
In the parent animals, observations of signs of reaction, mortalities, food consumption, bodyweight change, pregnancy rate, mating performance, and gestation period were made throughout the study. As soon as possible (< 12 hours) after birth, all young were counted, identified by toe amputation and examined for external abnormalities. Up to day 21 post partum, animals were examined daily for dead and abnormal young. Young of the first litters and surplus young of the second litters were sacrificed and examined for abnormalities internally and externally. Rats of the F_{3b} generation were killed at 3 weeks old and were also examined internally and externally for abnormalities. For the F_{3b} generation, tissue from the brain, liver, heart, pituitary, spleen, thyroid, kidneys, thymus, adrenals, lungs, gonads, pancreas, bladder, bone, bone marrow, sections of the stomach, and sections of the small and large intestines were removed and examined.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Commercial Light Duty liquid detergent (CLD) containing 17% LAS and 7% alkyl ether sulfate (Lion Oil and Fat Co., Ltd.)

Reference: Palmer, A.K., Cozens, D.D., Batham, P., and Cherry, C.P. 1974. Effect of CLD on reproductive function of multiple generations in the rat. Final Report. Report No. LF010/731029.

Reliability: 2 Valid with restrictions

(c)

Type: Fertility **[ ]**; One-generation study **[ ]**; Two-generation study **[ ]**;
Other **[X] :** 4-generation reproduction study

Species/strain: Rat/Wistar

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**

Administration: drinking water

Frequency of treatment: Daily

Duration of the test: 4 generations

Doses: 0.1% (70 mg/kg bw d)

Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOAEL Parental: 70 mg/kg bw d

NOAEL F1 Offspring: 70 mg/kg bw d

NOAEL F2 Offspring: 70 mg/kg bw d

Results: The administration of LAS had no adverse effects on fertility, parturition, gestation period, or lactation in any of the generations.

Method: Two groups of 20 rats of both sexes were given water containing LAS and the reproductive performance was investigated for 4 generations. Five to 10 rats of both the control and the experimental group were sacrificed at 12 weeks for pathological examinations. For successive reproduction, 15 males and 15 females produced by the first mating of rats were used.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: LAS; mean molecular weight 348; average alkyl chain length = $C_{12.0}$.
Remarks: Information as cited in the IUCLID Data Set and the IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Endo, T., Furuido, Y., Namie, K., Yamamoto, N., Hasunuma, H. and Ueda, K. 1980. Studies of the chronic toxicity and teratogenicity of synthetic surfactants. Ann. Rep. Tokyo Metrop. Res Inst. Environ. Prot. 236-246 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY

(a)
Species/strain: Rat (Wistar) and Rabbit (NZW)
Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Administration: drinking water
Exposure period: day 6-15 of pregnancy (rat); day 6-18 of pregnancy (rabbit)
Frequency of treatment: Daily
Doses: 0.1% (70 mg/kg bw d in rat; 250 mg/kg bw d in rabbit)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[ ]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL Maternal Toxicity: Rat > 0.1% (383 mg/rat); rabbit = 0.1% (3030 mg/rabbit).
NOAEL teratogenicity: 0.1% for rat.
LOAEL teratogenicity: 0.1% (3030 mg/rabbit)
Results: The only effect on the dams was a slight inhibition of body weight gain in the rabbits. The litter parameters of both species did not show any significant differences from those of the controls. Delayed ossification was observed in rabbits, but there was no increase in malformations in either the rabbits or the rats.
Method: LAS was given to 40 rats (20 controls) and 22 rabbits (11 controls) from day 6 to 15 (rats) and day 6 to 18 (rabbits) of pregnancy, respectively.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS; activity: 38.74%; average alkyl chain length = $C_{12.0}$; (mean molecular weight 348)
Remarks: Information as cited in the IUCLID Data Set and the IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Endo, T., Furuido, Y., Namie, K., Yamamoto, N., Hasunuma, H. and Ueda, K. 1980. Studies of the chronic toxicity and teratogenicity of synthetic surfactants. Ann. Rep. Tokyo Metrop. Res. Inst. Environ. Prot. 236-246 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(b)
Species/strain: Rat: CD
Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**

Administration: gavage
Duration of the test: sacrifice at day 20 of gestation
Exposure period: day 6 - 15 of pregnancy
Frequency of treatment: daily
Doses: 0.2, 2, 300, 600 mg/kg bw d
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL Maternal Toxicity: 300 mg/kg bw
NOAEL teratogenicity: 600 mg/kg bw
Results: Maternal toxicity:
Body weight gain was retarded in the highest dose group from the start of dosing and showed partial recovery toward the end of the dosing period. One animal died in this group but it could not be conclusively related to treatment. The toxic effects were associated with disturbance of the gastrointestinal tract. Pregnancy rate was comparable at all dosages.
Teratogenicity:
No differences were observed among dose groups and the control group with respect to number of litters, viable young, litter weight, foetal weight, embryonic deaths, implantations, corpora lutea, pre- and post implantation embryonic loss, major malformations, minor visceral or embryonic loss, major malformations, minor visceral or skeletal anomalies or incidence of pups with extra ribs.
Method: Animals received doses by gavage daily from days 6-15 of gestation. Twenty animals per dose group were used.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS
Reference: Palmer, A.K., Readshaw, M.A. and Neuff, A.M. 1975a. Assessment of the teratogenic potential of surfactants (Part I) – LAS, AS and CLD. Toxicology 3:91-106.
Reliability: 2 Valid with restrictions

(c)
Species/strain: Charles River CD strain rat
Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Administration: Oral in distilled water
Duration of the test: 20 days
Exposure period: day 6 to day 15 of pregnancy
Frequency of treatment: daily
Doses: 0.2, 2.0, 300 and 600 mg/kg
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL Maternal: 300 mg/kg
NOAEL teratogenicity: 300 mg/kg
Results: Maternal toxicity: Parent animals were observed daily. Change in bodyweight was not affected by treatment at 0.2, 2.0, and 300 mg/kg, but treatment at 600 mg/kg was associated with retarded weight gain and a transient diarrhea following initiation of treatment. The pregnancy rate was comparable at all dosages.
Pregnancy/litter data: The litter parameters assessed included litter size, fetal loss and litter weight. These parameters were not significantly affected by any dosage. Mean pup weights were statistically higher at 0.2, 2.0 and 300 mg/kg.
Teratogenicity: Embryonic and fetal development were assessed by the incidence of major malformations. The incidence of minor visceral anomalies was unaffected by treatment at any dosage. The distribution of

skeletal variants were not statistically significant with the exception of a marginal retardation of sternebral ossification at 600 mg/kg.

Method: After overnight mating, the rats were randomly allocated to five groups which included one control group and four different treatment groups. LAS was prepared daily as a series of graded aqueous solutions. Animals in all groups were dosed orally at the standard volume of 1.0 mL/100 g. Control animals were dosed in a similar manner with distilled water used as the vehicle. The dams were observed daily for signs of toxicity and weighed on days 1, 3, 6, 10, 14, 17 and 20 of pregnancy. On day 20, the rats were killed by CO_2 euthanasia. Their ovaries and uterine contents were examined immediately for number of copora lutea, number of viable young, number of resorption sites, litter weight, and fetal abnormalities.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: LAS (Na salt) as a slurry containing 64.0% w/v of active ingredient (Lion Oil and Fat Co., Ltd.); average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = $C_{11.7\text{-}12.3}$.

Reference: Palmer, A.K. and Lovell, M.R. 1971a. Effect of LAS detergent on pregnancy of the rat. Report No. 4331/71/487.

Reliability: 2 Valid with restrictions

(d)

Species/strain: Charles River Specific Pathogen Free mice of the CD-1 strain

Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**

Administration: Oral in distilled water

Duration of the test: 17 days

Exposure period: day 6 to day 15 of gestation

Frequency of treatment: daily

Doses: 0.2, 2.0, 300, 600 mg/kg

Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOAEL Maternal: 2.0 mg/kg

NOAEL teratogenicity: 600 mg/kg

Results: Maternal toxicity: After examining parent animals, treatment at 300 and 600 mg/kg was linked with increased mortality (35% and 90% respectively) and weight loss. At 600 mg/kg no dams bearing feasible young survived to termination. Autopsy revealed the consistent occurrence of tympanites sometimes associated with gastritis.
Pregnancy/litter data: The litter parameters were assessed by litter size, fetal loss and litter weight, none of which were significantly affected by treatment at any dosage. Mean pup weight was increased at 0.2 and 2.0 mg/kg.
Teratogenicity: Embryonic and fetal development was assessed by the incidence of major malformations and minor visceral anomalies and the distribution of skeletal variants. Any malformations and anomalities observed were not dose related. Development was not significantly affected at any dosage.

Method: After overnight mating, the mice were randomly allocated to five groups which included one control group and four different treatment groups. LAS was prepared daily as a series of graded aqueous solutions. Animals in all groups were dosed orally at the standard volume of 0.06 mL/10 g. Control animals were dosed in a similar manner with distilled water used as the vehicle. The dams were observed daily for signs of toxicity and weighed on days 1, 3, 6, 10, 14, and 17 of pregnancy. On day 17, the mice were killed by cervical dislocation. Their uterine contents were examined immediately for number of viable young, number of resorption sites, litter weight, and fetal abnormalities.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: LAS (Na salt), as a slurry containing 64.0% w/v of active ingredient (Lion Oil and Fat Co., Ltd.); average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = $C_{11.7-12.3}$.
Reference: Palmer, A.K. and Lovell, M.R. 1971b. Effect of LAS detergent on pregnancy of the mouse. Report No. 4330/71/486.
Reliability: 2 Valid with restrictions

(e)
Species/strain: Mouse/CD-1
Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Administration: gavage
Duration of the test: sacrifice at day 17 of pregnancy
Exposure period: days 6 - 15 of pregnancy
Frequency of treatment: daily
Doses: 0.2, 2, 300, 600 mg/kg bw d
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL Maternal Toxicity: 2 mg/kg bw d
NOAEL teratogenicity: 300 mg/kg bw d
Results: Maternal toxicity:
Among parent animals treatment at 300 and 600 mg/kg bw d was associated with increased mortality (35% and 90% respectively). At 300 mg/kg bw d weight gain was retarded only during the first four days. No assessment could be made at 600 mg/kg bw d, due to the high mortality rate. Necropsy revealed a ubiquitous occurrence of tympanites, sometimes associated with gastritis. Pregnancy rate was essentially comparable for all groups.
Teratogenicity:
At doses with no maternal toxicity, no differences were observed among the dose group and the control group with respect to number of litters, viable young, litter weight, foetal weight, embryonic deaths, implantations and post implantation embryonic loss. At these doses the incidences of major malformations and minor abnormalities were not affected. At doses with maternal toxicity there was an increased foetal loss and reduced litter size due almost entirely to total litter loss, which was considered to be a secondary effect due to the maternal toxicity. The incidences of major malformations was not affected; minor skeletal or visceral anomalies were increased at 300 mg/kg.
Method: Twenty female mice were administered 0.2, 2.0, 300, or 600 mg/kg bw of LAS by gavage at days 6-15 of gestation. All animals were sacrificed at day 17 of pregnancy.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS
Remarks: The maternal NOAEL of 2 mg/kg bw d is considered very conservative because the range (2-300 mg/kg bw d) was too wide.
Reference: Palmer, A.K., Readshaw, M.A. and Neuff, A.M. 1975a. Assessment of the teratogenic potential of surfactants (Part I) – LAS, AS and CLD. Toxicology 3:91-106.
Reliability: 2 Valid with restrictions

(f)
Species/strain: New Zealand white rabbit
Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Administration: Gavage
Exposure period: day 6 to 18 of pregnancy
Frequency of treatment: Daily

Duration of the test: sacrifice at day 29 of pregnancy
Doses: 0.2, 2, 300, 600 mg/kg
Control Group: Yes; concurrent
NOAEL maternal toxicity: 2 mg/kg bw
NOAEL teratogenicity: 2 mg/kg bw
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS
Results: Maternal toxicity:
At 300 and 600 mg/kg severe maternal toxicity was observed resulting in body weight loss and associated with diarrhoea, anorexia, and cachexia prior to death.
Teratogenicity:
At doses with no maternal toxicity, no differences were observed among the dose groups and the control group with respect to number of litters, viable young, litter weight, foetal weight, embryonic deaths, implantations and post implantation embryonic loss. At these doses the incidences of major malformations and minor abnormalities were not affected. Higher doses resulted in total litter which was considered to be a secondary effect due to the maternal toxicity. Since there were no survivors, malformations and anomalies were not assessed at these doses.
Remarks: Information as cited in the IUCLID Data Sheet and the IPCS document.
Reference: Palmer, A.K., Readshaw, M.A. and Neuff, A.M. 1975a. Assessment of the teratogenic potential of surfactants (Part I) – LAS, AS and CLD. Toxicology 3:91-106.
Reliability: 2 Valid with restrictions

(g)
Species/strain: New Zealand White rabbit
Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Administration: intragastric intubation
Duration of the test: 29 days
Exposure period: day 6 to day 18 of pregnancy
Frequency of treatment: daily
Doses: 0.2, 2.0, 300, 600 mg/kg
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL Maternal Toxicity: 2.0 mg/kg
NOAEL teratogenicity: 2.0 mg/kg
Results: Maternal toxicity: Daily assessment of bodyweight change and pregnancy rate determined that at 0.2 and 2.0 mg/kg the treatment did not adversely affect parent animals. At 300 and 600 mg/kg parent animals showed signs of severe anorexia, diarrhoea, weight loss and death. Respective mortality rates were 85 and 100% and autopsy consistently revealed changes in the gastrointestinal tract.
Pregnancy/litter data: The influence of maternal toxicity restricted assessment of effect on litter parameters to animals treated at 0.2 and 2.0 mg/kg. At these two dosages there were no adverse effects on litter parameters, as assessed by litter size and fetal loss, litter and mean pup weights.
Teratogenicity: Also at these two dosages there were no adverse effects on embryonic and fetal development, as assessed by the incidence of major and minor malformations, minor anomalies and skeletal variants.
Method: Thirteen rabbits were mated on a one-to-one basis with males of proven fertility. The does were then injected intraveneously with 10 i.u. luteinizing hormone to ensure that ovulation occurred. The rabbits were identified by an

ear tag and allocated to one control group and four treatment groups. LAS was prepared daily and administered by intragastric intubation by a series of graded solutions in distilled water so that all animals were dosed at the standard volume of 4 mL/kg. Control animals were dosed at the same rate with distilled water as the vehicle. The parent animals were observed daily for signs of toxicity and weighed on days 1, 6, 10, 14, 21, and 28. On day 29, the animals were killed by cervical dislocation and immediately examined to determine the numbers and uterine disposition of young and resorption sites. The number of corpora lutea were also counted. Any rabbit containing abnormal fetus and/or resorption sites was thoroughly examined for signs of natural disease. Viable young were weighed, sexed and examined internally and externally for abnormalities. All young were preserved in alcohol for subsequent clearing, staining and skeletal examination. Resorption sites were classified as early or late. Abnormalities were classified as major or variant.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: LAS (Na salt), as a slurry containing 64% active ingredient (Lion Oil and Fat Co., Ltd.); average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = $C_{11.7\text{-}12.3}$.

Remarks: The maternal NOAEL of 2 mg/kg bw d is considered very conservative because the range (2-300 mg/kg bw d) was too wide.

Reference: Palmer, A.K. and Neuff, A.M. 1971. Effect of LAS detergent on pregnancy of the New Zealand white rabbit. Report No. 4387/71/543.

Reliability: 2 Valid with restrictions

(h)

Species/strain: Mouse/ICR

Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**

Administration: gavage

Duration of the test: See method.

Exposure period: See method.

Frequency of treatment: daily

Doses: 0.4, 4.0% (40, 400 mg/kg bw d)

Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOAEL Maternal Toxicity: 40 mg/kg bw d

NOAEL teratogenicity 400 mg/kg bw d

Results: In mice given 400 mg/kg from day 0 to 6, the pregnancy rate was 46.2% compared to 92.9% in the controls. There was no increase in malformations. Although no information on maternal toxicity is available, it appears likely that maternal toxicity was present at the high dose group.

Method: LAS was administered from day 0 to day 6 of pregnancy or from day 7 to 13 of pregnancy. Thirteen to fourteen mice were used in each dose group.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Japan LAS; average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = $C_{11.7\text{-}12.3}$; activity: 99.5%

Remarks: Information as cited in the IUCLID Data Sheet and the IPCS document.

Reference: 1) European Commission. 2000a. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Takahashi, M., Sato, K., Ando, H., Kubo, Y. and Hiraga, K. 1975. Teratogenicity of some synthetic detergents and linear alkylbenzene sulfonate (LAS). Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 26: 67-78 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(i)
Species/strain: Mouse/ICR.
Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Administration: gavage
Duration of the test: see text.
Exposure period: day 6 through day 15 of pregnancy.
Frequency of treatment: daily.
Doses: 10, 100, 300 mg/kg bw d
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
LOAEL Maternal Toxicity: 10 mg/kg bw d
NOAEL teratogenicity: 300 mg/kg bw d
Results: The dams showed inhibition of body weight gains in all groups, especially in the high dose group. In this group, two dams died, and there was one case of premature delivery and death of all fetuses. There were findings such as decreased body weight and delayed ossification among the living fetuses, but there was no increase in malformations.
Method: LAS was administered by gavage to 25 to 33 mice per dose on days 6 through 15 of gestation.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Japan LAS; average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = $C_{11.7\text{-}12.3}$; activity: 48.6%
Remarks: Information as cited in the IUCLID Data Sheet and the IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Shiobara, S. and Imahori, A. 1976. Effects of linear alkylbenzene sulfonate orally administered to pregnant mice and their fetuses. J. Food Hyg. Soc. Jpn. 17:295-301 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(j)
Species/strain: Rat: SD-JCL
Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Administration: oral feed
Exposure period: from day 0 to 20 of gestation
Frequency of treatment: Daily
Doses: 0.1%, 1.0% (80, 780 mg/kg bw d)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL Maternal: 780 mg/kg bw d
NOAEL teratogenicity: 780 mg/kg bw d
Results: The LAS intake was about 780 mg/kg with the 1% diet, but there were no abnormalities in the body weight gains of the dams, or in the occurrence and maintenance of pregnancy. The values of the litter parameters did not differ from those of the controls and there was no evidence of teratogenicity. The numbers of offspring were rather low in the 1% group, and the weaning rate of 78.3% was lower than the 100% rate observed in the controls. However,

there were no abnormalities in body weight gain, organ weights or functions in the offspring.

Method: LAS was fed in the diet to 16 pregnant female rats/dose from day 0 to 20 of gestation.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Japan LAS; average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = $C_{11.7\text{-}12.3}$.

Remarks: Information as cited in IUCLID Data Sheet and IPCS document.

Reference: 1) European Commission. 2000a. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.

2) Tiba, S., Shiobara, S., Imahori, A. and Kitagawa, T. 1976. Effects of linear alkylbenzene sulfonate on dam, fetus and newborn rat. J. Food Hyg. Soc. Jpn. 17:66-71. (In Japanese); cited in IPCS. 1996. Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates and Related Compounds. World Health Organization, Geneva, Switzerland. Original article in Japanese.

Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(k)

Species/strain: Weanling Charles River CD Sprague-Dawley albino rats and New Zealand rabbits

Sex: Female **[ ]**; Male **[ ]**; Male/Female **[X]**; No data **[ ]**

Administration: oral in feed

Duration of the test: two generation (rats); one generation (rabbits)

Exposure period: Rat: continuously or during organogenesis period of six pregnancies
Rabbit: day 2-16 of gestation during a single pregnancy

Frequency of treatment: continuous

Doses: Rat: 0.1, 0.5 or 1.0% TAE_3S/LAS (equivalent to 50, 250 or 500 mg/kg/day in female rats corresponding to LAS doses of 22.5, 112.5 and 225 mg/kg bw d.)
Rabbit: 50, 100, or 300 mg/kg TAE_3S/LAS, corresponding to LAS doses of 22.5, 45, and 135 mg/kg bw d

Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOAEL Maternal: 225 mg/kg bw d LAS (rat)
135 mg/kg bw d LAS (rabbit)

NOAEL teratogenicity: 225 mg/kg bw d LAS (rat)
135 mg/kg bw d LAS (rabbit)

Results: Maternal toxicity: No treatment related adverse effects were observed in the maternal generation of either rats or rabbits. Fetal toxicity: No treatment-related adverse effects were observed on conception, fetal viability or post-natal survival in either generation of rats. Some statistically significant differences were observed in live-born and surviving pup numbers, but there were no consistent trend or patterns. Combined with the high lactation index in all groups, indicating a very low mortality among the suckling rats, these differences were considered due to causes not related to treatment with the test material. There were no statistical differences among the groups of rat fetuses taken by Caesarian section and examined for birth defects. Some minor soft-tissue and skeletal anomalies were observed in rat fetuses from both generations. Of the 1210 rat fetuses, the overall incidence of abnormal young was 9.0% and did not vary significantly between treatment groups or the controls. Similarly, no treatment-related adverse effects were seen in rabbits treated with the surfactant mixture. Of the 855 rabbit fetuses, 5.7% were abnormal, but the incidence of defective fetuses in the test groups were not significantly different from those in controls. Therefore, no test related

effects were seen on reproduction or embryonic development in either animal species.

Method: (A) Rat studies

The rats were divided into seven groups consisting of 25 males and 25 females after a five day acclimation period in the laboratory. The tallow alkyl ethoxy sulfate (55%)-LAS(45%) mixture (TAE_3S/LAS) was mixed into the ground commercial feed at levels of 0.1, 0.5 or 1.0% and fed to two generations of male and female rats continuously or only to females during each period of organogenesis (days 6-15) of pregnancy. A control group was fed the commercial feed with no additive. The parent animals body weights were recorded weekly for the first eight weeks in each generation and afterwards recorded only at each mating phase.

Once sexually mature, five rats of each sex per group were sacrificed for histology during each generation. The remaining rats were mated on a one-to-one basis three successive times during each generation. The first two pregnancies (F_{1a}, $_{1b}$, $_{2a}$ and $_{2b}$) in each generation were allowed to proceed to natural births. These pups were counted and inspected for abnormalities at birth. The third pregnancies in each generation (F_{1c} and F_{2c}) were used for teratology purposes. At weaning all pups except the F_{1b} litters, which became the second generation parents, were discarded. Animals for the second generation were selected on the same basis as previously described for the first generation. During the third pregnancies of both generations (F_{1c} and F_{2c}), one-half of each group of females was sacrificed on day 13 of gestation. A laparotomy was performed and the number of corpora lutea of pregnancy and the number of implantation and resorption sites were observed and recorded. On day 21 of gestation, the remaining dams were examined in a similar manner.

One-third of the fetuses in each of the third litters were examined for skeletal development and defects. The others were examined for soft tissue defects. During the teratology period, tissues were collected from five parent females of each group and from five parent males of the control and continuously treated groups. The heart, liver, kidneys and gonads were weighed, blood was taken for routine hemograms, and tissues were set in 10% formalin, paraffin-sectioned and stained with haemotoxylin-eosin for histopathy.

(B) Rabbit study

Five groups of 25 sexually mature does were distributed on the based on body weights and litter mates. The does were artificially inseminated with 0.25 mL of undiluted semen, collected from sperm-tested untreated males. Ovulation was induced by a 1 mg/kg injection of PLH immediately prior to insemination. The day of insemination was considered day 0 of gestation. The TAE_3S/LAS mixture was administered by gavage from day 2 through day 16 of gestation at daily doses of 50, 100, or 300 mg/kg of body weight. Distilled water was the vehicle and each doe received 2 mL of solution per kg of bodyweight. For the control groups, one received no treatment and the other received a treatment with water. In order to monitor the dose level, the females were weighed every three days. The dams were sacrificed on day 28 of gestation and the number of corpora lutea, resorptions and live or dead fetuses were observed and recorded. The fetuses were removed and treated and examined for abnormalities.

GLP: Yes **[ ]** No **[ ]** ? **[X]**

Test substance: A mixture of 55% tallow alkyl ethoxylate sulfate (TAE_3S) and 45% LAS (assumed Procter and Gamble products)

Remarks: The authors indicate that rats received up to 6000 times the estimated "worst-case" human exposure without causing any deleterious effects on the development or variability of the embryo or fetus. Rabbits also received

doses many times the "worst-case" human dose without causing significant effects.

Reference: Nolen, G.A., Klusman, L.W., Patrick, L.F. and Geil, R.G. 1975. Teratology studies of a mixture of tallow alkyl ethoxylate and linear alkylbenzene sulfonate in rats and rabbits. Toxicology. 4:231-243.

Reliability: 2 Valid with restrictions

(l)

Species/strain: Rat: CD

Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**

Administration: Dermal

Exposure period: days 2 through 15 of gestation

Frequency of treatment: daily

Doses: 0.03, 0.3, or 3% on the shaved skin as 0.5 ml aqueous solution.

Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOAEL Maternal: 0.3% (6 mg/kg bw d)

NOAEL teratogenicity: 3% (60 mg/kg bw d)

Results: Maternal toxicity:
At the high dose, local irritation was observed resulting in a slightly lower body weight gain and hypersensitivity (i.e., animals were increasingly irritable).
Teratogenicity:
No differences were observed among the dose groups and the control group with respect to number of litters, viable young, litter weight, foetal weight, embryonic deaths, implantations, corpora lutea, or pre- and post implantation embryonic loss. The incidences of major malformations, minor visceral or skeletal anomalies, and skeletal variants were not different between controls and dose groups even at maternal by toxic doses.

Method: The dosage volume was 0.5 mL which was applied to an area of skin (4x4 cm) from which the fur was removed. The nominal doses were 0.6, 6.0, and 60 mg/kg bw d.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: Japan LAS; average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = $C_{11.7}$.

Reference: Palmer, A.K., Readshaw, M.A. and Neuff, A.M. 1975b. Assessment of the teratogenic potential of surfactants (Part III) – Dermal application of LAS and soap. Toxicology 4:171-181.

Reliability: 2 Valid with restrictions

(m)

Species/strain: Rat/Wistar

Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**

Administration: Dermal

Duration of the test: sacrifice at day 21 of gestation

Exposure period: 21 days (days 0 through 21 of gestation)

Frequency of treatment: Daily

Doses: 0.05, 0.1, and 0.5% (0.1, 2 and 10 mg/kg bw d) or 1.0, 5.0, and 20% (20, 100, and 400 mg/kg bw d)

Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOAEL Maternal: 1% (20 mg/kg bw d)

NOAEL teratogenicity: 20% (400 mg/kg bw d)

Results: Maternal toxicity:
The dams treated with 20% and 5% showed inhibition of body weight gain and local skin effects.

Teratogenicity:
There were no indications of teratogenic or embryotoxic effects at any level in either group tested.

Method: LAS was applied to depilated areas on the chests and backs of female rats 12-18 weeks of age. Five to six hours prior to treatment an exposure site (roughly 24 cm^2) in the dorsothoracic region of each animal from group II through IX was clipped to a length of 1 mm. The animals were reclipped every 48 hr throughout the study. Group I animals were unclipped, group II animals were clipped but not treated and group III animals were clipped and treated with tap water. The mated female rats were treated daily from day 0 through day 20 of gestation. A 0.5-ml sample of the appropriate concentration of LAS and/or tap water was applied once daily to the clipped area and spread with a gloved finger over as much of the exposure site as possible. Each application was carried out slowly over a 3-min period. In the 1, 5 and 20% LAS groups (groups VII, VIII and IX, respectively corresponding to 20, 100 and 400 mg/kg/day) the test material was allowed to remain on the backs of the animals for 30 min. after which it was removed with warm tap water. The test material was not removed from the backs of the animals in the 0.05, 0.1 and 0.5% LAS groups (groups IV, V and VI corresponding to 1, 2 and 10 mg/kg/day). Animal body weight and food consumption were determined during the treatment period. Daily observations were also made for toxicological effects.

GLP: Yes **[ ]** No **[X]** ? **[ ]**

Test substance: LAS; mean chain length: 11.7; mean molecular weight: 344, activity: 20.5%

Reference: Daly, I.W., Schroeder, R.E. and Killeen, J.C. 1980. A teratology study of topically applied linear alkylbenzene sulphonate in rats. Fd. Cosmet. Toxicol. 18:55-58.

Reliability: 2 Valid with restrictions

(n)

Species/strain: Mouse/CD-1

Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**

Administration: Dermal

Exposure period: days 2 through 13 of gestation

Frequency of treatment: daily

Doses: 0.03, 0.3, or 3% LAS in aqueous solution onto the shaved skin (5, 50 and 500 mg/kg bw d)

Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**

NOAEL Maternal: 0.03% (5 mg/kg bw d)

NOAEL teratogenicity: 0.3% (50 mg/kg bw d)

Results: Maternal toxicity:
At the high dose, severe local irritation was observed resulting in body weight loss and hypersensitivity (i.e., animals were increasingly irritable), which was also observed at the medium dose. The conclusion of the authors was that LAS caused marked toxicity at the high dose and moderate or mild toxicity at the medium dose.
Teratogenicity:
At the lowest dose, the dose with no maternal toxicity, no differences were observed among the LAS group and the control group with respect to number of litters, viable young, litter weight, foetal weight, embryonic deaths, implantations, corpora lutea, pre- and post implantation embryonic loss. The incidences of major malformations, minor visceral or skeletal anomalies, and skeletal variants were not different between controls and the LAS group.

Maternally toxic dosages were associated with a significantly increased foetal loss and consequent reduction of litter size. This was due almost entirely to total litter losses as values, for the one surviving litter at 3% was similar to the control litters. At the medium dose, the moderate degree of maternal toxicity correlated with a moderate effect on litter values in that, whilst the higher incidence of embryonic deaths differed significantly from control values, the consequent reduction in litter size was not statistically significant. With regard to major malformations and minor skeletal or visceral anomalies, the assessment of litters was not possible in the highest dose group due to the low survival. At the low doses, no treatment related increase of the incidences of major malformations and minor skeletal and visceral anomalies were observed.

Method: The dosage volume was 0.5 mL which was applied to an area of skin (2 x 3 cm) from which the fur was removed. The nominal doses were 5, 50, and 500 mg/kg bw/day.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: Japan LAS; average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = $C_{11.7\text{-}12.3}$.
Reference: Palmer, A.K., Readshaw, M.A. and Neuff, A.M. 1975b. Assessment of the teratogenic potential of surfactants (Part III) Dermal application of LAS and soap. Toxicology. 4:171-181.
Reliability: 2 Valid with restrictions

(o)
Species/strain: mouse: ddy.
Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Administration: Dermal
Exposure period: day 0 through day 13 of pregnancy
Frequency of treatment: Daily
Doses: 2.2% (110 mg/kg bw d)
Control group: Yes **[ ]**; No **[ ]**; No data **[X]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL Maternal: 2.2% (110 mg/kg bw d)
NOAEL teratogenicity: 2.2% (110 mg/kg bw d)
Results: No abnormalities were seen in the dam or fetuses.
Method: An area of 4 x 4 cm on the backs of mice was depilated and LAS was applied at a dose of 0.5 ml/mouse/day. Sixteen animals were used per group.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS; molecular wt = 346; average alkyl chain length = 11.8; activity: 99.5%
Remarks: Information as cited in the IUCLID Data Sheet and the IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, $C_{10\text{-}13}$-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Sato, K., Ando, H., Yuzawa, K. and Hiraga, K. 1972. Studies on toxicity of synthetic detergents (III) Examination of teratogenic effects of alkyl benzene sulfonates spread on the skin of mice. Ann. Rep. Tokyo Metrop. Res. Lab. Public Health. Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(p)
Species/strain: mouse/ICR
Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Administration: dermal

Exposure period: from day 6 through day 15 of pregnancy
Frequency of treatment: daily
Doses: 0.03, 0.3, 3% (15, 150, and 1500 mg/kg bw d)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL Maternal: 0.3% (150 mg/kg bw d)
NOAEL teratogenicity: 3% (1500 mg/kg bw d)
Results: The 3% group showed a clear decrease in the pregnancy rate (67.9%) when compared with a rate of 96.3% in the controls. However, there were no decreases in the litter size, and no changes in the litter parameters with the exception of a slight decrease in fetal body weight. There were no significant increases in the incidence of malformations in the fetuses.
Method: Areas of 4 x 4 cm on the backs of the mice were depilated and aqueous solutions of LAS were applied.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: C_{10-14} LAS (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = $C_{11.7}$; activity: 46.6%
Remarks: Information as cited in the IUCLID Data Sheet and the IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Imahori, A., Kinagawa, T. and Shiobara, S. 1976. Effects of linear alkyl benzene sulfonate (LAS) applied dermally to pregnant mice and their fetuses. Jpn. J. Public Health. 23:68-72 (in Japanese); cited in IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(q)
Species/strain: mouse/ICR
Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Administration: Subcutaneous injection
Exposure period: Day 0 to 3 or day 8 to 11 of pregnancy
Frequency of treatment: daily
Doses: 0.35, 1% in water (20, 200 mg/kg bw d)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL Maternal: 0.35% (20 mg/kg bw d)
NOAEL teratogenicity : 1% (200 mg/kg bw d)
Results: When dams were administered the 1% solution from day 0 to 3 of pregnancy, there was an initial decrease in body weight and necrosis at the injection sites. The number of pregnancies decreased in the mice given the 1% solution compared to the controls (61.5% vs. 93.3%) There were no significant changes with respect to litter parameters, major malformations or minor abnormalities.
Method: LAS was injected at doses of 20 mL/kg/day from day 0 to 3 or day 8 to 11 of pregnancy. There were 12 - 19 mice in each treatment group.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS, activity: 99.5%
Remarks: Information as cited in the IUCLID Data Sheet and the IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Takahashi, M., Sato, K., Ando, H., Kubo, Y. and Hiraga, K. 1975. Teratogenicity of some synthetic detergents and linear alkylbenzene sulfonate (LAS) Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 26:67-78 (in

Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document

(r)

Species/strain: rabbit/New Zealand white
Sex: Female **[X]**; Male **[ ]**; Male/Female **[ ]**; No data **[ ]**
Administration: Dermal
Exposure period: 17 days (days 1 through 16 of gestation)
Frequency of treatment: Daily
Doses: 0.03, 0.3, or 3% (0.9, 9, or 90 mg/kg bw d)
Control group: Yes **[X]**; No **[ ]**; No data **[ ]**;
Concurrent no treatment **[X]**; Concurrent vehicle **[ ]**; Historical **[ ]**
NOAEL Maternal: 0.03% (0.9 mg/kg bw d)
NOAEL teratogenicity: 3% (90 mg/kg bw d)
Results: Maternal toxicity:
At the high dose, local irritation was observed resulting in body weight loss and hypersensitivity (i.e., animals were increasingly irritable). The medium dose caused retarded body weight gain and hypersensitivity.
Teratogenicity:
At the medium and low dose, no differences were observed among the dose groups and the control group with respect to number of litters, viable young, litter weight, foetal weight, embryonic deaths, implantations, corpora lutea, pre and post implantation embryonic loss. The high dose was associated with slightly, but not significantly, higher foetal loss and lower litter size. The incidences of major malformations, minor visceral or skeletal anomalies, and skeletal variants were not different between controls and dose groups even at maternal toxic doses.
Method: The dosage volume was 10 mL which was applied to an area of skin (12 x 20 cm) from which the fur was removed. The nominal doses were 0.9, 9.0, and 90 mg/kg bw/day. Thirteen rabbits per dose were used.
GLP: Yes **[ ]** No **[X]** ? **[ ]**
Test substance: LAS
Reference: Palmer, A.K., Readshaw, M.A. and Neuff, A.M. 1975b. Assessment of the teratogenic potential of surfactants (Part III) – Dermal application of LAS and soap. Toxicology 4:171-181.
Reliability: 2 Valid with restrictions

5.10 OTHER RELEVANT INFORMATION

(a)

Type: Toxicokinetics
Results: ^{35}S-LAS (15 x 10^8 cpm) was administered topically, once, onto the back skin of rats and guinea pigs. Absorption and distribution in major organs and blood were studied. Urine was collected 24 hours after topical application of the test substance. In the guinea pig, the amount of ^{35}S excreted in the urine was about 0.1% of the total administered dose. Organ distribution in the rat was about 5 times greater than in the guinea pig, and "relatively large amounts" of ^{35}S were noted in the liver and kidneys. Conclusion states that: "when 0.2 to 0.5% LAS was topically applied once, approximately 0.1 to 0.6% was absorbed"; there was no accumulation in specific organs; the "test chemical was quickly excreted in the urine after being metabolized".

Reference: Debane, C. 1978. National Hygiene Laboratory; in: "Report on Studies on Synthetic Detergents", October 1978, Japan's Science and Technology Agency [in Japanese].
Reliability: 4 Not assignable

(b)
Type: Toxicokinetics
Method: The absorption, distribution, metabolism and elimination of LAS (radioactively labelled with ^{35}S) were studied in male Charles River rats. LAS was administered as an aqueous solution.
Results: The compound was readily absorbed from the gastrointestinal tract (80-90% of the dose). Most of the absorbed ^{35}S was eliminated within 72 hours and 60-65% of the absorbed dose was eliminated in the urine, with sulfophenyl butanoic and sulfophenyl pentatonic acid as metabolites. These metabolites were not reabsorbed from the kidney tubules. 35% of the absorbed ^{35}S was excreted in the bile and were reabsorbed completely from the gastrointestinal tract. Although the metabolites in the bile were not identified, it was shown that no unchanged LAS was eliminated via this pathway.
Test substance: C_{10-13}, LAS (CAS #68411-30-3); alkyl chain length predominately C_{11}, C_{12} and C_{13}.
Remarks: The authors suggested that metabolism proceeded via omega oxidation with subsequent beta-oxidation. Retention of radioactivity was not observed in any organ.
Reference: Michael, W.R. 1968. Metabolism of linear alkylate sulfonate and alkyl benzene sulfonate in albino rats. Toxicol. Appl. Pharmacol. 12:473-485.
Reliability: 2 Valid with restrictions

(c)
Type: Toxicokinetics
Results: LAS is well absorbed by via the gastrointestinal tract of pigs treated with 3.3 mmol/animal 35S-Na-dodecylbenzene sulfonate. At 200 hours after oral administration, the radioactivity was relatively high in bristles and bones, while low in liver, kidney and spleen. After 10 weeks only traces of radioactivity were still in the body. 40 hours after the administration, 40% of the dose was excreted into the urine and 60% of the dose via the faeces.
Remarks: Information as cited in the IUCLID Data Sheet and the IPCS document.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Havermann, H. and Menke, K.H. 1959. Biological study of the water-soluble surface-active substances. Fette. Seifen. Anstrichmittel 61:429-434. (in German); cited in IPCS. 1996. Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates and Related Compounds. World Health Organization, Geneva, Switzerland. Original article in Japanese.
Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(d)
Type: Toxicokinetics
Results: Four (2 male, 2 female; 5 kg average body weight) adult rhesus monkeys (*Macaca mulatta*) were given single or repeated oral (30, 150 or 300 mg/kg) or subcutaneous (0.1, 0.5 or 1 mg/kg) doses of ^{14}C-LAS. After single 30 mg/kg oral doses the radioactivity was rapidly excreted, mostly during the first 24 hours. Means of 71.2% and 23.1% of the dose were excreted in the urine and feces, respectively, during 5 days. Similarly, after single 1 mg/kg subcutaneous doses, means of 64.1% and 10.9% were excreted in urine and

feces, respectively, during 5 days, mostly during the first 24 hours. After single oral doses of 30, 150 and 300 mg/kg, peak plasma concentrations (at 4 hours in all cases) were very similar, with levels of 34, 41 and 36 µg/mL, respectively. Concentrations declined during the period of 6-24 hours, with a biological half life of about 6.5 hours. After single subcutaneous doses of 0.1, 0.5 and 1 mg/kg, peak plasma concentrations increased almost proportionately, with levels of 0.16, 0.72 and 1.13 µg/mL, respectively. During the 120 hours after single oral (30 mg/kg) or subcutaneous doses (1 mg/kg) the average rate of excretion was between 63 and 74% in the urine and between 9 and 26% in the feces.

During seven consecutive daily oral (30 mg/kg/day) or subcutaneous (1 mg/kg/day) doses, there was no accumulation of radioactivity in plasma. Mean peak concentrations and biological half-lives were similar after the first and seventh doses. Two hours after the last dose, the highest radioactivity was observed in the stomach. Radioactivity was also observed in the intestinal tract, kidneys, liver, lung, pancreas, adrenals and pituitary. At 24 hours, concentrations were highest in the intestinal tract, probably indicating biliary excretion. Since the concentrations in the tissues in general were lower than in plasma, no specific accumulation of LAS occurred. When ^{14}C-LAS was injected into the skin, most of the radioactivity remained at the site of injection. No localization of radioactivity in any tissue occurred. No unchanged LAS was detected in urine samples after oral or subcutaneous doses (either single or repeated).

Five metabolites were excreted but they were not identified. Incubations with beta-glucuronidase/sulfatase did not affect the metabolites, indicating that the metabolites were probably not present as the corresponding conjugates.

Test substance: Alkyl benzene sulfonate, sodium salt; mean molecular weight 349 (supplied by the Japan Soap and Detergent Association)

Reference: Cresswell, D.G., Baldock, G.A., Chasseaud, L.F. and Hawkins, D.R. 1978. Toxicological studies of linear alkylbenzene sulfonate (LAS) in rhesus monkeys: (II) the disposition of [^{14}C] LAS after oral or subcutaneous administration. Toxicology 11:5-17.

Reliability: 2 Valid with restrictions

(e)

Type: Toxicokinetics

Results: Rats were dosed orally with ^{14}C-Na-LAS and radioactivity was detected 0.25 hr after administration, reaching a maximum at 2 hrs. The biologically half lives were calculated to be 10.9 hrs. The distribution was high in the digestive tract and in the bladder at 4 hours after administration. Concentrations were also high in the liver, kidney, testis, spleen and lung. 168 hours after the administration, the rates of excreted radioactivity were 47% in the urine and 50% in the faeces

Remarks: Information as cited in the IUCLID Data Sheet and the IPCS document.

Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.

2) Sunakawa, T., Ikida, Y. and Okamoto, K. 1979. Absorption, distribution, metabolism, and excretion of linear alkylbenzene sulfonate in rats. J. Jpn. Oil Chem. Soc. 39:59-68 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

Reliability: 4 This study is assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document.

(f)

Type:	Toxicokinetics
Method:	Studies were conducted with isolated human skin preparations as well as *in vivo* investigations of percutaneous administration of LAS to rats. Two C_{12} LAS solutions were tested: a 3 mM solution in 25% v/v polyethylene glycol 400 in water, and a 3 mM suspension in water prepared by homogenizing and equilibration in an all-glass homogenizer.
Results:	No radioactivity was detected in urine or faeces.
Test substance:	LAS (CAS #25155-30-0); activity: >99%
Remarks:	These studies demonstrated that penetration through skin and subsequent systemic absorption of this surfactant does not occur to any significant extent at 24 to 48 hrs.
Reference:	Howes, D. 1975. The percutaneous absorption of some anionic surfactants. J. Soc. Cosmet. Chem. 26:47-63.
Reliability:	2 Valid with restrictions

(g)

Type:	*in vitro* studies with fertilised eggs
Method:	Eggs from B6 x $C3F_1$ female mice, which were fertilised *in vitro* with sperm from C3 x $101F_1$ male mice, were treated with LAS for 1 hour at the pronucleus stage and then cultivated for 5 days.
Results:	Eggs treated with LAS at concentrations of less than 0.025% developed to the blastocyst stage as well as the untreated ones. At higher concentrations no egg developed beyond the 1-cell stage. The group that was treated with natural soap had no effect up to a concentration of 0.05%.
Test substance:	Commercial LAS detergent (Japan)
Remarks:	The authors suggest that LAS interrupts mouse pregnancy by killing fertilized eggs, however, the relevance of the results obtained in this assay for the *in vivo* situation has not been proven.
Reference:	Ishii, Y., Samejima, Y., Saji, F. and Nomura, T. 1990. Effect of alcohol sulfate, linear alkylbenzene sulfonate, and natural soap on the development of fertilized eggs of the mouse *in vitro*. Mutat. Res. 242:151-155.
Reliability:	2 Valid with restrictions

5.11 EXPERIENCE WITH HUMAN EXPOSURE

(a)

Type:	Human Repeat Insult Patch Test
Number of Subjects:	95 (at completion)
Methods:	LAS was applied at 0.10% (w/v) on the upper arms of volunteers, under occlusive patch conditions. Test material was applied for 24 hours, 3 times a week, for 3 weeks during the induction period. After a 14-17-day rest, a 24-hour challenge patch was applied on the original and alternate arm sites.
Results:	There was no evidence of skin sensitization on the 95 subjects who completed the test.
Test Material:	LAS; activity: 30.0%
Reference:	The Procter & Gamble Company, unpublished data, Report No. ISC-124-0470.
Reliability:	4 Not assignable

(b)

Type:	Human Repeat Insult Patch Tests.
Number of subjects:	2,294 (exposed to LAS as a raw material) 17,887 (exposed to LAS in formulations)
Results:	No evidence of skin sensitization.

Reference: Nusair, T.L., Danneman, P.J., Stotte, J., and Bay, P.H.S. 1988. Consumer products: Risk assessment process for contact sensitization. Toxicologist 8:258. (abstract).
Reliability: 4 Not assignable

(c)
Type: Occlusive epicutaneous
Results: LAS was applied at 1% once to middle Europeans for 24 hours. Test duration was 6 days. The authors concluded that LAS was sufficiently compatible to the skin.
Remarks: Information as cited in the IUCLID Data Sheet.
Reference: 1) European Commission. 2000a. Benzenesulfonic acid, C_{10-13}-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.
2) Matthies, W., Henkel KgaA, unpublished data, Report No. 890356 (1989).
Reliability: 4 Not assignable

(d)
Type: Comparison of human experience to eye exposure to surfactants with animal eye irritation studies
Methods: Summaries of human manufacturing accident and consumer accident eye irritation incidents over several years were collected for laundry, household and personal cleaning products. These summaries included the date the incident occurred, the exact product or formulation involved, the estimated time for the eyes to return to normal, and a brief description of the eye response. A total of 231 manufacturing employee incidents and 284 consumer incidents were usable, covering 24 and 23 different products, respectively. The results of these human contact incidents were compared to the results of studies conducted using two rabbit eye irritation procedures commonly used to assess eye irritation. These two methods are briefly summarized below:

1. The FHSA (modified Draize) test utilized albino rabbits, which were dosed into the conjunctival sac with 0.1 mL of liquid product or the weight of the solid product equivalent to 0.1 cc. The eyelids were held shut for one second after instillation. The animals were observed at 1, 2, 3, 4, 7, 14 and 21 days or longer.
2. The Griffith low-volume eye irritation test utilized albino rabbits, with the test substances dosed directly on the cornea with 0.01 mL of liquid product or the weight of solids equivalent to 0.01 cc. The eyelid was released immediately after dosing without forced closing. The animals were observed for the same time periods as above.

Results: Median days-to-clear for human accident eye exposure are minimal. Only one product was as high as 7 days and the rest were 2 days or less. A total of 88.1% of the eyes cleared in 4 days or less. There was no reported permanent eye damage. Both of the animal methods produced more severe eye responses than were reported from human eye accidents with the same consumer products (Freeberg et al. 1984).
Remarks: Animal studies consistently overestimated the human response to accidental exposure. Of the two animal methods, the low-volume rabbit test gave a closer correlation, while the FHSA test gave the least correlation. A follow-up study published in 1986 confirmed this conclusion. Finally, an additional paper published in 1995 compared consumer eye irritation comments from 1985 to 1992 with the results of low volume eye tests (LVET). The clinical data and consumer experience consistently showed less eye irritation in humans from exposure to products than was observed in animal studies.

Recovery in humans was similar to that reported previously, supporting milder irritation response and faster healing in humans than in rabbits.

Reference: Freeberg, F.E., Griffith, J.F., Bruce, R.D., and Bay, P.H.S. 1984. Correlation of animal test methods with human experience for household products. J. Toxicol.- Cut. & Ocular Toxicol. 1:53-64.
Freeberg, F.E., Hooker, D.T., and Griffith, J.F. 1986. Correlation of animal eye test data with human experience for household products: an update. J. Toxicol.- Cut. & Ocular Toxicol. 5:115-123.
Cormier, E.M., Hunter, J. E., Billhimer, W., May, J., and Farage, M.A. 1995. Use of clinical and consumer eye irritation data to evaluate the low-volume eye test. J. Toxicol.- Cut. & Ocular Toxicol. 14:197-205.

Reliability: 2 Valid with restrictions

(e)

Type: Characterization of aerosols generated from a consumer spray product

Methods: The study was designed to evaluate size distribution of aerosols suspended in air after normal use of consumer spray products. Size distribution of aerosols generated from six different consumer trigger spray product nozzles was measured using a laser diffraction particle sizer (Mastersizer Model X, Malvern Instruments Ltd). A 300 mm receiving lens was used, which covers a particle size range of 1.2-600 microns. The exit of the trigger sprayer was positioned at 20 mm from the lens to the center of the device to avoid vignetting, and 120 mm from the laser beam axis to the tip of the trigger sprayer to avoid its interference with the laser beam. Measurements were repeated 5 times for each sprayer.

Results: The overall mean (n=30) particle size is 0.11% particles under 10 microns, with a standard deviation of 0.21. The very highest observation was 0.80%. Under normal use conditions, the peak breathing zone concentration under 10 microns ranged from 0.13 to 0.72 mg/m^3.

Remarks: This testing only captured the spray particles that are under 600 microns, so the actual percentage of total volume sprayed is less than 0.1%.

Reference: Battelle. 1999. Measurement and Characterization of Aerosols Generated from a Consumer Spray Product – Pilot Study. Prepared for The Soap and Detergent Association. Battelle Study No. N003043A, January 18, 1999.

Reliability: 1 Valid without restriction

(f)

Type: Modeling of dose observed from inhalation of aerosols

Methods: The worst case air concentration of LAS resulting from use in surface cleaning spray products was modeled using methods recommended by the HERA Guidance Document (06/2001). In this modeling, HERA reports the results of experimental measurements of the concentration of aerosol particles from a 2001 Procter & Gamble study. The following algorithm was used to model the absorbed dose:

$$Exp_{sys} = F_1 \cdot C' \cdot Q_{inh} \cdot t \cdot n \cdot F_7 \cdot F_8/bw \text{ (mg/kg bw/day)}$$

Where:
Exp_{sys} = dose absorbed via inhalation
F_1 = weight fraction of substance in product = 6% (worst case assumption)
C' = product concentration = 0.35 mg/m^3
Q_{inh} = ventilation rate of user = 0.8 m^3/hr
t = duration of exposure = 0.17 hr (10 minutes)
n = product use frequency, in number of events per day = 1
F_7 = weight fraction respirable = 100%
F_8 = weight fraction absorbed or bioavailable = 75%

bw = body weight = 60 kg

Results: The modeling resulted in an Exp_{sys} (inhalation of aerosols) = 0.04 µg/kg bw/day. Measured aerosol particles under 6.4 microns in size were generated upon spraying with typical surface cleaning spray products, resulting in a product concentration of 0.35 mg/m^3.

Reference: HERA. 2002. HERA-LAS Human and Environmental Risk Assessment: Linear Alkylbenzene Sulphonates, LAS. CAS No. 68411-30-3, Draft, July 2002. http://www.heraproject.com/riskassessment.cfm

Reliability: 4 This score was assigned because the original Procter & Gamble study and the HERA model inputs were not available for review. However, the study and all assumptions were evaluated by HERA.

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APPENDIX A

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United States
Environmental Protection
Agency

Prevention, Pesticides
and Toxic Substances
(7510P)

EPA 739-R-06-006
July 2006

Reregistration Eligibility Decision for Alkylbenzene Sulfonates

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

OFFICE OF
PREVENTION, PESTICIDES
AND TOXIC SUBSTANCES

CERTIFIED MAIL

Dear Registrant:

This is to inform you that the Environmental Protection Agency (hereafter referred to as EPA or the Agency) has completed its review of the available data and public comments received related to the preliminary risk assessments for the antimicrobial alkylbenzene sulfonates (ABS). The enclosed Reregistration Eligibility Decision (RED) document was approved on July 27, 2006.

Based on its review, EPA is now publishing its Reregistration Eligibility Decision (RED) and risk management decision for alkylbenzene sulfonates and its associated human health and environmental risks. A Notice of Availability will be published in the *Federal Register* announcing the publication of the RED.

The RED and supporting risk assessments for alkylbenzene sulfonates are available to the public on the U.S. Federal Government website www.regulations.gov. The docket is EPA-HQ-OPP-2006-0156.

The alkylbenzene sulfonates RED was developed through EPA's public participation process, published in the Federal Register on September 10, 2004, which provides opportunities for public involvement in the Agency's pesticide tolerance reassessment and reregistration programs. Developed in partnership with USDA and with input from EPA's advisory committees and others, the public participation process encourages robust public involvement starting early and continuing throughout the pesticide risk assessment and risk mitigation decision making process. The public participation process encompasses full, modified, and streamlined versions that enable the Agency to tailor the level of review to the level of refinement of the risk assessments, as well as to the amount of use, risk, public concern, and complexity associated with each pesticide. Using the public participation process, EPA is attaining its strong commitment to both involve the public and meet statutory deadlines.

Please note that the alkylbenzene sulfonates risk assessment and the attached RED document concern only this particular pesticide. This RED presents the Agency's conclusions on the dietary, drinking water, occupational, residential and ecological risks posed by exposure to alkylbenzene sulfonates alone. This document also identifies both generic and product-specific data that the Agency intends to require in Data Call-Ins (DCIs). Note that DCIs, with all pertinent instructions, will be sent to registrants at a later date. Additionally, for product-specific DCIs, the first set of required responses will be due 90 days from the receipt of the DCI letter. The second set of required responses will be due eight months from the receipt of the DCI letter.

As part of the RED, the Agency has determined that alkylbenzene sulfonates will be eligible for reregistration provided that all the conditions identified in this document are satisfied. Sections IV and V of this RED document describe the necessary labeling amendments for end-use products and data requirements. Instructions for registrants on submitting the revised labeling can be found in the set of instructions for product-specific data that will accompany this DCI.

If you have questions on this document or the label changes relevant to this reregistration decision, please contact the Chemical Review Manager, Heather Garvie, at (703) 308-0034. For questions about product reregistration and/or the Product DCI that will follow this document, please contact Adam Heyward at (703) 308-6422.

Sincerely,

Frank T. Sanders
Director, Antimicrobials Division

REREGISTRATION ELIGIBILITY
DECISION
for
Alkylbenzene Sulfonates
List D
CASE 4006

Approved By:

Frank T. Sanders
Director, Antimicrobials Division
July 27, 2006

Attachment

Table of Contents

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GLOSSARY OF TERMS AND ABBREVIATIONS

a.i.	Active Ingredient
aPAD	Acute Population Adjusted Dose
APHIS	Animal and Plant Health Inspection Service
ARTF	Agricultural Re-entry Task Force
BCF	Bioconcentration Factor
CDC	Centers for Disease Control
CDPR	California Department of Pesticide Regulation
CFR	Code of Federal Regulations
ChEI	Cholinesterase Inhibition
CMBS	Carbamate Market Basket Survey
cPAD	Chronic Population Adjusted Dose
CSFII	USDA Continuing Surveys for Food Intake by Individuals
CWS	Community Water System
DCI	Data Call-In
DEEM	Dietary Exposure Evaluation Model
DL	Double layer clothing {i.e., coveralls over SL}
DWLOC	Drinking Water Level of Comparison
EC	Emulsifiable Concentrate Formulation
EDSP	Endocrine Disruptor Screening Program
EDSTAC	Endocrine Disruptor Screening and Testing Advisory Committee
EEC	Estimated Environmental Concentration. The estimated pesticide concentration in an environment, such as a terrestrial ecosystem.
EP	End-Use Product
EPA	U.S. Environmental Protection Agency
EXAMS	Tier II Surface Water Computer Model
FDA	Food and Drug Administration
FFDCA	Federal Food, Drug, and Cosmetic Act
FIFRA	Federal Insecticide, Fungicide, and Rodenticide Act
FOB	Functional Observation Battery
FQPA	Food Quality Protection Act
FR	Federal Register
GL	With gloves
GPS	Global Positioning System
HIARC	Hazard Identification Assessment Review Committee
IDFS	Incident Data System
IGR	Insect Growth Regulator
IPM	Integrated Pest Management
RED	Reregistration Eligibility Decision
LADD	Lifetime Average Daily Dose
LC_{50}	Median Lethal Concentration. Statistically derived concentration of a substance expected to cause death in 50% of test animals, usually expressed as the weight of substance per weight or volume of water, air or feed, e.g., mg/l, mg/kg or ppm.
LCO	Lawn Care Operator
LD_{50}	Median Lethal Dose. Statistically derived single dose causing death in 50% of the test animals when administered by the route indicated (oral, dermal, inhalation), expressed as a weight of substance per unit weight of animal, e.g., mg/kg.
LOAEC	Lowest Observed Adverse Effect Concentration
LOAEL	Lowest Observed Adverse Effect Level
LOC	Level of Concern
LOEC	Lowest Observed Effect Concentration
mg/kg/day	Milligram Per Kilogram Per Day
MOE	Margin of Exposure
MP	Manufacturing-Use Product

MRID	Master Record Identification (number). EPA's system of recording and tracking studies submitted.
MRL	Maximum Residue Level
N/A	Not Applicable
NASS	National Agricultural Statistical Service
NAWQA	USGS National Water Quality Assessment
NG	No Gloves
NMFS	National Marine Fisheries Service
NOAEC	No Observed Adverse Effect Concentration
NOAEL	No Observed Adverse Effect Level
NPIC	National Pesticide Information Center
NR	No respirator
OP	Organophosphorus
OPP	EPA Office of Pesticide Programs
ORETF	Outdoor Residential Exposure Task Force
PAD	Population Adjusted Dose
PCA	Percent Crop Area
PDCI	Product Specific Data Call-In
PDP	USDA Pesticide Data Program
PF10	Protections factor 10 respirator
PF5	Protection factor 5 respirator
PHED	Pesticide Handler's Exposure Data
PHI	Pre-harvest Interval
ppb	Parts Per Billion
PPE	Personal Protective Equipment
PRZM	Pesticide Root Zone Model
RBC	Red Blood Cell
RED	Reregistration Eligibility Decision
REI	Restricted Entry Interval
RfD	Reference Dose
RPA	Reasonable and Prudent Alternatives
RPM	Reasonable and Prudent Measures
RQ	Risk Quotient
RTU	(Ready-to-use)
RUP	Restricted Use Pesticide
SCI-GROW	Tier I Ground Water Computer Model
SF	Safety Factor
SL	Single layer clothing
SLN	Special Local Need (Registrations Under Section 24C of FIFRA)
STORET	Storage and Retrieval
TEP	Typical End-Use Product
TGAI	Technical Grade Active Ingredient
TRAC	Tolerance Reassessment Advisory Committee
TTRS	Transferable Turf Residues
UF	Uncertainty Factor
USDA	United States Department of Agriculture
USFWS	United States Fish and Wildlife Service
USGS	United States Geological Survey
WPS	Worker Protection Standard

EXECUTIVE SUMMARY

The Environmental Protection Agency (hereafter referred to as EPA or the Agency) has completed preliminary risk assessments and its review of error correction and public comments on the human health and environmental risk assessments for alkylbenzene sulfonates and is issuing its risk management decision. The Agency will accept public comments on this decision and supporting documents for 60 days following publication. The Agency has decided alkylbenzene sulfonates are eligible for reregistration provided all measures outlined in this document are implemented. If during the comment period the Agency receives new or additional information that substantially changes the risk assessment findings or the risk management decision, the Agency will issue an amendment to this document.

Alkylbenzene sulfonates are used largely as food-contact sanitizers in food processing plants and eating establishments. They are also used as disinfectants and sanitizers for agricultural, commercial, institutional, industrial, and public access uses. Approximately 300,000 pounds of alkylbenzene sulfonates are used in EPA registered antimicrobial products. However, the largest overall use of alkylbenzene sulfonates is in household laundry and dish detergents. The alkylbenzene sulfonates are listed on the EPA High Production Volume (HPV) Challenge Program. HPV chemicals are those that are manufactured or imported into the U.S. in production volumes greater than one million pounds per year.

Overall Risk Summary

An acute dietary assessment was not conducted because there are no adverse effects attributable to a single dose seen in animal studies. Chronic dietary risk estimates were provided for the general U.S. population and all population subgroups. All chronic dietary risk estimates are below the Agency's level of concern.

Because there are no adverse effects attributable to acute exposure, an acute aggregate assessment was not conducted. An intermediate-term aggregate assessment was not conducted because there are no residential exposures of this duration. Therefore, only short-term and chronic aggregate assessments were conducted. In addition, because there are no long-term residential exposures, the chronic aggregate assessment only considered food and drinking water exposures. The short-term aggregate assessment considers both the active and inert uses of the alkylbenzene sulfonates. The chronic aggregate assessment considers average dietary exposure (food and drinking water) from both the active food contact sanitizer uses and the inert uses on agricultural commodities. The dietary exposures from the fruit and vegetable wash were not considered because it would be overly conservative to assume simultaneous exposure to alkylbenzene sulfonates from three different use patterns. The short-term aggregate oral and inhalation risks are not of concern for adults or children. In addition, the chronic aggregate assessment found no risk of concern for children or adults.

The Agency's human heath risk assessment indicates that there are four occupational handler inhalation scenarios with MOEs less than the target of 100. These four scenarios have MOEs between 90 and 93. Although these MOEs are below the Agency target of 100, the

Agency is not requiring mitigation since the risk assessment is based on conservative assumptions and the MOEs are very close to the target so that the Agency does not have risk concerns.

Dermal exposures were not considered in the risk assessment because a toxicological endpoint was not established for this route of exposure.

An environmental risk assessment was also conducted for alkylbenzene sulfonates. Due to limited potential for environmental exposure, environmental risks are below the Agency's level of concern.

Dietary Risk

The Agency conducted three chronic dietary exposure and risk assessments for alkylbenzene sulfonates: (1) as an active ingredient in food contact sanitizing solutions; (2) as an active ingredient in a fruit and vegetable wash; and (3) as an inert ingredient in pesticide formulations that may be applied to growing agricultural crops, raw agricultural commodities after harvest, and to animals. An acute dietary assessment was not conducted because there are no adverse effects attributable to a single dose in animal studies.

The dietary risk estimates for the active ingredient, total food contact sanitizing uses are below the Agency's level of concern for the general U.S. population for all age groups (less than 11% of the cPAD). The dietary risk estimates for the fruit and vegetable wash are also below the Agency's level of concern for all age groups (less than 71.2% of the cPAD).

The dietary risk estimates for the inert ingredient uses are below the Agency's level of concern for the general U.S. population (24% of the cPAD) and all population subgroups (84% of the cPAD for children 1-2 years of age). There is no concern for aggregate food and drinking water exposures to the alkylbenzene sulfonates resulting from their use as inert ingredients in pesticide products.

The chronic dietary risk assessment concludes that risk estimates are below the Agency's level of concern for the general U.S. population and all subpopulations. Therefore, no mitigation measures are necessary.

Drinking Water Risk

There are no currently registered outdoor uses of alkylbenzene sulfonates as active ingredients. However, the potential exists for transport into drinking water resulting from the pesticidal inert ingredient uses of alkylbenzene sulfonates. Therefore, the Agency estimated drinking water concentrations resulting from the inert ingredient uses of these substances. The Agency did not estimate acute drinking water risks for the inert ingredient use because an acute dietary endpoint (i.e., aPAD) was not selected as there were no effects attributable to a single dose exposure in animal studies. The Agency concluded that there are no risk concerns for the

general U.S. population and all population subgroups for drinking water exposures to the alkylbenzene sulfonates as pesticide inert ingredients.

Residential Risk

Residential handler and post-application exposure scenarios were assessed using high end exposure scenarios, end-use product application methods and use rates for inert uses. For each of the use scenarios, the Agency assessed residential handler (applicator) inhalation exposure and post application incidental ingestion by toddlers. All margins of exposure (MOEs) for short-term inhalation exposure for residential handlers are above the target MOE of 100 and, therefore, not of concern, with the exception of the flea and tick product where the MOE was 87. However, this screening level assessment was conducted using conservative assumptions because it assumes a person treats his/her pet with 0.5 cans of flea product that contains 24% alkylbenzene sulfonates every day for a month. All MOEs for residential post-application exposure are above the target of MOE of 100 and, therefore, are not of concern. Therefore the Agency does not have risk concerns.

Aggregate Risk

The chronic aggregate assessment considers average dietary exposure (food and drinking water) from both the active food contact sanitizer uses and the inert uses on agricultural commodities. The dietary exposures from the fruit and vegetable wash were not considered because it would be overly conservative to assume simultaneous exposure to alkylbenzene sulfonates from three different use patterns. Oral and inhalation exposure and risk estimates were conservatively combined for the aggregate risk assessment. Both short-term and chronic aggregate assessments were conducted. The short-term aggregate oral and inhalation risks are not of concern for adults, as the total aggregate MOE is 340 which is greater than the target of 100. For children, the aggregate risk estimate is very close to the target MOE of 100 (MOE=99). Because of the conservative nature of the assessment, the Agency does not have any risks of concern for children. The chronic aggregate assessment found no risk of concern for children or adults.

Occupational Risk

The Agency's human heath risk assessment indicates that there are four occupational handler inhalation scenarios with MOEs less than the target of 100. These four scenarios have MOEs between 90 and 93. The Agency is not requiring mitigation because the conservative assumptions used in the risk assessment, combined with the nearness of the MOE to the target, do not suggest concerns.

For most of the occupational scenarios, postapplication dermal exposure is not expected to occur or is expected to be negligible based on the application rates and chemical properties of alkylbenzene sulfonates.

Alkylbenzene sulfonates are dermal irritants at concentrations greater than 20%. Almost all of the labels require the use of gloves by workers.

Ecological Risk

Minimal or no environmental exposure to terrestrial or aquatic organisms is expected to occur from the majority of alkylbenzene sulfonate antimicrobial indoor pesticide uses given that only a very small number of total alkylbenzene sulfonates pounds are used for these purposes. Available data suggest that the alkylbenzene sulfonates may be more toxic to aquatic organisms as the number of carbons in the chain increase. Available data also indicate that the alkylbenzene sulfonates are slightly toxic to green algae.

The inert agricultural uses of alkylbenzene sulfonates are not expected to adversely affect avian or mammalian species on an acute or chronic basis. Aquatic organisms are also not expected to be adversely affected by inert alkylbenzene sulfonates use acutely or chronically due to the low estimated level of alkylbenzene sulfonates in water.

Use of alkylbenzene sulfonates in agricultural pesticide formulations is not expected to result in significant environmental exposure, therefore, no adverse effects (NE) to listed species are anticipated.

Regulatory Decision

The Agency has completed its review and has determined that the data are sufficient to support reregistration of all supported products containing alkylbenzene sulfonates. The Agency is issuing this RED for alkylbenzene sulfonates, as announced in a Notice of Availability published in the *Federal Register*. The RED and supporting risk assessment documents for alkylbenzene sulfonates are available to the public on the U.S. Federal Government website www.regulations.gov. The docket is EPA-HQ-OPP-2006-0156.

This RED document includes guidance and time frames for making any necessary label changes for products containing alkylbenzene sulfonates.

Summary of Mitigation Measures

Since no risks of concern were identified, no specific mitigation measures are needed for alkylbenzene sulfonates.

Data Requirements

Additional confirmatory data is required to complete the reregistration of alkylbenzene sulfonates. A complete list of data gaps is presented Section V and Appendix B (Table of Generic Data Requirements). In addition, product-specific data is required for all products containing alkylbenzene sulfonates as described in Section V of this document.

I. Introduction

The Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) was amended in 1988 to accelerate the reregistration of products with active ingredients registered prior to November 1, 1984 and amended again by the Pesticide Registration Improvement Act of 2003 to set time frames for the issuance of Reregistration Eligibility Decisions. The amended Act calls for the development and submission of data to support the reregistration of an active ingredient, as well as a review of all submitted data by the U.S. Environmental Protection Agency (EPA or the Agency). Reregistration involves a thorough review of the scientific database underlying a pesticide's registration. The purpose of the Agency's review is to reassess the potential hazards arising from the currently registered uses of the pesticide; to determine the need for additional data on health and environmental effects; and to determine whether or not the pesticide meets the "no unreasonable adverse effects" criteria of FIFRA.

On August 3, 1996, the Food Quality Protection Act of 1996 (FQPA) was signed into law. This Act amends FIFRA to require tolerance reassessment. The Agency has decided that, for those chemicals that have tolerances and are undergoing reregistration, the tolerance reassessment will be initiated through this reregistration process. The Act also requires that by 2006, EPA must review all tolerances in effect on the day before the date of the enactment of the FQPA. FQPA also amends the Federal Food, Drug, and Cosmetic Act (FFDCA) to require a safety finding in tolerance reassessment based on factors including consideration of cumulative effects of chemicals with a common mechanism of toxicity. This document presents the Agency's revised human health and ecological risk assessments and the Reregistration Eligibility Decision (RED) for alkylbenzene sulfonates (ABS).

The alkylbenzene sulfonates case is comprised of three active ingredients: sodium dodecylbenzene sulfonate, dodecylbenzene sulfonic acid and alklybenzene sulfonic acid. Sodium dodecylbenzene sulfonate and dodecylbenzene sulfonic acid (DDBSA) were first registered with the EPA on September 25, 1968 and February 24, 1969. C10-16 alkylbenzene sulfonic acid was registered on September 20, 1988.

As the case currently stands, sodium dodecylbenzene sulfonate (PC Code 079010) has three active products. Dodecylbenzene sulfonic acid (PC Code 098002) has 18 active products. C10-16-alkylbenzene sulfonic acid (PC Code 190116) has one active product. For a list of all the current products, please see Appendix A. In addition, these chemicals are also used as inert ingredients in other pesticide products.

Alkylbenzene sulfonates are antimicrobial pesticides that are used largely as food-contact sanitizers in food processing plants and eating establishments. They are also used as disinfectants and sanitizers for agricultural, commercial, institutional, industrial, and public access uses.

Tolerance exemptions for the active food-contact sanitizer uses of these ingredients have been established and can be found at 40 CFR 180.940(b) and (c).

The Agency has concluded that the FQPA Safety Factor for alkylbenzene sulfonates should be removed (equivalent to 1X), based on the available data and the risk assessment that does not underestimate risks for infants and children. A number of developmental studies via the oral route have been performed with alkylbenzene sulfonates in rats, mice and rabbits. The available information in these studies does not suggest any qualitative or quantitative evidence for susceptibility between the fetuses and maternal animals. The alkylbenzene sulfonates were tested in several multigeneration studies in rats, and there were no effects on offspring in any of these tests at doses up to 250 mg/kg/day.

The Food Quality Protection Act (FQPA) requires that the Agency consider available information concerning the cumulative effects of a particular pesticide's residues and other substances that have a common mechanism of toxicity. The reason for consideration of other substances is due to the possibility that low-level exposures to multiple chemical substances that cause a common toxic effect by a common toxic mechanism could lead to the same adverse health effect that would occur at a higher level of exposure to any of the substances individually. Unlike other pesticides for which EPA has followed a cumulative risk approach based on a common mechanism of toxicity, EPA has not made a common mechanism of toxicity finding for alkylbenzene sulfonates and any other substances. Alkylbenzene sulfonates do not appear to produce a toxic metabolite produced by other substances. For the purposes of this action, therefore, EPA has not assumed that alkylbenzene sulfonates have a common mechanism of toxicity with other substances. For information regarding EPA's efforts to determine which chemicals have a common mechanism of toxicity and to evaluate the cumulative effects of such chemicals, see the policy statements released by EPA's Office of Pesticide Programs concerning common mechanism determinations and procedures for cumulating effects from substances found to have a common mechanism on EPA's website at http://www.epa.gov/pesticides/cumulative.

This document presents the Agency's decision regarding the reregistration eligibility of the registered uses of alkylbenzene sulfonates. In an effort to simplify the RED, the information presented herein is summarized from more detailed information which can be found in the technical supporting documents for alkylbenzene sulfonates referenced in this RED. The revised risk assessments and related addenda are not included in this document, but are available in the Public Docket at www.regulations.gov.

This document consists of six sections. Section I is the Introduction. Section II, Chemical Overview, provides regulatory history, a profile of the use and usage of alkylbenzene sulfonates and a basic overview of the chemical. Section III, Summary of Alkylbenzene Sulfonates Risk Assessments, gives an overview of the human health and environmental assessments, based on the data available to the Agency. Section IV, Risk Management, Reregistration, and Tolerance Reassessment Decision, presents the reregistration eligibility and risk management decisions. Section V, What Registrants Need to Do, summarizes the necessary label changes based on the risk mitigation measures, if any, outlined in Section IV. Finally, the Appendices list all use patterns eligible for reregistration, bibliographic information, related documents and how to access them, and Data Call-In (DCI) information.

II. Chemical Overview

A. Regulatory History

The alkylbenzene sulfonates case is comprised of three active ingredients. Sodium dodecylbenzene sulfonate (PC Code 079010) and dodecylbenzene sulfonic acid or DDBSA (PC Code 098002) were first registered with the EPA on September 25, 1968 and February 24, 1969, respectively. C10-16-alkylbenzene sulfonic acid (PC Code 190116) was not registered until 1988. According to the unregistered technical manufacturers, at least some of the technical material contains a carbon mixture (C10-16) in the alkyl string and not pure C12 (as the name dodecyl- implies). As the case currently stands, sodium dodecylbenzene sulfonate has three active products. Dodecylbenzene sulfonic acid has 18 active products. C10-16-alkylbenzene sulfonic acid has one active product.

These chemicals are antimicrobials used largely as food-contact sanitizers in food processing plants and eating establishments. They are also used as disinfectants and sanitizers for agricultural, commercial, institutional, industrial, and public access uses. In addition to the pesticidal uses, the linear alkylbenzene sulfonate (LAS) surfactants are used in laundry and dish detergents as well as many other common uses. As inert ingredients in pesticide products, the chemicals are used in residential and outdoor agricultural settings.

The DDBSA Steering Committee/Joint Venture ("Joint Venture") formed on January 23, 1992 in response to EPA's October 23, 1989 notice initiating reregistration under FIFRA § 4 for List D of active pesticide ingredients. Current Joint Venture Members include: Acuity Specialty Products/Zep; Alex C. Fergusson, Inc.; Anderson Chemical Co.; DeVere Chemical Co., Inc.; Ecolab, Inc.; Hydrite Chemical Co.; JohnsonDiversey, Inc.; Morgan-Gallacher, Inc.; Oakite Products, Inc.; Quadra Chemical, Inc.; Thatcher Company; and West Agro, Inc.

Exemptions from the requirement of a tolerance for the active food-contact sanitizer uses of these ingredients have been established in the 40 CFR 180.940(b) and (c).

B. Chemical Identification

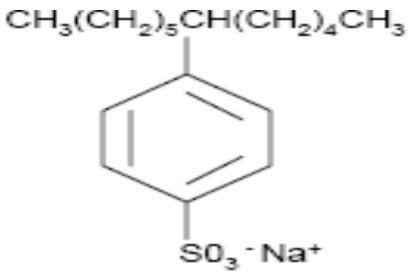

Figure 1: Sodium Dodecylbenzene Sulfonate (also named as dodecylbenzene sulfonic acid, sodium salt)

1. Sodium Dodecylbenzene Sulfonate (079010)

a. Chemical Overview

Common Name:	Sodium dodecylbenzene sulfonate
Chemical Name:	Alkyl(C12) benzenesulfonic acid, sodium salt Benzenesulfonic acid, dodecyl-, sodium salt Dodecylbenzene sodium sulfonate Dodecylbenzenesulfonic acid, sodium salt Sodium laurylbenzenesulfonate
OPP Chemical Codes:	079010
CAS Registry No.:	25155-30-0
Case Number:	4006
Empirical Formula:	$C_{18}H_{29}NaO_3S$ / $C_{12}H_{25}C_6H_4SO_3Na$
Molecular Weight:	348.5
Highest Percentage of Active:	3.6%
End-Use Product Distributors:	Oakite Products Inc. Microcide Inc.

b. Use Profile

Type of pesticide:	Disinfectant	Sanitizer
	Microbiocide	Microbiostat
	Bacteriocide	Bacteriostat

Use Sites:
FOOD HANDLING/STORAGE ESTABLISHMENT PREMISES AND EQUIPMENT
Fruit and Vegetable Wash Water
Food Processing, Handling, and Storage Plant Surfaces, Equipment, and Premises
Milk and Dairy Processing Plant Surfaces, Equipment, and Premises
Meat and Poultry Processing Plant Surfaces, Equipment, and Premises
Eating Establishment Food Contact Surfaces, Equipment and Utensils
Food Dispensing Equipment
Vending Machines
Soft Custard Equipment

COMMERCIAL, INSTITUTIONAL, INDUSTRIAL PREMISES AND EQUIPMENT
Mine Acid Control

2. Dodecylbenzene Sulfonic Acid (098002)

a. Chemical Overview

Common Name:	Dodecylbenzene sulfonic acid
Chemical Name:	Dodecylbenzene sulfonic acid
OPP Chemical Codes:	098002
CAS Registry No.:	27176-87-0
Case Number:	4006
Empirical Formula:	$C_{18}H_{30}O_3S$ / $C_{12}H_{25}C_6H_4{\cdot}SO_3H$
Molecular Weight:	326.5
Highest Percentage of Active:	15.67%
End-Use Product Distributors:	Anderson Chemical Co. ZEP Manufacturing Co. Hydrite Chemical Co. Devere Company Inc. Morgan-Gallacher Inc. FiveStar Affiliates Inc Alex C. Fergusson, Inc. International Chemical Corp. Chemical Systems of Florida Inc. Diverseylever Ecolab, Inc. West Argo Inc. US Chemical Corp. Drexel Chemical Co.

b. Use Profile:

Type of Pesticide:	Sanitizer	Disinfectant
	Virucide	Bacteriocide
	Bacteriostat	

Use Sites:

AGRICULTURAL PREMISES AND EQUIPMENT
Dairy Farms (enclosed premise treatment)
Milking Equipment
Teat Liner

FOOD HANDLING/STORAGE ESTABLISHMENTS PREMISES AND EQUIPMENT
Dairy Equipment, Premises, and Utensils
Milk Storage (bulk)
Fruit and Vegetable Wash Water
Food/Milk Transportation Vehicles
Food Processing Plant Equipment, Premises, and Surfaces
Bakery Processing Equipment
Brewery Process Plant Equipment and Surfaces
Cannery Processing Equipment
Milk and Dairy Processing Plant Equipment, Premises, and Surfaces
Potato Washing Machines
Fruit and Vegetable Processing Equipment
Meat and Poultry Processing Plant Equipment, Premises, and Surfaces
Winery Processing Equipment
Egg Processing Equipment
Beverage Processing Equipment and Surfaces
Fish Processing Equipment
Eating Establishment Equipment, Glassware, Utensils, Surfaces
Food Vending Machines
Food Dispensing Equipment
Food Store/Market/Supermarket Premises
Seed Houses/Stores/Storage Areas/Warehouses

COMMERCIAL, INSTITUTIONAL, INDUSTRIAL PREMISES AND EQUIPMENT
Research Animal Facilities (enclosed premise treatment)
Zoo Premises (enclosed premise treatment)
Airports
Campgrounds
Commercial Transportation Facilities
Aircraft (non feed/food)
Buses (non feed/food)

Ships
Railroad Trains
Commercial Premises and Equipment
Shower Stalls
Urinals
Toilet Bowls

RESIDENTIAL AND PUBLIC ACCESS PREMISES
Boat Premises
Automobiles

MEDICAL PREMISES AND EQUIPMENT
Sickroom Premises

3. Benzenesulfonic acid, C10-16-alkyl derivatives (190116)

a. Chemical Overview

Common Name:	Benzenesulfonic acid, C10-16-alkyl derivs.
Chemical Name:	C10-16-Alkylbenzene sulfonic acid
OPP Chemical Codes:	190116
CAS Registry No.:	68584-22-5
Case Number:	4006
Empirical Formula:	$C_{16\text{-}22}H_{30}O_3S$ / $C_{10\text{-}16}H_{25}C_6H_4{\cdot}SO_3H$
Molecular Weight:	324
Highest Percentage of Active:	25.6%
End-Use Product Distributors:	Kay Chemical Co. Quadra Chemicals, Inc.

b. Use Profile:

Type of Pesticide:	Sanitizer	Bacteriocide
	Bacteriostat	

Use Sites:
AGRICULTURAL PREMISES AND EQUIPMENT
Dairy/Milking Equipment and Utensils

FOOD HANDLING/STORAGE ESTABLISHMENTS PREMISES AND EQUIPMENT

Milk Storage (bulk)
Food Processing Plant Equipment and Surfaces
Meat and Poultry Processing Plant Equipment and Premises
Milk and Dairy Processing Plant Equipment and Premises
Beverage Processing Plant Equipment, Premises, and Surfaces
Eating Establishment Equipment, Utensils, and Surfaces

III. Summary of Alkylbenzene Sulfonates Risk Assessments

The purpose of this summary is to assist the reader by identifying the key features and findings of these risk assessments and to help the reader better understand the conclusions reached in the assessments. The human health and ecological risk assessment documents and supporting information listed in Appendix C were used to formulate the safety finding and regulatory decision for alkylbenzene sulfonates. While the risk assessments and related addenda are not included in this document, they are available from the U.S. Federal Government Public Docket at www.regulations.gov. The docket identification number is EPA-HQ-OPP-2006-0156. Hard copies of these documents may be found in the OPP public docket which is located in Room S-4400, One Potomac Yard, 2777 South Crystal Drive, Arlington, VA, and is open Monday through Friday, excluding Federal holidays, from 8:30 a.m.to 4:00 p.m.

A. Human Health Risk Assessment

The Agency's use of human studies in the alkylbenzene sulfonates risk assessment is in accordance with the Agency's Final Rule promulgated on January 26, 2006, related to Protections for Subjects in Human Research, which is codified in 40 CFR Part 26.

1. Toxicity of Alkylbenzene Sulfonates

A brief overview of the toxicity studies used for determining endpoints in the risk assessments are outlined below in Table 1. Further details on the toxicity of alkylbenzene sulfonates can be found in the "Alkylbenzene Sulfonates (ABS) Toxicology Chapter for the Reregistration Eligibility Decision (RED) Document," dated July 06 , 2006; and "Sulfonates (ABS) Revised Risk Assessment for the Reregistration Eligibility Decision (RED) Document," dated July 19, 2006. These documents are available on the U.S. Federal Government Public Docket website at www.regulations.gov.

The Agency has reviewed all toxicity studies submitted for alkylbenzene sulfonates and has determined that the toxicological database is sufficient for reregistration. The studies have been submitted to support guideline requirements. Major features of the toxicology profile are presented in Table 1.

Table 1. Acute Toxicity Studies for Alkylbenzene Sulfonates			
Guideline No./ Study Type	**MRID No.**	**Results**	**Toxicity Category**
870.1100 Acute oral toxicity	43498402 43498408 43498430	LD_{50} = range from 404 to over 5000 mg/kg	III-IV
870.1200 Acute dermal toxicity	94032006	LD_{50} = 1200 mg/kg	II
870.1300 Acute inhalation toxicity	Open Literature	LC_{50} = 0.31 mg/L	II
870.2400 Acute eye irritation	43498405	Corneal opacity not reversed at 72 hours.	I
870.2500 Acute dermal irritation	40359306	Severe irritation at 72 hours	II
870.2600 Skin sensitization	Open Literature	Non-Sensitizer	

The doses and toxicological endpoints selected by the Agency for the various exposure scenarios are summarized below in Table 2.

Table 2. Summary of Toxicological Dose and Endpoints for Alkylbenzene Sulfonates			
Exposure Scenario	**Dose Used in Risk Assessment, UF**	**Special FQPA SF*, endpoint and Level of Concern for Risk Assessment**	**Study and Toxicological Effects**
Acute Dietary (All populations)	No endpoint was selected. No effects are attributable to a single dose in animal studies.		

Table 2. Summary of Toxicological Dose and Endpoints for Alkylbenzene Sulfonates			
Exposure Scenario	**Dose Used in Risk Assessment, UF**	**Special FQPA SF*, endpoint and Level of Concern for Risk Assessment**	**Study and Toxicological Effects**
Chronic Dietary (All populations)	Systemic/ Reproductive NOAEL= 50 mg/kg/day UF = 100 **Chronic RfD** = 0.5 mg/kg/day	FQPA SF = 1X **cPAD** = chronic RfD / FQPA SF = 0.5 mg/kg/day	NOAEL = 40 mg/kg/day (0.07%) and LOAEL= 114 mg/kg/day (0.2%) based on increased caecum weight and slight kidney damage in a 6 month rat dietary study (Yoneyama et al 1972 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 24:409-440) **plus** Systemic/Reproductive NOAEL = 50 mg/kg/day and LOAEL = 250 mg/kg/day based on decreased Day 21 female pup body weight (Buehler, E. et al. 1971. Tox. Appl. Pharmacol. 18:83-91) **plus** NOAEL = 85 mg/kg/day and LOAEL= 145 mg/kg/day from 9 month drinking water rat study based on decreased body weight gain, and serum/ biochemical and enzymatic changes in the liver and kidney (Yoneyama et al. 1976 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 27(2):105-112)

General Toxicity Observations

Acute Toxicity. Alkylbenzene sulfonates exhibit a wide range of acute toxicity via the oral route in rats (LD_{50}s of 404 – 1980 mg/kg), with a narrower range in mice (LD_{50}s of 1259-2300 mg/kg). This spans the acute oral toxicity categories of III-IV. Alkylbenzene sulfonates are classified as acute toxicity category II for the dermal and inhalation routes of exposure. They are irritants to the eye (category I) and skin (category II), and are not skin sensitizers.

Absorption, Distribution, Metabolism, Excretion. In animal tests (oral – monkeys, pigs, rats), alkylbenzene sulfonates are readily absorbed from the gastrointestinal tract, are distributed throughout the body, and are extensively metabolized. Excretion is via both the urine and feces. Available dermal absorption data (rats and guinea pigs) indicate that alkylbenzene sulfonates are poorly absorbed from the skin, although prolonged contact may lead to irritation and thus compromise the skin to permit more absorption (WHO, 1996 and HERA, 2004).

Repeated Dose Toxicity (Subchronic and Chronic). There have been many oral repeated dose studies performed with alkylbenzene sulfonates ranging from a 28-day study in monkeys to nine month studies conducted with rats and mice. There have also been repeated dose dermal (guinea pigs, rabbits, and rats) and inhalation studies (dogs and monkeys). Collectively, animal data suggests that the liver, kidney and caecum (for oral studies) are the major target organs for toxicity. The liver and kidney effects were dose and duration related in that mild effects (organ weight changes and serum enzyme/clinical chemistry changes indicative of mild organ effects) were seen at lower doses, but increased in severity with both dose and time.

For the purposes of this hazard assessment, several studies were considered collectively to determine a no-observable adverse effect level (NOAEL) of 50 mg/kg/day for the chronic dietary endpoint. This is based on: increased caecum weight and slight kidney damage (at a NOAEL of 40 mg/kg/day and at a LOAEL of 114 mg/kg/day in the six month rat study); reduced body weight in 21-day old pups (at a NOAEL of 50 mg/kg/day and a LOAEL of 250 mg/kg/day in a reproductive toxicity rat study); and significant decreases in renal biochemical parameters (at a NOAEL of 85 mg/kg/day and a LOAEL of 145 mg/kg/day in a nine month drinking water study in rats).

Developmental Toxicity. A number of developmental studies via the oral and dermal routes have been performed with alkylbenzene sulfonates in rats, mice and rabbits; there were also several subcutaneous injection developmental studies reported in mice (WHO, 1996). In these developmental studies, there is varying quality in the more than 20 studies submitted. However, it is concluded that some developmental effects (including some terata) were observed at high doses at which maternal toxicity was observed and the available information does not suggest any qualitative or quantitative susceptibility differences between fetuses and maternal animals.

Reproductive Toxicity. Alkylbenzene sulfonates were tested in several multigeneration studies in rats. There were no effects on reproductive parameters in any of these tests at doses up to 250 mg/kg/day.

Carcinogenicity. The available long-term studies that assessed carcinogenicity were older studies (pre-1970) that would not be acceptable under current standards due to low number of animals used, insufficient number of doses and duration of dosing, and limited histopathological examinations. However, the limited studies provide no evidence of carcinogenicity in animals given alkylbenzene sulfonates orally.

Genotoxicity. The toxicological data show that alkylbenzene sulfonates were not genotoxic in vitro or in vivo.

Neurotoxicity. There is no evidence in the available toxicity studies or scientific literature to indicate neurotoxic effects of the alkylbenzene sulfonates in humans or laboratory animals.

Endocrine Disruption Potential. EPA is required under the Federal Food Drug and Cosmetic Act (FFDCA), as amended by FQPA, to develop a screening program to determine whether certain substances (including all pesticide active and other ingredients) "may have an effect in humans that is similar to an effect produced by a naturally occurring estrogen, or other such endocrine effects as the Administrator may designate." Following recommendations of its Endocrine Disruptor and Testing Advisory Committee (EDSTAC), EPA determined that there was a scientific basis for including, as part of the program, the androgen and thyroid hormone systems, in addition to the estrogen hormone system. EPA also adopted EDSTAC's recommendation that the Program include evaluations of potential effects in wildlife. For pesticide chemicals, EPA will use FIFRA and, to the extent that effects in wildlife may help determine whether a substance may have an effect in humans, FFDCA authority to require the wildlife evaluations. As the science develops and resources allow, screening of additional hormone systems may be added to the Endocrine Disruptor Screening Program (EDSP). When the appropriate screening and/or testing protocols being considered under the Agency's Endocrine Disrupting Screening Program (EDSP) have been developed, alkylbenzene sulfonates may be subjected to additional screening and/or testing to better characterize effects related to endocrine disruption.

2. FQPA Safety Factor

The FQPA Safety Factor (as required by the Food Quality Protection Act of 1996) is intended to provide an additional 10-fold safety factor (10X), to protect for special sensitivity in infants and children to specific pesticide residues in food, drinking water, or residential exposures, or to compensate for an incomplete database. The FQPA Safety Factor has been removed (i.e., reduced to 1X) for alkylbenzene sulfonates based on: (1) a lack of evidence that alkylbenzene sulfonates will induce neurotoxic effects, (2) no quantitative or qualitative evidence of increased susceptibility to the fetus following *in utero* exposure in the prenatal developmental toxicity studies, and (3) no quantitative or qualitative evidence of increased susceptibility to the offspring when adults are exposed in the two-generation reproductive study. The FQPA Safety Factor assumes that the exposure databases (food, drinking water, and residential) are complete and that the risk assessment does not underestimate the potential risk for infants and children. These criteria have been met for alkylbenzene sulfonates. Based on the analysis of submitted developmental toxicity studies, the Agency determined that no special FQPA Safety Factor was needed since there were no residual uncertainties for pre- and/or postnatal toxicity.

3. Population Adjusted Dose (PAD)

Dietary risk is characterized in terms of the Population Adjusted Dose (PAD), which reflects the reference dose (RfD), either acute or chronic, that has been adjusted to account for the FQPA Safety Factor (SF). This calculation is performed for each population subgroup. A risk estimate that is less than 100% of the acute or chronic PAD is not of concern.

a. Acute PAD

Acute dietary risk is assessed by comparing acute dietary exposure estimates (in mg/kg/day) to the acute Population Adjusted Dose (aPAD). Acute dietary risk is expressed as a percent of the aPAD. An acute dietary assessment for alkylbenzene sulfonates was not conducted because there are no adverse effects attributable to a single dose exposure in animal studies.

b. Chronic PAD

Chronic dietary risk for alkylbenzene sulfonates is assessed by comparing chronic dietary exposure estimates (in mg/kg/day) to the chronic Population Adjusted Dose (cPAD). Chronic dietary risk is expressed as a percent of the cPAD. The cPAD is the chronic reference dose (0.5 mg/kg/day) modified by the FQPA safety factor. The chronic RfD is 0.5 mg/kg/day for all populations, using a NOAEL of 50 mg/kg/day based on a weight of evidence from three toxicological studies that observed decreased pup body weight at 250 mg/kg/day and increased caecum weight, slight kidney damage at 114 mg/kg/day and significant decreases in renal biochemical parameters at 145 mg/kg/day. The NOAELs in the three studies used to develop the chronic endpoint are 40, 50 and 85 mg/kg/day as shown in Table 2. An uncertainty factor of 100 (10X for interspecies extrapolation, 10X for intraspecies variability) was applied to the NOAEL to obtain the chronic RfD. The alkylbenzene sulfonates cPAD is 0.5 mg/kg/day based on a reference dose of 0.5 mg/kg/day, which includes the incorporation the FQPA safety factor (1X) for the overall U.S. population or any population subgroups.

4. Dietary Exposure Assumptions

Chronic dietary exposure assessments for alkylbenzene sulfonates were conducted for the following uses: (1) as active ingredients in food contact sanitizing solutions; (2) as active ingredients in a fruit and vegetable wash; and (3) as inert ingredients in pesticide formulations that may be applied to growing agricultural crops, raw agricultural commodities after harvest, and to animals (pet product).

In the absence of residue data for residues of alkylbenzene sulfonates on treated food contact surfaces, the Agency estimated residue levels that may occur in food from the application rates on food contact surfaces. As mentioned previously, to determine the Estimated Daily Intake (EDI), the Agency has used an FDA model. The maximum percentage of active ingredient for dodecylbenzene sulfonates in food handling establishments from the various labels is 400 ppm. The Agency estimates that use of this product results in food residues of 530 ppb (µg/kg). The Agency assumed that food can contact 4000 cm^2 of treated surfaces, utensils, glassware, or pots and pans and that 100% of the pesticide migrates to food based on the standard assumptions used in the FDA Sanitizing Solution Guidelines. It was assumed that an adult and child consume 3000 and 1500 grams of food per day, respectively that will contact the treated surfaces.

The Agency used the FDA milk truck model to estimate residues in milk that could result from the use of alkylbenzene sulfonates in the food processing equipment, as representative of the potential uses in the food processing industry. As a conservative measure, the Agency assessed the maximum application rate of 400 ppm for dodecylbenzene sulfonates, as listed on the labels, although the current tolerance exemption has a limitation of 5.5 ppm for dairy processing equipment. The Agency estimates that use of this product results in maximum milk residues of 10 ppb (µg/kg). The Agency will be proposing a change to the 40 CFR 180.940(b) to have the end-use concentration not to exceed 400 ppm, rather than the current limitation of 5.5 ppm.

The Agency also estimated dietary exposure from the fruit and vegetable wash of the alkylbenzene sulfonates. This use is regulated by the FDA in 21 CFR 173.315, which permits the wash solution to contain dodecylbenzene sulfonic acid up to a maximum application rate of 0.2% (2000 ppm), without a potable rinse. The Agency assumed this maximum application rate of 2000 ppm in wash solution, along with assumptions for Thompson Seedless grapes as a surrogate to represent residues on all treated fruits and vegetables. The model estimates dodecylbenzene sulfonic acid residues of 9.25 ppm. Most of the pesticide labels are in compliance with this limitation. One label however, allows a vegetable wash solution containing 0.31% (3100 ppm) dodecylbenzene sulfonic acid, but requires a potable rinse following washing. The Agency plans to establish 0.2% as the maximum application rate that can be used without a potable rinse.

As inert ingredients in pesticide formulations, a conservative screening level dietary exposure model, Exposure Evaluation Model (DEEM™), was used that assumed 100% of all commodities, and 100% of all crops were treated with the alkylbenzene sulfonates, with no limitation on the fraction of inert ingredient. A complete explanation of the assumptions used in the generic screening model for estimating inert ingredient dietary exposure is given in Appendix A of the Inert Ingredient Dietary Risk Assessment for Linear Alkyl Benzenesulfonate.

5. Dietary (Food) Risk Assessment

a. Acute and Chronic Dietary Risk

Generally, a dietary risk estimate that is less than 100% of the acute or chronic PAD does not exceed the Agency's risk concerns. A summary of chronic risk estimates for active uses is shown in Table 3. A summary of chronic risk estimates for inert uses is shown in Table 4. Based on the pesticide labels, the Agency assessed dietary exposure that could result from the use of alkylbenzene sulfonates in the food service industry (treated surfaces, dishes, utensils, glassware, pots and pans), in the food processing industry (food processing equipment such as breweries and beverage plants, meat and poultry processing plants, milk and dairy products/packing plants etc), and as a fruit and vegetable wash. For additional information, please see the Dietary Exposure Assessments for the Reregistration Eligibility Decision and the Inert Ingredient Dietary Risk Assessment for Linear Alkyl Benzenesulfonate documents.

The daily estimates for food handling establishments, food processing equipment and the fruit and vegetable wash were conservatively used to assess chronic dietary risks, which are shown below in Table 3. As noted previously, an acute dietary assessment was not conducted because there were no adverse effects attributable to a single dose exposure in animal studies.

The dietary risk estimates for the total food contact sanitizing uses are below the Agency's level of concern for all age groups (less than 11% of the cPAD). In addition, the dietary risk estimates for the fruit and vegetable wash for adults and young children are below the Agency's level of concern for all age groups (less than 71.2% of the cPAD). These risk estimates are based on a number of conservative assumptions, and thus may overestimate the actual risks.

Table 3. Summary of Dietary Exposure and Risk for Alkylbenzene Sulfonates Pesticidal Active Uses

Use	Population Subgroup	Chronic Dietary	
		Dietary Exposure (mg/kg/day) a	% cPAD b
Food Service Industry (treated surfaces, utensils, glassware, etc)	adult male	0.023	4.6
	females (13-50 years)	0.027	5.4
	infants/children	0.053	10.6
Food Processing Industry (Food Processing Equipment)	adult male	0.00043	0.086
	females (13-50 years)	0.0005	0.1
	infants/children	0.001	0.2
Total Food Contact Surface Sanitizing Uses	adult male	0.023	4.6
	females (13-50 years)	0.027	5.4
	infants/children	0.054	10.8
Fruit and Vegetable Wash	U.S population	0.0979	19.6
	children 1-2 yrs	0.3558	71.2
	children 3-5 yrs	0.2573	51.5

NA=not applicable

a-- chronic exposure analysis based on body weights of 70 kg, 60 kg, and 15 kg for adult males, females and children, respectively.

b-- %PAD = dietary exposure (mg/kg/day) / cPAD, where cPAD=0.5 mg/kg/day for all populations.

b. Dietary Exposure for Inert Ingredient Uses

Included in this RED is the reassessment of alkylbenzene sulfonates when used as an inert ingredient in pesticide products. Alkylbenzene sulfonates are used as solvents, surfactants, dispersants, detergents, or wetting agents. Some of these products are designed for use in agricultural settings (pre- and post-harvest and when applied to animals), where there is a potential for dietary exposure.

Inert Dietary Exposure Assumptions

A dietary exposure analysis for the inert ingredient use of the alkylbenzene sulfonates was conducted using a screening model for estimating inert ingredient dietary exposure. The dietary assessment is unrefined and extremely conservative in nature because the screening model assumes that the inert ingredient is used on all commodities, and that 100 percent of crops are treated with the inert ingredient. Further, the model assumes residues will be present for every consumed commodity (including meat, milk, poultry and eggs) that is included in the Dietary Exposure Evaluation Model (DEEM™). The conservative nature of this assessment is believed to capture all potential dietary exposures, including those from direct application to animals.

The alkylbenzene sulfonates assessed in this document are constituents of a larger group of compounds that have a tolerance exemption as an inert ingredient in 40 CFR 180.910 and 180.930. The tolerance exemption is listed as Alkyl (C8-C24) benzenesulfonic acid and its ammonium, calcium, magnesium, potassium, sodium and zinc salts.

Inert Dietary Risk from Food

Table 4 provides a summary of the results of the chronic dietary risk estimates for alkylbenzene sulfonates as an inert ingredient.

Based on the use of the screening level inert ingredient dietary exposure model, there are no risk concerns associated with dietary exposures as the estimated dietary exposures for the U.S. population and all population subgroups are below 100% of the cPAD. As noted, a number of conservative assumptions were used in this screening level dietary risk assessment of inert uses.

Table 4. Summary of Dietary Exposure and Risk for Alkylbenzene Sulfonates as Inert Ingredients		
Population Subgroup	Chronic Dietary	
	Dietary Exposure (mg/kg/day)	% cPAD a
U.S. population	0.12	24
females (13-50 years)	0.087	17
children 1-2 yrs	0.422	84
children 3-5 yrs	0.31	62

a-- %PAD = dietary exposure (mg/kg/day) / cPAD, where cPAD=0.5 mg/kg/day for all population

c. Dietary Risk from Drinking Water

The drinking water exposure analysis is based on a derivation of estimated upper bound drinking water concentrations from these substances' use as pesticidal inert ingredient from the FQPA Index Reservoir Screening Tool (FIRST). The results of the FIRST modeling analysis and the conservative assumptions utilized as inputs into the inert ingredient drinking water exposure assessment model are provided in Appendix B of the Inert Ingredient Dietary Risk Assessment for Linear Alkyl Benzenesulfonate.

For chronic drinking water exposures to linear alkylbenzene sulfonates as inert ingredients, the Drinking Water Level of Comparison (DWLOC) range for chronic exposure is 38-1500 µg/L for the general U.S. population and 8-500 µg/L for children 1-2 years old. The Estimated Drinking Water Concentration (EDWC) used to assess chronic (non-cancer) dietary risk from drinking water is 6.6 µg/L. The chronic estimated concentration is below the DWLOCs for the general U.S. population and all population subgroups. Drinking water risks, therefore, are not of concern.

The Agency did not estimate acute drinking water risks for the inert ingredient use because an acute dietary endpoint (i.e., aPAD) was not selected as there were no effects attributable to a single dose exposure.

The estimated chronic drinking water concentration and drinking water level of concern for chronic exposure to linear alkyl benzenesulfonates is given in Table 5.

Table 5. Chronic Drinking Water Exposure Estimates for Inert Ingredient Uses of Alkylbenzene Sulfonates			
Population Subgroup	**EDWC[1] (µg/L)**	**%cPAD[2]**	**DWLOC[3] (µg/L)**
U.S. Population (total)	6.6	<0.1%	38 -1,500
Children (1-2 years)	6.6	<0.1%	8 - 500

1 Estimated Drinking Water Concentration (EDWC) for chronic drinking water exposure as determined by the use of FIRST modeling analysis described above for inert ingredient use. [The EDWC for linear alkyl benzenesulfonates is the value reported as the "Adjusted Annual Average (Chronic) Untreated Water Concentration"]

2 %cPAD = drinking water exposure (mg/kg/day) / cPAD, where cPAD=0.5 mg/kg/day for all populations. It was assumed that a 15 kg child ingests 1 L water per day and that a 70 kg adult ingests 2L water per day.

3 Drinking Water Level of Comparison (DWLOC) is the maximum contribution from water allowed in the diet based on food and drinking water from inert use only. In this case, since the allowable risk contribution from food is based on a screening level model, the use of a single, deterministic value for the DWLOC is not appropriate. Rather a DWLOC range is given, with the values in the range corresponding to an upper value of range of drinking water concentrations ranging from 100% of the cPAD (i.e., assuming no food exposure) to a lower value that considers food exposures to be at the dietary screening level value.

6. Residential Risk Assessment

Residential exposure assessment considers all potential pesticide exposure, other than exposure due to residues in food or in drinking water. Exposure may occur during treatment of outdoor residential turf, while cleaning indoor hard surfaces, or while using pet flea and tick products. Each route of exposure (oral, dermal, inhalation) is assessed, where appropriate, and risk is expressed as a Margin of Exposure (MOE), which is the ratio of estimated exposure to an appropriate NOAEL. Based on its use patterns, alkylbenzene sulfonates has been assessed for the residential mixing/loading/applicator (or "handler") exposure for applications by homeowners using an aerosol spray or by using a ready-to-use liquid with a low pressure hand wand, a hose or a sprinkling can. An inhalation post-application assessment was not conducted because the vapor pressure of the alkylbenzene sulfonates is extremely low ($5.1x10^{-10}$ to $6x10^{-15}$ mmHg). In addition, a dermal assessment was not conducted because of the lack of a dermal toxicological endpoint. Post application incidental ingestion by toddlers that may contact turf, hard surfaces or a pet treated with pesticide products containing alkylbenzene sulfonates is expected to be minimal, and all the scenarios evaluated have MOEs above 100.

a. Toxicity

The toxicological endpoints and associated uncertainty factors used for assessing the non-dietary risks for alkylbenzene sulfonates are listed in Table 6.

A MOE greater than or equal to 100 is considered adequately protective for the residential exposure assessment for the incidental oral and inhalation routes of exposure. The MOE of 100 includes 10X for interspecies extrapolation and 10X for intraspecies variation.

Table 6. Summary of Toxicological Dose and Endpoints for Assessing Occupational and Residential Risk for Alkylbenzene Sulfonates			
Exposure Scenario	**Dose Used in Risk Assessment, UF**	**Special FQPA SF*, endpoint and Level of Concern for Risk Assessment**	**Study and Toxicological Effects**
Short-Term Incidental Oral (1-30 days)	Oral NOAEL= 50 mg/kg/day UF = 100	**Residential** LOC for MOE < 100	NOAEL = 40 mg/kg/day (0.07%) and LOAEL= 114 mg/kg/day (0.2%) based on increased caecum weight and slight kidney damage in a 6 month rat dietary study (Yoneyama et al 1972 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 24:409-440) **plus** Systemic/Reproductive NOAEL = 50 mg/kg/day and LOAEL = 250 mg/kg/day based on decreased Day 21 female pup body weight (Buehler, E. et al. 1971. Tox. Appl. Pharmacol. 18:83-91) **plus** NOAEL = 85 mg/kg/day and LOAEL= 145 mg/kg/day from 9 month drinking water rat study based on decreased body weight gain, and serum/ biochemical and enzymatic changes in the liver and kidney (Yoneyama et al. 1976 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 27(2):105-112)
Short-, Intermediate- and Long-Term Inhalation (1 to 30 days, 1-6 months, >6 months)	Inhalation study NOAEL= 1mg/m^3 detergent dust combined with up to 0.1 mg/m^3 enzyme dust Equivalent to approximately 0.14 mg/kg/day (a) (inhalation absorption rate = 100%) purity= 13% active ingredient UF = 100	**Residential** LOC for MOE < 100 **Occupational** LOC for MOE < 100	Subchronic Inhalation Monkey Study LOAEL = 10 mg/m^3 detergent combined with 0.1 mg/m^3 enzyme dust. Toxicological effect is weight loss and decreased weight gain (W. Coates, et al 1978. Tox. Appl. Pharmacol. 45: 477-496) This air concentration is equivalent to approximately 1.4 mg/kg/day (a)

Table 6. Summary of Toxicological Dose and Endpoints for Assessing Occupational and Residential Risk for Alkylbenzene Sulfonates			
Exposure Scenario	**Dose Used in Risk Assessment, UF**	**Special FQPA SF*, endpoint and Level of Concern for Risk Assessment**	**Study and Toxicological Effects**
Dermal Endpoint	Quantification of dermal risk is not required since: 1) the alkylbenzene sulfonates are surfactants that are dermal irritants at concentrations generally greater than 20% solution. The requirement of the dermal toxicity studies with the end-use products will determine the personal protective clothing necessary to protect against irritation during product use; 2) no systemic toxicity was seen following repeated dermal applications to rabbits at 200 mg/kg/day (with an end use product), and 3) no developmental toxicity concerns were seen following repeated dermal applications to pregnant mice, rats or rabbits (developmental effects were seen either in the presence of maternal toxicity or at doses higher than those that caused maternal toxicity).		
Cancer (oral, dermal, inhalation)	No evidence of carcinogenicity in reported studies in rats		

(a) Equation used to convert inhalation air concentration to a dose= mg/L* absorption*respiratory volume (L/hr)*duration (hrs) * activity factor / body weight. Thus, 0.001 mg/L * 1*67.94 L/hr (based on default respiratory volumes for a New Zealand Rabbit which is used as a surrogate for a cynomolgus monkey) * 6 hrs * 1 / 2.98 kg (body weight for New Zealand Rabbit used as a surrogate for cynomolgus monkey, study reports monkey body weight ranges from 1.6 to 3.7 kg).

b. Residential Handler

i. Exposure Scenarios, Data and Assumptions

Residential exposure may occur for alkylbenzene sulfonates during applications of turf treatment, hard surface cleaners and pet flea and tick products. A number of assumptions, or estimates, such as adult body weight and area treated per application, are made by the Agency for residential risk assessment. Also, note that residential handlers are sometimes addressed somewhat differently than occupational handlers in that homeowners are assumed to complete all elements of an application (mix/load/apply) without the use of personal protective equipment.

The quantitative exposure/risk assessment developed for residential handlers is based on these scenarios:

1) outdoor residential turf treatment (ready to use liquid),
2) indoor hard surface cleaner (ready to use liquid), and
3) pet flea and tick products (aerosol can spray).

For the purposes of this screening level assessment, the Agency selected representative scenarios for the vast majority of products, based on end-use product application methods and use amounts. The above scenarios reflect high-end exposure and risk estimates for all products represented in a residential setting.

For most residential scenarios, the Agency used EPA's Pesticide Inert Risk Assessment Tool (PiRat) to estimate residential applicator and post-application exposures and risks from the use of alkylbenzene sulfonates as an inert ingredient in representative residential products. For the assessment of the pet products and hard surface cleaners, the Agency used assumptions in the Residential Standard Operating Procedures (SOPs). Typically, most products used in a residential setting result in exposures occurring over a short-term duration. Thus, the residential handler and postapplication scenarios are assumed to be of short- term duration (1-30 days).

An inhalation post-application assessment was not conducted because the vapor pressure of the alkylbenzene sulfonates is extremely low ($5.1x10^{-10}$ to $6x10^{-15}$ mmHg) and not expected to result in inhalation exposure. In addition, a dermal assessment was not conducted because of the lack of a dermal toxicological endpoint was not identified in animal studies.

ii. Residential Handler Risk Estimates

Based on toxicological criteria and potential for exposure, the Agency has conducted incidental oral and inhalation exposure assessments. As noted previously, MOEs greater than or equal to 100 for the inhalation route of exposure and 100 for incidental oral exposure are considered adequately protective for the residential exposure assessment.

A summary of the residential handler exposures and risk are presented in Table 7. For residential handlers that handle products containing alkylbenzene sulfonates as inert ingredients, the short-term inhalation MOEs were above the target MOE of 100, and thus, do not exceed the Agency's level of concern, with the exception of the flea and tick product where the MOE was 87 for the high-end formulation containing 24% alkylbenzene sulfonates. This scenario is conservative because it assumes a person treats their pet with 0.5 cans of flea product that contains 24% alkylbenzene sulfonates every day for a month. It is unlikely that a person would treat his/her pet every day for one month. Therefore, the Agency is not requiring risk mitigation. In addition, there are no risk concerns for the majority of pet products containing 2% alkylbenzene sulfonates.

Table 7. Estimates of Inhalation Exposures and Risks to Residential Handlers of Alkylbenzene Sulfonates as Inert Ingredients (Short-Term Duration)				
Product Use	**Application Method**	**Area Treated/Quantity Handled[a]**	**Inhalation Exposure (mg/kg/day)**	**Inhalation MOEs[c] (Target MOE ≥ 100)**
Outdoor Products				
Ready to Use Liquid Turf spot/gardens[b]	Low pressure handwand; MLAP	1000 ft^2/day (spot)	$7.07x10^{-6}$	20,000
	Hose end sprayer; MLAP	$2x10^4$ ft^2/day (full broadcast)	$4.48x10^{-5}$	3,100
	Backpack; MLAP	1000 ft^2/day (spot)	$7.07x10^{-6}$	20,000
	Sprinkling can; MLAP		$2.24x10^{-6}$	63,000
Indoor Products				
Ready to Use Liquid (hard surface cleaner)[d,e]	Low pressure handwand; MLAP	0.5 gallons/day	$1.37x10^{-4}$	1.000
Pet Flea and Tick Product[f]	Aerosol Can Spray	0.5 6 oz can	$1.61x10^{-3}$	87

a: Standard PiRat model input parameters, except for pet products and hard surface cleaner, which are based on an AD assumption.
b: percent formulation used = 11%; an application rate of 0.00015 lb product/ft^2 was assumed for all scenarios and the body weight = 70kg.
c: MOEs = NOAEL / exposure where inhalation NOAEL = 0.14 mg/kg/day and the target MOE ≥ 100
d: % formulation used = 8%
e: An application rate of 8 lb/gallon, which is the density of water, was assumed for all scenarios and the body weight =70kg.
f= % formulation = 24%.

c. Residential Post-Application

Residential post application exposures occur when bystanders contact areas in which the antimicrobial end use product has recently been applied. For alkylbenzene sulfonates there are no residential postapplication risk concerns for the household products that contain alkylbenzene sulfonates as an inert ingredient as shown on Table 8. All of the scenarios evaluated have short-term MOEs above 100, and thus are not of concern including postapplication incidental oral risks to children that may contact turf, hard surfaces or a pet treated with pesticide products containing alkylbenzene sulfonates as an inert ingredient. The postapplication MOEs range from 106 to 7,400.–

Table 8. Summary of Short-Term Residential Postapplication Exposure and Risk Estimates from Alkylbenzene Sulfonates as Inert Ingredients[a]

Product Use	Route of Exposure	Exposure mg/kg/day[b]	MOEs[c] (Target MOE ≥ 100
Ready to Use Liquid Turf spot/gardens[d]	Incidental ingestion: hand to mouth	1.08×10^{-2}	4,600
Ready to Use Liquid (hard surface cleaner)[a, e]		0.0068	7,400
Pet Flea and Tick Product[f]	Incidental ingestion: hand to mouth	0.4739	106

a: The representative use sites assessed through using PiRAT for incidental oral post application exposures to toddlers are turf products. Exposure from hard surface cleaner and pet products was based on AD assumptions.
b: The body weight used in this calculation was 15kg, which is assumed to be the body weight of a toddler.
c: MOEs = NOAEL / exposure where incidental oral NOAEL = 50 mg/kg/day. Target MOE ≥ 100.
d: % formulation used = 11%
e: % formulation used = 8%
f: % formulation used = 24%

7. Aggregate Risk

The Food Quality Protection Act amendments to the Federal Food, Drug, and Cosmetic Act (FFDCA, Section 408(b)(2)(A)(ii)) require "that there is a reasonable certainty that no harm will result from aggregate exposure to pesticide chemical residue, including all anticipated dietary exposures and other exposures for which there are reliable information." Aggregate exposure will typically include exposures from food, drinking water, residential uses of a pesticide, and other non-occupational sources of exposure. Aggregate exposure is the total exposure to a single chemical (or its residues) that may occur from dietary (i.e., food and drinking water), residential, and other non-occupational sources, and from plausible exposure routes (oral, dermal, and inhalation).

In performing aggregate exposure and risk assessments, the Office of Pesticide Programs has published guidance outlining the necessary steps to perform such

assessments (General Principles for Performing Aggregate Exposure and Risk Assessments, November 28, 2001; available at: http://www.epa.gov/pesticides/trac/science/aggregate.pdf . Steps for deciding whether to perform aggregate exposure and risk assessments are listed and include: identification of toxicological endpoints for each exposure route and duration; identification of potential exposures for each pathway (food, water, and/or residential); reconciliation of durations and pathways of exposure with durations and pathways of health effects; determination of which possible residential exposure scenarios are likely to occur together within a given time frame; determination of magnitude and duration of exposure for all exposure combinations; determination of the appropriate technique (deterministic or probabilistic) for exposure assessment; and determination of the appropriate risk metric to estimate aggregate risk.

Typically, aggregate risk assessments are conducted for acute (1 day), short-term (1-30 days), intermediate-term (1-6 months) and chronic (6 months to lifetime) exposures. However, an acute aggregate assessment was not conducted because there are no adverse effects attributable to acute exposure. An intermediate-term aggregate assessment was not conducted because there are no residential exposures of this duration. In addition, because there are no long-term residential exposures, the chronic aggregate assessment only considered food and drinking water. Thus, only short-term and chronic aggregate assessments were conducted. Oral and inhalation exposure and risk estimates were conservatively combined for the aggregate risk assessment because these endpoints both identify adverse effects on body weight. Dermal exposures were not considered in the risk assessment because a toxicological endpoint was not established.

a. Short- Term Aggregate Risk

This assessment considers both the active and inert uses of the alkylbenzene sulfonates. For children, the short-term aggregate assessment includes average dietary exposure (food and drinking water) from both the active food contact sanitizer uses and the inert uses on agricultural commodities, in addition to estimated incidental oral exposures to children from residential uses such as hard surface cleaning products as an inert ingredient. For adults, the aggregate assessment includes dietary (food and drinking water) from both active and inert uses and residential inhalation exposures from wiping a hard surface cleaning products since this scenario represents the highest exposure from the inert use. The residential handler scenario for pet flea and tick products (inhalation MOE of 87) was not included in the aggregate assessment. The pet flea and tick product assumes a person treats his/her pet with 0.5 cans of flea product that contains 24% alkylbenzene sulfonates every day for a month. The Agency does not have any risks of concern for this scenario because it is very conservative in nature.

The aggregate oral and inhalation risks are not of concern for adults, as the total aggregate MOE is 340 which is greater than the target of 100. For children, the aggregate risk estimate is very close to the target MOE of 100 (MOE = 99). As noted previously, several conservative assumptions were used in this assessment, and thus the Agency does

not have any risk concerns. The assumptions and equations are presented in the footnotes on Table 9.

Table 9 presents a summary of the short-term aggregate risk MOEs.

Table 9. Summary of Short-Term Aggregate Risk Estimates				
Exposure Scenario	**Dose [a] (mg/kg/day)**		**Total MOE[b] (Target MOE≥100)**	
	Child	**Adult**	**Child**	**Adult**
Oral Exposure				
Dietary Exposure				
Food Contact Sanitizer	0.054	0.027	926 (10.8% of cPAD)	1,850 (5.4% of cPAD)
Inert Ingredient Uses (Food)	0.422	0.12	118 (84% of cPAD)	417 (24% of the cPAD)
Drinking Water Exposure (Inert) c	0.00044	0.000189	114,000 (<1% of cPAD	227,000 (<1% of cPAD)
Hard Surface Cleaner (2% Inert)	0.0068	NA	7,400	NA
Inhalation Exposure				
Handler of hard surface cleaning products (2% Inert)	NA	0.000137	NA	1,000
Total Aggregate Dose and MOE	0.5	0.147	99	340

NA= Not applicable

(a) Chronic dietary exposure for females 13-50 years for sanitizer use. The total general population dietary exposure was used to assess inerts, since this population has higher exposure than females 13-50 years.

(b) MOE = NOAEL (mg/kg/ day) / potential dose rate (mg/kg/day) [Where short-term oral NOAEL = 50 mg/kg/day]. Target MOE ≥ 100.

(c) Exposure estimates assume a 15 kg child ingests 1L water/day and that a 60 kg adult female ingests 2L water per day of 6.6 ppb (the chronic estimated drinking water concentration (EDWC) based on the inert ingredient use.

b. Chronic Aggregate Risk

The chronic aggregate assessment considers average dietary exposure (food and drinking water) from both the active food contact sanitizer uses and the inert uses on agricultural commodities. The dietary exposures from the fruit and vegetable wash were not considered because it would be overly conservative to assume simultaneous exposure to alkylbenzene sulfonates from three different use patterns. As shown on Table 10, the dietary aggregate risk is 95% of the cPAD for children, while for adults it is 29% of the cPAD.

It should also be recognized that the majority of the uses of alkylbenzene sulfonates are not in pesticide products, but rather are used in household laundry and dish detergents. Over 800 million pounds of these compounds are produced each year, while only 300,000 pounds are used in EPA registered antimicrobial products. The Agency did

not consider potential exposure and risks from the numerous other residential exposures to alkylbenzene sulfonates because the Agency lacks reliable information at this time.

Table 10 presents a summary of the chronic aggregate risk estimates.

Table 10.
Summary of Chronic Aggregate Risk Estimates

Exposure Scenario	Dose [a] (mg/kg/day)		%cPAD[b]	
	Child (15 kg)	Adult	Child (15 kg)	Adult
Oral Exposure				
Dietary Exposure				
Food Contact Sanitizer	0.054	0.027	10.8%	5.4%
Inert Ingredient Uses (Food)	0.422	0.12	84%	24%
Drinking Water Exposure (Inert) c	0.00044	0.000189	<1%	<1%
Total Aggregate Dose and Risk	0.476	0.147	95%	29%

NA= Not applicable

(a) Chronic dietary exposure for females 13-50 years for sanitizer use. The total general population dietary exposure was used to assess inerts, since this population has higher exposure than females 13-50 years.

(b) %cPAD = dietary exposure (mg/kg/day) / cPAD, where cPAD -= 0.5 mg/kg/day for all populations.

(c) Exposure estimates assume a 15 kg child ingests 1L water/day and that a 60 kg adult female ingests 2L water per day containing 6.6 ppb alkylbenzene sulfonates. The 6.6 ppb estimate is based on the chronic estimated drinking water concentration (EDWC)) resulting from agricultural use of products that contain the alkylbenzene sulfonates as an inert ingredient.

8. Occupational Exposure and Risk

Workers can be exposed to a pesticide through mixing, loading, and/or applying a pesticide, or re-entering treated sites. Occupational handlers of alkylbenzene sulfonates include workers in a variety of occupational settings. Additionally, postapplication exposures are likely to occur in these settings. The representative scenarios selected for assessment were evaluated using maximum application rates as recommended on the product labels for alkylbenzene sulfonates.

Occupational risk is assessed for exposure at the time of application (termed "handler" exposure) and is assessed for exposure following application, or post-application exposure. Application parameters are generally defined by the physical nature of the formulation (e.g., formula and packaging), by the equipment required to deliver the chemical to the use site, and by the application rate.

Occupational risk for all of these potentially exposed populations is measured by a Margin of Exposure (MOE) which determines how close the occupational exposure comes to a No Observed Adverse Effect Level (NOAEL) from toxicological studies. In the case for alkylbenzene sulfonates, MOEs greater than 100 for inhalation exposures

are not of concern to the Agency for short- and intermediate-term exposures. For workers entering a treated site, MOEs are calculated for each day after application to determine the minimum length of time required before workers can safely re-enter.

a. Occupational Toxicity

Table 6 provides a listing of the toxicological endpoints used in the occupational risk assessment for alkylbenzene sulfonates.

b. Occupational Handler Exposure

The Agency has determined that there is potential for dermal and inhalation worker exposure to alkylbenzene sulfonates at various use sites when used at various use sites including agricultural premises, food handling, and commercial/institutional/industrial premises. Representative scenarios were selected for evaluation based on the use sites and maximum application rates for all three of the active ingredients in this assessment. As noted previously, the Agency did not select a dermal endpoint, and thus only inhalation exposure and risk estimates are presented.

To assess the handler risks, the Agency used surrogate unit exposure data from both the proprietary Chemical Manufacturers Association (CMA) antimicrobial exposure study and the Pesticide Handlers Exposure Database (PHED). Short-, and intermediate-term inhalation risks to occupational handlers for sanitizing scenarios, and estimated risks are presented in Table 11.

The Agency also calculated a total MOE for one of the active ingredients, sodium dodecylbenzene sulfonate based on the label use directions, which recommend the same product be used for both cleaning and sanitizing. Short-, and intermediate-term inhalation risks to occupational handlers cleaning and sanitizing with products that contain sodium dodecylbenzene sulfonate are shown in Table 12.

c. Occupational Handler Risk Summary

The occupational handler risk assessment included only inhalation exposures because the Agency did not select a dermal endpoint. For the occupational handler inhalation risk assessment, the short- and intermediate- term risks calculated at baseline exposure (no respirators) were above target MOEs for all scenarios (i.e., inhalation MOEs were >100), except:

- Short-Term and Intermediate-Term inhalation exposure from cleaning hard surfaces via wiping in the food handling category, inhalation MOE = 93.

Due to the conservative nature of the assessment, the Agency does not have a risk concern for this scenario.

The Agency also calculated a total MOE for one of the active ingredients, sodium

dodecylbenzene sulfonate based on the label use directions, which recommend the same product be used for both cleaning and sanitizing. As shown on Table 12, all total inhalation MOEs for cleaning and sanitizing (baseline) were above the target MOE of 100 for all scenarios, except the following:

- Short-Term and Intermediate-Term inhalation exposure from cleaning indoor hard surfaces via wiping and then following with sanitizing via immersion/flooding in the food handling premises category, inhalation MOE = 93.
- Short-Term and Intermediate-Term inhalation exposure from cleaning indoor hard surfaces via wiping and then following with sanitizing via low pressure spray in the food handling premises category, inhalation MOE = 90.
- Short-Term and Intermediate-Term inhalation exposure from cleaning indoor hard surfaces via sponge/mesh/wiping and then sanitizing via immersion/flooding in the food handling premises category, inhalation MOE = 90.

Again, due to the conservative nature of the assessment, risk estimates making a lot of assumptions, and the MOEs being so close to the target, the Agency does not have a risk concern for these scenarios.

Table 11. Short-, and Intermediate-Term Inhalation Risks for Occupational Handlers for Sanitizing (Representative Scenarios)

Exposure Scenario	Method of Application	Application Rate (lb ai/ gallon)	Quantity Handled/ Treated per day (gallons)	Baseline Inhalation MOE (a) (Target MOE≥100)
Agricultural Premises and Equipment				
Application to hard surfaces	Brush	0.0667	0.26	2,000
	Mechanical Foam	0.0667	0.26	430
	Flooding	0.00183	10	280
	Cleaning in place (CIP)	0.00195	10,000	1,200
	High Pressure spray	0.00326	40	630
	Immersion	0.00334	10	160
	Low pressure spray	0.00334	10	430
	Trigger Pump Spray	0.00334	0.26	8,700
Food Handling				
Application to indoor hard surfaces	Brush	0.0667	0.26	2,000
	Mechanical Foam	0.0667	0.26	430
	Immersion	0.00334	10	160
	Trigger Pump Spray	0.00334	0.26	8,700
	Low pressure handwand (clean)	0.00603	2	1,200

Table 11. Short-, and Intermediate-Term Inhalation Risks for Occupational Handlers for Sanitizing (Representative Scenarios)				
Exposure Scenario	**Method of Application**	**Application Rate (lb ai/ gallon)**	**Quantity Handled/ Treated per day (gallons)**	**Baseline Inhalation MOE (a) (Target MOE≥100)**
	High pressure spray (sanitize)	0.0115	40	180
	Immersion, flooding for RTU (sanitize)	0.003	10	170
	Mopping	0.00244	2	840
	Wiping (clean)	0.00603	0.26	93
	Sponge/mesh wipe (clean)	0.003	0.26	190
	Cleaning in Place (CIP) (clean and sanitize)	0.00358	10,000	680
Food dispensing equipment	Cleaning in Place (CIP) (clean)	0.00603	10,000	400
	Cleaning in Place (CIP) (sanitize)	0.00302	10,000	810
Fruits and vegetables	Immersion	0.00455	10	110
	Trigger pump spray	0.003	0.26	9,700
Commercial/Institutional Premises				
Application to indoor hard surfaces (includes utensils and silverware)	Brush	0.0667	0.26	2,000
	Mechanical Foam	0.0667	0.26	430
	Immersion	0.00334	10	160
	Low Pressure Handwand	0.00334	2	2,200
	Trigger Pump Spray	0.00334	0.26	8,700
Shower stalls and toilets	Mopping	0.0177	2	120
	Swabbing after a liquid pour	0.0177	0.26	1,100

(a) MOE = NOAEL (mg/kg/day) / Daily Dose [Where short-and intermediate-term NOAEL = 0.14 mg/kg/day for inhalation exposure] Target MOE is ≥ 100.

Table 12. Short, and Intermediate Term Inhalation Risks to Occupational Handlers Cleaning and Sanitizing with Products That Contain Sodium Dodecylbenzene Sulfonate			
Representative Use	**Method of CLEANING Application (Baseline MOE)**	**Method of SANITIZING Application (Baseline MOE)**	**Total Inhalation MOE (Baseline) (Target MOE≥100)**
Food Handling/Storage Establishments Premises and Equipment			
Indoor Hard Surfaces (includes dishes and silverware)	High pressure spray (1,100)	High pressure spray (180)	150
		Brush (12,000)	1,000
	Brush (75,000)	High pressure spray (180)	180
		Brush (12,000)	10,000
	Low pressure spray (1,200)	Immersion/Flooding ($1.4X10^6$)	1,200
		Low pressure spray (2,400)	800
	Wiping (93)	Immersion/Flooding ($1.4X10^6$)	93
		Low pressure spray (2,400)	90
	Foam (4,000)	Immersion/Flooding ($1.4X10^6$)	4,800
		Low pressure spray (2,400)	1,600
	Brush (22,000)	Immersion/Flooding ($1.4X10^6$)	22,000
		Low pressure spray (2,400)	2,000
	Sponge/Mesh/Wiping (190)	Immersion/Flooding (170)	90
		Trigger Pump (9,700)	190
	Low Pressure Spray (2,400)	Immersion/Flooding (170)	160
		Trigger Pump (9,700)	1,900
	Brush (45,000)	Immersion/Flooding (170)	170
		Trigger Pump (9,700)	8,000
	CIP (680)	CIP (680)	340
Food dispensing equipment	CIP(400)	CIP (810)	270

d. Occupational Post-Application Exposure

For most of the occupational scenarios, postapplication dermal exposure is not expected to occur or is expected to be negligible based on the application rates and chemical properties of these chemicals. The alkylbenzene sulfonates have a low vapor pressure ($5.1x10^{-10}$ to $6.02x10^{-15}$ mmHg), so that any standing solutions that may result in post application exposure were deemed negligible. For additional information, please see the Occupational and Residential Exposure Assessment for Alkylbenzene Sulfonates for the Reregistration Eligibility Decision document, dated July 6, 2006.

B. Environmental Risk Assessment

A summary of the Agency's environmental risk assessment is presented below. The following risk characterization is intended to describe the magnitude of the estimated environmental risks for alkylbenzene sulfonates use sites and any associated uncertainties.

For detailed discussions of all aspects of the environmental risk assessment, see the Environmental Fate Assessment of Alkylbenzene Sulfonates for the Reregistration Eligibility Decision and the Ecological Hazard and Environmental Risk Assessment of Alkylbenzene Sulfonates for the Reregistration Eligibility Decision document, dated July 12, 2006.

1. Environmental Fate and Transport

No fate studies for alkylbenzene sulfonates are available in US EPA's files. Thus, the Agency has relied on scientific literature and the Agency's EPI Suite model to obtain different environmental properties for the alkylbenzene sulfonates. The EPI Suite model predicts that alkylbenzene sulfonates are not likely to persist in water or microbial soils and sediments. The Agency also conducted a literature search to further support the output parameters that were provided by the EPI Suite model. Extensive literature are available that describe the fate and significance of alkylbenzene sulfonates in the environment from a long history of detergent use.

Environmental exposure modeling was not conducted for alkylbenzene sulfonic acids and sulfonates because the currently registered uses are indoor spray applications. Uses such as urinals and toilet bowls could result in minimal exposure to the environment when flushed, however, significant environmental exposure is not expected for the following reasons: total alkylbenzene sulfonate usage for these industrial applications is very minor - a very small percentage of the total pounds is used in antimicrobials; commercial only use precludes broad environmental exposures that might occur with residential use; applications are mostly sprayed on and allowed to air dry; alkylbenzene sulfonate breakdown and degrade rapidly in the environment; alkylbenzene sulfonates are significantly reduced by sewage treatment; and industrial water treatment requires a NPDES permit in order to discharge effluents.

2. Ecological Risk

The ecological risk assessment integrates the results of the exposure and ecotoxicity data to evaluate the likelihood of adverse ecological effects.

Alkylbenzene sulfonates demonstrate low acute toxicity to birds, moderate acute toxicity to freshwater fish, and low to high acute toxicity to freshwater aquatic invertebrates depending on the length of the carbon chain. Supplemental acute studies indicate that alkylbenzene sulfonates are moderately toxic to freshwater fish and slightly to highly toxic to freshwater aquatic invertebrates depending on the length of the carbon chain. A summary of submitted data is provided in Table 13.

Table 13. Acute Toxicity of Alkylbenzene Sulfonates

Species	Chemical, % active ingredient (ai)	Endpoint	Toxicity Category (TGAI)	Satisfies Guidelines/ Comments	MRID
Birds					
Northern bobwhite *(Colinus virginianus)*	87.6%Carbon chain not identified. (Nacconal 90G used)	LD_{50} > 1382 mg/kg NOEL = 279 mg/kg	Slightly toxic	Yes. Acceptable. 14 day test	41143901
Freshwater Fish					
Fathead Minnow (*Pimephales promelas*)	14.0% (Carbon chain not identified.)	96hr LC50 = 3.4 mg/L	Moderately toxic	Yes. Supplemental study.	44260002
Rainbow trout *Oncorhynchus mykiss*)	65.0% C11, C12	96 hr LC50 = 1.68 mg/L	Moderately toxic	Yes. Supplemental study.	44260009
Freshwater Invertebrates					
Waterflea *(Daphnia magna)*	Not reported.	48-hr. EC_{50} = LAS-C10 = 29.5 mg/L, LAS-C12 = 6.84 mg/L, LAS-C14 = 0.80 mg/L, LAS-C16 = 0.20 mg/L.	C-10 = Slightly toxic, C14 = highly toxic.	Yes. Supplemental study.	47025025
Green Algae					
Selenastrum capricornutum	Not Reported. (Carbon chain not identified.)	96 hr. EC50 = 70.27 ppm	Slightly toxic	Supplemental study.	42439803

The alkylbenzene sulfonates are used as inert ingredients in agricultural herbicide formulations. Preplant incorporated and preemergence herbicide treatments are typically

applied once per year to the tilled, minimally tilled or no-tilled field before planting or before crop emergence in the spring. Spray applications are primarily via ground boom spray and occasionally by aircraft. Movement of the alkylbenzene sulfonates from the treated field to the aquatic environment can occur at the time of application due to spray drift, or following application via surface water/soil flow or by percolation to groundwater. The FIRST model has predicted a maximum potential concentration of 6.6 ppb alkylbenzene sulfonates in drinking water from inert agricultural uses. Available modeling and literature suggest that these chemicals will most likely biodegrade rapidly in soil due to microbial degradation. In addition, aquatic organisms are also not expected to be adversely affected by inert alkylbenzene sulfonates use acutely or chronically due to the low estimated level of alkylbenzene sulfonates in water.

3. Risk to Listed Species

Section 7 of the Endangered Species Act, 16 U.S.C. Section 1536(a)(2), requires all federal agencies to consult with the National Marine Fisheries Service (NMFS) for marine and anadromous listed species, or the United States Fish and Wildlife Services (FWS) for listed wildlife and freshwater organisms, if they are proposing an "action" that may affect listed species or their designated habitat. Each federal agency is required under the Act to insure that any action they authorize, fund, or carry out is not likely to jeopardize the continued existence of a listed species or result in the destruction or adverse modification of designated critical habitat. To jeopardize the continued existence of a listed species means "to engage in an action that reasonably would be expected, directly or indirectly, to reduce appreciably the likelihood of both the survival and recovery of a listed species in the wild by reducing the reproduction, numbers, or distribution of the species." 50 C.F.R. § 402.02.

To facilitate compliance with the requirements of the Endangered Species Act subsection (a)(2) the Environmental Protection Agency, Office of Pesticide Programs has established procedures to evaluate whether a proposed registration action may directly or indirectly reduce appreciably the likelihood of both the survival and recovery of a listed species in the wild by reducing the reproduction, numbers, or distribution of any listed species (U.S. EPA 2004). After the Agency's screening-level risk assessment is performed, if any of the Agency's Listed Species LOC Criteria are exceeded for either direct or indirect effects, a determination is made to identify if any listed or candidate species may co-occur in the area of the proposed pesticide use. If determined that listed or candidate species may be present in the proposed use areas, further biological assessment is undertaken. The extent to which listed species may be at risk then determines the need for the development of a more comprehensive consultation package as required by the Endangered Species Act.

For certain use categories, the Agency assumes there will be minimal environmental exposure, and only a minimal toxicity data set is required (Overview of the Ecological Risk Assessment Process in the Office of Pesticide Programs U.S. Environmental Protection Agency Endangered and Threatened Species Effects Determinations, 1/23/04, Appendix A, Section IIB, pg.81). Chemicals in these categories

therefore do not undergo a full screening-level risk assessment, and are considered to fall under a "No Effect" determination. The active ingredient uses of alkylbenzene sulfonic acids and sulfonates fall into this category for the following reasons:

1. The amount that will actually reach the environment is very small based on usage data for down-the-drain uses.
2. Use for toilets and urinals is limited (no home-owner or residential uses are registered).
3. Breakdown of alkylbenzene sulfonate in the environment and via sewage treatment is rapid and well documented in the literature.

The labeled antimicrobial uses of alkylbenzene sulfonic acids and sulfonates are not expected to result in significant environmental exposure. Therefore, no adverse effects (NE) to listed species are anticipated. Use of alkylbenzene sulfonates as inert ingredients in agricultural pesticide formulations is not expected to result in significant environmental exposure. Therefore, no adverse effects (NE) to listed species are anticipated.

IV. Risk Management, Reregistration, and Tolerance Reassessment Decision

A. Determination of Reregistration Eligibility

Section 4(g)(2)(A) of FIFRA calls for the Agency to determine, after submission of relevant data concerning an active ingredient, whether or not products containing the active ingredient are eligible for reregistration. The Agency has previously identified and required the submission of the generic (i.e., active ingredient-specific) data required to support reregistration of products containing alkylbenzene sulfonates as an active ingredient. The Agency has completed its review of these generic data and has determined that the data are sufficient to support reregistration of all supported products containing alkylbenzene sulfonates.

The Agency has completed its assessment of the dietary, residential, occupational, drinking water, and ecological risks associated with the use of pesticide products containing the active ingredient alkylbenzene sulfonates. Based on a review of these data and on public comments on the Agency's assessments for the active ingredient alkylbenzene sulfonates, the Agency has sufficient information on the human health and ecological effects of alkylbenzene sulfonates to make decisions as part of the tolerance reassessment process under FFDCA and reregistration process under FIFRA, as amended by FQPA. The Agency has determined that alkylbenzene sulfonates-containing products are eligible for reregistration provided that current data gaps and confirmatory data needs are addressed. Appendix A summarizes the uses of alkylbenzene sulfonates that are eligible for reregistration. Appendix B identifies the generic data requirements that the Agency reviewed as part of its determination of reregistration eligibility of alkylbenzene sulfonates and lists the submitted studies that the Agency found acceptable. Data gaps are identified as generic data requirements that have not been satisfied with acceptable data.

B. Public Comments and Responses

Through the Agency's public participation process, EPA worked with stakeholders and the public to reach the regulatory decision for alkylbenzene sulfonates. During the public comment period on the risk assessments, which closed on June 19, 2006, the Agency received numerous comments from The DDBSA Steering Committee/Joint Venture (JV) and The Council for LAB/LAS Environmental Research (CLER) and the European Centre on Studies on LAB/LAS (ECOSOL) in response to EPA's draft risk assessment (RA) for alkylbenzene sulfonates. The comments submitted include areas of toxicology, chemical structure, risks, production volumes, and exposure. The Agency's responses to these comments are incorporated into the risk assessment and revised chapters, which are available on the U.S. Federal Government website at: www.regulations.gov (EPA-HQ-OPP-2006-0156). A Response to Comment document will be made available on the public docket in the future. In addition, comments received by the registrants during Phase I of the RED process, are available on the docket.

The Agency is providing a 60-day public comment period on this RED.

C. Regulatory Position

1. Food Quality Protection Act Findings

a. "Risk Cup" Determination

As part of the FQPA tolerance reassessment process, EPA assessed the risks associated with alkylbenzene sulfonates. The Agency has concluded that the tolerance exemptions for the use of alkylbenzene sulfonates as an active and as an inert ingredient meet the FQPA safety standards and that the risk from dietary exposure (food sources only) is within the "risk cup." An acute aggregate assessment was not conducted because there are no adverse effects attributable to acute exposure. An intermediate-term aggregate assessment was not conducted because there are no residential exposures of this duration. In addition, because there are no long-term residential exposures, the chronic aggregate assessment only considered food and drinking water. Thus, only short-term and chronic aggregate assessments were conducted.

The Agency has determined that the human health risks from these combined exposures are within acceptable levels. In reaching this determination, EPA has considered the available information on the special sensitivity of infants and children, as well as aggregate exposure from food, drinking water and residential uses.

b. Determination of Safety to U.S. Population

As part of the FQPA tolerance reassessment process, EPA assessed the risks associated with alkylbenzene sulfonates. The Agency has determined that the established tolerance exemptions for alkylbenzene sulfonates meet the safety standards under the FQPA amendments to section 408(b)(2)(D) of the FFDCA, and that there is a reasonable certainty no harm will result to the general population or any subgroup from it's use. In reaching this conclusion, the Agency has considered all available information on alkylbenzene sulfonates.

Typically, aggregate risk assessments are conducted for acute (1 day), short-term (1-30 days), intermediate-term (1-6 months) and chronic (6 months to lifetime) exposures. However, an acute aggregate assessment was not conducted because there are no adverse effects attributable to acute exposure of alkylbenzene sulfonates. An intermediate-term aggregate assessment was not conducted because there are no residential exposures of this duration. In addition, because there are no long-term residential exposures, the chronic aggregate assessment only considered food and drinking water. Thus, only short-term and chronic aggregate assessments were conducted. The short-term and chronic aggregate risk estimates associated with alkylbenzene sulfonates are well below the Agency's level of concern. Oral and inhalation exposure and risk estimates were conservatively combined for the aggregate risk assessment because these endpoints both identify adverse effects on body weight. The aggregate oral and inhalation risks are not of concern for adults or children. Dermal exposures were not considered in the risk assessment because a toxicological endpoint was not established.

c. Determination of Safety to Infants and Children

EPA has determined that the currently registered uses of alkylbenzene sulfonates, with changes as specified in this document, meet the safety standards under the FQPA amendments to section 408(b)(2)(C) of the FFDCA, that there is a reasonable certainty of no harm for infants and children. The safety determination for infants and children considers factors of the toxicity, use practices, and environmental behavior noted above for the general population, but also takes into account the possibility of increased susceptibility to the toxic effects of alkylbenzene sulfonates residues in this population subgroup.

No Special FQPA Safety Factor is necessary to protect the safety of infants and children. In determining whether or not infants and children are particularly susceptible to toxic effects from alkylbenzene sulfonates residues, the Agency considered the completeness of the database for developmental and reproductive effects, the nature of the effects observed, and other information. The FQPA Safety Factor has been removed (i.e., reduced to 1X) for alkylbenzene sulfonates based on: (1) there is no concern for developmental neurotoxicity resulting from exposure to alkylbenzene sulfonates because there is no evidence alkylbenzene sulfonates will induce neurotoxic effects; (2) there is no quantitative or qualitative evidence of increased susceptibility to the fetus following *in utero* exposure in the prenatal developmental toxicity studies or to the offspring when adults are exposed in the two-generation reproductive study; and (3) the risk assessment does not underestimate the potential exposure for infants and children.

d. Endocrine Disruptor Effects

EPA is required under the FFDCA, as amended by FQPA, to develop a screening program to determine whether certain substances (including all pesticide active and other ingredients) "may have an effect in humans that is similar to an effect produced by a naturally occurring estrogen, or other endocrine effects as the Administrator may designate." Following recommendations of its Endocrine Disruptor Screening and Testing Advisory Committee (EDSTAC), EPA determined that there was a scientific basis for including, as part of the program, the androgen and thyroid hormone systems, in addition to the estrogen hormone system. EPA also adopted EDSTAC's recommendation that EPA include evaluations of potential effects in wildlife. For pesticides, EPA will use FIFRA and, to the extent that effects in wildlife may help determine whether a substance may have an effect in humans, FFDCA authority to require the wildlife evaluations. As the science develops and resources allow, screening of additional hormone systems may be added to the Endocrine Disruptor Screening Program (EDSP).

When the appropriate screening and/or testing protocols being considered under the EDSP have been developed, alkylbenzene sulfonates may be subject to additional screening and/or testing to better characterize effects related to endocrine disruption.

e. Cumulative Risks

Risks summarized in this document are those that result only from the use of alkylbenzene sulfonates. The Food Quality Protection Act (FQPA) requires that the Agency consider "available information" concerning the cumulative effects of a particular pesticide's residues and "other substances that have a common mechanism of toxicity." The reason for consideration of other substances is due to the possibility that low-level exposures to multiple chemical substances that cause a common toxic effect by a common toxic mechanism could lead to the same adverse health effect as would a higher level of exposure to any of the substances individually. Unlike other pesticides for which EPA has followed a cumulative risk approach based on a common mechanism of toxicity, EPA has not made a common mechanism of toxicity finding for alkylbenzene sulfonates. For information regarding EPA's efforts to determine which chemicals have a common mechanism of toxicity and to evaluate the cumulative effects of such chemicals, see the policy statements released by EPA's Office of Pesticide Programs concerning common mechanism determinations and procedures for cumulating effects from substances found to have a common mechanism on EPA's website at http://www.epa.gov/pesticides/cumulative/.

2. Tolerance Summary

Active Ingredient Uses

Exemptions from the requirement of a tolerance for the active food-contact sanitizer uses of these ingredients have been established in the 40 CFR 180.940(b) and (c).

Table 14. Tolerance Exemptions for Food Contact Sanitizer Uses (Active Uses)

Tolerance Exemption Expression/ Chemical Name	CAS No.	PC Code	40 CFR Citation	Use Pattern (Pesticidal)
Benzenesulfonic acid, dodecyl-	27176-87-0	098002	180.940 (b)	food contact sanitizing solutions for dairy processing equipment, and food processing equipment and utensils; end use concentration not to exceed 5.5 ppm NOTE: The Agency will be proposing a change to 40 CFR 180.940(b) to make the end use concentration not to exceed 400 ppm.
			180.940 (c)	food contact sanitizing solutions for food processing equipment and utensils; end use concentration not to exceed 400 ppm
Benzenesulfonic acid dodecyl-, sodium salt	25155-30-0	079010	180.940 (c)	food contact sanitizing solutions for food processing equipment and utensils; end use concentration not to exceed 430 ppm

Dodecylbenzenesulfonic acid (27176-87-0) and sodium dodecylbenzene sulfonate (25155-30-0) have uses in food-contact surface sanitizing solutions with tolerance exemptions as specified in 40 CFR 180.940 (b) and (c), and summarized in Table 14. Residues for these compounds are exempt from the requirement of a tolerance when used in accordance with good manufacturing practice as ingredients in an antimicrobial pesticide formulation, provided that the substance is applied on a semi-permanent or permanent food-contact surface (other than being applied on food packaging) with adequate draining before contact with food. Both dodecylbenzene sulfonic acid, and sodium dodecylbenzene sulfonate have limitations for the ready-to-use end-use concentration not to exceed 400 ppm and 430 ppm, respectively for food processing equipment and utensils. However, dodecylbenzene sulfonic acid has a much lower limitation of 5.5 ppm for use on dairy processing equipment. The Agency estimates that the 430 ppm limitation for the sodium salt is equivalent to approximately 400 ppm of the free acid form. The Agency will be proposing a change to the 40 CFR 180.940(b) to establish a maximum of 400 ppm for the end-use concentration of dodecylbenzenesulfonic acid, rather than the current limitation of 5.5 ppm. As previously stated, the Agency used the FDA milk truck model to estimate residues in milk that could result from the use of alkylbenzene sulfonates in the food processing equipment. The Agency assessed the maximum application rate of 400 ppm for dodecylbenzene sulfonates (as listed on the labels), although the current tolerance exemption has a limitation of 5.5 ppm for dairy processing equipment. This assessment indicated that risks are not of concern for all subpopulations.

Inert Ingredient Uses

Included in this document is the reassessment of the alkylbenzene sulfonates when used as an inert ingredient in pesticidal products. As noted previously, some of the inert functions of alkylbenzene sulfonates in the registered products are listed as solvent, surfactant, dispersant, detergent, or wetting agent. Some of these products are designated for use in agricultural settings (i.e., pre- and post-harvest and when applied to animals), where there is a potential for dietary exposure. The alkylbenzene sulfonates assessed in this document are constituents of a larger group of compounds that have a tolerance exemption as an inert ingredient in 40 CFR 180.910 and 180.930. As shown in Table 15, the tolerance exemption is listed as Alkyl (C8-C24) benzenesulfonic acid and its ammonium, calcium, magnesium, potassium, sodium and zinc salts.

Table 15. Tolerance Exemptions for Inert Use		
Tolerance Exemption Expression	**40 CFR Citation**	**Use Pattern**
Alkyl (C8-C24) benzenesulfonic acid and its ammonium, calcium, magnesium, potassium , sodium and zinc salts	180.910 (a)	Surfactants, related adjuvants of surfactants
	180.930 (a)	Surfactants, emulsifier, related adjuvants of surfactants

(a) Residues listed in 40 CFR §180.910 are exempted from the requirement of a tolerance when used as inert ingredients in pesticidal formulations when applied to growing crops or to raw agricultural commodities after harvest (i.e., pre- and post-harvest). Residues listed in 40 CFR §180.930 are exempted from the requirement of a tolerance when used as inert ingredients in pesticidal formulations when applied to animals only.

D. Regulatory Rationale

The Agency has determined that alkylbenzene sulfonates are eligible for reregistration provided that additional required data confirm this decision.

1. Human Health Risk Management

a. Dietary (Food) Risk Mitigation

The chronic dietary exposure estimates for both the active and inert ingredient uses are below the Agency's level of concern for all age groups. Therefore, no mitigation measures are necessary at this time.

b. Drinking Water Risk Mitigation

The chronic drinking water exposure estimates for the inert ingredient uses are below the Agency's level of concern. Significant drinking water exposure is not expected to result from the active ingredient uses of alkylbenzene sulfonates. Therefore, no mitigation measures are necessary at this time.

c. Residential Risk Mitigation

Residential risk estimates for the uses of alkylbenzene sulfonates as inert ingredients are below the Agency's level of concern. Therefore, no mitigation measures are needed at this time for these uses, as none present a risk of concern.

d. Occupational Risk Mitigation

i. Handler Risk Mitigation

The calculated short and intermediate-term inhalation MOEs are greater than 100, and therefore, are not of concern with the exception of the following scenarios:

- Short-Term and Intermediate-Term inhalation exposure from cleaning hard surfaces via wiping in the food handling category, inhalation MOE = 93.
- Short-Term and Intermediate-Term inhalation exposure from cleaning indoor hard surfaces via wiping and then following with sanitizing via immersion/flooding in the food handling premises category, inhalation MOE = 93.
- Short-Term and Intermediate-Term inhalation exposure from cleaning indoor hard surfaces via wiping and then following with sanitizing via low pressure spray in the food handling premises category, inhalation MOE = 90**.**
- Short-Term and Intermediate-Term inhalation exposure from cleaning indoor hard surfaces via sponge/mesh/wiping and then sanitizing via immersion/flooding in the food handling premises category, inhalation MOE = 90.

Due to the conservative nature of the assessment, risk estimates making a lot of assumptions, and the MOEs being so close to the target, the Agency does not have a risk concern for these scenarios.

ii. Post-Application Risk Mitigation

At this time, EPA does not foresee post-application exposures for the occupational uses of alkylbenzene sulfonates; therefore, no mitigation measures are necessary.

2. Environmental Risk Management

The Agency considers the uses of alkylbenzene sulfonates assessed in this RED to be unlikely to result in any appreciable exposure to terrestrial or aquatic organisms. Therefore, no risk mitigation measures are required.

3. Listed Species Considerations

a. The Endangered Species Act

Section 7 of the Endangered Species Act, 16 U.S.C. Section 1536(a)(2), requires all federal agencies to consult with the National Marine Fisheries Service (NMFS) for marine and anadromous listed species, or the United States Fish and Wildlife Services (FWS) for listed wildlife and freshwater organisms, if they are proposing an "action" that may affect listed species or their designated habitat. Each federal agency is required under the Act to insure that any action they authorize, fund, or carry out is not likely to jeopardize the continued existence of a listed species or result in the destruction or adverse modification of designated critical habitat.

To jeopardize the continued existence of a listed species means "to engage in an action that reasonably would be expected, directly or indirectly, to reduce appreciably the likelihood of both the survival and recovery of a listed species in the wild by reducing the reproduction, numbers, or distribution of the species." 50 C.F.R. § 402.02.

To facilitate compliance with the requirements of the Endangered Species Act subsection (a)(2) the Environmental Protection Agency, Office of Pesticide Programs has established procedures to evaluate whether a proposed registration action may directly or indirectly reduce appreciably the likelihood of both the survival and recovery of a listed species in the wild by reducing the reproduction, numbers, or distribution of any listed species (U.S. EPA 2004). After the Agency's screening-level risk assessment is performed, if any of the Agency's Listed Species LOC Criteria are exceeded for either direct or indirect effects, a determination is made to identify if any listed or candidate species may co-occur in the area of the proposed pesticide use. If determined that listed or candidate species may be present in the proposed use areas, further biological assessment is undertaken. The extent to which listed species may be at risk then determines the need for the development of a more comprehensive consultation package as required by the Endangered Species Act.

For certain use categories, the Agency assumes there will be minimal environmental exposure, and only a minimal toxicity data set is required (Overview of the Ecological Risk Assessment Process in the Office of Pesticide Programs U.S. Environmental Protection Agency - Endangered and Threatened Species Effects Determinations, 1/23/04, Appendix A, Section IIB, pg.81). Chemicals in these categories therefore do not undergo a full screening-level risk assessment, and are considered to fall under a "no effect" determination. Due to the low likelihood of exposure and low toxicity of alkylbenzene sulfonates, the Agency expects no effects to listed species or critical habitat and therefore makes a "No Effect" determination for this chemical.

b. General Risk Mitigation

Alkylbenzene sulfonates end-use products (EPs) may also contain other registered pesticides. Although the Agency is not proposing any mitigation measures for products containing alkylbenzene sulfonates specific to federally listed species, the Agency needs to address potential risks from other end-use products. Therefore, users should adopt all listed species risk mitigation measures for all active ingredients in the product. If a product contains multiple active ingredients with conflicting listed species risk mitigation measures, the more stringent measure(s) should be adopted.

V. What Registrants Need to Do

The Agency has determined that alkylbenzene sulfonates are eligible for reregistration provided that additional data that the Agency intends to require confirm this decision. The additional data requirements that the Agency intends to obtain will include, among other things, submission of the following:

For end-use products containing the active ingredient alkylbenzene sulfonates, the registrants need to submit the following items as there are no registered technical manufacturers:

Within 90 days from receipt of the generic data call-in (DCI):

1. completed response forms to the generic DCI (i.e., DCI response form and requirements status and registrant's response form); and

2. submit any time extension and/or waiver requests with a full written justification.

Within the time limit specified in the generic DCI:

1. cite any existing generic data which address data requirements or submit new generic data responding to the DCI.

Please contact Adam Heyward at (703) 308-6422 with questions regarding generic reregistration.

By US mail:
Document Processing Desk
Adam Heyward
Office of Pesticide Programs (7510P)
U.S. Environmental Protection Agency
1200 Pennsylvania Ave., NW
Washington, DC 20460-0001

By express or courier service:
Document Processing Desk
Adam Heyward
Office of Pesticide Programs (7510P)
U.S. Environmental Protection Agency
Room S-4900, One Potomac Yard
2777 South Crystal Drive
Arlington, VA 22202

For end-use products containing the active ingredient alkylbenzene sulfonates, the registrants need to submit the following items for each product:

Within 90 days from the receipt of the product-specific data call-in (PDCI):

1. completed response forms to the PDCI (i.e., PDCI response form and requirements status and registrant's response form); and

2. submit any time extension or waiver requests with a full written justification.

Within eight months from the receipt of the PDCI:

1. two copies of the confidential statement of formula (EPA Form 8570-4);

2. a completed original application for reregistration (EPA Form 8570-1). Indicate on the form that it is an "application for reregistration";

3. five copies of the draft label incorporating all label amendments outlined in Table 13 of this document;

4. a completed form certifying compliance with data compensation requirements (EPA Form 8570-34);

5. if applicable, a completed form certifying compliance with cost share offer requirements (EPA Form 8570-32); and

6. the product-specific data responding to the PDCI.

Please contact Adam Heyward at (703) 308-6422 with questions regarding product reregistration and/or the PDCI. All materials submitted in response to the PDCI should be addressed as follows:

By US mail:
Document Processing Desk
Adam Heyward
Office of Pesticide Programs (7510P)
U.S. Environmental Protection Agency
1200 Pennsylvania Ave., NW
Washington, DC 20460-0001

By express or courier service:
Document Processing Desk
Adam Heyward
Office of Pesticide Programs (7510P)
U.S. Environmental Protection Agency
Room S-4900, One Potomac Yard
2777 South Crystal Drive
Arlington, VA 22202

A. Manufacturing Use Products

There are no currently registered alkylbenzene sulfonates manufacturing-use products. However, additional generic data requirements have been identified.

1. Additional Generic Data Requirements

The generic database supporting the reregistration of alkylbenzene sulfonates has been reviewed and determined to be substantially complete. However, the following additional data requirements have been identified by the Agency as confirmatory data requirements. A generic data call-will be issued at a later date.

The risk assessment noted deficiencies in the surrogate inhalation exposure data available from the Chemical Manufacturers Association (CMA) data base. Therefore, the Agency is requiring confirmatory data to support the uses assessed with the CMA exposure data within this risk assessment. The risk assessment also noted that many of the use parameters (e.g., amount handled and duration of use) were based on professional judgments. Therefore, descriptions of human activities associated with the uses assessed are required as confirmatory. A 90-day nose-only rat inhalation study using DDBSA (Guideline 870.3465) is required due to limitations with the monkey inhalation study, which used 13% LAS, in addition to the presence of enzyme.

Table 16. Confirmatory Data Requirements for Reregistration

Guideline Study Name	New OPPTS Guideline No.	Old Guideline No.
90-Day Inhalation – Rat	870.3465	82-4
Indoor Inhalation Exposure and Applicator Exposure Monitoring Data Reporting	875.1400 and 875.1600	234 and 236
Descriptions of Human Activity	875.2800	133-1
Product Use Information	875.1700/2700	N/A

2. Labeling for Technical and Manufacturing Use Products

There are no registered technical or manufacturing use products.

B. End-Use Products

1. Additional Product-Specific Data Requirements

Section 4(g)(2)(B) of FIFRA calls for the Agency to obtain any needed product-specific data regarding the pesticide after a determination of eligibility has been made. The registrant must review previous data submissions to ensure that they meet current EPA acceptance criteria and if not, commit to conduct new studies. If a registrant believes that previously submitted data meet current testing standards, then the study MRID numbers should be cited according to the

instructions in the Requirement Status and Registrants Response Form provided for each product.

A product-specific data call-in, outlining data requirements, will be sent to registrants at a later date. Possible efficacy studies that the Agency may call-in are listed in Table 17 below. The PDCI will be based upon current efficacy-related requirements for antimicrobial pesticide products, claims, or patterns of use. A summary of these requirements can be found on the Agency's Antimicrobials Science Policy website at http://www.epa.gov/oppad001/sciencepolicy.htm.

Table 17. Efficacy Data Requirements for Product Reregistration

Claim	Use Pattern	Guideline Study Name	New OPPTS Guideline No.	Old Guideline No.
Sanitizer	(non-food contact surfaces – non-residual)	Sanitizer Test for Hard Inanimate Non—food contact surfaces	810.2100(l)	91-2(j)
Sanitizer	previously cleaned food-contact surfaces (non residual)	AOAC Germicidal and Detergent Sanitizers Method	810.2100 (m)(2)	91-2 (l)(2)
Disinfectant	Toilet bowl, urinal surfaces	AOAC Use Dilution Test (hard water and organic soil) Or AOAC Germicidal Spray Test Or AOAC Hard Surface Carrier Test (distilled water only)	91-7 (a) (1)	810.2600 (b) (1)
Virucidal Claim in Conjunction with Disinfectant Claim	Any site/application	Virucidal Activity Method used in conjunction with modifications of: AOAC Hard Surface Carrier Test (distilled water only) Or AOAC Germicidal Spray Test	810.2100(g)	91-2(f)
Fungicidal Claim	Any site/application	AOAC Fungicidal Test or AOAC Hard Surface Carrier Test (distilled water only) Or AOAC Germicidal Spray Products Test	810.2100(f)	91-2(e)

2. Labeling for End-Use Products that Contain Alkylbenzene Sulfonates as an Inert Ingredient

All products that contain alkylbenzene sulfonates as an inert ingredient and make a sanitization claim must contain an active ingredient that is a sanitizer. If a product containing alkylbenzene sulfonates as an inert ingredient makes a sanitization claim and does not contain an active ingredient that is a sanitizer, the sanitization claim will have to be removed from the label. If the registrant wishes to keep the sanitization claim, alkylbenzene sulfonates will need to be listed as an active ingredient rather than an inert ingredient. All relevant data will need to be submitted and reviewed in order to make this change.

VI. APPENDICES

Appendix A. Table of Use Patterns for Alkylbenzene Sulfonates

PC Code 079010

Use Site	Formulation/ EPA Reg No.	Method of Application	Application Rate/ No. of applications[1]	Use Limitations
Food handling/ storage establishments premises and equipment				
Eating Establishments & Equipment (utensils, cutting boards, counter tops, sinks, etc.), Food handling areas	Soluble Concentrate 1020-13	Brush or Spray	2 oz / gallon of water	Prepare fresh solutions daily
	Soluble Concentrate 71094-1 Ready to Use 71094-2	Immersion, flooding or spraying	1%(one pouch/ 8 gallons) to 2%(one pouch/ 4 gallons) One minute contact time	None Stated
Dairy and Food Processing Plants & Equipment, Food Contact	Soluble Concentrate 1020-13	Brush or Spray	2 oz / gallon of water	Prepare fresh solutions daily
	Soluble Concentrate 71094-1 Ready to Use 71094-2	Immersion, flooding or spraying	1%(one pouch/ 8 gallons) to 2%(one pouch/ 4 gallons) One minute contact time	None Stated
Fruit and Vegetable Rinses	Soluble Concentrate 71094-1 Ready to Use 71094-2	Immersion, gentle hand scrub	1%(one pouch/ 8 gallons) to 2%(one pouch/ 4 gallons) 2 to 5 minute wash	Prepare cleaning solution with potable water
Soft Ice Cream, Juice and Vending Machines	Soluble Concentrate 71094-1	Circulate in system	5 to 10 minute circulation to clean 2 to 5 minute circulation	Maintain sanitizer solution pH of 2.2-2.8; discard sanitizer if it becomes visibly dirty or its pH increases/ solution may not be

Use Site	Formulation/ EPA Reg No.	Method of Application	Application Rate/ No. of applications[1]	Use Limitations
			to sanitize	reused for sanitizing
	Ready to Use 71094-2			

[1] Application rate is given in terms of end-use product, not active ingredient.

Appendix A. Table of Use Patterns for Alkylbenzene Sulfonates

PC Codes 098002 and 190116

Use Site	Formulation/ EPA Reg No.	Method of Application	Application Rate/ No. of applications[2]	Use Limitations
Agricultural premises and equipment				
Dairy Farm milking machines, milk handling equipment and facilities	Soluble Concentrate 833-75 875-85 875-184 1270-254 4959-29 9152-18 64328-1 74210-1	Immersion, brush, spray, flushing or circulation	To clean: 1 oz. to 1.5-5 gallons of water To sanitize: 1 oz. to 1-6 gallons of water. 1-5 minute contact time. (200-400ppm)	Pre-clean and pre-soak prior to use. For cleaning follow with a potable water rinse. For sanitization, wash pre-cleaned surfaces with approved alkaline cleaner and potable water rinse before use.
	Soluble Concentrate 875-185	Immersion, brush, spray, flushing or circulation	1:30 to 1:40 dilution for foam cleaning and de-scaling	
			To sanitize: 1:200 dilution, ten minute contact time	

Use Site	Formulation/ EPA Reg No.	Method of Application	Application Rate/ No. of applications[2]	Use Limitations
Food handling/storage establishments premises and equipment				
Diary/Cheese processing plant equipment	Soluble Concentrate 150-61 833-75 875-85 875-184 1270-254 1677-169 2686-10 9152-18 19713-299 64328-1 65001-1 71695-1 74210-1	Immersion, brush, spray, flushing or circulation	To clean: 1 oz. to 1.5-5 gallons of water To sanitize: 1 oz. to 1-6 gallons of water. 1-5 minute contact time. (200-400ppm)	Pre-clean and pre-soak prior to use. For cleaning follow with a potable water rinse. For sanitization, wash pre-cleaned surfaces with approved alkaline cleaner and potable water rinse before use.
Diary/Cheese processing plant equipment	Soluble Concentrate 875-185	Immersion, brush, spray, flushing or circulation	1:30 to 1:40 dilution for foam cleaning and de-scaling To sanitize: 1:200 dilution, ten minute contact time	Pre-clean and pre-soak prior to use. For cleaning follow with a potable water rinse. For sanitization, wash pre-cleaned surfaces with approved alkaline cleaner and potable water rinse before use.
Ice Cream processing plant equipment	Soluble Concentrate 9152-18	Immersion, brush, spray, flushing or circulation	To sanitize: 1 oz. to two gallons of water, five minute contact time.	For sanitization, wash pre-cleaned surfaces with approved alkaline cleaner and potable water rinse before use.
	Soluble Concentrate 74210-1	Immersion, brush, spray, flushing or	To sanitize: 1 – 2 oz per 10 gallons of water, two minute contact time.	

Use Site	Formulation/ EPA Reg No.	Method of Application	Application Rate/ No. of applications[2]	Use Limitations
		circulation		
Egg processing and packing equipment and surfaces	Soluble Concentrate 1270-254	Circulation, flushing	To sanitize: 1 oz. to 6 gallons of water, one minute contact time.	For sanitization, wash pre-cleaned surfaces with approved alkaline cleaner and potable water rinse before use. NOTE: EPA Reg. No. 74210-1 has shell egg grading and egg products on its label but no specific directions for how to use the product on the site.
	Soluble Concentrate 74210-1	Immersion, brush, spray, flushing or circulation	To sanitize: 1 – 2 oz per 10 gallons of water, two minute contact time.	
Eating establishments equipment, glassware and utensils	Soluble Concentrate 833-75 875-184 1270-254 4959-29 64328-1	Immersion, brush, spray, flushing or circulation	To clean: 1 oz. to 1.5-5 gallons of water To sanitize: 1 oz. to 1-6 gallons of water. 1-5 minute contact time. (200-400ppm)	Pre-clean and pre-soak prior to use. For cleaning follow with a potable water rinse. For sanitization, wash pre-cleaned surfaces with approved alkaline cleaner and potable water rinse before use.
	Soluble Concentrate 875-185	Immersion, brush, spray, flushing or circulation	1:30 to 1:40 dilution for foam cleaning and de-scaling	
			To sanitize: 1:200 dilution, ten minute contact time	
Food processing equipment and surfaces	Soluble Concentrate 150-61 833-75 875-85	Immersion, brush, spray, flushing or circulation	To clean: 1 oz. to 1.5-5 gallons of water To sanitize: 1 oz. to 1-6 gallons of water. 1-5 minute contact time. (200-400ppm)	Pre-clean and pre-soak prior to use. For cleaning follow with a potable water rinse. For sanitization, wash pre-cleaned surfaces with approved alkaline cleaner and potable water rinse before use.
Food processing equipment and surfaces	Soluble Concentrate 875-184 1270-254	Immersion, brush, spray, flushing or	To clean: 1 oz. to 1.5-5 gallons of water To sanitize: 1 oz. to 1-6	Pre-clean and pre-soak prior to use. For cleaning follow with a potable water rinse.

Use Site	Formulation/ EPA Reg No.	Method of Application	Application Rate/ No. of applications[2]	Use Limitations
	1677-169 2686-10 4959-29 7546-4 9152-18 19713-299 64328-1 65001-1 71695-1	circulation	gallons of water. 1-5 minute contact time. (200-400ppm)	For sanitization, wash pre-cleaned surfaces with approved alkaline cleaner and potable water rinse before use.
	Soluble Concentrate 875-185	Immersion, brush, spray, flushing or circulation	1:30 to 1:40 dilution for foam cleaning and de-scaling	
			To sanitize: 1:200 dilution, ten minute contact time	
Meat and poultry processing plants	Soluble Concentrate 833-75 875-184 1270-254 4959-29 64328-1 74210-1	Immersion, brush, spray, flushing or circulation	To clean: 1 oz. to 1.5-5 gallons of water To sanitize: 1 oz. to 1-6 gallons of water. 1-5 minute contact time. (200-400ppm)	Pre-clean and pre-soak prior to use. For cleaning follow with a potable water rinse. For sanitization, wash pre-cleaned surfaces with approved alkaline cleaner and potable water rinse before use.
	Soluble Concentrate 875-185	Immersion, brush, spray, flushing or circulation	1:30 to 1:40 dilution for foam cleaning and de-scaling	

Use Site	Formulation/ EPA Reg No.	Method of Application	Application Rate/ No. of applications[2]	Use Limitations
			To sanitize: 1:200 dilution, ten minute contact time	
Carbonated beverage and brewery processing equipment and surfaces	Soluble Concentrate 150-61 833-75 875-184 9152-18 19713-299 64328-1 65001-1 71695-1 74210-1	Immersion, brush, spray, flushing or circulation	To clean: 1 oz. to 1.5-5 gallons of water To sanitize: 1 oz. to 1-6 gallons of water. 1-5 minute contact time. (200-400ppm)	Pre-clean and pre-soak prior to use. For cleaning follow with a potable water rinse. For sanitization, wash pre-cleaned surfaces with approved alkaline cleaner and potable water rinse before use
	Soluble Concentrate 875-185	Immersion, brush, spray, flushing or circulation	1:30 to 1:40 dilution for foam cleaning and de-scaling To sanitize: 1:200 dilution, ten minute contact time	
Wineries, carbonated beverage and brewery processing equipment and surfaces	Soluble Concentrate 1270-254	Immersion, brush, spray, flushing or circulation	To clean: 1 oz. to 1.5-5 gallons of water To sanitize: 1 oz. to 1-6 gallons of water. 1-5 minute contact time. (200-400ppm)	Pre-clean and pre-soak prior to use. For cleaning follow with a potable water rinse. For sanitization, wash pre-cleaned surfaces with approved alkaline cleaner and potable water rinse before use

Use Site	Formulation/ EPA Reg No.	Method of Application	Application Rate/ No. of applications[2]	Use Limitations
Seafood processing plants	Soluble Concentrate 1270-254	Immersion, brush, spray, flushing or circulation	To sanitize: 1 oz. to 6 gallons of water, one minute contact time.	For sanitization, wash pre-cleaned surfaces with approved alkaline cleaner and potable water rinse before use.
Fruit and vegetable rinses	Soluble Concentrate 71695-1		1 oz. per 5 gallons of water. Rinse with potable water after the wash cycle.	Use a test kit to assure proper concentration of product in the wash water. At no time should the concentration of product exceed 2 oz. per 5 gallons of water.
Residential and public access premises				
Toilets, Porcelain Urinals and Shower Stalls	Soluble Concentrate/ Ready to Use 3625-279	Mop, brush or sponge	Ready to Use: Add 1 oz. to toilet bowl, ten minute contact time.	
			Concentrate: 1 oz. per gallon of water, ten minute contact time.	
	Soluble Concentrate 65001-1	Mop, brush or sponge	1 oz. per 5 gallons of water	

[2] Application rate is given in terms of end-use product, not active ingredient.

Appendix B. Table of Generic Data Requirements and Studies Used to Make the Reregistration Decision

Guide to Appendix B

Appendix B contains listing of data requirements which support the reregistration for active ingredients within case #4006 (alkylbenzene sulfonates) covered by this RED. It contains generic data requirements that apply to alkylbenzene sulfonates in all products, including data requirements for which a "typical formulation" is the test substance.

The data table is organized in the following formats:

1. Data Requirement (Column 1). The data requirements are listed in the order in which they appear in 40 CFR part 158. The reference numbers accompanying each test refer to the test protocols set in the Pesticide Assessment Guidance, which are available from the National technical Information Service, 5285 Port Royal Road, Springfield, VA 22161 (703) 487-4650.

2. Use Pattern (Column 4). This column indicates the use patterns for which the data requirements apply. The following letter designations are used for the given use patterns.

(1) Agricultural premises and equipment
(2) Food handling/ storage establishment premises and equipment
(3) Commercial, institutional and industrial premises and equipment
(4) Residential and public access premises
(5) Medical premises and equipment
(6) Human water systems
(7) Materials preservatives
(8) Industrial processes and water systems
(9) Antifouling coatings
(10) Wood preservatives
(11) Swimming pools
(12) Aquatic areas

3. Bibliographic Citation (Column 5). If the Agency has acceptable data in its files, this column list the identify number of each study. This normally is the Master Record Identification (MRID) number, but may be a "GS" number if no MRID number

has been assigned. Refer to the Bibliography appendix for a complete citation of the study.

DATA REQUIREMENT				CITATION(S)
New Guideline Number	**Old Guideline Number**	**Study Title**	**Use Pattern**	**MRID Number**
PRODUCT CHEMISTRY				
830.1550	61-1	Product Identity and Composition	1,2,3	42439801
830.1600 830.1620 830.1650	61-2a	Starting Materials and Manufacturing Process	1,2,3	42439801
830.1670	61-2b	Formation of Impurities	1,2,3	42439801
830.1700	62-1	Preliminary Analysis	1,2,3	42439801
830.1750	62-2	Certification of Limits	1,2,3	43729701; 43741101; 43752001; 43750401; 43748801; 43761801
830.1800	62-3	Analytical Method	1,2,3	42439802
830.6302	63-2	Color	1,2,3	00161997
830.6303	63-3	Physical State	1,2,3	43656401
830.6304	63-4	Odor	1,2,3	43656401
830.7200	63-5	Melting Point	1,2,3	00161997
830.7220	63-6	Boiling Point	1,2,3	Not required
830.7300	63-7	Density	1,2,3	43656401
830.7840 830.7860	63-8	Solubility	1,2,3	00161997
830.7950	63-9	Vapor Pressure		Waived
830.7370	63-10	Dissociation Constant in Water	1,2,3	00161997; 00161996

DATA REQUIREMENT				CITATION(S)
New Guideline Number	**Old Guideline Number**	**Study Title**	**Use Pattern**	**MRID Number**
830.7550 830.7560 830.7570	63-11	Partition Coefficient (Octanol/Water)		Waived
830.7000	63-12	pH	1,2,3	00161997
830.6313	63-13	Stability	1,2,3	43656402; 43656403; 43656401; 43787401
830.6314	63-14	Oxidizing/Reducing Action		Not required
830.6315	63-15	Flammability		Not required
830.6316	63-16	Explodability		Not required
830.6317	63-17	Storage Stability	1,2,3	41221301
830.7100	63-18	Viscosity		Not required
830.6319	63-19	Miscibility		Not required
830.6320	63-20	Corrosion Characteristics		Not required
830.6321	63-21	Dielectric breakdown voltage		Not required
ECOLOGICAL EFFECTS				
850.2100	71-1	Avian Acute Oral Toxicity Test	1,2,3	41143901
850.2200	71-2	Avian Dietary Toxicity		Not required
850.1075	72-1	Acute Freshwater Fish (rainbow trout or bluegill sunfish)	1,2,3	44260002, 44260009

DATA REQUIREMENT				CITATION(S)
New Guideline Number	**Old Guideline Number**	**Study Title**	**Use Pattern**	**MRID Number**
850.1010	72-2	Acute Freshwater Invertebrate (daphnia magna)	1,2,3	47025025
TOXICOLOGY				
870.1100	81-1	Acute Oral – Rat	1,2,3	43498402; 43498408; 43498430
870.1200	81-2	Acute Dermal – Rabbit	1,2,3	94032006
870.1300	81-3	Acute Inhalation – Rat	1,2,3	Open literature
870.2400	81-4	Primary Eye Irritation – Rabbit	1,2,3	43498405
870.2500	81-5	Primary Dermal Irritation – Rabbit	1,2,3	40359306
870.2600	81-6	Dermal Sensitization	1,2,3	Open literature
870.3100	82-1a	90-Day Feeding-Rodent	1,2,3	43498412; 43498402; 43498409; 43498413 & 43511401; open literature
	82-1b	90-Day Feeding-Non-Rodent		Not required
870.3200	82-2	21/28-Day Dermal Toxicity – Rat	1,2,3	43498411; Open literature
870.3250	82-3	90-day Dermal Toxicity – Rodent		Not required; Reserved
870.3465	82-4	90-Day Inhalation – Rat	1,2,3	Data gap
870.3700a		Developmental Toxicity – rodent	1,2,3	Open literature; 43498423; 43498424; 43498425; 43498426; 43511403
870.3700	83-3b	Teratogenicity – Rabbit	1,2,3	43498426

DATA REQUIREMENT				CITATION(S)
New Guideline Number	Old Guideline Number	Study Title	Use Pattern	MRID Number
870.3800	83-4	Reproduction and Fertility Effects - 2 Generation Repro	1,2,3	43498416; Open literature
870.4100	83-1a	Chronic Feeding Toxicity – Rodent	1,2,3	43498416; Open literature
	83-1b	Chronic Feeding Toxicity - Non-Rodent (dog)		Not required
870.4200	83-2a	Oncogenicity – Rat	1,2,3	43498421; 43498422; 43498419; 43498420; 43498416; Open literature
	83-2b	Oncogenicity – Mouse		Waived
870.4300	83-5	Combined Chronic Toxicity/Carcinogenicity		Not required
870.5100		Bacterial reverse mutation test	1,2,3	Open literature; 43498429
870.5300		In Vitro mammalian cell gene mutation test	1,2,3	Open literature; 43498427
870.5265	84-2a	Gene Mutation – ames	1,2,3	43498428
870.5385	84-2b	Structural Chromosome Aberration	1,2,3	43498429; 43498428; Open literature
870.5395		Mammalian erythrocyte micronucleus test	1,2,3	Open literature
870.5450		Rodent dominant lethal assay	1,2,3	Open literature
	84-4	Other genotoxic effects	1,2,3	43498429
870.7485	85-1	General Metabolism	1,2,3	43498431; 43498410; Open literature
870.7600	85-2	Dermal Absorption	1,2,3	42565201; 43498407

DATA REQUIREMENT				CITATION(S)
New Guideline Number	**Old Guideline Number**	**Study Title**	**Use Pattern**	**MRID Number**
OCCUPATIONAL/RESIDENTIAL EXPOSURE				
875.2800	133-1	Description of Human Activity	1,2,3	Data gap
875.1200 875.1600	233	Dermal Indoor Exposure	1,2,3	Waived
875.1400 875.1600	234	Inhalation Indoor Exposure	1,2,3	Data gap
875.1700 875.2700		Product Use Information	1,2,3	Data gap
ENVIRONMENTAL FATE				
835.2120	161-1	Hydrolysis	1,2,3	Open literature

Appendix C. Technical Support Documents

Additional documentation in support of this RED is maintained in the OPP docket, located in Room S-4400, One Potomac Yard, 2777 South Crystal Drive, Arlington, VA, and is open Monday through Friday, excluding Federal holidays, from 8:30 a.m. to 4:00 p.m.

The docket initially contained the April 19, 2006 preliminary risk assessment and the related supporting science documents. EPA then considered comments on the risk assessment and revised the risk assessment and supporting chapters as necessary. The revised risk assessment will be posted in the docket at the same time as the RED.

All documents, in hard copy form, may be viewed in the OPP docket room or downloaded or viewed via the Internet at the following site:

http://www.regulations.gov

These documents include:

- Alkylbenzene Sulfonates Preliminary Risk Assessment; Notice of Availability, 4/19/06.

Preliminary Risk Assessment and Supporting Science Documents (RED Supporting Documents):

- Alkylbenzene Sulfonates (ABS) Preliminary Risk Assessment for the Reregistration Eligibility Decision (RED) Document. PC Code: 079010, 190116 and 098002. Case No. 4006. DP Barcode: D323972
- Occupational and Residential Exposure Assessment for Alkylbenzene Sulfonates for the Reregistration Eligibility Decision Document (RED) (Active Uses). T. Milano. March 23. D327732
- Residential Exposure Inert Assessment of Alkylbenzene Sulfonates for the Reregistration Eligibility Decision Document (RED). T. Milano/C. Walls**,** March 23, 2006. D327733
- Environmental Fate Assessment of Alkylbenzene Sulfonates for the Reregistration Eligibility Document (RED). T. Milano. March 23, 2006. D323968
- Product Chemistry Science Chapter for Benzene Sulfonic Acid, C_{10}-C_{16} Derivatives and Sodium Salt. A. N. Shamim. March 2006. D323976.
- Ecological Hazard and Environmental Risk Assessment of Alkylbenzene Sulfonates for the Registration Eligibility Document (RED). R. Petrie. January 2006. D323970.
- Dietary Exposure Assessments for the Reregistration Eligibility Decision. R. Quick. March 23, 2006. D327731.
- Toxicology Disciplinary Chapter for the Reregistration Eligibility Decision (RED) Document, A.Assaad/W.Dyksra/L.Scarano, March 23, 2006. D327886.
- Inert Ingredient Dietary Risk Assessment for Linear Alkyl Benzenesulfonate. K. Leifer. March 23, 2006. D324036

Revised Risk Assessment and Revised Supporting Science Documents (RED Supporting Documents):

- Alkylbenzene Sulfonates (ABS) Revised Risk Assessment for the Reregistration Eligibility Decision (RED) Document. PC Code: 079010, 190116 and 098002. Case No. 4006. DP Barcode: D330338
- Occupational and Residential Exposure Assessment for Alkylbenzene Sulfonates for the Reregistration Eligibility Decision Document (RED) (Active Uses). T. Milano. July 6, 2006. D330329
- Residential Exposure Inert Assessment of Alkylbenzene Sulfonates for the Reregistration Eligibility Decision Document (RED). T. Milano/C. Walls**,** July 6, 2006. D330330
- Product Chemistry Science Chapter for Benzene Sulfonic Acid, C_{10}-C_{16} Derivatives and Sodium Salt. A. N. Shamim. July 11, 2006. D330332.
- Ecological Hazard and Environmental Risk Assessment of Alkylbenzene Sulfonates for the Registration Eligibility Document (RED). R. Petrie. July 12, 2006. D330326.
- Toxicology Disciplinary Chapter for the Reregistration Eligibility Decision (RED) Document, A.Assaad/W.Dyksra/L.Scarano, July 6, 2006. D330328.
- Environmental Fate Assessment of Alkylbenzene Sulfonates for the Registration Eligibility Document (RED). T. Milano. July 6, 2006. D323968.

Appendix D. Citations Considered to be Part of the Data Base Supporting the Reregistration Decision (Bibliography)

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Linear Alkyl Benzenesulfonate Modeling Input Parameters for FIRST and GENEEC

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Appendix E. Generic Data Call-In

The Agency intends to issue a Generic Data Call-In at a later date. See Chapter V of the Alkylbenzene Sulfonates RED for a list of studies that the Agency plans to require.

Appendix F. Product Specific Data Call-In

The Agency intends to issue a Product Specific Data Call-In at a later date.

Appendix G. Batching of Alkylbenzene Sulfonates Products for Meeting Acute Toxicity Data Requirements for Reregistration

The Agency will complete the batching at a later date.

Appendix H. List of All Registrants Sent the Data Call-In

A list of registrants sent the data call-in will be posted at a later date.

Appendix I. List of Available Related Documents and Electronically Available Forms

Pesticide Registration Forms are available at the following EPA internet site: http://www.epa.gov/opprd001/forms/.

Pesticide Registration Forms (These forms are in PDF format and require the Acrobat reader)

Instructions

1. Print out and complete the forms. (Note: Form numbers that are bolded can be filled out on your computer then printed.)

2. The completed form(s) should be submitted in hardcopy in accord with the existing policy.

3. Mail the forms, along with any additional documents necessary to comply with EPA regulations covering your request, to the address below for the Document Processing Desk.

DO NOT fax or e-mail any form containing 'Confidential Business Information' or 'Sensitive Information.'

If you have any problems accessing these forms, please contact Nicole Williams at (703) 308-5551 or by e-mail at williams.nicole@epamail.epa.gov.

The following Agency Pesticide Registration Forms are currently available via the internet at the following locations:

8570-1	Application for Pesticide Registration/Amendment	http://www.epa.gov/opprd001/forms/8570-1.pdf
8570-4	Confidential Statement of Formula	http://www.epa.gov/opprd001/forms/8570-4.pdf
8570-5	Notice of Supplemental Registration of Distribution of a Registered Pesticide Product	http://www.epa.gov/opprd001/forms/8570-5.pdf
8570-17	Application for an Experimental Use Permit	http://www.epa.gov/opprd001/forms/8570-17.pdf
8570-25	Application for/Notification of State Registration of a Pesticide To Meet a Special Local Need	http://www.epa.gov/opprd001/forms/8570-25.pdf
8570-27	Formulator's Exemption Statement	http://www.epa.gov/opprd001/forms/8570-27.pdf
8570-28	Certification of Compliance with Data Gap Procedures	http://www.epa.gov/opprd001/forms/8570-28.pdf
8570-30	Pesticide Registration Maintenance Fee Filing	http://www.epa.gov/opprd001/forms/8570-30.pdf
8570-32	Certification of Attempt to Enter into an Agreement with other Registrants for Development of Data	http://www.epa.gov/opprd001/forms/8570-32.pdf
8570-34	Certification with Respect to Citations of Data (in PR Notice 98-5)	http://www.epa.gov/opppmsd1/PR_Notices/pr98-5.pdf
8570-35	Data Matrix (in PR Notice 98-5)	http://www.epa.gov/opppmsd1/PR_Notices/pr98-5.pdf

8570-36	Summary of the Physical/Chemical Properties (in PR Notice 98-1)	http://www.epa.gov/opppmsd1/PR_Notices/pr98-1.pdf
8570-37	Self-Certification Statement for the Physical/Chemical Properties (in PR Notice 98-1)	http://www.epa.gov/opppmsd1/PR_Notices/pr98-1.pdf

Pesticide Registration Kit
www.epa.gov/pesticides/registrationkit/.

Dear Registrant:

For your convenience, we have assembled an online registration kit that contains the following pertinent forms and information needed to register a pesticide product with the U.S. Environmental Protection Agency's Office of Pesticide Programs (OPP):

1. The Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) and the Federal Food, Drug and Cosmetic Act (FFDCA) as Amended by the Food Quality Protection Act (FQPA) of 1996.

2. Pesticide Registration (PR) Notices

   a. 83-3 Label Improvement Program—Storage and Disposal Statements

   b. 84-1 Clarification of Label Improvement Program

   c. 86-5 Standard Format for Data Submitted under FIFRA

   d. 87-1 Label Improvement Program for Pesticides Applied through Irrigation Systems (Chemigation)

   e. 87-6 Inert Ingredients in Pesticide Products Policy Statement

   f. 90-1 Inert Ingredients in Pesticide Products; Revised Policy Statement

   g. 95-2 Notifications, Non-notifications, and Minor Formulation Amendments

   h. 98-1 Self Certification of Product Chemistry Data with Attachments (This document is in PDF format and requires the Acrobat reader.)

Other PR Notices can be found at http://www.epa.gov/opppmsd1/PR_Notices.

3. Pesticide Product Registration Application Forms (These forms are in PDF format and will require the Acrobat reader.)

   a. EPA Form No. 8570-1, Application for Pesticide Registration/Amendment

b. EPA Form No. 8570-4, Confidential Statement of Formula

c. EPA Form No. 8570-27, Formulator's Exemption Statement

d. EPA Form No. 8570-34, Certification with Respect to Citations of Data

e. EPA Form No. 8570-35, Data Matrix

4. General Pesticide Information (Some of these forms are in PDF format and will require the Acrobat reader.)

a. Registration Division Personnel Contact List

b. Biopesticides and Pollution Prevention Division (BPPD) Contacts

c. Antimicrobials Division Organizational Structure/Contact List

d. 53 F.R. 15952, Pesticide Registration Procedures; Pesticide Data Requirements (PDF format)

e. 40 CFR Part 156, Labeling Requirements for Pesticides and Devices (PDF format)

f. 40 CFR Part 158, Data Requirements for Registration (PDF format)

g. 50 F.R. 48833, Disclosure of Reviews of Pesticide Data (November 27, 1985)

Before submitting your application for registration, you may wish to consult some additional sources of information. These include:

1. The Office of Pesticide Programs' Web Site

2. The booklet "General Information on Applying for Registration of Pesticides in the United States", PB92-221811, available through the National Technical Information Service (NTIS) at the following address:

National Technical Information Service (NTIS)
5285 Port Royal Road
Springfield, VA 22161

The telephone number for NTIS is (703) 605-6000. Please note that EPA is currently in the process of updating this booklet to reflect the changes in the registration program resulting from the passage of the FQPA and the reorganization of the Office of Pesticide Programs. We anticipate that this publication will become available during the Fall of 1998.

3. The National Pesticide Information Retrieval System (NPIRS) of Purdue University's Center for Environmental and Regulatory Information Systems. This service does charge a fee for subscriptions and custom searches. You can contact NPIRS by telephone at (765) 494-6614 or through their Web site.

4. The National Pesticide Telecommunications Network (NPTN) can provide information on active ingredients, uses, toxicology, and chemistry of pesticides. You can contact NPTN by telephone at (800) 858-7378 or through their Web site: ace.orst.edu/info/nptn.

The Agency will return a notice of receipt of an application for registration or amended registration, experimental use permit, or amendment to a petition if the applicant or petitioner encloses with his submission a stamped, self-addressed postcard. The postcard must contain the following entries to be completed by OPP:

Date of receipt
EPA identifying number
Product Manager assignment

Other identifying information may be included by the applicant to link the acknowledgment of receipt to the specific application submitted. EPA will stamp the date of receipt and provide the EPA identifying File Symbol or petition number for the new submission. The identifying number should be used whenever you contact the Agency concerning an application for registration, experimental use permit, or tolerance petition.
To assist us in ensuring that all data you have submitted for the chemical are properly coded and assigned to your company, please include a list of all synonyms, common and trade names, company experimental codes, and other names which identify the chemical (including "blind" codes used when a sample was submitted for testing by commercial or academic facilities). Please provide a CAS number if one has been assigned.

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

WASHINGTON, D.C. 20460

OFFICE OF
PREVENTION, PESTICIDES
AND TOXIC SUBSTANCES

Date: July 19, 2006

MEMORANDUM

SUBJECT: **Alkylbenzene Sulfonates (ABS) Risk Assessment** for the Reregistration Eligibility Decision (RED) Document. PC Codes: 079010, 190116 and 098002.(active); 790102, 790116, 790101 (inert) Case No. 4006. DP Barcode: D330338

Regulatory Action: Reregistration Eligibility Decision (RED) (Phase I)
Risk Assessment Type: Single Chemical Aggregate

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Attached is the Risk Assessment for the Alkylbenzene Sulfonates (ABS) for the purpose of issuing a Reregistration Eligibility Decision (RED). This document has been revised to address public comments. The disciplinary science chapters and other supporting documents for the Alkylbenzene Sulfonates RED are also included as attachments as follows:

Occupational and Residential Exposure Assessment for Alkylbenzene Sulfonates for the Reregistration Eligibility Decision Document (RED) (Active Uses). T. Milano. July 6, 2006. D330329

Residential Exposure Inert Assessment of Alkylbenzene Sulfonates for the Reregistration Eligibility Decision Document (RED). T. Milano/C. Walls**,** July 6, 2006. D330330

Environmental Fate Assessment of Alkylbenzene Sulfonates for the Reregistration Eligibility Document (RED). T. Milano.July 6, 2006. D323968

Product Chemistry Science Chapter for Benzene Sulfonic Acid, C_{10}-C_{16} Derivatives and Sodium Salt. A. N. Shamim. July 11, 2006. D330332.

Ecological Hazard and Environmental Risk Assessment of Alkylbenzene Sulfonates for the Registration Eligibility Document (RED). R. Petrie. July 12, 2006. D330326.

Dietary Exposure Assessments for the Reregistration Eligibility Decision. R. Quick. March 23, 2006. D327731.

Toxicology Disciplinary Chapter for the Reregistration Eligibility Decision (RED) Document, A.Assaad/W.Dyksra/L.Scarano, July 6, 2006, D330328

Inert Ingredient Dietary Risk Assessment for Linear Alkyl Benzenesulfonate. K. Leifer. March 23, 2006.

1.0 EXECUTIVE SUMMARY

The alkylbenzene sulfonates evaluated in this risk assessment are: (1) sodium dodecylbenzene sulfonate (CAS # 25155-30-0), (2) dodecylbenzene sulfonic acid (CAS # 27176-87-0), and (3) benzenesulfonic acid, C10-C16 alkyl derivatives (CAS # 68584-22-5). These compounds are collectively called DDBSA by the DDBSA Joint Venture Task Force. Dodecylbenzene sulfonic acid is not considered to be a pure compound, and is included in the mixture of benzenesulfonic acid, C10-16 alkyl derivatives.

The alkylbenzene sulfonates are both active and inert ingredients in pesticide products. As active ingredients, there are currently twenty-three registered end-use products used as a disinfectant, food-contact sanitizer, bacteriocide/bacteriostat, microbiocide/microbiostat, fungicide/fungistat, and virucide. Alkylbenzene sulfonates are in cleaners and sanitizers that are designated for use in agricultural, food handling and commercial/institutional/industrial settings. Examples of registered uses for alkylbenzene sulfonates include, but are not limited to: application to indoor hard surfaces (e.g. urinals, shower stalls, toilet bowls, etc.), food dispensing equipment (e.g. pre-mix and post-mix vending machines), food contact surfaces (glasses, dishes, silverware, countertops, etc.), agricultural tools, and fruits and vegetables (post-harvest). As active ingredients, there are no residential or outdoor uses currently registered. Concentrations of alkylbenzene sulfonates as an active ingredient in products range from 0.036% to 25.6%. Products containing alkylbenzene sulfonates are formulated as soluble concentrates, flowable concentrates, ready-to-use solutions, or water soluble packaging.

As inert ingredients, there are approximately 350 registered end-use products containing these chemicals. Many of these products are used in residential settings, and outdoors in agricultural settings. The percent formulations for most of the products that contain alkylbenzene sulfonates as an inert ingredient range from 0.01% to 5%. However, the majority of the labels in this range contain 2% alkylbenzene sulfonates. It should be noted that a few sanitizing products have inert levels as high as 30% and the highest concentration of alkylbenzene sulfonates are found in wood preservative products up to 65 %.

Approximately 300,000 pounds of alkylbenzene sulfonates are used in EPA registered antimicrobial products, which is a small fraction of the approximately 860 million pounds produced each year. The majority of uses of alkylbenzene sulfonates are as household laundry and dish detergents. The alkylbenzene sulfonates are listed on the EPA High Production Volume (HPV) Challenge Program. HPV chemicals are those that are manufactured or imported into the U.S. in production volumes greater than one million pounds per year. The alkylbenzene sulfonates are sponsored by the Linear Alkylbenzene (LAB) Sulfonic Acids Coalition, which has generated data for these chemicals.

Hazard: The toxicology database for the alkylbenzene sulfonates consists almost entirely of published literature, and is essentially complete and of acceptable quality to assess the potential hazard to humans. The alkylbenzene sulfonates are readily absorbed following oral ingestion, but not following dermal exposure. Following oral exposure, they are readily metabolized, excreted fairly rapidly, and do not accumulate in any tissues. Available acute toxicity data show that alkylbenzene sulfonates are not highly acutely toxic (Categories III-IV) following oral exposure,

but are moderately toxic via dermal and inhalation exposure (Category II), are irritating to the eye and skin (categories I and II, respectively), and they are not skin sensitizers. Subchronic and chronic exposures show that the liver, kidney and intestinal tract (following oral exposures) are the major target organs of toxicity. Both *in vitro* and *in vivo* genotoxicity data show that alkylbenzene sulfonates are not genotoxic. The alkylbenzene sulfonates did not cause reproductive or developmental toxicity in acceptable studies. Early (pre-GLP) carcinogenicity studies indicate that alkylbenzene sulfonates do not cause an increase in tumor incidence.

Toxicity Endpoints: The toxicity endpoints used in this document to assess potential risks include chronic dietary, short-term incidental oral, and short-, intermediate- and/or long-term inhalation exposure scenarios. The Health Effects Division's Toxicity Advisory Clinic (TAC) was consulted and agreed with the choice of toxicity endpoints of concern selected for the aforementioned exposure scenarios in December 2005 for the alkylbenzene sulfonates as a group.

Acute and Chronic Reference Dose (RfDs): No acute dietary endpoint was selected because there were no effects attributable to a single dose exposure.

The chronic RfD is 0.5 mg/kg/day for all populations, using a no-observable adverse effect level (NOAEL) of 50 mg/kg/day based on a weight of evidence from three toxicological studies that observed decreased pup body weight at 250 mg/kg/day and increased caecum weight and slight kidney damage at 114 mg/kg/day. An uncertainty factor of 100 (10X for interspecies extrapolation, 10X for intraspecies variability) was applied to the NOAEL to obtain the chronic RfD.

Incidental oral Exposure: For the short-term incidental oral exposure, a NOAEL of 50 mg/kg/day was selected based on a weight of evidence from three toxicological studies that observed decreased pup body weight at 250 mg/kg/day and increased caecum weight and slight kidney damage at 114 mg/kg/day. The target margin of exposure (MOE) is 100 (10X for interspecies extrapolation, 10X for intraspecies variability, and 1X FQPA factor discussed below).

Dermal Exposure: The Agency determined that quantitation of dermal risk is not required because: (1) the alkylbenzene sulfonates are surfactants that are dermal irritants at concentrations generally greater than 20% solution (WHO 1996). Thus, dermal exposure would be self-limiting to preclude dermal irritation. Most pesticide formulations have less than 5% alkylbenzene sulfonates as an inert ingredient, with the vast majority of household products containing approximately 2%. Additionally, the requirement of the dermal toxicity studies with the end-use product will determine whether personal protective clothing would be necessary to protect against irritation during product use; (2) no systemic toxicity was seen following repeated dermal applications to rabbits at 200 mg/kg/day (with an end use product); (3) no developmental toxicity concerns were seen following repeated dermal applications to pregnant mice, rats or rabbits (developmental effects were seen either in the presence of maternal toxicity or at doses higher than those that caused maternal toxicity); and (4) there is no residential exposure to alkylbenzene sulfonates as an active ingredient, however, residential exposure from its use as an inert ingredient in pesticide formulations is expected to be of an intermittent nature (i.e, no continuous, constant contact, multi-day exposure) from household products.

Inhalation Exposure: For the short-, intermediate- and long-term inhalation exposure a NOAEL of 1 mg/m^3 was selected (equivalent to 0.14 mg/kg/day) from a subchronic inhalation monkey study that noted weight loss and decreased weight gain at 10 mg/m^3 (1.4 mg/kg/day) following exposure to a detergent dust containing 13% active ingredient of alkylbenzene sulfonates. In the absence of data, it was conservatively assumed that inhalation absorption is 100% to convert the air concentration into a dose equivalent. The target MOE is 100 for both residential and occupational exposures (10X for interspecies extrapolation, 10X for intraspecies variability, includes 1X FQPA factor discussed below).

FQPA Safety Factor. The TAC agreed that the FQPA safety factor should be **removed (1X).** A number of developmental studies via the oral route have been performed with alkylbenzene sulfonates in rats, mice and rabbits. The available information in these studies does not suggest any qualitative or quantitative evidence for susceptibility between the fetuses and maternal animals. The alkylbenzene sulfonates were tested in several multigeneration studies in rats, and there were no effects on offspring toxicity in any of these tests at doses up to 250 mg/kg/day.

Based on OPP policy, the cRfD modified by a FQPA safety factor is a population adjusted dose (PAD)[1]. OPP calculated a chronic PAD and used this value to estimate chronic dietary risk.

Dietary (Food/Drinking Water) Exposure and Risk: The Agency has conducted three chronic dietary exposure and risk assessments for the alkylbenzene sulfonates: (1) as active ingredients in food contact sanitizing solutions; (2) as active ingredients in a fruit and vegetable wash; and (3) as inert ingredients in pesticide formulations that may be applied to growing agricultural crops, raw agricultural commodities after harvest, and to animals. An acute dietary assessment was not conducted because there are no adverse effects attributable to a single dose.

In assessing the food contact sanitizing uses, the Agency believes that a counter top, utensils or glassware that are treated with these products may come into contact with food, which in turn may be ingested. This is considered to be an indirect food use. Dodecylbenzene sulfonic acid (27176-87-0) and sodium dodecylbenzene sulfonate (25155-30-0) have tolerance exemptions as specified in 40 CFR 180.940 (b) and (c). Both dodecylbenzene sulfonic acid and sodium dodecylbenzene sulfonate have limitations for the ready-to-use end-use concentration not to exceed 400 ppm and 430 ppm, respectively for food processing equipment and utensils. However, dodecylbenzene sulfonic acid has a much lower limitation of 5.5 ppm for use on dairy processing equipment.

When assessing chronic (non-cancer) dietary risk, the Agency considered potential dietary exposure to the U.S. population including infants and children, as well as to females of childbearing age (13-50 years). EPA expresses dietary risk estimates as a percentage of the

[1] PAD = Population Adjusted Dose = $\frac{\text{Chronic RfD}}{\text{FQPA Safety Factor}}$

chronic PAD. Dietary exposures that are less than 100% of the cPAD are below the Agency's level of concern.

Active Ingredient Dietary Risk Estimates. There are no currently registered outdoor uses of alkylbenzene sulfonates that are being supported by the registrant as an active ingredient. Thus, the dietary assessment for active uses was limited to potential food exposures. The risk analysis assumes daily exposure from the hard surface sanitation of counter tops, utensils, glassware and food processing equipment (i.e., beverage plants, meat and poultry processing plants, milk and dairy plants). The dietary risk estimates for the fruit and vegetable wash were considered separately, because this use is regulated by the Food and Drug Administration (FDA). The dietary risk estimates for the total food contact sanitizing uses are below the Agency's level of concern for all age groups (less than **11% of the cPAD**). In addition, the dietary risk estimates for the fruit and vegetable wash are below the Agency's level of concern for all age groups (less than **71.2% of the cPAD**). These risk estimates are based on a number of conservative assumptions, and thus may overestimate the actual risks.

Inert Ingredient Dietary Risk Estimates. The alkylbenzene sulfonates have some uses as inert ingredients in food-use pesticide products that are used outdoors on agricultural crops. Thus, the inert assessment considered both food and drinking water exposures. The Agency utilized a conservative screening level dietary exposure model [Dietary Exposure Evaluation Model (DEEM™)] that assumed 100% of all commodities, and 100% of all crops were treated with the alkylbenzene sulfonates, with no limitation on the fraction of inert ingredient. The highest dietary risk estimate is **84% of the cPAD** for children 1-2 years of age, which is below the Agency's level of concern. The conservative screening-level drinking water assessment predicted chronic Estimated Drinking Water Concentrations (EDWC) of 6.6 ppb using the FQPA Index Reservoir Screening Tool (FIRST), which represents **<0.1% of the cPAD**. The Agency concludes there is no concern for aggregate food and drinking water exposures to the alkylbenzene sulfonates resulting from their use as pesticide inert ingredients.

Residential (Non-Occupational) Exposure and Risk: There are no residential use sites for the alkylbenzene sulfonates as active ingredients. However, alkylbenzene sulfonates are formulated as inert ingredients in approximately 350 registered end-use products, many of which are used in residential settings. Some examples of the specified use sites on the products consist of indoor hard non-porous surfaces (e.g. floors, walls etc.), carpets, food contact surfaces (glasses, dishes, silverware, countertops, etc.), agricultural tools and crops, lawns and turfs, fruits and vegetables (post-harvest), wood preservatives, materials preservatives, metalworking fluids, and pet products. In this screening level assessment, the Agency selected representative scenarios for the vast majority of products, based on end-use product application methods and use amounts. The Agency evaluated the following high end exposure scenarios: (1) outdoor residential turf treatment (ready to use liquid); (2) indoor hard surface cleaner (ready to use liquid; and (3) pet flea and tick products (aerosol can spray). For each of the use sites, the Agency assessed residential handler (applicator) inhalation exposure and post application incidental ingestion by toddlers.

For most scenarios, the Agency utilized EPA's Pesticide Inert Risk Assessment Tool (PiRat) to estimate residential applicator and post-application exposures from the use of alkylbenzene sulfonates as inert ingredients in residential products. For the pet product scenario and the hard surface cleaner post application exposure assessment, the Agency used assumptions based on the Residential Exposure Assessment Standard Operating Procedures (SOPs). Because there are a large number of products that contain alkylbenzene sulfonates as an inert ingredient, and to be conservative the Agency assessed a representative high end formulation product. A dermal assessment was not conducted because a dermal endpoint was not selected. An inhalation post-application assessment was not conducted because the vapor pressure of the sulfonates is extremely low. The duration of exposure was assumed to be short-term (1-30 days) for all residential scenarios assessed.

Residential Handler Risk Estimates. For residential handlers that handle products containing alkylbenzene sulfonates as inert ingredients, the short-term inhalation MOEs were above the target MOEs (i.e., >100) and thus, do not exceed the Agency's level of concern, with the exception of the flea and tick product where the MOE was 87 for the high-end formulation containing 24% alkylbenzene sulfonates. However, this scenario is conservative because it assumes a person treats his/her pet with 0.5 cans of flea product that contains 24% alkylbenzene sulfonates every day for a month.

Residential Postapplication Risk Estimates. There are no residential postapplication risk concerns for the household products that contain alkylbenzene sulfonates as an inert ingredient. All of the scenarios evaluated have short-term MOEs above 100, and thus are not of concern including postapplication incidental oral risks to children that may contact turf, hard surfaces or a pet treated with pesticide products containing alkylbenzene sulfonates as an inert ingredient.

The alkylbenzene sulfonates caused dermal irritation following repeated dermal exposure, generally to concentrations greater than 20%. Thus, dermal exposure would be self-limiting to preclude dermal irritation. The majority of residential products contain less than 5% alkylbenzene sulfonates. The Agency intends to consider the potential for irritation in recommended labeling language of pesticide products containing the alkylbenzene sulfonates, and consider available dermal toxicity data on a diluted end-use formulation.

Aggregate Exposure and Risk: In order for a pesticide registration to continue, it must be shown that the use does not result in "unreasonable adverse effects on the environment". Section 2 (bb) of FIFRA defines this term to include "a human dietary risk from residues that result from a use of a pesticide in or on any food inconsistent with standard under section 408..." of FFDCA. As mandated by the FQPA amendments to FIFRA and the Federal Food, Drug and Cosmetic Act (FFDCA), the Agency must consider total aggregate exposure from food, drinking water and residential sources of exposure to alkylbenzene sulfonates.

An acute aggregate assessment was not conducted because there are no adverse effects attributable to acute exposure. An intermediate-term aggregate assessment was not conducted because there are no residential exposures of this duration. In addition, because there are no long-term residential exposures, the chronic aggregate assessment only considered food and drinking water exposures from the inert uses that were previously determined to not be of risk

concern. Thus, only short-term and chronic aggregate assessments were conducted. Oral and inhalation exposure and risk estimates were conservatively combined for the aggregate risk assessment because these endpoints both identify adverse effects on body weight. Dermal exposures were not considered in the risk assessment because a toxicological endpoint was not established.

Short-Term. This assessment considers both the active and inert uses of the alkylbenzene sulfonates. For children, the short-term aggregate assessment includes average dietary exposure (food and drinking water) from both the active food contact sanitizer uses and the inert uses on agricultural commodities, in addition to estimated incidental oral exposures to children from residential uses such as hard surface cleaning products as an inert ingredient. For adults, the aggregate assessment includes dietary (food and drinking water) from both active and inert uses and residential inhalation exposures from wiping a hard surface cleaning products since this scenario represents the highest exposure from the inert use. Individual scenarios that had risks of concern were not included in the aggregate assessment.

The aggregate oral and inhalation risks are not of concern for adults, as the total aggregate MOE is 340 which is greater than the target of 100. For children, the aggregate risk estimate is very close to the target MOE of 100 (MOE=99). As noted previously, several conservative assumptions were used in this assessment.

Chronic Aggregate. The chronic aggregate assessment considers average dietary exposure (food and drinking water) from both the active food contact sanitizer uses and the inert uses on agricultural commodities. The dietary exposures from the fruit and vegetable wash were not considered because it would be overly conservative to assume simultaneous exposure to alkylbenzene sulfonates from three different use patterns. For children, the dietary aggregate risk is **95% of the cPAD**, while for adults it is **29% of the cPAD**.

It should also be recognized that the majority of the uses of alkylbenzene sulfonates are not in pesticide products, but rather are used in household laundry and dish detergents. Over 800 millions pounds of these compounds are produced each year, while only 300,000 pounds are used in EPA registered antimicrobial products. The Agency did not consider potential exposure and risks from the numerous other residential exposures to alkylbenzene sulfonates because the Agency lacks reliable information at this time to assess the consumer product uses of these chemicals.

Occupational Exposure and Risk. Based on examination of product labels describing uses for the product, it has been determined that exposure to handlers can occur in a variety of occupational environments. The representative scenarios selected by the Agency for assessment were evaluated using maximum application rates as recommended on the product labels for the three alkylbenzene sulfonate active ingredients assessed in this report.

To assess the handler risks, the Agency used surrogate unit exposure data from both the proprietary Chemical Manufacturers Association (CMA) antimicrobial exposure study and the Pesticide Handlers Exposure Database (PHED). Only inhalation risks were evaluated because a dermal toxicity endpoint was not selected. For the occupational handler inhalation risk

assessment, the short- and intermediate-term risks calculated at baseline exposure (no respirators) were above target MOEs for all scenarios (i.e., inhalation MOEs were >100) for all scenarios except the following:

- ST and IT inhalation exposure from cleaning hard surfaces via wiping in the food handling category, inhalation MOE = 93.

Many product labels have use directions that recommend both cleaning and sanitizing with the same product. Thus, the Agency estimated total risks resulting from use of these specific products. The following scenarios had risks of concern (i.e., MOE < 100).

- ST and IT inhalation exposure from cleaning indoor hard surfaces via wiping and then following with sanitizing via immersion/flooding in the food handling premises category, inhalation MOE = 93.
- ST and IT inhalation exposure from cleaning indoor hard surfaces via wiping and then following with sanitizing via low pressure spray in the food handling premises category, inhalation MOE = 90**.**
- ST and IT inhalation exposure from cleaning indoor hard surfaces via sponge/mesh/wiping and then sanitizing via immersion/flooding in the food handling premises category, inhalation MOE = 90.

Although all the inhalation risks of concern are for baseline exposures, the Agency does not believe it is practicable to require the use of respiratory protection on cleaning products used in janitorial situations. In addition, engineering controls are not feasible for the current use patterns on the labels.

As noted previously, the alkylbenzene sulfonates are dermal irritants at concentrations greater than 20%. Thus, dermal exposure would be self-limiting to preclude dermal irritation. The Agency intends to consider the potential for irritation in recommended labeling language of pesticide products containing the alkylbenzene sulfonates, and consider available dermal toxicity data on a diluted end-use formulation. The Agency should confirm that all products with greater than 20% require the use of gloves.

For most of the occupational scenarios, postapplication dermal exposure is not expected to occur or is expected to be negligible based on the application rates and chemical properties of the chemical. The alkylbenzene sulfonates have a low vapor pressure (less than 10^{-9} mmHg), so that any standing solutions that may result in post application exposure were deemed negligible.

Environmental Hazard and Risk. The alkylbenzene sulfonates are slightly toxic to the Northern bobwhite quail, and moderately toxic to freshwater fish and freshwater invertebrates following acute exposure. The available data indicate that the alkylbenzene sulfonates are slightly toxic to green algae.

Available literature for linear alkylbenzene sulfonate (LAS) detergent use indicates that the alkylbenzene sulfonates are not expected to bioaccumulate in the environment or aquatic organisms (i.e. fish) and are expected to be soluble in water such that they will exhibit mobility

through the soil. The model-calculated linear and non-linear biodegradation probabilities suggest that these chemicals will most likely biodegrade rapidly. The short half life indicates that if these chemicals are present in the soil, they are not likely to be volatile and are expected to degrade rapidly in the environment.

Minimal or no environmental exposure is expected to occur from the majority of alkylbenzene sulfonate antimicrobial pesticide uses because a very small number of pounds of this chemical are sold for antimicrobial use per data provided by the manufacturers.

The inert agricultural uses of alkylbenzene sulfonates are not expected to adversely affect avian or mammalian species on an acute or chronic basis. Aquatic organisms are also not expected to be adversely affected by inert alkylbenzene sulfonates use acutely or chronically due to the low predicted level of alkylbenzene sulfonates in water. A chronic freshwater fish toxicity test NOAEC of 400 ug/L alkylbenzene sulfonates is considered protective of ecosystem structure and function in experimental streams. Therefore, the predicted concentration of 6.6 ppb in water is well below the Agency's chronic Level of Concern (LOC).

Use of alkylbenzene sulfonates in agricultural pesticide formulations is not expected to result in significant environmental exposure. Therefore, no adverse effects (NE) to listed species are anticipated.

2.0 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties for the three alkylbenzene sulfonates assessed in this document: (1) sodium dodecylbenzene sulfonate, (2) benzene sulfonic acid, C10-16-alkyl derivatives, and (3) dodecylbenzene sulfonic acid are provided in Table 1. The product chemistry chapter (memo from N. Shamim, July 2006, D330332) provides a comprehensive list of the different physical/chemical properties. Below is the chemical structure for a representative C12-linear alkylbenzene sulfonate (LAS).

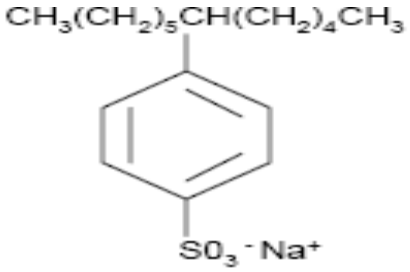

Figure 1: Sodium Dodecylbenzene Sulfonate (also named as dodecylbenzene sulfonic acid, sodium salt)

Table 1 Physical/Chemical Properties of Linear Alkylbenzene Sulfonates			
Parameter	**Sodium Dodecylbenzene Sulfonate**	**Benzene Sulfonic Acid, C10-16-alkyl derivatives**	**Dodecylbenzene Sulfonic Acid (DDBSA)**
PC Chemical Code	079010 (active) 790102 (inert)	190116 (active) 790116 (inert)	098002 (active) 790101 (inert)
Cas Number	25155-30-0	68584-22-5	27176-87-0
Molecular Formula	$C_{18}H_{29}O_3S$ Na	$C_{18}H_{20}O_3S$	$C_{18}H_{30}O_3S$
Synonyms	Alkyl(C12)benzenesulfonic acid, sodium salt Benzenesulfonic acid, dodecyl-, sodium salt Dodecylbenzene sodium sulfonate Dodecylbenzenesulfonic acid, sodium salt Sodium laurylbenzenesulfonate		Benzenesulfonic acid, dodecyl
Molecular Weight	348.48 g/mol	326.6 g/mol	326.50 g/mol
Henry Law Constant	6.02×10^{-17} atm.-m^3/mol	2.8×10^{-11} atm- m^3/mol	4.8×10^{-11} atm- m^3/mol
Melting Point	287.6^{O}C	$167.7\ ^{O}$C	$178\ ^{O}$C
Boiling Point	660^{O}C	$437\ ^{O}$C	$460\ ^{O}$C
Water Solubility	800 mg/L	400 g/L (25 ^{O} C)	400 g/L (25 ^{O} C)
log K_{ow}	1.96	3.80	4.78
Vapor Pressure	6.02×10^{-15} mm Hg	5.1×10^{-10} mm Hg (25^{o} C)	7.9×10^{-11} mm Hg (25^{o} C)
Half-life in air	0.66 days = 7.9 hours	0.79 days = 9.48 hours	0.654 days = 7.85 hours

3.0. ENVIRONMENTAL FATE

Detailed information on environmental fate is presented in the attached memo from T. Milano (July 6, 2006, D323968). A brief summary is provided below.

The environmental fate properties of dodecylbenzene sulfonic acid are assumed to be represented by the conclusions made pertaining to benzenesulfonic acid, C10-C16 alkyl derivatives. This is because dodecylbenzene sulfonic acid (DDBSA) is not considered to be a pure compound, and is actually included in the mixture of benzenesulfonic acid, C10-16 alkyl derivatives. These compounds will be addressed as a group, DDBSA.

The environmental fate assessment for DDBSA is based on US EPA's Estimation Programs Interface (EPI) Suite. EPI Suite provides estimations of physical/chemical properties and environmental fate properties.

Based on the output of the model, sodium dodecylbenzene sulfonate is highly unlikely to bioaccumulate in the environment or aquatic organisms (i.e. fish) because the low value for the log Kow (1.96). This also supports that the chemical is soluble in water such that it will exhibit mobility through the soil. In addition, the low log Koc (4.22) further supports the expected soil mobility. The model-calculated linear and non-linear biodegradation probabilities suggest that the linear carbon chain will biodegrade rapidly, whereas the benzene ring is not expected to biodegrade as rapidly. The extremely low vapor pressure along with the short half life of approximately 7.9 hours indicates that if this chemical is present in the soil, it is not likely to be volatile and is expected to degrade rapidly.

Based on the output of the model, DDBSA is expected to behave very similarly as what is projected for sodium dodecylbenzene sulfonate. Based on the low Kow value (3.8), DDBSA is highly unlikely to bioaccumulate in the environment or aquatic organisms (i.e. fish). The chemical is also expected to be soluble in water such that it will exhibit mobility through the soil. In addition, the log Koc (3.69) is low, and this further supports the expected soil mobility. The model-calculated linear and non-linear biodegradation probabilities suggest that the chemical will most likely biodegrade rapidly. The extremely low vapor pressure along with the short half life of approximately 9.48 hours indicates that this chemical is not likely to be volatile and is expected to degrade rapidly.

The output parameters from the EPI Suite model support that any potential impacts of these chemicals are expected to be very short-lived. This is because they are not likely to persist in water or microbial soils and sediments. As a result, the environmental fate of alkylbenzene sulfonate is not likely to be of concern.

4.0 HAZARD CHARACTERIZATION

4.1 Hazard Profile

The toxicology database for the alkylbenzene sulfonates consists almost entirely of published literature, is essentially complete and of acceptable quality to assess the potential hazard to humans.

A detailed Toxicology Assessment for the linear alkylbenzene sulfonates is presented in the attached memorandum (memo from A. Assaad/W. Dykstra/L. Scarano, July 2006). Table 2 highlights the acute toxicity studies for the alkylbenzene sulfonates. A detailed summary of the key toxicological studies is presented in Appendix A because of the large number of available toxicological information on these compounds. A brief hazard assessment is presented below.

Acute Toxicity. Alkylbenzene sulfonates exhibit a wide range of acute toxicity via the oral route in rats (LD_{50}s of 404 – 1980 mg/kg), with a narrower range in mice (LD_{50}s of 1259-2300 mg/kg). This spans the acute oral toxicity categories of III-IV. Alkylbenzene sulfonates are classified as acute toxicity category II for the dermal and inhalation routes of exposure. They are irritants to the eye (category I), and skin (category II), and are not skin sensitizers.

Absorption, Distribution, Metabolism, Excretion. In animal tests (oral – monkeys, pigs,

rats), alkylbenzene sulfonates are readily absorbed from the gastrointestinal tract, are distributed throughout the body, and are extensively metabolized. Excretion is via both the urine and feces. Available dermal absorption data (rats and guinea pigs) indicate that alkylbenzene sulfonates are poorly absorbed from the skin, although prolonged contact may lead to irritation and thus compromise the skin to permit more absorption (WHO, 1996 and HERA, 2004).

Repeated Dose Toxicity (Subchronic and Chronic). There have been many oral repeated dose studies performed with alkylbenzene sulfonates ranging from a 28-day study in monkeys to nine month studies conducted with rats and mice. There have also been repeated dose dermal (guinea pigs, rabbits, and rats) and inhalation studies (dogs and monkeys). Collectively, the animal data suggest that the liver, kidney and caecum (for oral studies) are the major target organs for toxicity. The liver and kidney effects were dose and duration related in that mild effects (organ weight changes and serum enzyme/clinical chemistry changes indicative of mild organ effects) were seen at lower doses, but increased in severity with both dose and time.

For the purposes of this hazard assessment, several studies were considered collectively to determine a NOAEL of 50 mg/kg/day for the chronic dietary endpoint. The NOAELs in the three studies used to develop the chronic endpoint are 40, 50 and 85 mg/kg/day, as shown on Table 3. The chronic endpoint is based on: increased caecum weight and slight kidney damage (at a LOAEL of 114 mg/kg/day in the six month rat study); reduced body weight in 21-day old pups (at a LOAEL of 250 mg/kg/day in a reproductive toxicity rat study); and significant decreases in renal biochemical parameters (at a LOAEL of 145 mg/kg/day in a nine month drinking water study in rats).

Developmental Toxicity. A number of developmental studies via the oral and dermal routes have been performed with alkylbenzene sulfonates in rats, mice and rabbits; there were also several subcutaneous injection developmental studies reported in mice (WHO, 1996). There is a spectrum of quality in the 20+ studies in terms of dosing (some had only one or two doses), purity of alkylbenzene sulfonates used (some used formulated products that ranged from 1-45% alkylbenzene sulfonates content), and overt toxicity to the pregnant females in the dermal studies due to severe irritating effects. It is concluded that some developmental effects (including some terata) were observed at high doses at which maternal toxicity was observed and the available information does not suggest any qualitative or quantitative susceptibility differences between fetuses and maternal animals.

Reproductive Toxicity. Alkylbenzene sulfonates were tested in several multigeneration studies in rats. There were no effects on reproductive parameters in any of these tests at doses up to 250 mg/kg/day.

Carcinogenicity. The available long-term studies that assessed carcinogenicity were older studies (pre-1970) that would not be acceptable under current standards (due to low number of animals used, insufficient number of doses and duration of dosing, and limited histopathological examinations. However, the limited studies provide no evidence of carcinogenicity in animals given alkylbenzene sulfonates orally.

Genotoxicity. The toxicological data show that alkylbenzene sulfonates were not

genotoxic in vitro or in vivo.

Neurotoxicity. There is no evidence in the available toxicity studies or scientific literate to indicate neurotoxic effects of the alkylbenzene sulfonates in humans or laboratory animals.

Table 2 Acute Toxicity Studies for Alkylbenzene Sulfonates

Guideline No./ Study Type	MRID No.	Results	Toxicity Category
870.1100 Acute oral toxicity	Multiple	LD_{50} = range from 404 to over 5000 mg/kg	III-IV
870.1200 Acute dermal toxicity	94032006	LD_{50} = 1200 mg/kg	II
870.1300 Acute inhalation toxicity	Literature (HERA 2004)	LC_{50} = 310 mg/m3	II
870.2400 Acute eye irritation	0033443*	Corneal opacity not reversed at 72 hours.	I
870.2500 Acute dermal irritation	003444*	Severe irritation at 72 hours	II
870.2600 Skin sensitization	Open Literature	Non-Sensitizer	

* Toxicity record No.

4.2 FQPA Considerations

Under the Food Quality Protection Act (FQPA), P.L. 104-170, which was promulgated in 1996 as an amendment to the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) and the Federal Food, Drug and Cosmetic Act (FFDCA), the Agency was directed to "ensure that there is a reasonable certainty that no harm will result to infants and children" from aggregate exposure to a pesticide chemical residue. The law further states that in the case of threshold effects, for purposes of providing this reasonable certainty of no harm, "an additional tenfold margin of safety for the pesticide chemical residue and other sources of exposure shall be applied for infants and children to take into account potential pre- and post-natal toxicity and completeness of the data with respect to exposure and toxicity to infants and children. Notwithstanding such requirement for an additional margin of safety, the Administrator may use a different margin of safety for the pesticide residue only if, on the basis of reliable data, such margin will be safe for infants and children."

The toxicology database is complete with respect to assessing the increased susceptibility to infants and children as required by FQPA for alkylbenzene sulfonates. The prenatal developmental and reproduction studies showed no qualitative or quantitative evidence of increased susceptibility (i.e., developmental NOAELs/LOAELs were the higher than those for maternal effects). Therefore, the FQPA factor was reduced to 1X.

Several reproduction and many developmental studies have been performed with

alkylbenzene sulfonate in a number of animal species. In the developmental studies, whenever toxicity was observed in adults, it was generally for mild effects (slight body weight changes, intestinal disturbances) except for severe dermal irritation effects in dermal developmental studies. Any developmental toxicity observed in these same studies included minor increases in visceral/skeletal anomalies and some fetal losses; but only at maternally toxic doses.

In one reproduction study (Buehler et al., 1971), there were slight changes in hematology and histopathology (both within historical control ranges) and slight decreases in body weight in the offspring at the highest dose of 250 mg/kg/d (at which there were no effects on the parental generation). There were no effects in either the parents or offspring in the other two reproductive toxicity studies (see Toxicity Profile Table) – high doses of 70 or 170 mg/kg/day.

There is no evidence in the available toxicity studies or scientific literature to indicate neurotoxic effects of the alkylbenzene sulfonates in humans or laboratory animals.

Based on hazard data, the Agency recommended the special FQPA SF be reduced to 1X because there are no concerns and no residual uncertainties with regard to pre- and/or postnatal toxicity. The risk assessment team evaluated the quality of the exposure data; and based on these data the team also recommended that the special FQPA SF be reduced to 1X. There is no need for a special FQPA factor because the mid-dose level of 50 mg/kg/day (NOAEL for offspring effects) in a reproduction study (Buehler et al. 1971) is the basis for the chronic RfD of 0.5 mg/kg/day. Thus, the chronic hazard value is based on slight pup effects and is protective of laboratory animals of all ages in this hazard assessment.

4.3 Dose-Response Assessment

The Health Effects Division's Toxicity Advisory Clinic (TAC) was consulted and agreed with the choice of toxicity endpoints of concern in December 2005 for the alkylbenzene sulfonates as a group.

Table 3. Summary of Toxicological Dose and Endpoints for Alkylbenzene Sulfonates

Exposure Scenario	Dose Used in Risk Assessment, UF	Special FQPA SF*, endpoint and Level of Concern for Risk Assessment	Study and Toxicological Effects
Acute Dietary (All populations)	No endpoint was selected. No effects are attributable to a single dose.		

Table 3. Summary of Toxicological Dose and Endpoints for Alkylbenzene Sulfonates			
Exposure Scenario	**Dose Used in Risk Assessment, UF**	**Special FQPA SF*, endpoint and Level of Concern for Risk Assessment**	**Study and Toxicological Effects**
Chronic Dietary (All populations)	Systemic/ Reproductive NOAEL= 50 mg/kg/day UF = 100 **Chronic RfD** = 0.5 mg/kg/day	FQPA SF = 1X **cPAD** = chronic RfD / FQPA SF = 0.5 mg/kg/day	Systemic/Reproductive NOAEL= 50 mg/kg/day; LOAEL = 250 mg/kg/day based on decreased Day 21 female pup body weight (Buehler, E. et al. 1971. Tox. Appl. Pharmacol. 18:83-91) **plus** NOAEL = 85 mg/kg/day; LOAEL= 145 mg/kg/day from 9 month drinking water rat study based on decreased body weight gain, and serum/ biochemical and enzymatic changes in the liver and kidney (Yoneyama et al. 1976 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 27(2):105-112) **plus** NOAEL= 40 mg/kg/day (0.07%) LOAEL= 114 mg/kg/day (0.2%) based on increased caecum weight and slight kidney damage in a 6 month rat dietary study (Yoneyama et al 1972 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 24:409-440)
Short-Term Incidental Oral (1-30 days)	Oral NOAEL= 50 mg/kg/day	**Residential** LOC for MOE < 100	Systemic/Reproductive NOAEL= 50 mg/kg/day; LOAEL = 250 mg/kg/day based on decreased Day 21 female pup body weight (Buehler, E. et al. 1971. Tox. Appl. Pharmacol. 18:83-91) **plus** NOAEL = 85 mg/kg/day; LOAEL= 145 mg/kg/day from 9 month drinking water rat study based on decreased body weight gain, and serum/ biochemical and enzymatic changes in the liver and kidney (Yoneyama et al. 1976 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 27(2):105-112) **plus** NOAEL= 40 mg/kg/day (0.07%); LOAEL= 114 mg/kg/day (0.2%) based on increased caecum weight and slight kidney damage in a 6 month rat dietary study (Yoneyama et al 1972 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 24:409-440)

Table 3. Summary of Toxicological Dose and Endpoints for Alkylbenzene Sulfonates			
Exposure Scenario	**Dose Used in Risk Assessment, UF**	**Special FQPA SF*, endpoint and Level of Concern for Risk Assessment**	**Study and Toxicological Effects**
Short-, intermediate- and Long-Term Inhalation (1 to 30 days, 1-6 months, >6 months)	Inhalation study NOAEL= 1mg/m^3 detergent dust combined with up to 0.1 mg/m^3 enzyme dust Equivalent to approximately 0.14 mg/kg/day (a) (inhalation absorption rate = 100%) purity= 13% active ingredient	**Residential** LOC for MOE < 100 **Occupational** LOC for MOE < 100	Subchronic Inhalation Monkey Study LOAEL = 10 mg/m^3 detergent combined with 0.1 mg/m^3 enzyme dust based on weight loss and decreased weight gain (W. Coates, et al 1978. Tox. Appl. Pharmacol. 45: 477-496) This air concentration is equivalent to approximately 1.4 mg/kg/day (a)
Dermal Endpoint	Quantification of dermal risk is not required since: 1) the alkylbenzene sulfonates are surfactants that are dermal irritants at concentrations generally greater than 20% solution (WHO 1996). Thus, dermal exposure would be self-limiting to preclude dermal irritation. Most pesticide formulations have less than 5% alkylbenzene sulfonates as an inert ingredient, with the vast majority of household products containing approximately 2%. Additionally, the requirement of the dermal toxicity studies with the end-use product will determine whether personal protective clothing would be necessary to protect against irritation during product use; 2) no systemic toxicity was seen following repeated dermal applications to rabbits at 200 mg/kg/day (with an end use product); 3) no developmental toxicity concerns were seen following repeated dermal applications to pregnant mice, rats or rabbits (developmental effects were seen either in the presence of maternal toxicity or at doses higher than those that caused maternal toxicity); and 4) there is no residential exposure to alkylbenzene sulfonates as an active ingredient, however, residential exposure from its use as an inert ingredient in pesticide formulations is expected to be of an intermittent nature (i.e, no continuous, constant contact, multi-day exposure) from household products.		
Cancer (oral, dermal, inhalation)	No evidence of carcinogenicity in reported studies in rats done before 1980 GLPs		

UF = uncertainty factor, FQPA SF = Special FQPA safety factor, NOAEL = no observed adverse effect level, LOAEL = lowest observed adverse effect level, PAD = population adjusted dose (a = acute, c = chronic) RfD = reference dose, MOE = margin of exposure, LOC = level of concern, NA = Not Applicable

(a) Equation used to convert inhalation air concentration to a dose= mg/L* absorption*respiratory volume (L/hr)*duration (hrs) * activity factor / body weight. Thus, 0.001 mg/L * 1*67.94 L/hr (based on default respiratory volumes for a New Zealand Rabbit which is used as a surrogate for a cynomolgus monkey) * 6 hrs * 1 / 2.98 kg (body weight for New Zealand Rabbit used as a surrogate for cynomolgus monkey, study reports monkey body weight ranges from 1.6 to 3.7 kg).

4.4 Endocrine Disruption

EPA is required under the FFDCA, as amended by FQPA, to develop a screening program

to determine whether certain substances (including all pesticide active and other ingredients) "may have an effect in humans that is similar to an effect produced by a naturally occurring estrogen, or other such endocrine effects as the Administrator may designate." Following recommendations of its Endocrine Disruptor and Testing Advisory Committee (EDSTAC), EPA determined that there was a scientific basis for including, as part of the program, the androgen and thyroid hormone systems, in addition to the estrogen hormone system. EPA also adopted EDSTAC's recommendation that the Program include evaluations of potential effects in wildlife. For pesticide chemicals, EPA will use FIFRA and, to the extent that effects in wildlife may help determine whether a substance may have an effect in humans, FFDCA authority to require the wildlife evaluations. As the science develops and resources allow, screening of additional hormone systems may be added to the Endocrine Disruptor Screening Program (EDSP).

In the available toxicity studies on the alkylbenzene sulfonates, there was no estrogen, androgen, and/or thyroid mediated toxicity. When additional appropriate screening and/or testing protocols being considered under the Agency's EDSP have been developed, alkylbenzene sulfonates may be subjected to further screening and/or testing to better characterize effects related to endocrine disruption.

5.0 PUBLIC HEALTH DATA

Incident Reports. There are no human incident reports associated with alkylbenzene sulfonates. The Agency consulted the following databases for poisoning incident data for alkylbenzene sulfonates:

(1) **OPP Incident Data System (IDS)** - The Incident Data System of The Office of Pesticide Programs (OPP) of the Environmental Protection Agency (EPA) contains reports of incidents from various sources, including registrants, other federal and state health and environmental agencies and individual consumers, submitted to OPP since 1992. Reports submitted to the Incident Data System represent anecdotal reports or allegations only, unless otherwise stated. Typically no conclusions can be drawn implicating the pesticide as a cause of any of the reported health effects. Nevertheless, sometimes with enough cases and/or enough documentation risk mitigation measures may be suggested.

(2) **Poison Control Centers (1993-2003)** - as the result of a data purchase by EPA, OPP received Poison Control Center data covering the years 1993 through 2003 for all pesticides. Most of the national Poison Control Centers (PCCs) participate in a national data collection system, the Toxic Exposure Surveillance System, which obtains data from about 65-70 centers at hospitals and universities. PCCs provide telephone consultation for individuals and health care providers on suspected poisonings, involving drugs, household products, pesticides, etc.

(3) **California Department of Pesticide Regulation (1982-2004)** - California has collected uniform data on suspected pesticide poisonings since 1982. Physicians are required, by statute, to report to their local health officer all occurrences of illness suspected of being related to exposure to pesticides. The majority of the incidents involve workers. Information on exposure (worker activity), type of illness (systemic, eye, skin, eye/skin and respiratory), likelihood of a causal relationship, and number of

days off work and in the hospital are provided.

(4) **National Pesticide Telecommunications Network (NPTN)** - NPTN is a toll-free information service supported by OPP. A ranking of the top 200 active ingredients for which telephone calls were received during calendar years 1984-1991, inclusive, has been prepared. The total number of calls was tabulated for the categories human incidents, animal incidents, calls for information, and others.

6.0 EXPOSURE ASSESSMENT AND CHARACTERIZATION

Dietary exposure to alkylbenzene sulfonates can occur from its use in food contact sanitizing solutions as an active ingredient, and as an inert ingredient in food-use pesticide products applied to agricultural crops, and animals. There are no currently registered products used in residential settings where alkylbenzene sulfonates are considered to be an active ingredient. However, alkylbenzene sulfonates are used as an inert ingredient in pesticide products used in residential settings, including hard surface and carpet cleaners, lawn products, and pet products. Postapplication residential exposure can occur in children from hand-to-mouth incidental oral exposure from treated surfaces, and contacting pets treated with flea and tick products. Occupational exposure to alkylbenzene sulfonates can occur from mixing/loading/application activities in various use sites, including agricultural food handling, and commercial/institutional/industrial premises.

Approximately 300,000 pounds of alkylbenzene sulfonates are used in EPA registered antimicrobial products, which is a small fraction of the approximately 860 million pounds produced each year. The majority of uses of alkylbenzene sulfonates are as household laundry and dish detergents. The alkylbenzene sulfonates are listed on the EPA HPV Challenge Program. HPV chemicals are those that are manufactured or imported into the U.S. in production volumes greater than one million pounds per year. The HPV Challenge Program is a voluntary partnership between industry, environmental groups, and the EPA which invites chemical manufacturers and importers to provide basic hazard data on the HPV chemicals they produce/import. The goal of this program is to facilitate the Public's right-to-know about the potential hazards of chemicals found in their environment, their homes, their workplace, and in consumer products. The alkylbenzene sulfonates are sponsored by the Linear Alkylbenzene (LAB) Sulfonic Acids Coalition, which has generated data for these chemicals.

6.1 Summary of Registered Uses

The alkylbenzene sulfonates are both active and inert ingredients in pesticide products. As active ingredients, they are currently in twenty-three registered end-use products as a disinfectant, food-contact sanitizer, bacteriocide/bacteriostat, microbiocide/microbiostat, fungicide/fungistat, and virucide. Alkylbenzene sulfonates are in cleaners and sanitizers that are designated for use in agricultural, food handling and commercial/institutional/industrial settings. Examples of registered uses for alkylbenzene sulfonates include, but are not limited to: application to indoor hard surfaces (e.g. urinals, shower stalls, toilet bowls, etc.), food dispensing equipment (e.g. pre-mix and post-mix vending machines), food contact surfaces (glasses, dishes, silverware,

countertops, etc.), agricultural tools, and fruits and vegetables (post-harvest). As active ingredients, there are no residential or outdoor uses currently registered. As active ingredients, concentrations of alkylbenzene sulfonates in products range from 0.036% to 25.6%. Products containing alkylbenzene sulfonates are formulated as soluble concentrates, flowable concentrates, ready-to-use solutions, or water soluble packaging. The application rates used in this assessment were the maximum application rates as recommended on the product labels.

As inert ingredients, there are approximately 350 registered end-use products containing these chemicals. Some of the inert functions of alkylbenzene sulfonates in the registered products are listed as solvent, surfactant, dispersant, detergent, and wetting agent. Products that contain alkylbenzene sulfonates as an inert are designated for use in agricultural settings, food handling premises, medical premises, commercial/institutional/industrial settings, and residential settings. Some examples of the specified use sites of the products consist of indoor hard non-porous surfaces (e.g. floors, walls etc.), carpets, food contact surfaces (glasses, dishes, silverware, countertops, etc.), agricultural tools and crops, lawns and turfs, fruits and vegetables (post-harvest), wood preservatives, materials preservatives, metalworking fluids, and pet products. Many of these products are formulated as soluble concentrates, flowable concentrates, ready-to-use solutions, or water-soluble packaging.

As inert ingredients, the percent formulations for most of the products that contain alkylbenzene sulfonates as an inert ingredient range from 0.01% to 5%. However, the majority of the labels in this range contain 2% alkylbenzene sulfonates. Because there are a large number of pesticide products that contain alkylbenzene sulfonates as an inert ingredient, the Agency assessed risks at an appropriate high-end formulation, which is dependent upon the product type. It should be noted that a few sanitizing products have inert levels as high as 30% and the highest concentration of alkylbenzene sulfonates are found in wood preservative products up to 65 %.

6.2 Dietary Exposure and Risk

6.2.1 Dietary Exposure for Active Ingredient Uses

Estimates of dietary risk from the use of alkylbenzene sulfonates as active ingredients in pesticide products are based upon the detailed analysis in the Dietary Exposure Assessment memorandum (memo from R. Quick, March 2006, D327731) and are summarized here for completeness. Dodecylbenzenesulfonic acid (27176-87-0) and sodium dodecylbenzene sulfonate (25155-30-0) have uses in food-contact surface sanitizing solutions with tolerance exemptions as specified in 40 CFR 180.940 (b) and (c), and summarized in the Table below. Residues for these compounds are exempt from the requirement of a tolerance when used in accordance with good manufacturing practice as ingredients in an antimicrobial pesticide formulation, provided that the substance is applied on a semi-permanent or permanent food-contact surface (other than being applied on food packaging) with adequate draining before contact with food. Both dodecylbenzene sulfonic acid, and sodium dodecylbenzene sulfonate have limitations for the ready-to-use end-use concentration not to exceed 400 ppm and 430 ppm, respectively for food processing equipment and utensils. However, dodecylbenzene sulfonic acid has a much lower limitation of 5.5 ppm for use on dairy processing equipment. The Agency estimates that the 430

ppm limitation for the sodium salt is equivalent to approximately 400 ppm of the free acid form.

Table 4. Tolerance Exemptions for Food Contact Sanitizer Uses (Active Uses)				
Tolerance Exemption Expression/ Chemical Name	**CAS No.**	**PC Code**	**40 CFR ◊ 180.**	**Use Pattern (Pesticidal)**
Benzenesulfonic acid, dodecyl-	27176-87-0	098002	940 (b)	food contact sanitizing solutions for dairy processing equipment, and food processing equipment and utensils; end use concentration not to exceed 5.5 ppm
			940 (c)	food contact sanitizing solutions for food processing equipment and utensils; end use concentration not to exceed 400 ppm
Benzenesulfonic acid dodecyl-, sodium salt	25155-30-0	079010	940 (c)	food contact sanitizing solutions for food processing equipment and utensils; end use concentration not to exceed 430 ppm

Based on the pesticide labels, the Agency assessed dietary exposure that could result from the use of alkylbenzene sulfonates in the food service industry (treated surfaces, dishes, utensils, glassware, pots and pans), in the food processing industry (food processing equipment such as breweries and beverage plants, meat and poultry processing plants, milk and dairy products/packing plants etc), and as a fruit and vegetable wash.

Food Handling Establishments. In the absence of residue data for residues of alkylbenzene sulfonates on treated food contact surfaces, the Agency estimated residue levels that may occur in food from the application rates on food contact surfaces. To determine the Estimated Daily Intake (EDI), the Agency has used an FDA model. The maximum ingredient percentage for dodecylbenzene sulfonates in food handling establishments from the various labels is 400 ppm. The Agency estimates that use of this product results in food residues of 530 ppb (µg/kg). The Agency assumed that food can contact 4000 cm^2 of treated surfaces, utensils, glassware, or pots and pans and that 100% of the pesticide migrates to food based on the standard assumptions used in the FDA Sanitizing Solution Guidelines. It was assumed that an adult and child consume 3000 and 1500 grams of food per day, respectively that will contact the treated surfaces.

Food Processing Equipment. The Agency used the FDA milk truck model to estimate residues in milk that could result from the use of alkylbenzene sulfonates in the food processing equipment, as representative of the potential uses in the food processing industry. As a conservative measure, the Agency assessed the maximum application rate of 400 ppm for dodecylbenzene sulfonates, as listed on the labels, although the current tolerance exemption has a limitation of 5.5 ppm for dairy processing equipment. The Agency estimates that use of this product results in maximum milk residues of 10 ppb (µg/kg).

Fruit and Vegetable Wash. The Agency also estimated dietary exposure from the fruit and vegetable wash of the alkylbenzene sulfonates. This use is regulated by the FDA in 21 CFR 173.315, which permits the wash solution to contain dodecylbenzene sulfonic acid up to 0.2% (2000 ppm), without a potable rinse. Most of the pesticide labels are in compliance with this limitation. One label however, allows a vegetable wash solution containing 0.31% (3100 ppm) dodecylbenzene sulfonic acid, but requires a potable rinse following washing.

In the absence of data for residues on fruits and vegetables, the Agency developed a model and used a number of conservative assumptions. The Agency assumed the maximum application rate of 2000 ppm in wash solution, along with assumptions for Thompson Seedless grapes as a surrogate to represent residues on all treated fruits and vegetables. The model estimates dodecylbenzene sulfonic acid residues of 9.25 ppm, which were used to estimated dietary exposure using the Dietary Exposure Evaluation Model (DEEM-FDIC™), Version 2.03 which uses food consumption data from the USDA's Continuing Surveys of Food Intake by Individuals (CSFII) from 1994-1996 and 1998. This assessment is Tier 1, conservative (assumes 100% of fruits and vegetables are washed) and uses the deterministic approach.

The daily estimates for the above three use patterns were conservatively used to assess chronic dietary risks, which are shown below in Table 5. As noted previously, an acute dietary assessment was not conducted because there are no adverse effects attributable to a single dose exposure.

The dietary risk estimates for the total food contact sanitizing uses are below the Agency's level of concern for all age groups (less than 11% of the cPAD). In addition, the dietary risk estimates for the fruit and vegetable wash for adults and young children are below the Agency's level of concern for all age groups (less than 71.2% of the cPAD). These risk estimates are based on a number of conservative assumptions, and thus may overestimate the actual risks.

Table 5. Summary of Dietary Exposure and Risk for Alkylbenzene Sulfonates

Pesticidal Active Uses

Use	Population Subgroup	Chronic Dietary	
		Dietary Exposure (mg/kg/day) a	% cPAD b
Food Service Industry (treated surfaces, utensils, glassware, etc)	adult male	0.023	4.6
	females (13-50 years)	0.027	5.4
	infants/children	0.053	10.6
Food Processing Industry (Food Processing Equipment)	adult male	0.00043	0.086
	females (13-50 years)	0.0005	0.1
	infants/children	0.001	0.2
	adult male	0.023	4.6

Table 5. Summary of Dietary Exposure and Risk for Alkylbenzene Sulfonates Pesticidal Active Uses			
Use	**Population Subgroup**	**Chronic Dietary**	
		Dietary Exposure (mg/kg/day) a	**% cPAD b**
Total Food Contact Surface Sanitizing Uses	females (13-50 years)	0.027	5.4
	infants/children	0.054	10.8
Fruit and Vegetable Wash	U.S population	0.0979	19.6
	children 1-2 yrs	0.3558	71.2
	children 3-5 yrs	0.2573	51.5

NA=not applicable

a-- chronic exposure analysis based on body weights of 70 kg, 60 kg, and 15 kg for adult males, females and children, respectively.

b-- %PAD = dietary exposure (mg/kg/day) / cPAD, where cPAD=0.5 mg/kg/day for all populations.

6.2.2 Dietary Exposure for Inert Ingredient Uses

Included in this risk assessment is the reassessment of the alkylbenzene sulfonates when used as an inert ingredient in pesticide products. Estimates of dietary risk from the inert uses of alkylbenzene sulfonates are based upon the detailed analysis in the Inert Ingredient Dietary Risk Assessment memorandum (memo from K. Leifer, March 2006, D327731). As noted previously, some of the inert functions of alkylbenzene sulfonates in the registered products are listed as solvent, surfactant, dispersant, detergent, and wetting agent. Some of these products are designated for use in agricultural settings (i.e., pre- and post-harvest and when applied to animals), where there is a potential for dietary exposure.

The alkylbenzene sulfonates assessed in this document are constituents of a larger group of compounds that have a tolerance exemption as an inert ingredient in 40 CFR 180.910 and 180. 930. As shown in Table 6, the tolerance exemption is listed as Alkyl (C8-C24) benzenesulfonic acid and its ammonium, calcium, magnesium, potassium, sodium and zinc salts.

Table 6. Tolerance Exemptions for Inert Use		
Tolerance Exemption Expression	**40 CFR ◊ 180. (a)**	**Use Pattern**
Alkyl (C8-C24) benzenesulfonic acid and its ammonium, calcium, magnesium, potassium , sodium and zinc salts	910	Surfactants, related adjuvants of surfactants
	930	Surfactants, emulsifier, related adjuvants of surfactants

(a) Residues listed in 40 CFR §180.910 are exempted from the requirement of a tolerance when used as inert

ingredients in pesticide formulations when applied to growing crops or to raw agricultural commodities after harvest (i.e., pre- and post-harvest). Residues listed in 40 CFR §180.930 are exempted from the requirement of a tolerance when used as inert ingredients in pesticide formulations when applied to animals only.

Inert Dietary Exposure Assumptions and Risk Estimates

A dietary exposure analysis for the inert ingredient use of the alkylbenzene sulfonates was conducted using the generic screening model for estimating inert ingredient dietary exposure. The dietary assessment is unrefined and extremely conservative in nature because the screening model assumes that the inert ingredient is used on all commodities, and that 100 percent of crops are treated with the inert ingredient, with no limitation on the fraction of inert ingredient. Further, the model assumes residues will be present for every consumed commodity (including meat, milk, poultry and eggs) that is included in the Dietary Exposure Evaluation Model (DEEM™). The conservative nature of this assessment is believed to capture all potential dietary exposures, including those from direct application to animals.

Based on the use of the screening level inert ingredient dietary exposure model, there are no risk concerns associated with dietary exposures as the estimated dietary exposures for the U.S. population and all population subgroups are below 100% of the cPAD. As noted, a number of conservative assumptions were used in this screening level dietary risk assessment[1] of inert uses.

Table 7. Summary of Dietary Exposure and Risk for Alkylbenzene Sulfonates as Inert Ingredients

Population Subgroup	Chronic Dietary	
	Dietary Exposure (mg/kg/day)	% cPAD a
U.S. population	0.12	24
females (13-50 years)	0.087	17
children 1-2 yrs	0.422	84
children 3-5 yrs	0.31	62

a-- %PAD = dietary exposure (mg/kg/day) / cPAD, where cPAD=0.5 mg/kg/day for all populations.

6.3 Drinking Water Exposure and Risk for Inert Ingredient Uses

There are no currently registered outdoor uses of the alkylbenzene sulfonates as active ingredients that are being supported by the registrant. However, these compounds are inert

[1] A review of those products listed as containing ingredients Benzenesulfonic acid, dodecyl- (CAS Reg. No. 27176-87-0); Sodium dodecylbenzenesulfonate (CAS Reg. No. 25155-30-0); and Benzenesulfonic acid, C10-16-alkyl derivs (CAS Reg. No.68584-22-5) was conducted. The results of that review indicate that the linear alkylbenzenesulfonates are primarily used in low concentrations (typically less than 5% w/w) in herbicide products that typically are applied in a preemergent or early post-emergent fashion.

ingredients in many residential and agricultural products that are used outdoors. The majority of these products contain alkylbenzene sulfonates at low concentrations that are generally less than 5%. Based on the "Environmental Fate Assessment of Alkylbenzene Sulfonates for the Registration Eligibility Document (RED)" (T. Milano, March 2006), linear alkyl benzenesulfonates are water soluble, nonvolatile and mobile, but also readily biodegradable. There are no readily available data on the occurrence of linear alkyl benzenesulfonates in ambient or treated drinking water. No ambient water quality criteria, drinking water maximum contaminant levels or health advisory levels have been established for these compounds by EPA's Office of Water. The potential for transport into drinking water resulting from pesticide inert ingredient uses of these substances do exist, therefore the Agency estimated drinking water concentrations resulting from the inert ingredient uses of these substances. Details of this analysis are presented in the Inert Ingredient Dietary Risk Assessment memorandum from K. Leifer, March 23, 2006.

The drinking water analysis is based on a derivation of estimated upper bound Tier I drinking water concentrations from these substances' use as pesticide inert ingredients from the FQPA Index Reservoir Screening Tool (FIRST). A number of conservative assumptions were utilized as inputs into the inert ingredient drinking water exposure assessment model. For example, it was assumed that the linear alkylbenzene sulfonates were stable, and pesticide products were applied via aerial spray. The results of the model were scaled to account for a linear alkylbenzene sulfonate weight fraction of 5% (which is a 95th percentile value). The Estimated Drinking Water Concentration (EDWC) for chronic drinking water exposure is 6.6 ug/L (ppb).

The Agency did not estimate acute drinking water risks for the inert ingredient use because an acute dietary endpoint (i.e., aPAD) was not selected as there were no effects attributable to a single dose exposure. The estimated chronic drinking water concentration and drinking water level of concern for chronic exposure to linear alkyl benzenesulfonates is given in Table 8 below.

Table 8. Chronic Drinking Water Exposure Estimates for Inert Ingredient Uses of Alkylbenzene Sulfonates

Population Subgroup	EDWC[1] (µg/L)	%cPAD[2]	DWLOC[3] (µg/L)
U.S. Population (total)	6.6	<0.1%	38 -1,500
Children (1-2 years)	6.6	<0.1%	8 - 500

1 Estimated Drinking Water Concentration (EDWC) for chronic drinking water exposure as determined by the use of FIRST modeling analysis described above for inert ingredient use. [The EDWC for linear alkyl benzenesulfonates is the value reported as the "Adjusted Annual Average (Chronic) Untreated Water Concentration"]

2 %cPAD = drinking water exposure (mg/kg/day) / cPAD, where cPAD=0.5 mg/kg/day for all populations. It was assumed that a 15 kg child ingests 1 L water per day and that a 70 kg adult ingests 2L water per day.

3 Drinking Water Level of Comparison (DWLOC) is the maximum contribution from water allowed in the diet based on food and drinking water from inert use only. In this case, since the allowable risk contribution from food is based on a screening level model, the use of a single, deterministic value for the DWLOC is not appropriate. Rather a DWLOC range is given, with the values in the range corresponding to an upper value of range of drinking water concentrations ranging from 100% of the cPAD (i.e., assuming no food exposure) to a lower value that considers food exposures to be at the dietary screening level value.

For chronic drinking water exposures to linear alkyl benzenesulfonates as inert ingredients,

the Drinking Water Level of Comparison (DWLOC) range for chronic exposure is 38-1500 µg/L for the general U.S. population and 8-500 µg/L for children 1-2 years old. The EDWC used to assess chronic (non-cancer) dietary risk from drinking water is 6.6 µg/L. The chronic estimated concentration is below the DWLOCs for the general U.S. population and all population subgroups. Drinking water risks, therefore, are not of concern.

The Agency concludes that there are no risk concerns for chronic aggregate dietary and drinking water exposures to the alkylbenzene sulfonates as pesticide inert ingredients. This is based on the conservative assumptions used in the screening level dietary exposure model, as well as the estimated upper bound drinking water concentrations from these substances' use as pesticide inert ingredients derived from FIRST.

6.4 Residential Exposure and Risks from Inert Ingredient Use

Exposure Scenarios

As noted previously, there are no residential use sites for the alkylbenzene sulfonates as active ingredients. However, alkylbenzene sulfonates are formulated as inert ingredients in approximately 350 registered end-use products, many of which are used in residential settings. Some examples of the specified use sites on the products consist of indoor hard non-porous surfaces (e.g. floors, walls etc.), carpets, food contact surfaces (glasses, dishes, silverware, countertops, etc.), agricultural tools and crops, lawns and turfs, fruits and vegetables (post-harvest), wood preservatives, materials preservatives, metalworking fluids, and pet products. Details of the residential inert exposure assessment can be found within the companion memorandum (memorandum from T. Milano/C. Walls, July 2006, D330330). A summary of the residential assessment is presented below.

For the purposes of this screening level assessment, the Agency selected representative scenarios for the vast majority of products, based on end-use product application methods and use amounts. These scenarios reflect high-end exposure and risk estimates for all products represented. The following residential use sites were assumed to be the high-end representative scenarios for inert uses of alkylbenzene sulfonates. These include:

1) outdoor residential turf treatment (ready to use liquid),
2) indoor hard surface cleaner (ready to use liquid), and
3) pet flea and tick products (aerosol can spray).

For each of the use sites, the Agency assessed residential handler (applicator) inhalation exposure and post application incidental ingestion by toddlers. Residential postapplication exposures result when bystanders, such as children come in contact with alkylbenzene sulfonates in areas where end-use products have recently been applied (e.g., treated hard surfaces/floors), or when children incidentally ingest the residues through mouthing the treated end products/treated articles (i.e., hand-to-mouth or object-to-mouth contact). Although the alkylbenzene sulfonates are also present in carpet cleaners as an inert ingredient, the Agency believes that the risk associated with a toddler contacting treated hard surfaces are representative of risks associated

with a toddler contacting a treated carpet. As previously mentioned, there is no dermal endpoint, and therefore, there were no dermal assessments conducted (handler or post application).

Exposure Data and Assumptions

For most residential scenarios, the Agency used EPA's Pesticide Inert Risk Assessment Tool (PiRat) to estimate residential applicator and post-application exposures and risks from the use of alkylbenzene sulfonates as an inert ingredient in representative residential products. Background information and the downloadable executable file for PiRat can be found at http://www.epa.gov/opptintr/exposure/docs/pirat.htm. The Agency utilized all of PiRat's default values, along with high-end percent formulations based on the review of the Confidential Statements of Formula (CSFs) for the various residential products that contain the alkylbenzene sulfonates as inert ingredients. For the assessment of the pet products and hard surface cleaners, the Agency used assumptions in the Residential Standard Operating Procedures (SOPs). Typically, most products used in a residential setting result in exposures occurring over a short-term duration. Thus, the residential handler and postapplication scenarios are assumed to be of short- term duration (1-30 days).

Because there are a large number of products that contain alkylbenzene sulfonates as an inert ingredient, the Agency assessed a representative high-end formulation product to be conservative.

An inhalation post-application assessment was not conducted because the vapor pressure of the alkylbenzene sulfonates is extremely low ($5.1x10^{-10}$ to $6x10^{-15}$ mmHg). In addition, a dermal assessment was not conducted because of the lack of a dermal toxicological endpoint.

Risk Characterization

A summary of the residential handler exposure and risk estimates are presented on Table 9, while the postapplication incidental oral exposure and risk estimates are presented in Table 10. The non-cancer risk estimates are expressed in terms of the MOE. For residential handlers that handle products containing alkylbenzene sulfonates as inert ingredients, the short-term inhalation MOEs were above the target MOEs (i.e., >100) and thus, do not exceed the Agency's level of concern, with the exception of the flea and tick product where the MOE was 87 for the high-end formulation containing 24% alkylbenzene sulfonates. This scenario is conservative because it assumes a person treats their pet with 0.5 cans of flea product that contains 24% alkylbenzene sulfonates every day for a month. However, there are no risk concerns for the majority of pet products containing 2% alkylbenzene sulfonates.

There are no residential postapplication risk concerns for the household products that contain alkylbenzene sulfonates as an inert ingredient as shown on Table 10. All of the scenarios evaluated have short-term MOEs above 100, and thus are not of concern including postapplication incidental oral risks to children that may contact turf, hard surfaces or a pet treated with pesticide products containing alkylbenzene sulfonates as an inert ingredient. The postapplication MOEs range from 106 to 7,400.

Alkylbenzene sulfonates are considered to be dermal irritants in formulations that have

listed amounts generally greater than 20%. Thus, dermal exposure would be self-limiting due to dermal irritation. The vast majority of residential products contain less than 5% alkylbenzene sulfonates. The Agency intends to consider the potential for irritation in recommended labeling language of pesticide products containing the alkylbenzene sulfonates, and consider available dermal toxicity data on a diluted end-use formulation. The Agency should confirm that all products with greater than 20% require the use of gloves.

Table 9.
Estimates of Inhalation Exposures and Risks to Residential Handlers of Alkylbenzene Sulfonates as Inert Ingredients
(Short-Term Duration)

Product Use	Application Method	Area Treated/Quantity Handled[a]	Inhalation Exposure (mg/kg/day)	Inhalation MOEs[c] (Target MOE ≥ 100)
Outdoor Products				
Ready to Use Liquid Turf spot/gardens[b]	Low pressure handwand; MLAP	1000 ft^2/day (spot)	$7.07x10^{-6}$	20,000
	Hose end sprayer; MLAP	$2x10^4$ ft^2/day (full broadcast)	$4.48x10^{-5}$	3,100
	Backpack; MLAP	1000 ft^2/day (spot)	$7.07x10^{-6}$	20,000
	Sprinkling can; MLAP		$2.24x10^{-6}$	63,000
Indoor Products				
Ready to Use Liquid (hard surface cleaner)[d,e]	Low pressure handwand; MLAP	0.5 gallons/day	$1.37x10^{-4}$	1.000
Pet Flea and Tick Product[f]	Aerosol Can Spray	0.5 6 oz can	$1.61x10^{-3}$	**87**

a: Standard PiRat model input parameters, except for pet products and hard surface cleaner, which are based on an AD assumption.
b: percent formulation used = 11%; an application rate of 0.00015 lb product/ft^2 was assumed for all scenarios and the body weight = 70kg.
c: MOEs = NOAEL / exposure where inhalation NOAEL = 0.14 mg/kg/day and the target MOE ≥ 100
d: % formulation used = 8%
e: An application rate of 8 lb/gallon, which is the density of water, was assumed for all scenarios and the body weight =70kg.
f= % formulation = 24%.

Table 10. Summary of Short-Term Residential Postapplication Exposure and Risk Estimates from Alkylbenzene Sulfonates as Inert Ingredients[a]			
Product Use	**Route of Exposure**	**Exposure mg/kg/day[b]**	**MOEs[c] (Target MOE ≥ 100**
Ready to Use Liquid Turf spot/gardens[d]	Incidental ingestion: hand to mouth	1.08×10^{-2}	4,600
Ready to Use Liquid (hard surface cleaner)[a, e]		0.0068	7,400
Pet Flea and Tick Product[f]	Incidental ingestion: hand to mouth	0.4739	106

a: The representative use sites assessed through using PiRAT for incidental oral post application exposures to toddlers are turf products. Exposure from hard surface cleaner and pet products was based on AD assumptions.
b: The body weight used in this calculation was 15kg, which is assumed to be the body weight of a toddler.
c: MOEs = NOAEL / exposure where incidental oral NOAEL = 50 mg/kg/day. Target MOE ≥ 100.
d: % formulation used = 11%
e: % formulation used = 8%
f: % formulation used = 24%

7.0 AGGREGATE RISK ASSESSMENTS AND RISK CHARACTERIZATION

In order for a pesticide registration to continue, it must be shown that the use does not result in "unreasonable adverse effects on the environment". Section 2 (bb) of FIFRA defines this term to include "a human dietary risk from residues that result from a use of a pesticide in or on any food inconsistent with standard under section 408..." of FFDCA. As mandated by the FQPA amendments to FIFRA and the Federal Food, Drug and Cosmetic Act (FFDCA), the Agency must consider total aggregate exposure from food, drinking water and residential sources of exposure to alkylbenzene sulfonates. Aggregate exposure is the total exposure to a single chemical (or its residues) that may occur from dietary (i.e., food and drinking water), residential, and other non-occupational sources, and from plausible exposure routes (oral, dermal, and inhalation).

Typically, aggregate risk assessments are conducted for acute (1 day), short-term (1-30 days), intermediate-term (1-6 months) and chronic (6 months to lifetime) exposures. However, an acute aggregate assessment was not conducted because there are no adverse effects attributable to acute exposure. An intermediate-term aggregate assessment was not conducted because there are no residential exposures of this duration. In addition, because there are no long-term residential exposures, the chronic aggregate assessment only considered food and drinking water. Thus, only short-term and chronic aggregate assessments were conducted. Oral and inhalation exposure and risk estimates were conservatively combined for the aggregate risk assessment because these endpoints both identify adverse effects on body weight. Dermal exposures were not considered in the risk assessment because a toxicological endpoint was not established.

In performing aggregate exposure and risk assessments, the Office of Pesticide Programs has published guidance outlining the necessary steps to perform such assessments (General Principles for Performing Aggregate Exposure and Risk Assessments, November 28, 2001; available at http://www.epa.gov/pesticides/trac/science/aggregate.pdf). Steps for deciding whether to perform aggregate exposure and risk assessments are listed, which include: identification of toxicological endpoints for each exposure route and duration; identification of potential exposures for each pathway (food, water, and/or residential); reconciliation of durations and pathways of exposure with durations and pathways of health effects; determination of which possible residential exposure scenarios are likely to occur together within a given time frame; determination of magnitude and duration of exposure for all exposure combinations; determination of the appropriate technique (deterministic or probabilistic) for exposure assessment; and determination of the appropriate risk metric to estimate aggregate risk.

Short-Term Aggregate Risk. Aggregate short term risk assessments are designed to provide estimates of risk likely to result from exposures to the pesticide or pesticide residues in food, water, and from residential (or other non-occupational) pesticide uses. This assessment considers both the active and inert uses of the alkylbenzene sulfonates. For children, the short-term aggregate assessment includes average dietary exposure (food and drinking water) from both the active food contact sanitizer uses and the inert uses on agricultural commodities, in addition to estimated incidental oral exposures to children from residential uses such as hard surface cleaning products as an inert ingredient. For adults, the aggregate assessment includes dietary (food and drinking water) from both active and inert uses and residential inhalation exposures from wiping a hard surface cleaning products since this scenario represents the highest exposure from the inert use.

Individual scenarios that had risks of concern were not included in the aggregate assessment. These include exposure to some of the high-end formulation products such as the residential handler of pet flea and tick products (inhalation MOE is 87 compared to target MOE>100). As noted previously, a number of very conservative assumptions were used to derive these risk estimates.

Aggregate risks were calculated using the total MOE approach outlined in OPP guidance for aggregate risk assessment (August 1, 1999, Updated "Interim Guidance for Incorporating Drinking Water Exposure into Aggregate Risk Assessments"). The assumptions and equations are presented in the footnotes on Table 11.

Table 11 presents a summary of the short-term aggregate risk MOEs. The aggregate oral and inhalation risks are not of concern for adults, as the total aggregate MOE is 340 which is greater than the target of 100. For children, the aggregate risk estimate is very close to the target MOE of 100 (MOE=99. As noted previously, several conservative assumptions were used in this assessment. For example, dietary exposure from both the active sanitizer use and the inert uses were considered together to estimate an upper-bound exposure estimate, since these use patterns are very different and thus could co-occur. To compensate for this conservative assumption, the Agency only included one representative residential use scenario in the aggregate assessment even though these compounds are used extensively as inert ingredients in approximately 350 pesticide

products.

It should also be recognized that the majority of the uses of alkylbenzene sulfonates are not in pesticide products, but rather are used in household laundry and dish detergents. Over 800 millions pounds of these compounds are produced each year, while only 300,000 pounds are used in EPA registered antimicrobial products. The Agency did not consider potential exposure and risks from the numerous other residential exposures to alkylbenzene sulfonates because the Agency lacks reliable information at this time.

Table 11
Summary of Short-Term Aggregate Risk Estimates

Exposure Scenario	Dose [a] (mg/kg/day)		Total MOE[b] (Target MOE≥100)	
	Child (15 kg)	Adult	Child (15 kg)	Adult
Oral Exposure				
Dietary Exposure				
Food Contact Sanitizer	0.054	0.027	926 (10.8% of cPAD)	1,850 (5.4% of cPAD)
Inert Ingredient Uses (Food)	0.422	0.12	118 (84% of cPAD)	417 (24% of the cPAD)
Drinking Water Exposure (Inert) c	0.00044	0.000189	114,000 (<1% of cPAD	227,000 (<1% of cPAD)
Hard Surface Cleaner	0.0068	NA	7,400	NA
Inhalation Exposure				
Handler of hard surface cleaning products	NA	0.000137	NA	1,000
Total Aggregate Dose and MOE	0.5	0.147	**99**	340

NA= Not applicable

(a) Chronic dietary exposure for females 13-50 years for sanitizer use. The total general population dietary exposure was used to assess inerts, since this population has higher exposure than females 13-50 years.

(b) MOE = NOAEL (mg/kg/day) / potential dose rate (mg/kg/day) [Where short-term oral NOAEL = 50 mg/kg/day]. Target MOE ≥ 100.

(c) Exposure estimates assume a 15 kg child ingests 1L water/day and that a 60 kg adult female ingests 2L water per day of 6.6 ppb (the chronic estimated drinking water concentration (EDWC) based on the inert ingredient use.

Chronic Aggregate Risk. The chronic aggregate assessment considers average dietary exposure (food and drinking water) from both the active food contact sanitizer uses and the inert uses on agricultural commodities. The dietary exposures from the fruit and vegetable wash were not considered because it would be overly conservative to assume simultaneous exposure to alkylbenzene sulfonates from three different use patterns. As shown on Table 12, the dietary aggregate risk is **95% of the cPAD for children**, while for adults it is **29% of the cPAD**.

Table 12 Summary of Chronic Aggregate Risk Estimates				
Exposure Scenario	Dose [a] (mg/kg/day)		%cPAD[b]	
	Child (15 kg)	Adult	Child (15 kg)	Adult
Oral Exposure				
Dietary Exposure				
Food Contact Sanitizer	0.054	0.027	10.8%	5.4%
Inert Ingredient Uses (Food)	0.422	0.12	84%	24%
Drinking Water Exposure (Inert) c	0.00044	0.000189	<1%	<1%
Total Aggregate Dose and Risk	0.476	0.147	95%	29%

NA= Not applicable

(a) Chronic dietary exposure for females 13-50 years for sanitizer use. The total general population dietary exposure was used to assess inerts, since this population has higher exposure than females 13-50 years.

(b) %cPAD = dietary exposure (mg/kg/day) / cPAD, where cPAD -= 0.5 mg/kg/day for all populations.

(c) Exposure estimates assume a 15 kg child ingests 1L water/day and that a 60 kg adult female ingests 2L water per day containing 6.6 ppb alkylbenzene sulfonates. The 6.6 ppb estimate is based on the chronic estimated drinking water concentration (EDWC)) resulting from agricultural use of products that contain the alkylbenzene sulfonates as an inert ingredient.

8.0 CUMULATIVE EXPOSURE AND RISK

Another standard of section 408 of the FFDCA which must be considered in making an unreasonable adverse effect determination is that the Agency considers "available information" concerning the cumulative effects of a particular pesticide's residues and "other substances that have a common mechanism of toxicity."

Unlike other pesticides for which EPA has followed a cumulative risk approach based on a common mechanism of toxicity, EPA has not made a common mechanism of toxicity finding as to the alkylbenzene sulfonates and any other substances and the alkylbenzene sulfonates do not appear to produce a toxic metabolite produced by other substances. For the purposes of this tolerance action, therefore, EPA has not assumed that alkylbenzene sulfonates have a common mechanism of toxicity with other substances. For information regarding EPA's efforts to determine which chemicals have a common mechanism of toxicity and to evaluate the cumulative effects of such chemicals, see the policy statements released by EPA's Office of Pesticide Programs concerning common mechanism determinations and procedures for cumulating effects from substances found to have a common mechanism on EPA's website at http://www.epa.gov/pesticides/cumulative/.

9.0 OCCUPATIONAL EXPOSURE AND RISK

The Agency has assessed the exposures and risks to occupational workers that handle alkylbenzene sulfonates (memorandum from T. Milano, July 6, 2006, D330329). This section

summarizes the results of the occupational exposure assessment.

Based on examination of product labels describing uses for the product, it has been determined that exposure to handlers can occur in a variety of occupational settings. Additionally, postapplication exposures are likely to occur in these settings. The representative scenarios selected by the Agency for assessment were evaluated using maximum application rates as recommended on the product labels for alkylbenzene sulfonates.

Occupational Handlers. The Agency has determined that there is potential for dermal and inhalation worker exposure to alkylbenzene sulfonates at various use sites including agricultural premises, food handling, and commercial/institutional/industrial premises. Representative scenarios were selected for evaluation based on the use sites and maximum application rates for all three of the active ingredients in this assessment.

As noted previously, the Agency did not select a dermal endpoint, and thus only inhalation exposure and risk estimates are presented. The alkylbenzene sulfonates are dermal irritants, and all of the labels require the use of gloves by workers, except for Reg. #71094-2 (0.036% ai, ready to use product). The occupational exposure scenarios, and estimated risks are presented in Table 13.

To assess the handler risks, AD used surrogate unit exposure data from both the proprietary Chemical Manufacturers Association (CMA) antimicrobial exposure study and the Pesticide Handlers Exposure Database (PHED).

For the occupational handler inhalation risk assessment, the short- and intermediate- term risks calculated at baseline exposure (no respirators) were above target MOEs for all scenarios (i.e., inhalation MOEs were >100), except the following:

- ST and IT inhalation exposure from cleaning hard surfaces via wiping in the food handling category, inhalation MOE = 93.

The Agency also calculated a total MOE for one of the active ingredients, sodium dodecylbenzene sulfonate (25155-30-0) based on the label use directions, which recommend the same product be used for both cleaning and sanitizing. As shown on Table 14, all total inhalation MOEs for cleaning and sanitizing (baseline) were above the target MOEs for all scenarios (i.e., inhalation MOEs were >100), except the following:

- ST and IT inhalation exposure from cleaning indoor hard surfaces via wiping and then following with sanitizing via immersion/flooding in the food handling premises category, inhalation MOE = **93.**
- ST and IT inhalation exposure from cleaning indoor hard surfaces via wiping and then following with sanitizing via low pressure spray in the food handling premises category, inhalation MOE = **90.**

- ST and IT inhalation exposure from cleaning indoor hard surfaces via sponge/mesh/wiping and then sanitizing via immersion/flooding in the food handling premises category, inhalation MOE = **90.**

Although all the inhalation risks of concern are for baseline exposures, the Agency does not believe it is practicable to require the use of respiratory protection on cleaning products used in janitorial situations. In addition, engineering controls are not feasible for the current use patterns on the labels.

Table 13
Short-, and Intermediate-Term Inhalation Risks for Occupational Handlers
(Representative Scenarios)

Exposure Scenario	Method of Application	Application Rate (lb ai/ gallon)	Quantity Handled/ Treated per day (gallons)	Baseline Inhalation MOE (a) (Target MOE≥100)
Agricultural Premises and Equipment				
Application to hard surfaces	Brush	0.0667	0.26	2,000
	Mechanical Foam	0.0667	0.26	430
	Flooding	0.00183	10	280
	Cleaning in place (CIP)	0.00195	10,000	1,200
	High Pressure spray	0.00326	40	630
	Immersion	0.00334	10	160
	Low pressure spray	0.00334	10	430
	Trigger Pump Spray	0.00334	0.26	8,700
Food Handling				
Application to indoor hard surfaces	Brush	0.0667	0.26	2,000
	Mechanical Foam	0.0667	0.26	430
	Immersion	0.00334	10	160
	Trigger Pump Spray	0.00334	0.26	8,700
	Low pressure handwand (clean)	0.00603	2	1,200
	High pressure spray (sanitize)	0.0115	40	180
	Immersion, flooding for RTU (sanitize)	0.003	10	170
	Mopping	0.00244	2	840
	Wiping (clean)	0.00603	0.26	**93**
	Sponge/mesh wipe (clean)	0.003	0.26	190

Table 13 Short-, and Intermediate-Term Inhalation Risks for Occupational Handlers (Representative Scenarios)				
Exposure Scenario	**Method of Application**	**Application Rate (lb ai/ gallon)**	**Quantity Handled/ Treated per day (gallons)**	**Baseline Inhalation MOE (a) (Target MOE≥100)**
	Cleaning in Place (CIP) (clean and sanitize)	0.00358	10,000	680
Food dispensing equipment	Cleaning in Place (CIP) (clean)	0.00603	10,000	400
	Cleaning in Place (CIP) (sanitize)	0.00302	10,000	810
Fruits and vegetables	Immersion	0.00455	10	110
	Trigger pump spray	0.003	0.26	9,700
Commercial/Institutional Premises				
Application to indoor hard surfaces (includes utensils and silverware)	Brush	0.0667	0.26	2,000
	Mechanical Foam	0.0667	0.26	430
	Immersion	0.00334	10	160
	Low Pressure Handwand	0.00334	2	2,200
	Trigger Pump Spray	0.00334	0.26	8,700
Shower stalls and toilets	Mopping	0.0177	2	120
	Swabbing after a liquid pour	0.0177	0.26	1,100

(a) MOE = NOAEL (mg/kg/day) / Daily Dose [Where short-and intermediate-term NOAEL = 0.14 mg/kg/day for inhalation exposure] Target MOE is ≥ 100.

Table 14 Short, and Intermediate Term Inhalation Risks to Occupational Handlers Cleaning and Sanitizing with Products That Contain Sodium Dodecylbenzene Sulfonate				
Representative Use	**Registration #**	**Method of CLEANING Application (Baseline MOE)**	**Method of SANITIZING Application (Baseline MOE)**	**Total Inhalation MOE (Baseline) (Target MOE≥100)**
Food Handling/Storage Establishments Premises and Equipment				
Indoor Hard Surfaces (includes dishes and silverware)	1020-13	High pressure spray (1,100)	High pressure spray (180)	150
			Brush (12,000)	1,000
		Brush (75,000)	High pressure spray (180)	180
			Brush (12,000)	10,000
	71094-1	Low pressure spray (1,200)	Immersion/Flooding ($1.4X10^6$)	1,200

Table 14 Short, and Intermediate Term Inhalation Risks to Occupational Handlers Cleaning and Sanitizing with Products That Contain Sodium Dodecylbenzene Sulfonate				
Representative Use	**Registration #**	**Method of CLEANING Application (Baseline MOE)**	**Method of SANITIZING Application (Baseline MOE)**	**Total Inhalation MOE (Baseline) (Target MOE≥100)**
			Low pressure spray (2,400)	800
		Wiping (93)	Immersion/Flooding ($1.4X10^6$)	**93**
			Low pressure spray (2,400)	**90**
		Foam (4,800)	Immersion/Flooding ($1.4X10^6$)	4,800
			Low pressure spray (2,400)	1,600
		Brush (22,000)	Immersion/Flooding ($1.4X10^6$)	22,000
			Low pressure spray (2,400)	2,000
	71094-2	Sponge/Mesh/Wiping (190)	Immersion/Flooding (170)	**90**
			Trigger Pump (9,700)	190
		Low Pressure Spray (2,400)	Immersion/Flooding (170)	160
			Trigger Pump (9,700)	1,900
		Brush (45,000)	Immersion/Flooding (170)	170
			Trigger Pump (9,700)	8,000
	1020-13	CIP (680)	CIP (680)	340
Food dispensing equipment	71094-1	CIP (400)	CIP (810)	270

Postapplication Exposure and Risk. For most of the occupational scenarios, postapplication dermal exposure is not expected to occur or is expected to be negligible based on the application rates and chemical properties of these chemicals. The alkylbenzene sulfonates have a low vapor pressure ($5.1x10^{-10}$ to $6.02x10^{-15}$ mmHg), so that any standing solutions that may result in post application exposure were deemed negligible.

10.0 ENVIRONMENTAL RISK

10.1 Active Ingredient Uses

A detailed ecological hazard and environmental risk assessment for the alkylbenzene sulfonates is presented in the attached memorandum for the active ingredient pesticidal uses (memo from R. Petrie, July 12, 2006). A brief summary is presented below.

Ecological Toxicity Data.

Acute toxicity to terrestrial organisms: As shown in the acute toxicity summary Table 15, alkylbenzene sulfonates are slightly toxic to the Northern bobwhite quail on an acute oral basis. The avian acute oral LD50 is > 500 ppm, therefore, an avian environmental hazard statement for birds is not required on manufacturing use product labels. No evidence of endocrine disrupting effects was observed in mammalian toxicity studies. No data are available or required for terrestrial plants.

Acute toxicity to aquatic organisms: As shown in Table 15, supplemental acute studies indicate that alkylbenzene sulfonates are moderately toxic to freshwater fish and freshwater aquatic invertebrates. In addition, 11 acute freshwater fish studies using commercially relevant LAS and LAB formulations indicate the LC50 values range from 1.67 to 7.7 mg/L [LAS SIDS Initial Assessment Report, (SIAR)]. Data using LAB sulfonic acids in the LAS SIAR report range in toxicity from 3.0 to 10.0 mg/L. Research by Fairchild et al. (1993) indicates that "Degradation processes rapidly reduce chain lengths of LAS in the environment to averages lower than C12. Thus, hazard assessments of LAS to aquatic organisms should focus on environmentally relevant mixtures of average chain lengths of C12 or less." Based on study results above (MRIDs 44260002, 44260009) and studies presented in LAS SIAR, an environmental hazard statement for fish is not required on manufacturing use products under consideration in this RED.

In aquatic invertebrates, LAS toxicity is variable, depending on the length of the carbon chain. LAS/SIAR (page 37) summarizes 11 *Daphnia* magna studies on commercially relevant LAS that range in EC50 values from 1.62 to 9.3 mg/L. Data on the LAB sulfonic acids give EC50 values for *Daphnia* magna ranging from 2.9 to 12 mg/L. Formulations tested included the C10-C16 benzene sulfonic acid and the dodecylbenzene sulfonic acid. Even though the higher carbon chains are more toxic, the CLER (Council for LAB/LAS Environmental Research) ensures that the typical LAS or LAB formulations contain less than 1 - 10% carbon chains C14 or greater. The LAS SIAR report cites 11 *Daphnia magna* studies on commercial LAS formulations with EC50 values ranging from 1.62 to 9.3 mg/L. LAB formulations ranged in toxicity from 2.9 to 12 mg/L. Research by Fairchild et al. (1993) states: "Degradation processes rapidly reduce chain lengths of LAS in the environment to averages lower than C12. Thus, hazard assessments of LAS to aquatic organisms should focus on environmentally relevant mixtures of average chain lengths of C12 or less." Based on study results above (MRID 47025025) and studies presented in LAS SAIR, an environmental hazard statement for aquatic invertebrates is not required on manufacturing use products under consideration in this RED.

Chronic toxicity to aquatic organisms: Chronic toxicity testing (Fish early life stage, 850.1300/72-4a and aquatic invertebrate life cycle, 850.1400/72-4b) is required for pesticides when certain conditions of use and environmental fate apply. Chronic aquatic organism tests are not required for alkylbenzene sulfonates because the currently registered uses are indoor applications. A 28 day chronic freshwater fish toxicity test was found in the literature. The NOAEC was 0.7 mg/L for a carbon chain C11.7 (Fairchild et al, 1993). Scientists studying

alkylbenzene sulfonates have concluded that a laboratory derived NOAEC of 0.4 mg/L alkylbenzene sulfonates is protective of ecosystem structure and function in experimental streams. Alkylbenzene sulfonates literature indicates slight toxicity to green algae.

Table 15. Acute Toxicity of Alkylbenzene Sulfonates

Species	Chemical, % active ingredient (ai)	Endpoint	Toxicity Category (TGAI)	Satisfies Guidelines/Comments	Reference
Birds					
Northern bobwhite *(Colinus virginianus)*	87.6%Carbon chain not identified. (Nacconal 90G used)	LD_{50} > 1382 mg/kg NOEL = 279 mg/kg	Slightly toxic	Yes. Acceptable. 14 day test	MRID: 41143901
Freshwater Fish					
Fathead Minnow (*Pimephales promelas*)	14.0% (Carbon chain not identified.)	96hr LC50 = 3.4 mg/L	Moderately toxic	Yes. Supplemental study.	44260002
Rainbow trout *Oncorhynchus mykiss*)	65.0% C11, C12	96 hr LC50 = 1.68 mg/L	Moderately toxic	Yes. Supplemental study.	44260009
Freshwater Invertebrates					
Waterflea *(Daphnia magna)*	Not reported.	48-hr. EC_{50} = LAS-C10 = 29.5 mg/L, LAS-C12 = 6.84 mg/L, LAS-C14 = 0.80 mg/L, LAS-C16 = 0.20 mg/L.	C-12 = Moderately toxic	Yes. Supplemental study.	47025025
Green Algae					
Selenastrum capricornutum	Not Reported. (Carbon chain not identified.)	96 hr. EC50 = 70.27 ppm	Slightly toxic	No. Supplemental.	42439803

Data Requirements: There are no outstanding ecological data requirements. The guideline requirements for a freshwater fish acute test (Guideline 850.1075), and freshwater invertebrate (Guideline 850.1010) have been fulfilled. Acute estuarine/marine tests, chronic toxicity testing (Fish early life stage, 850.1300/72-4a and aquatic invertebrate life cycle, 850.1400/72-4b) and non-target plant phytotoxicity tests are not required for indoor uses.

Environmental Fate and Exposure Assessment.

No fate studies for alkylbenzene sulfonates are available in US EPA's files. Thus, the Agency has relied on scientific literature and the Agency's EPI Suite model to obtain different environmental properties for the alkylbenzene sulfonates. The EPI Suite model predicts that alkylbenzene sulfonates are not likely to persist in water or microbial soils and sediments. The Agency also conducted a literature search to further support the output parameters that were provided by the EPI Suite model. Extensive literature are available that describe the fate and significance of alkylbenzene sulfonates in the environment from a long history of detergent use.

Environmental exposure modeling was not conducted for alkylbenzene sulfonic acids and sulfonates because the currently registered uses are indoor spray applications. Uses such as urinals and toilet bowls could result in minimal exposure to the environment when flushed, however, significant environmental exposure is not expected for the following reasons: total alkylbenzene sulfonate usage for these industrial applications is very minor - a very small percentage of the total pounds used in antimicrobials; commercial only use precludes broad environmental exposures that might occur with residential use; applications are mostly sprayed on and allowed to air dry; alkylbenzene sulfonate breakdown and degrade rapidly in the environment; alkylbenzene sulfonates are significantly reduced by sewage treatment; and industrial water treatment requires a NPDES permit in order to discharge effluents.

Ecological Risk Characterization.

Sodium dodecylbenzene sulfonate, and DDBSA are unlikely to bioaccumulate in the environment or aquatic animals and are expected to be soluble in water such that they will exhibit mobility through the soil. Available modeling and literature suggest that these chemicals will most likely biodegrade rapidly in soil due to microbial degradation. Minimal or no environmental exposure to terrestrial or aquatic organisms is expected to occur from the majority of alkylbenzene sulfonate antimicrobial indoor pesticide uses given that only a very small number of total DDBSA pounds are used for these purposes.

Linear alkyl benzene sulfonates (LAS) have been the principal ingredient in laundry detergent for 30+ years. Volume 12 (10) of the 1993 issue of Environmental Toxicology and Chemistry featured a series of papers on environmental impacts of LAS in a special symposium: Surfactants and Their Environmental Safety - convened by R.A. Kimerle, N.T. De Oude and T.W. La Point. Two papers provide excellent summaries of ecotoxicity endpoints from literature, and feature laboratory vs field analysis of detergent generated LAS impacts on aquatic organisms. An assessment of short and long-term impacts of LAS detergents on the environment was conducted. Increases and decreases in natural periphyton community abundance were observed, but determined to be insignificant for the three major species evaluated: *Amphora perpusilla, Navicula minima, and Schizothrix calcicola* (Lewis et al, 1993). Monitoring indicates that concentrations of 0.230 mg/L (continuous criterion concentration) and 0.625 mg/L (criterion maximum concentration) are rarely exceeded in aquatic systems protected by activated sludge treatment systems. Ecotoxicity studies indicate that a laboratory derived NOAEC value of 0.40 mg/L for LAS is protective of structure and function of experimental streams (Fairchild et al, 1993).

No environmental exposure is expected to occur from the majority of linear alkylbenzene sulfonate uses and it is unlikely that any appreciable exposure to terrestrial or aquatic organisms would occur from limited commercial down-the-drain use because of the very small number of pounds sold for these uses plus rapid degradation in the environment.

Endangered Species Considerations

Section 7 of the Endangered Species Act, 16 U.S.C. Section 1536(a)(2), requires all federal agencies to consult with the National Marine Fisheries Service (NMFS) for marine and andronomus listed species, or the United States Fish and Wildlife Services (FWS) for listed wildlife and freshwater organisms, if they are proposing an "action" that may affect listed species or their designated habitat. Each federal agency is required under the Act to insure that any action they authorize, fund, or carry out is not likely to jeopardize the continued existence of a listed species or result in the destruction or adverse modification of designated critical habitat. To jeopardize the continued existence of a listed species means "to engage in an action that reasonably would be expected, directly or indirectly, to reduce appreciably the likelihood of both the survival and recovery of a listed species in the wild by reducing the reproduction, numbers, or distribution of the species." 50 C.F.R. § 402.02.

To facilitate compliance with the requirements of the Endangered Species Act subsection (a)(2) the Environmental Protection Agency, Office of Pesticide Programs has established procedures to evaluate whether a proposed registration action may directly or indirectly reduce appreciably the likelihood of both the survival and recovery of a listed species in the wild by reducing the reproduction, numbers, or distribution of any listed species (U.S. EPA 2004). After the Agency's screening-level risk assessment is performed, if any of the Agency's Listed Species LOC Criteria are exceeded for either direct or indirect effects, a determination is made to identify if any listed or candidate species may co-occur in the area of the proposed pesticide use. If determined that listed or candidate species may be present in the proposed use areas, further biological assessment is undertaken. The extent to which listed species may be at risk then determines the need for the development of a more comprehensive consultation package as required by the Endangered Species Act.

For certain use categories, the Agency assumes there will be minimal environmental exposure, and only a minimal toxicity data set is required (Overview of the Ecological Risk Assessment Process in the Office of Pesticide Programs U.S. Environmental Protection Agency - Endangered and Threatened Species Effects Determinations, 1/23/04, Appendix A, Section IIB, pg.81). Chemicals in these categories therefore do not undergo a full screening-level risk assessment, and are considered to fall under a "no effects" determination. The active ingredient uses of alkylbenzene sulfonic acids and sulfonates fall into this category for the following reasons:

1. The amount that will actually reach the environment is very small based on usage data for down-the-drain uses.
2. Use for toilets and urinals is limited (no home-owner or residential uses are registered).
3. Breakdown of alkylbenzene sulfonate in the environment and via sewage treatment is rapid and well documented in the literature.

The labeled antimicrobial uses of alkylbenzene sulfonic acids and sulfonates are not expected to result in significant environmental exposure. Therefore, no adverse effects (NE) to listed species are anticipated. Use of alkylbenzene sulfonates as inert ingredients in agricultural pesticide formulations is not expected to result in significant environmental exposure. Therefore, no adverse effects (NE) to listed species are anticipated.

10.2 Inert Ingredient Use

The alkylbenzene sulfonates are used as "inert" ingredients in agricultural herbicide formulations. Preplant incorporated and preemergence herbicide treatments are typically applied once per year to the tilled, minimally tilled or no-tilled field before planting or before crop emergence in the spring. Spray applications are primarily via ground spray boom and occasionally by aircraft if a wet spring. Movement of the alkylbenzene sulfonates from the treated field to the aquatic environment can occur at the time of application due to spray drift, or following application via surface water/soil flow or by percolation to groundwater. The FIRST model has predicted a maximum potential concentration of 6.6 ppb alkylbenzene sulfonates in drinking water from inert agricultural uses (memo from K. Leifer, 2006). Available modeling and literature suggest that these chemicals will most likely biodegrade rapidly in soil due to microbial degradation.

The inert agricultural uses of alkylbenzene sulfonates are not expected to adversely affect avian or mammalian species on an acute or chronic basis. Aquatic organisms are also not expected to be adversely affected by inert alkylbenzene sulfonates use acutely or chronically due to the low predicted level of alkylbenzene sulfonates in water by FIRST. A chronic freshwater fish toxicity test NOAEC of 400 ug/L alkylbenzene sulfonates is considered protective of ecosystem structure and function in experimental streams. Therefore, the predicted concentration of 6.6 ug/L in water is well below our chronic Level of Concern (LOC).

11.0 DEFICIENCIES/DATA NEEDS

Hazard Data Gaps. The toxicology database for the alkylbenzene sulfonates consists almost entirely of published literature, is essentially complete and of acceptable quality to assess the potential hazard to humans. Due to limitations with the monkey inhalation study, which used 13% LAS, in addition to the presence of enzyme, the Agency requests a 90-day nose only rat inhalation study using DDBSA.

Ecological Data Gaps. There are no outstanding ecological data requirements

Label Hazard Statements for Terrestrial and Aquatic Organisms

Manufacturing and end-use products must state:

"Do not discharge effluent containing this product into lakes, streams, ponds, estuaries, oceans, or other waters unless in accordance with the requirements of a National Pollutant Discharge Elimination System (NPDES) permit and the permitting authorities are notified in writing prior to discharge. Do not discharge effluent containing this product to sewer systems without previously notifying the local sewage treatment plant authority. For guidance contact your State Water Board or Regional Office of the EPA."

Residential/Occupational Data Gaps. Confirmatory worker exposure data are necessary, due to the significant limitations of the existing exposure data used in this assessment. The Agency is requesting worker exposure studies that evaluate inhalation (Guideline 875.1400) exposure for indoor uses.

12.0 REFERENCES

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Appendix A
Toxicity Profile for Alkylbenzene Sulfonates

Table A-1 Toxicity Profile of Alkylbenzene Sulfonates			
Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
Subchronic Toxicity			
870.3100 Oral Subchronic (rodent)	Bornmann et al (1963) Study of a Detergent Based on Dodecylbenzene Sulfonate. Fette Seifen Anstrichm, 65 (10): 818-824. (EHC 169) **Open Literature**	0.01% of a preparation containing 51% LAS was administered in the drinking water for 100 weeks Rats (60/sex) Purity: Not Reported	No detrimental effects on body weight and no pathological effects, including tumors, were reported
870.3100 Oral Subchronic (rodent)	Ikawa et al., (1980)/ Ann. Rep. Tokyo Metrop. Res. Lab. Public Health. 29(2): 51-54(Z). 1978 (in Japanese, see WHO, 1996 and HERA, 2004). **Open Literature**	LAS was administered for 2, 4, or 12 weeks at a single dose of 1.5% in the diet (750 mg/kg/d). Male rats (five/group) Purity not reported.	LAS suppressed body weight gain and the relative liver weight was increased after two weeks. Serum biochemical alterations included: significant increases in ALP, GTP (at 2, 4, 12 weeks); significant decreases in cholesterol and protein (4 weeks); decreases in liver enzymes G6Pase and G6PDH and increases in isocitrate DH (all at 2, 4, 12 weeks). The following enzymes associated with kidney function were also altered: decreases in G6Pase, 5'nucleotidase (at 2, 4, 12 weeks) and Na,K-ATPase (12 wks); increase in LDH (12 wks) and IDH (2,4 wks).
870.3100 Oral Subchronic (rodent)	Ito, et al. (1978) Acute, Subacute, and Chronic Toxicity of Magnesium LAS (LAS-Mg). J. Med. Soc. Toho Univ. 25: 850-875. **Open Literature**	Administration by oral gavage at doses of 0, 155, 310, or 620 mg/kg/day (LAS-Mg) and 125, 250, and 500 mg/kg/day (LAS-Na) for one month Sprague-Dawley Rats (12/sex/group) Purity: 99.5%	LAS-Na: Body weight increase was suppressed; feed-efficacy was decreased, and liver weight increased at 500 mg/kg/day. NOAEL: 125 mg/kg bw/d.
870.3100 Oral Subchronic (rodent)	**MRID No. 43498412** Kay et al. (1965) Subacute Oral Toxicity of a Biodegradable, Linear Alkylbenzene Sulfonate. Toxicol Appl. Pharmacol. 7: 812-818 (HERA) **Acceptable** Guideline	SDDBS administered in the diet at dietary levels of 0, 200, 1000, and 5000 ppm for 90 days Weanling Sprague-Dawley Rat (10/sex/dose) Purity: 87.9% a.i.	NOEL: 5000 ppm (HDT) Two low dose males died early in the study from respiratory illness There was no compound-related effects in body weight, food consumption, hematology, urine analysis, organ weight, and histopathology.
870.3100 Oral Subchronic (rodent)	MRID No. 43511401 Mathur et al. (1986) Toxicological Evaluation of a Synthetic Detergent after Repeated Oral Ingestion in Rats. Industrial Toxicology Research Centre, Mahatma Ganghi Marg, Lucknow Study **No. DDBSA JV-RP-013.** Acceptable	LAS was administered as a commercial synthetic detergent solution at doses of 0, 50, 100, or 250 mg/kg/day in the feed for 10 weeks F Albino Rat (9/group) Purity: Not Reported	NOEL: < 50 mg/kg/d LOEL: 50 mg/kg/d based on alterations of several enzymes indicative of liver and kidney damage

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Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
870.3100 Oral Subchronic (rodent)	MRID No. 43498402 Oser et al. (1965) Toxicologic Studies with Branched and Linear Alkyl Benzene Sulfonates in the Rat. Toxicol. Appl. Pharmacol. 7: 819-825. (HERA) **Acceptable** Guideline	LAS and ABS were administered at dietary levels of 0, 50, or 250 mg/kg/day, adjusted for bw and fc, for 90 days FDRL Strain (Wistar-derived) Rat (15/sex/dose) Purity: Not Reported	NOEL: 50 mg/kg/d LEL: 250 mg/kg/d for increased absolute and relative liver weight in both sexes (21%) and increased relative cecal weight (21%) in males
870.3100 Oral Subchronic (rodent)	Watari et al. (1977) Ultrastructural Observations of the Protective Effect of Glycyrrhizin for Mouse Liver Injury Caused by Oral Administration of Detergent Ingredients (LAS), J. Clin. Electron. Microscopy (Nihon Rinsho Denshikenbikyo Kaishi) 10 (1-2): 121-139. **Open Literature**	Benzenesulfonic acid, C10-13- alkyl derivatives, sodium salt was administered in the drinking water for 6 months at 0 and 100 ppm with 2 months recovery (M: 0 and 17 mg/kg bw, F: 0 and 20 mg/kg bw) M/F ddy Mouse Purity: Not Reported	Liver effects were observed at the only dose tested (17-20 mg/kg/d), but they disappeared following the 2-month recovery period.
870.3100 Oral Subchronic (rodent)	Yoneyama & Hiraga (1977) Effect of Linear Alkylbenzene Sulfonate on Serum Lipid in Rats, J Ann Rep Tokyo Metrop Res Lab, Public Health 28(2): 109-111. (HERA) **Open Literature**	LAS was administered in the diet at concentrations of 180, 360, or 540 mg/kg bw/d for two and four weeks M Wistar Rat (5/group) Purity: 60% a.i.	Body weight gain was suppressed in the group receiving 540 mg/kg bw/d at four weeks, and the relative liver weight was increased at two weeks and thereafter in the groups receiving 360 mg/kg bw/d and 540 mg/kg bw/d. The levels of triglyceride and total lipids in the serum had decreased markedly at two weeks in all the experimental groups, and the levels of phospholipids and cholesterol in the serum had decreased significantly at two weeks in the groups given 360 and 540 mg/kg bw/d. These changes were less apparent at four weeks, but triglyceride, phospholipid, and cholesterol levels in serum were significantly decreased in the group given 540 mg/kg bw. Significant increases in triglyceride levels were seen in the liver after two weeks in the groups receiving 180 and 540 mg/kg bw/d, and in cholesterol levels in the group given 180 mg/kg bw.
870.3100 Oral Subchronic (rodent)	Yoneyama et al. (1978) Effects of LAS on Incorporation of Acetate-1-14C in Liver Lipids in Rats. J Ann Rep Tokyo Metrop Res Lab Public Health, 29 (2): 55-57. **Open Literature**	LAS was administered at a concentration of 200 mg/kg bw/d in the diet or in drinking water (560 mg/kg bw/d) for two weeks to determine the effect on the synthesis of lipids in the liver M Wistar Rat (5/group) Purity: Not Reported	Uptake of acetate-1-14C by lipids in the liver was increased in both groups; uptake of phospholipids and triglycerides tended to increase, and that of phospholipids increased significantly in rats given LAS in the diet.
870.3100 Oral Subchronic (rodent)	MRID No. 43498413 Heywood et al. (1978) Toxicology Studies of Linear Alkyl Sulphonate	LAS was given to four groups of three males and three females at doses of 30, 150, 300 mg/kg bw/day	At 300 (po) and 1.0 (sc) mg/kg bw/day, the monkeys vomited frequently and usually within 3 hours of administration. An increased frequency of loose or liquid faeces was recorded for animals receiving 150

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Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
	(LAS) in Rhesus Monkeys I. Simultaneous Oral and Subcutaneous Administration for 28 Days. Toxicol. Appl. Pharmacol. 11: 245-250. (HERA) Acceptable Guideline	per gavage (po) and simultaneously with 0.1, 0.5, or 1.0 mg/kg bw/day subcutaneously (sc). Control groups were used. Rhesus Monkey (3/sex/dose), 18-36 months old Purity: Not Reported	(po) and 0.5 (sc) mg/kg bw/day. These effects are probably related to the inherent irritative effects of LAS rather than to its systemic toxicity. Fibrosis of the injection sites was found among the entire test group, the incidence and severity being dose related. Ophthalmoscopy, laboratory examination of blood and urine, organ weight analysis and histopathological investigation did not detect any further treatment-related responses. The LOAEL is 150 mg/kg bw/day (po) + 0.5 mg/kg bw/day (sc) based on an increase in liquid feces and the NOAEL is 30 mg/kg/d
870.3200 21-Day Dermal	Mathur et al. (1992) Effect of Dermal Exposure to LAS Detergent and HCH Pesticide in Guinea Pigs: Biochemical and Histopathologic Changes in Liver and Kidney. J Toxicol Cutan Ocular Toxicol, 11(1): 3-13. (WHO 1996) **Open Literature**	A solution of LAS in distilled water equivalent to 60 mg/kg bw was applied to a 4-cm2 area of clipped dorsal skin daily for 30 days 12 Guinea Pigs Purity: Not Reported	The activities of B-glucuronidase, gamma- glutamyl transpeptidase, 5-nucleotidase, and sorbitol dehydrogenase were increased in liver and kidney. Lipid peroxidation was increased in the kidney but not in liver, and the glutathione content was unchanged in both organs. Extensive fatty changes were found in hepatic lobules, with dilation of sinusoids; tubular lesions were found in the kidney, predominantly in the proximal and distal portions.
870.3200 21-Day Dermal	Tox Record No. 003441 Subchronic (28-day) Percutaneous Toxicity (Rabbit) of Compound: B0002.01, (Bio/dynamics Inc., Project No. 4717-77, March 17, 1978, submitted by Procter and Gambel Company, May 10, 1978). **Unacceptable** Core-Minimum Data	SDDBS (end use product Comet Cleanser) was applied to the skin of rabbits for 28 days at 200 mg/kg/d. The hair of each rabbit was clipped from its trunk, so as to expose approximately 25% of the total body surface area and the skin was abraded daily just prior to treatment. 20 M/F Albino New Zealand White Rabbits (5/sex/group) Purity: 10%	NOEL: > 200 mg/kg/d
870.3465 90-Day Inhalation	MRID No. 43498403 Coate et al. (1978) Respiratory Toxicity of Enzyme Detergent Dust. Toxicol. Appl. Pharmacol., 45: **477-496.** Acceptable Guideline	SDDBS was administered a SDDBS mixture at levels of 0, 100(detergent), and [.001, .01, 0.1 and 1 (enzyme)] together with [+0, 1, 10, and 100 (detergent)] mg/m3 for 6 hours daily, 5 days a week, for 6 months 12 groups of 5 M/4 F Cynomolgus Monkeys Purity: 13%	NOEL: 1 mg/m3 detergent dust combined with up to 0.1 mg/m3 enzyme dust. The detergent dust alone at 100 mg/m^3 caused gross signs of respiratory distress, pulmonary histopathological effects, and pulmonary function impairment indicative of constricted bronchioles. Exposure to 10 or 100 mg/m^3 together with 0.01 and 0.1 mg/m^3 enzyme dust produced the same effects along with weight loss and decreased weight gain.
Developmental Toxicity			

Table A-1 Toxicity Profile of Alkylbenzene Sulfonates			
Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
870.3700a Developmental Toxicity (rodent)	Daly et al. (1980) A Teratology Study of Topically Applied LAS in Rats, Fd. Cosmet. Toxicol. 18: 55-58. (HERA) **Open Literature**	LAS was applied to the skin on days 0 through 21 of gestation at doses of 20, 100, and 400 mg/kg bw/d Rat Purity: Not Reported	NOAEL (maternal): 20 mg/kg bw/d NOAEL (fetuses): 400 mg/kg bw/d Maternal toxicity: the dams treated with 400 mg/kg bw/day and 100 mg/kg bw/day showed inhibition of body weight gain and llocal skin effects that compromised the integrity of the skin and caused overt toxicity, like inhibition of the body weight gain. Teratogenicity: there were no findings indicative of effects of LAS on the foetal parameters evaluated. There were no indications of teratogenic or embryotoxic effects.
870.3700a Developmental Toxicity (rodent)	Endo et al. (1980) Studies of the Chronic Toxicity and Teratogenicity of Synthetic Surfactants, Ann. Rep. Tokyo Metrop. Res. Inst. Environ. Prot. (Tokyo Kogai Kenkyujo Nempo), 236-246. (HERA) **Open Literature**	LAS was administered in the drinking water at 0.1%, corresponding to 383 mg/kg bw/d for rats and up to 3030 mg/kg bw/d for rabits from day 6 to 15 (rats) and day 6 to 18 (rabbits) of pregnancy. F Rat and Rabbit Purity: Not Reported	NOAEL (maternal): 383 mg/kg bw/d (rat) LOAEL (maternal): 3030 mg/kg bw/d (rabbit) NOAEL (fetuses): 383 mg/kg bw/d (rat) LOAEL (fetuses): 3030 mg/kg bw/d (rabbit) The effect on the dams was a slight inhibition of body weight gain in the rabbits. The litter parameters of both species did not show any significant differences from those of the controls. Delayed ossification was observed in rabbits, but there was no increase in malformations in either the rabbits or the rats.
870.3700a Developmental Toxicity (rodent)	Imahori et al. (1976) Effects of LAS Applied Dermally to Pregnant Mice on the Pregnant Mice and their Fetuses, J. Jpn. J. Public Health (Nihon Koshueisei Zasshi) 23(2): 68-72. (HERA) **Open Literature**	LAS was applied daily at dermal doses of 15, 150, and 1500 mg/kg bw/d on days 6 through day 15 of pregnancy F Mouse Purity: Not Reported	NOAEL (maternal): 150 mg/kg bw/d NOAEL (fetuses): 1500 mg/kg bw/d The 1500 mg/kg bw/day group showed a clear decrease in the pregnancy rate (67.9%) when compared with a rate of 96.3% in the controls. However, there were no decreases in the litter size, and no changes in the litter parameters with the exception of a slight decrease in foetal body weight. There were no significant increases in the incidence of malformations in the foetuses.
870.3700a Developmental Toxicity (rodent)	**MRID No. 43498423** Masuda et al. (1974) Effects of LAS Applied Dermally to Pregnant Mice on the Development of their Fetuses. 15: 349-355. **Acceptable** Guideline	LAS was applied dermally at a level of 0.5 ml. The ICR-JCL strain received doses of 0, 0.85, 1.7, 2.55, and 3.4% solutions daily from days 1 to 13 of gestation and the ddY strain received doses of 0, 0.017, 0.17, and 1.7% solutions daily from days 2 to 14 of gestation. Mouse (ICR-JCL strain and ddY strain) Purity: Not Reported	NOEL (maternal and developmental toxicity - ddY): 1.7% (HDT) NOEL (maternal toxicity - ICR-JCL): 2.55% NOEL (developmental toxicity - ICR-JCL): 1.7% At 3.4% LAS, maternal body weight and the absolute weight of liver, kidney, spleen were significantly increased over control.. Pregnancy rates were significantly less (33.35) compared to controls (69%). The number of implantations, live fetuses, sex ratio, dead or resorbed fetuses, placenta weight and external malformations were comparable with control. Fetal body weights of 2.55% and 3.4% LAS-treated groups were significantly less than controls.
870.3700a Developmental	MRID 43498424 and 43498425	LAS (0.1 ml) was applied at a concentration of 20%	Development was retarded and cleavage of eggs was interrupted. Significantly higher numbers of embryos

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Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
Toxicity (rodent)	Nomura, T et al. (1980) The Synthetic Surfactants AS and LAS Interrupt Pregnancy in Mice. Life Sciences, 26: 49-54. (HERA) Nomura, T. et al. (1987) Killing of Preimplantation Mouse Embryos by AS and LAS. Mutation Research 190: 25-29. (HERA) **Acceptable** Guideline	to the dorsal skin of pregnant mice during the pre-implantation period twice a day from day 0 to day 3 of pregnancy Female ICR/Jcl Mouse, 9-10 weeks old Purity: 20%	were found to be deformed in the LAS group in comparison to controls, and most of these embryos were in the morula stage, whereas they were mostly in the last blastocyst stage in controls. Some dead, deformed, and growth-retarded embryos were observed in the treated group. Although the authors stated that these effects were not due to maternal toxicity since no maternal organs were affected, this statement is probably not correct in view of the high concentration of LAS and its irritation effects. A secondary effect due to maternal toxicity appears much more likely.
870.3700a Developmental Toxicity (rodent)	**MRID 43498426** Palmer et al. (1975) Assessment of the Teratogenic Potential of Surfactants, (Part I), Toxicology 3: 91-106. **Acceptable** Guideline	LAS was administered by gavage on days 6-15 of pregnancy in rats and mice and days 6-18 of pregnancy in rabbits at doses of 0.2, 2, 300, and 600 mg/kg bw/d 20 CD Rats, 20 CD-1 Mice, and 13 New Zealand White Rabbits Purity: 17%	NOAEL (rat - maternal): 300 mg/kg bw/d NOAEL (mouse - maternal): 2.0 mg/kg bw/d (However, there is a large difference between this dose and the next highest dose of 300 mg/kg bw/d, this study does not allow determination of a reliable maternal NOAEL for mice) NOAEL (rabbit - maternal): 2.0 mg/kg b/d (However, the study does not allow determination of reliable NOAELs, given the large difference between the maternal no-effects doses of 2 mg/kg bw/d and the maternal LOAEL dose (300 mg/kg bw/d) that is also the dose for which effects on litters could not be determined due to the high mortality rate in parent animals) NOAEL (rat - developmental): 300 mg/kg bw/d NOAEL (mouse - developmental): 2.0 mg/kg bw/d NOAEL (rabbit - developmental): 2.0 mg/kg bw/d NOAEL (rat - fetal): 600 mg/kg bw/d NOAEL (mouse - fetal): 300 mg/kg bw/d (Due to a high mortality rate of parent animals, no assessment was possible at 600 mg/kg bw/d) NOAEL (rabbit - fetal): could not be determined
870.3700a Developmental Toxicity (rodent)	**MRID 43511403** Palmer, et al. (1975) Assessment of the Teratogenic Potential of Surfactants, (Part III) - Dermal Application of LAS and Soap. Huntingdon Research Centre, Huntingdon, Great Britain. Study No. DDBSA JV-RP4-029. Toxicology 4: 171-181. **Acceptable** Guideline	LAS was administered percutaneously to shaved skin at solutions of 0.03%, 0.3%, and 3% during pregnancy on days 2-13 in mice, 2-15 in rats, and 1-16 in rabbits. Dosages employed were 0.5 ml/rat or mouse/day and 10 ml/rabbit/day CD-1 Mice (20/group), CD Rats (20/group), N2W Rabbits (13/group) Purity: 0.03%, 0.3%, and 3%	LOEL (maternal toxicity, mice): 0.3% (50 mg/kg/d) LOEL (maternal toxicity, rats): 3.0% (60 mg/kg/d) LOEL (maternal toxicity, rabbits): 0.3% (9.0 mg/kg/d) NOEL (maternal toxicity, mice): 0.03% (5.0 mg/kg/d) NOEL (maternal toxicity, rats): 0.3% (6.0 mg/kg/d) NOEL (maternal toxicity, rabbits): 0.03% ((0.9 mg/kg/d) LOEL (developmental toxicity): 0.3% (50 mg/kg/d) LOEL (developmental toxicity): 3.0% (60 mg/kg/d) LOEL (developmental toxicity): 3.0% (90 mg/kg/d) NOEL (developmental toxicity): 0.03% (5.0 mg/kg/d) NOEL (developmental toxicity): 0.3% (6.0 mg/kg/d) NOEL (developmental toxicity): 0.3% (9.0 mg/kg/d) Marked local skin reaction, irritability, weight loss and failure to maintain or establish pregnancy was evident in mice treated with LAS 3% soap, 3 or 30%: marked local

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			reaction and weight loss also occurred in rabbits receiving LAS 3%. Moderate maternal toxicity was observed among mice treated with LAS, 0.3% and mild maternal toxicity in rats receiving LAS 3% or soap 30% and rabbits receiving LAS 0.3%. Effects on litter parameters were dose-dependent, causing marked maternal toxicity in mice, the principal higher fetal loss, reduction in viable litter size. LAS at 3% showed marked maternal toxicity in the rabbit The moderate maternal toxicity of LAS, 0.3% in the mouse correlated with a higher incidence of embryonic deaths and lower litter size but only the former differed significantly from the corresponding control value.
870.3700a Developmental Toxicity (rodent)	Sato et al. (1972) Studies on the Toxicity of Synthetic Detergents: (III), Examination of Teratogenic Effects of Alkylbenzene Sulfonates Spread on the Skin of Mice. Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 24: 441-448. (HERA) **Open Literature**	LAS was applied to the skin of female mice daily on days 0 through 13 of pregnancy with a single LAS dose of 110 mg/kg bw/d. Control group not specified. F Mouse Purity: Not Reported	NOAEL (maternal): 110 mg/kg bw/d No abnormalities were seen in the dam or foetuses.
870.3700a Developmental Toxicity (rodent)	Shiobara S., Imahori A. (1976) Effects of LAS Orally Administered to Pregnant Mice on the Pregnant Mice and their Fetuses. J.Food Hyg. Soc. Jpn. (Shokuhin Eiseigaku Zasshi) 17(4): 295-301. **Open Literature**	LAS was administered by gavage at doses of 10, 100, and 300 mg/kg bw/d at day 6 through 15 of gestation ICR-SLC Mouse (25-33/dose) Purity: Not Reported	LOAEL (maternal): 10 mg/kg bw/d NOAEL (fetuses): 300 mg/kg bw/d 1. Marked maternal and embryonic toxicities, such as maternal death, premature delivery, total litter loss and high fetal death rate, were observed at 300 mg/kg group. 2. Slight suppression of maternal body weight gain and slight body weight suppression of live fetuses were observed in each treated group. 3. External malformations such as cleft palate and exencephaly were observed sporadically both in the control and the treated groups. However, the incidence of these malformations was not significant, and considered to be within the spontaneous incidence of ICR mice.
870.3700a Developmental Toxicity (rodent)	Takahashi et al. (1975) Teratogenicity of Some Synthetic Detergent and LAS. Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 26(2): 67-78. (HERA) **Open Literature**	LAS doses of 40, and 400 mg/kg bw/d were administered daily from day 0 to day 6 of pregnancy or from day 7 to 13 of pregnancy by gavage Mouse (13-14/group) Purity: not reported	NOAEL (maternal): 40 mg/kg bw/d NOAEL (fetuses): 400 mg/kg bw/d At 400 mg/kg bw/day, the pregnancy rate was 46.2% compared to 92.9% in the controls. There was no increase in malformations. Although no information on maternal toxicity is available, it appears likely that maternal toxicity was present at the high dose group.
870.3700a Developmental Toxicity	Tiba et al. (1976) Effects of LAS on Dam, Fetus, and Newborn Rat. J. Food Hyg. Soc. Jpn.	LAS was administered in the diet at doses of 80 and 780 mg/kg bw/d from day 0	NOAEL (maternal): 780 mg/kg bw/d NOAEL (fetuses): 780 mg/kg bw/d At 780 mg/kg bw/day there were no abnormalities in the body weight gains of the dams, or in the occurrence and

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(rodent)	(Shokuhin Eiseigaku Zassh) 17(1): 66-71. (HERA) **Open Literature**	to 20 of gestation F Rat (16/dose) Purity: Not Reported	maintenance of pregnancy. The values of the litter parameters did not differ from those of the controls and there was no evidence of teratogenicity. The number of offsprings was rather low in the highest dose group, and the weaning rate of 78.3% was lower than the 100% rate observed in the controls. However, there were no abnormalities in body weight gain, organ weights or functions in the offsprings.
Reproduction Toxicity			
870.3800 Reproduction	**MRID 43498416** Buehler, E., Newmann, E., and King, W. (1971) Two Year Feeding and Reproduction Study in Rats with Linear Alkylbenzene Sulfonate (LAS). Tox. Appl. Pharm. 18: 83-91. (HERA) **Acceptable** Guideline	LAS was administered in the diet at doses of 0, 0.02, 0.1, and 0.5% , equivalent to (0, 10, 50, 250 mg/kg bw/day) for 84 days. Weanling Charles River CD Rat (20/sex/dose) Purity: 98.1%	NOAEL Parental: 250 mg/kg bw/day NOAEL Offspring: 50 mg/kg/d. The LOAEL of 250 mg/kg/day in the offspring is due to slight (non-significant) changes in hematology and histopathology and slight decrease in day 21 body weights.
870.3800 Reproduction	Endo et al. (1980) Studies of the Chronic Toxicity and Teratogenicity of Synthetic Surfactants, Ann. Rep. Tokyo Metrop. Res. Inst. Environ. Prot. (Tokyo Kogai Kenkyujo Nempo), 236-246. (HERA) **Open Literature**	LAS was administered at 70 mg/kg bw/day in the drinking water in a four generation rat study. M/F Wistar Rat Purity: Not Reported	NOAEL: > 70 mg/kg (only dose tested) No effects of LAS administration were observed
870.3800 Reproduction	Palmer et al. (1974) Effect of CLD Reproductive Function of Multiple Generations in the Rat, Report LFO10/731029, Unpublished results. (HERA) **Open Literature**	A commercial light duty liquid detergent of LAS (17%) and alkyl ethoxylate sulphate (7%) was continuously administered in the diet for three generations 60 days prior to mating at concentrations of 0, 40, 200, and 1000 mg/kg bw/d. The corresonding administration of LAS was of 0, 6.8, 34, and 170 mg/kg bw/d. Rat Purity: 17%	NOAEL: 170 mg/kg bw/d Among parental animals over the three generations there were no signs of adverse effects of treatment. Food consumption and bodyweight changes showed no consistent relationship to dosage. Necroscopy revealed no changes due to treatment. The mating performance, the pregnancy rate and the duration of gestation were unaffected. Among litter parameters, organ weight analysis, histopathology and skeletal staining of representative young from the F3b generation revealed no changes that could be conclusively related to treatment.
Chronic Toxicity			
870.4100a Chronic Toxicity	Taniguchi et al. (1978) Results of Studies on Synthetic Detergents.	LAS were applied to the dorsal skin of rats three times per week at doses of	Treatment had no effect on organ weights or histopathological appearance, and there was no evidence of toxicity or carcinogenicity.

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Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
(rodent)	Tokyo, Science and Technology Agency, Research and Coordination Bureau, pp. 18-54. (WHO 1996) **Open Literature**	1, 5, or 25 mg/rat for 24 months. Each application was washed from the skin with warm water after 24 hours. SLC-Wistar Rats Purity: 19.7% a.i.	
870.3100 Chronic Toxicity (rodent)	Yoneyama et al. (1976) Subacute Toxicity of LAS, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health27(2): 105-112, See: IPCS, 1996. (HERA) **Open Literature**	LAS was administered in the diet at concentrations of 500 and 1000 mg/kg bw/d and in drinking water at concentrations of 100, 250, 600 mg/kg bw/d for males and 100, 250, 900 mg/kg bw/d for females for 9 months Mouse (8 or 9/sex/dose) Purity: Not Reported	LOAEL: 500 mg/kg bw/d (in diet) NOAEL: 250 mg/kg bw/d (in water) LAS in diet: in the mice given 500 mg/kg bw/day, body weight gain was not suppressed, but the weight of the liver increased in male and female mice. Enzymatic examinations revealed significant decreases in LDH of the liver and in acid phosphatase of the kidneys in the male mice. LAS in drinking water: body weight was depressed at the highest dose for male and females, increase in liver weight in females, significant decreases in renal Na,K-ATPase.
870.3100 Chronic Toxicity (rodent)	Yoneyama et al. (1976) Subacute Toxicity of LAS, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health27(2): 105-112, See: IPCS, 1996. (HERA) **Open Literature**	LAS was administered for 9 months in the drinking water at doses of 85, 145, 430 mg/kg bw/day M/F Wistar Rat Purity: Not Reported	NOAEL: 85 mg/kg bw/d LOAEL: 145 mg/kg bw/d Haematological examination revealed no significant changes in any experimental group and no organ weight changes were observed. Body weight gain was suppressed in the males of the highest dose group and also serum-biochemical and enzymatic parameters of the liver and kidney were affected. A significant decrease in renal Na,K-ATPase was seen in the group given 145 mg/kg bw/day of LAS.
870.4100a Chronic Toxicity (rodent)	Yoneyama et al. (1972) Studies on the Toxicity of Synthetic Detergents. (II) Subacute Toxicity of Linear and Branched Alkyl Benzene Sulfonates in Rats. Ann Rep Tokyo Metrop Res Lab Public Health, 24: 409-440. **Open Literature**	Technical-grade LAS was administered in the feed for 6 months at a concentration of 0, 0.07, 0.2, 0.6, or 1.8% Wistar SLC Strain Rat (10/sex/dose) Purity: Not Reported	NOAEL: 0.07% (40 mg/kg bw/day) At 1.8%, diarrhea, decrease in body weight gain and tissue damage in caecum liver and kidney were observed. The damage to the kidney was especially remarkable. At 0.6% of the LAS or ABS, the adverse effects observed were a slight decrease of body weight, increase of ceacum weight, increased activity of alkaline phosphatase, decrease of total protein in blood, and the tissue damage in the kidney. At 0.2% of the LAS or ABS, an increase of caecum weight and a slight damage to the kidney were observed.
Carcinogenicity			
870.4200a Oncogenicity (Rat)	**MRID 43498416** Buehler, E., Newmann, E., and King, W. (1971) Two Year Feeding and Reproduction Study in Rats with Linear Alkylbenzene Sulfonate (LAS). Tox. Appl. Pharm. 18: 83-91.	LAS was administered in the diet at doses of 10, 50, and 250 mg/kg/day for 2 years Weanling Charles River CD Rats (50/sex/group) Purity: Not Reported	Negative at 250 mg/kg/day (HDT)

Table A-1 Toxicity Profile of Alkylbenzene Sulfonates			
Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
	(HERA) **Acceptable** Guideline		
870.4200a Oncogenicity (Rat)	Endo et al. (1980) Studies of the Chronic Toxicity and Teratogenicity of Synthetic Surfactants, Ann. Rep. Tokyo Metrop. Res. Inst. Environ. Prot. (Tokyo Kogai Kenkyujo Nempo), 236-246. (HERA) **Open Literature**	LAS was administered in the drinking water at the dose of 200 mg/kg bw/d 62 M/F Wistar Rat Purity: 38.74% a.i.	The administration of LAS had no effect on the intake of water, mortality, body weight gain, or general condition. In pathological examinations, looseness, atrophy, and fatty change of the hepatic cells in the liver were found in the experimental control group at 6 months, together with significant increases in GOT, GTP and bilirubin. In hematological examinations no effects due to LAS were observed.
870.4200a Oncogenicity (Rat)	Fujii et al. (1977) Pathological Examination of Rats Fed with LAS for their Lifespan, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 28(2): 85-108. (HERA) Yoneyama et al. (1977) Toxicity of LAS by Dietary Administration for Life-Span to Rats, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 28(2): 73-84. (HERA) **Open Literature**	LAS was administered in the feed at a concentration of 0.04, 0.16, and 0.60% for 24 months or lifespan Wistar Weanling Rat (15/sex/dose) Purity: Not Reported	Histopathological examination revealed that there was no evidence of a treatment-related effect on any tissue examined. Whereas a variety of tumors were observed in both linear alkylbenzene sulfonate treated and control rats, none was attributed for the exposure to linear alkylbenzene sulfonate. There was no relationship among the dosage groups, sex, type of tumor, or the site of occurrence.
870.4200a Oncogenicity (Rat)	**MRID 43498420** Takahasi et al. (1969) Effect of Alkylbenzenesulfonate as a Vehicle for 4-Nitroquinoline-1-Oxide on Gastric Carcinogenesis in Rats. GANN: 8, 241-261. **Acceptable** Guideline	For 560 days; Group I (79 rats): 1 mg 4-NQO and 80 mg SDDBS 2-3x per week for 18 weeks; Group I' (17 rats): same as Group 1, but fasted for 12 hours prior to dosing,; Group II (37 rats): 1 mg 4-NQO only; Group III (28 rats): 80 mg SDDBS only 97 M Wistar Rats Purity: Not Reported	In Groups I and I', the presence of SDDBS shifts the incidence of benign papillomas to malignant papillomas of the forestomach and the incidence of adenocarcinoma and sarcoma of the stomach were increased in comparison to Group II with only 4-NQO. The administration of SDDBS by itself has no effect on gastric tumors (Group III). The study authors concluded that the increased carcinogenicity produced by SDDBS was due to the better uptake of 4-NQO via LAS's surfactive/detersive effects on the protective mucous barrier which is normally found in the glandular stomach and other gastric compartments of the rat. The effect of SDDBS was physical rather than chemical in promoting the increased tumorigenicity.
870.4200a Oncogenicity (Rat)	**MRID 43498419** Takahasi et al. (1970) Effect of 4-Nitroquinoline-1-Oxide with Alkylbenzenesulfonate on Gastric Carcinogenesis in Rats. GANN: 61, 27-33. **Acceptable**	Rats were divided into three groups and gavaged with the following regimen for 560 days: Group I (37 rats) - 1 mg 4-NQO + 80 mg SDDBS + 20 mg ethanol in a 1 ml gavage for 18 weeks; Group II (13 rats) - 4-NQO and ethanol for 18 weeks; Group III (13 rats) - SDDBS + ethanol for	Survival: Mortality was 59% in Group I, 31% in Group II, and 23% in Group III Tumors: Group III - no gastric tumors; Group II - 9 benign papillomas of forestomach; Group I - 8 benign papillomas of forestomach, 2 malignant papillomas of forestomach, 1 hemangiosarcoma of forestomach. In glandular stomach, 2 adenocarcinomas, 1 hemangiosarcoma, 1 hemangioma, 5 squamous cell carcinomas, and 2 rats exhibited atrophic gastritis.

Table A-1 Toxicity Profile of Alkylbenzene Sulfonates			
Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
	Guideline	18 weeks 64 M Motoyama Strain Rat Purity: Not Reported	The increased toxicity in Group I produced increased mortality and increased numbers of malignant tumors. The role of SDDBS in the tumorigenesis of 4-NQO was to promote increased absorption of 4-NQO through the forestomach and glandular stomach.
870.4200a Oncogenicity (Rat)	**MRID 43498421, -22** Takahasi et al. (1973) Carcinogenic Effect of N-Methyl-N'-Nitro-N-N itrosoguanidine with Various Kinds of Surfactant in the Glandular Stomach of Rats. **Acceptable** Guideline	SDDBS was administered to 5 groups of rats: (I) 13 rats received 0.1g of MNNG + 4000 mg Tween 60 per L of drinking water for 36 weeks; (II) 16 rats received 0.1 g MNNG + 2000 mg nonipol per L of drinking water for 36 weeks; (III) 15 rats received 0.1 g of MNNG + 1000 mg branched ("hard") SDDBS per L of drinking water for 63 weeks; (IV) 10 rats received 0.1 g MNNG + 1000 mg of linear ("soft") SDDBS per L of drinking water for 63 weeks; (V) 14 rats received o.1 g MNNG per L of drinking water for 63 weeks M Wistar Rats Purity: Not Reported	Survivial was 100% in Groups I, III, and IV, and 93% and 94% in Groups V and II, respectively. The Group I and II rats had more tumors than the controls (Group V), whereas, the rats in Group III, ("hard" SDDBS, and particularly, Group IV (linear "soft" SDDBS) had the fewest tumors in comparison to controls.
870.4200a Oncogenicity (Rat)	Tiba S (1972) Studies on the Acute and Chronic Toxicity of LAS, J. Food Hyg. Soc. Jpn. (Shokuhin Eiseigaku Zasshi) 13(6): 509-516. (HERA) **Open Literature**	LAS was administered in drinking water for 2 years at doses of 20, 100, and 200 mg/kg bw/d M Wistar Rat (20/group) Purity: Not Reported	There were no changes due to the administration of LAS in regard to growth, mortality, the weight of major organs, or histopathological findings
Mutagenicity			
870.5100 Bacterial reverse mutation test	Huls, Report No. AM-93/12, Unpublished data, 1993. (As cited in HERA-2004) **Open Literature**	LAS was tested at 8-5000 ug/plate with and without metabolic activation. The cytotoxicity concentration was >5000 ug/plate. Salmonella typhimurium, strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538 Purity: Not Reported	Negative results
870.5100 Bacterial reverse mutation test	**MRID 43498429** Inoue et al. (1980) Studies of In Vitro Cell Transformation and Mutagenicity by Surfactants and other Compounds, Food.	SDDBS was tested at cytotoxic levels or limit concentrations of 2,000-30,000 ug/plate for 2 days (Salmonella) or 8 days (SHE)	Negative (both with and without S-9 metabolic activation)

Table A-1 Toxicity Profile of Alkylbenzene Sulfonates			
Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
	Cosmet. Toxicol 18: 289-296. (HERA) **Acceptable** Guideline	Strain: Salmonella typhimurium - TA 98 and TA 100 cells and Embryonic Syrian Golden Hamster cells (SHE) Purity: Not Reported	
870.5100 Bacterial reverse mutation test	Sunakawa et al. (1981) Studies on the Mutagenicity of Surfactants Following Activation with Various Liver Homogenates (S-9) and Mutagenicity in the Presence of Norharman, Hyg. Chem. (Eisei Kagaku) 27(4): 204-211, See: WHO, 1996. **Open Literature**	LAS was tested at up to 500 ug/plate Salmonella typhimurium Purity: Not Reported	Negative Results
870.5300 In Vitro mammalian cell gene mutation test	Inoue, K. et al. (1977) Osaka-furitsu Koshu Eisei Kenkyusho Kenkyu Hokoku, Shokuhin Eisei Hen 8: 25-8. (HERA) **Open Literature**	Sodium alkylbenzenesulfonate was added to culture at 62.5 ug/ml and 125 ug/l Hamster Lung Cell Purity: Not Reported	At 62.5 ug/ml: induced cell mutation, no effect on sister chromatid exchange At 125 ug/ml: destroyed the cells completely
870.5300 In Vitro cell transformation	***MRID No. 43498427*** K. Inoue et al (1980) Food Cosmetic Toxicol. 18:289-296 *Acceptable* **Open Literature**	Duplicate primary cultures of embryonic SHE and Salmonella typhimurium strain TA 98 and TA 100 cells were exposed to SDDBS and positive and negative controls for 8 days.	SDDBS was negative for transformation up to cytotoxic levels and did not induce mutation in either strains of Salmonalla when allplied up to cytotoxic levels or limit concentration of 2000-3000 ug/plate. SDDBS was tested negative at cytotoxic levels or limit concentrations (both with and without S-9 metabolic activation) of 2,000-30,000 ug/plate for 2 days (Salmonella) or 8 days (SHE)
870.5385 Mammalian bone marrow chomosomal aberration test	Inoue K, et al. (1979) In vivo Cytogenetic Tests of Some Synthetic Detergents in Mice, Ann. Rep. Osaka Perfect. Inst. Public Health 8: 17-24 (in Japanese), See: IPCS, 1996. (HERA) **Open Literature**	LAS was administered at doses of 200, 400, and 800 mg/kg bw/d by gavage for 1 and 5 days M Mouse Purity: Not Reported	There was no significant difference in the incidence of chromosomal aberrations between any of the groups
870.5385 Mammalian bone marrow chomosomal aberration test	Inoue, K. et al. (1977) In Vivo Cytogenetic Tests of Some Synthetic Detergents in Mice. Ann Rep Osaka Prefect Inst Public Health, 8: 17-24. (HERA) **Open Literature**	LAS was administered at a dose of 200, 400, and 800 mg/kg bw/d by gavage for 5 days. One commercial preparation containing 19.0% LAS was also given, at a dose of 800, 1600, or 3200 mg/kg bw, and another containing 17.1% LAS at a dose of 1000, 2000, or 4000 mg/kg bw once only by gavage.	There was no significant difference between any of the groups given LAS and the negative control group in the incidence of chromosomal aberrations

Table A-1 Toxicity Profile of Alkylbenzene Sulfonates			
Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
		M ICR:JCL Mouse Purity: Not Reported	
870.5385 Mammalian bone marrow chomosomal aberration test	**MRID 43498428** J. Hope (1977) Absence of Chromosome Damage in the Bone Marrow of Rats Fed Detergent Actives for 90 Days. Mutation Research, 56: 47-50. **Acceptable** Guideline	SDDBS was administered in the diet for 90 days at 0, 280, and 565 mg/kg bw/d Colworth/Wistar Weanling Rat (6/sex/dose) Purity: Not Reported	All test preparations were negative for increased chromosomal damage over controls.
870.5385 Mammalian bone marrow chomosomal aberration test	Masabuchi et al. (1976) Cytogenetic Studies and Dominant Lethal Tests with Long Term Administration of Butylated Hydroxytoluene (BHT) and LAS in Mice and Rats, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 27(2): 100-104. (HERA) **Open Literature**	LAS was administered in the diet for 9 months at a dose of 0.9% in rats (450 mg/kg bw/d) and in mice (1170 mg/kg bw/d) Male Rat and Male Mouse Purity: Not Reported	There were no significant differences in the incidences of chromosomal aberrations between the experimental and control groups
870.5395 Mammalian erthrocyte micronucleus test	Kishi et al. (1984) Effects of Surfactants on Bone Marrow Cells, Bull. Kanagawa Public Health Lab. 14: 57-58. (HERA) **Open Literature**	LAS was administered as a single intraperitoneal injection at a dose of 100 mg/kg bw 3 M ddY Mice Purity: Not Reported	There were no differences in the incidences of polychromatic erythrocytes with micronuclei in the bone marrow cells between the treated group and the control group
870.5395 Mammalian erthrocyte micronucleus test	Koizumi et al. (1985) Implantation Disturbance Studies with LAS in Mice, Arch. Environ. Contam. Toxicol. 14: 73-81. (HERA) **Open Literature**	LAS were administered as a single oral dose of 2 mg to pregnant mice on day 3 of gestation. On day 17 of gestation, each animal received a subcutaneous dose of 1, 2, or 10 mg and were killed 24 h later. Pregnant ICR Mice Purity: Not Reported	There was no difference among treated groups in the incidence of polychromatic erythrocytes with micronuclei in maternal bone marrow or fetal liver or blood. No mutagenetic effect was found in any of the groups.
870.5450 Rodent dominant lethal assay	Masubuchi MA et al. (1976) Cytogenetic Studies and Dominant Lethal Tests with Long Term Administration of Butylated Hydroxytoluene (BHT) and Linear	A diet containing 0.6% LAS at 300 mg/kg bw/d was administered to mice for 9 months. Each of the male mice was then mated with two female mice that had not been given LAS, and 11 of the 14 females	There were no significant differences in fertility, mortality of ova and embryos, the number of surviving fetuses, or the index of dominant lethal induction (Roehrborn) between the experimental and control groups.

Table A-1 Toxicity Profile of Alkylbenzene Sulfonates			
Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
	Alkylbenzene Sulfonate (LAS) in Mice and Rats. Ann Rep Tokyo Metrop Res Lab Public Heath, 27(2): 100-104. (HERA) **Open Literature**	became pregnant. The pregnant mice were laparotomized on day 13 of gestation 7 M ICR:JCL Mice Purity: Not Reported	
Metabolism			
870.7485 General Metabolism	**MRID 43498410** Creswell et al. (1978) Toxicology Studies of Linear Alkylbenzene Sulphonate (LAS) in Rhesus Monkeys II. The Disposition of C14-LAS After Oral or Subcutaneous Administration. Toxicology, 11: 5-17. **Acceptable** Guideline	Single oral doses of C14-LAS (SDDBS; 25 ucuries) were administered to each animal, following 2-3 weeks between dose levels, at levels of 30, 150, and 300 mg/kg. Following 2-3 weeks after the last single oral dose, each monkey received 7 consecutive daily oral doses of 30 mg/kg/d of C14-LAS. 2 M/2 F Rhesus Monkeys Purity: Not Reported	After single 30 mg/kg doses the radioactivity was rapidly excreted, mostly during the first 24 hours. Feces and urine contained 23.1% and 71.2%, respectively, in the first 5 days after oral dosing. Plasma concentrations were comparable after the oral doses and averaged 34, 41, and 36 u/ml, respectively. Peak plasma concentrations increased proportional to the dose and were 0.16, 0.72, 1.13 u/ml, respectively. In urine samples analyzed for metabolites, there was no unchanged SDDBS and the 5 metabolites detected were polar, but were not sulphate or glucuronide conjugates.
870.7485 General Metabolism	Lay JP, et al. (1983) Toxicol. Letters 17 (1-2): 187-192 **Open Literature**	(14)C-labeled sodium dodecylbenzenesulfonate was administered daily in the diet at a concentration of 1.4 mg/kg for 5 weeks M Rat Purity: not reported	From a total uptake of 1.213 + or - 0.08 mg/animal of DBS, 81.8% was excreted during the dosing period: 52.4% in feces and 29.4% in urine. Low levels of (14)C-DBS-derived residues were detected in all tissues analyzed on day 35 of the study. Following 1 week on a normal diet, only 7.8% of the nominally stored amount of (14)C was found in the excreta.
870.7485 General Metabolism	Sunakawa et al. (1979) Yakuzaigaku 39 (2): 59-68 **Open Literature**	Sodium-para-dodecylbenzenesulfonate Rat Purity: Not Reported	Blood levels were max at 2 hr, negligible at 48 hr Excretion rate of radioactive label was 99.4% after 48 hr
870.7485 General Metabolism	The Royal Society of Chemistry. (1981) Foreign Compound Metabolism in Mammals. Volume 6: A Review of the Literature Published during 1978 and 1979. London: The Royal Society of Chemistry, p.354. **Open Literature**	(35)S-labeled sodium dodecylbenzenesulfonate was administered as a single oral dose Rat Purity: Not Reported	Rats excreted 64% and 24% of the dose in urine and feces, respectively
870.7485 General Metabolism	The Royal Society of Chemistry. (1981) Foreign Compound Metabolism in Mammals. Volume 6: A	Repeated doses of (14)C-labeled alkylbenzenesulfonate were orally administered	Radioactivity did not accumulate in the tissues

Table A-1 Toxicity Profile of Alkylbenzene Sulfonates			
Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
	Review of the Literature Published during 1978 and 1979. London: The Royal Society of Chemistry, p.354.	Rhesus Monkey Purity: Not Reported	
870.7485 General Metabolism	**MRID 43498431** W. Michael (1968) Metabolism of Linear Alkylate Sulfonate and Alkyl Benzene Sulfonate. Toxicol. Appl. Pharmacol. 12: 473-485. **Acceptable** Guideline	LAS-S35 was administered orally to fasted rats at doses of 0.6, 1.2, 8, and 40 mg Charles River CD M Rat Purity: Not Reported	The rate and distribution of the excreted dose was independent of concentration. Similar levels of radioactivity were found in urine and feces and within 3 days, 85.2% - 96.6% of the label was recovered. In the high dose rats, no detectable radioactivity was found in the carcasses after 3 days. Following methylation, one urinary metabolite was identified as 4-(4'-methylsulfophenyl) pentanoate. LAS-S35 in the feces remained unmetabolized.
Special Studies			
870.3700a Developmental Toxicity (rodent)	Koizumi et al. (1985) Implantation Disturbance Studies with LAS in Mice, Arch. Environ. Contam. Toxicol. 14: 73-81. (HERA) **Open Literature**	LAS was administered as a single oral dose of 350 mg/kg bw on day 3 of gestation Pregnant ICR Mice Purity: Not Reported	LAS was not detected in the uterus
Other	Inoue K, T Sunakawa. (1979) Mutagenicity Tests of Surfactants, Jpn. Fragr. J. 38: 67-75, (in Japanese), See: IPCS, 1996. (HERA) **Open Literature**	LAS tested in a recombination assay at concentrations up to 50 ug/plate Bacillus subtilis Purity: 99.5%	Negative results with and without metabolic activation
Other	Fujise, H. and Aoyama, M. (1984) Nagoya Med J, 28 (3-4): 211-5 **Open Literature**	The proliferation rate of the connective tissue was examined by measuring the activity of proline hydroxylase. The dorsal neck skin of rats was coated with sodium laurylbenzenesulfonate for 4 days, and on the 5th day, the enzyme activity in the skin was measured. Rat Purity: Not Reported	The proline hydroxylase in the part of the skin coated with the irritants showed clearly higher activity than normal skin, although it was still lower than the injured skin region prepared as a positive control.
Other	**MRID 43498430 and 43498408** Kimura et al. (1982) Mechanisms of Toxicities of Some Detergents Added to a Diet and the	Ringer's bicarbonate (containing sodium lauryl benzene sulfonate) at 0.5 ml/min was used to perfuse a 10 cm length of jejunal segment for 150 minutes; equilibrated for 30 minutes and then the perfusates	Alkaline phosphatase was released by an increase of 15-fold in comparison to Ringer's alone (controls without added sodium lauryl benzene sulfonate) and 3-7 times greater than other surfactants tested in Ringer's. The authors conclude that SDDBS has an exfoliative effect on the intestinal brush border

Table A-1 Toxicity Profile of Alkylbenzene Sulfonates			
Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
	Ameliorating Effects of Dietary Fiber in the Rat. J. Nutrit. Science and Science and Vitaminology, 28: 483-489. Kimura et al. (1982) Toxicity for Detergent Feeding and Effect of the Concurrent Feeding of Dietary Fiber in the Rat. Nutrition Reports International, 26(2): 271-279. **Acceptable** Guideline	were collected in 30 minute aliqouts for 120 minutes M Wistar Rat Purity: 0.5%	
Other	Oba et al. (1968) Biochemical Studies of n-alpha-olefin sulfonates: (II) Acute Toxicity, Skin and Eye Irritation, and Some Other Physiological Properties. J Jpn Oil Chem Soc, 17 (11): 628-634. (EHC 169) **Open Literature**	Solutions of various concentrations of LAS were mixed with red blood cells from rabbits at room temperature for 3 hours Rabbit Red Blood Cell Purity: Not Reported	The 50% haemolytic concentration of LAS was 9 mg/litre
Other	Samejima Y (1991) Effects of Synthetic Surfactants and Natural Soap on the Development of Mouse Embryos In Vitro and the Fertilizing Capacity of Mouse and Human Sperm. J Osaka Univ Med Sch, 3 (12): 675-682. (EHC 169) **Open Literature**	Eggs were fertilized in vitro and incubated in culture medium containing LAS at concentrations between 0.015 and 0.03%. F B6C3F1 Mouse Egg Purity: Not Reported	Concentrations of LAS less than 0.025%: Eggs exposed for 1 hr, washed, and then cultured for 5 days developed normally to the blastocyst stage Concentrations of LAS higher than 0.03%: The eggs did not develop beyond the one-cell stage With continuous exposure to LAS for five days, a concentration of 0.01% slightly impaired development to the blastocyst stage, and 0.025% prevented development to the one-cell stage
Other	Takahashi et al. (1974) Inhibition of Thrombin by Linear Alkylbenzene Sulfonate (LAS). Ann Rep Tokyo Metrop Res Lab Public Health, 25: 637-645. (HERA) **Open Literature**	Purified LAS at various concentrations were added to 10 ul of plasma from rats and prothrombin time was determined M Rat Purity: Not Reported	Prothrombin time was prolonged; the 50% inhibitory concentration was about 0.6 mmol/litre. When LAS at various concentrations were added to a mixture of 1% fibrinogen and thrombin, the time of formation of a mass of fibrin was prolonged by inhibition of thrombin activity. The 50% inhibitory concentration was about 0.05 mmol/litre.
Other	Yanagisawa et al. (1964) Biochemical Studies of Dodecylbenzene Sulfonates; Differences Between Soft and Hard Detergents. Jpn. J Public Health, 11(13):	The haemolytic action of LAS was investigated by mixing red blood cells from rabbits with solutions of LAS at concentrations of 1-1000 mg/litre at 38 C for 30 min	Haemolysis occurred at concentrations >= 5 mg/litre.

Table A-1 Toxicity Profile of Alkylbenzene Sulfonates			
Guideline No./ Study Type	**MRID No./ Reference Information/ Study Classification**	**Dosing and Animal Information**	**Results**
	859-864. (EHC 169) **Open Literature**	Rabbit Red Blood Cell Purity: Not Reported	

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

WASHINGTON, D.C. 20460

OFFICE OF
PREVENTION, PESTICIDES
AND TOXIC SUBSTANCES

TXR No. 0054267

Date: July 6, 2006

MEMORANDUM

SUBJECT: **Alkylbenzene Sulfonates (ABS) Toxicology Chapter** for the Reregistration Eligibility Decision (RED) Document. PC Code: 079010, 190116 and 098002. Case No. 4006. DP Barcode: D330328.

FROM: Ayaad Assaad, D.V.M., PhD. Toxicologist
And
William Dykstra, PhD., Toxicologist
Health Effects Division (HED) (7509C)

THRU: Alberto Protzel, Ph.D.
Senior Branch Scientist, Tox Branch
Health Effects Division (HED) (7509 C)

TO: Deborah Smegal, MPH, Toxicologist/Risk Assessor
Health Effects Division (HED) (7509 C)

Attached is the Toxicology Disciplinary Chapter for the Alkylbenzene Sulfonates (ABS) for the purpose of issuing a Reregistration Eligibility Decision (RED) Document.

SODIUM DODECYLBENZENE SULFONATE
DODECYL BENZENESULFONIC ACID
BENZENE SULFONIC ACIDS, C_{10-16} ALKYL DERIVS.

PC Code: 079010, 098002, 190116

Toxicology Disciplinary Chapter for the
Re-registration Eligibility Decision (RED)Document

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1.0 HAZARD CHARACTERIZATION

Linear alkylbenzene Sulfonate (LAS) is an anionic surfactant which was introduced in 1964 as a more biodegradable replacement for highly branched alkylbenzene Sulfonates (ABS). LAS is a mixture of closely related isomers and homologues, each containing an aromatic ring Sulfonated at the para position and attached to a linear alkyl chain. Their primary use is as a detergent for cleaning (residential, commercial, and on surfaces where food contact occurs).
The presence of LAS in many commonly used household detergents gives rise to a variety of possible consumer contact scenarios such as: direct and indirect skin contact, inhalation, and oral ingestion derived either from residues deposited on dishes, from accidental product ingestion, or indirectly from drinking water.

In addition to EPA Office of Pesticide Programs reviews, this toxicology chapter draws heavily from the following sources: WHO (1996); and HERA (2004). The toxicology database consists almost entirely of published literature, is essentially complete and of acceptable quality to assess the potential hazard to humans.

LAS are readily absorbed following oral ingestion, but not following dermal exposure. LAS are readily metabolized, excreted fairly rapidly, and do not accumulate in tissues. Available acute toxicity data show that LAS are not highly acutely toxic (Categories III-IV) following oral exposure, but are moderately toxic via dermal and inhalation exposure (Category II), are irritating to the eye and skin, and they are not skin sensitizers. Subchronic and chronic exposures show that the liver, kidney and intestinal tract (following oral exposures) are the major target organs of toxicity. Both in vitro and in vivo genotoxicity data show that LAS are not toxic to the gene or the chromosome. LAS did not cause reproductive or developmental toxicity in acceptable studies. Early (pre-GLP) carcinogenicity studies indicate that LAS is not likely to be carcinogenic.

The hazard endpoints chosen for use in this risk assessment are:

- Acute dietary endpoint – there were no effects attributable to a single dose of LAS exposure and so no acute dietary endpoint was chosen.
- Chronic dietary endpoint and short-term incidental oral endpoint – a NOAEL of 50 mg/kg/day was chosen based on three different studies (see below). There were no susceptibility concerns for infants/children and so the special FQPA factor of 10x may be removed and the traditional uncertainty factors of 10 (intraspecies) and 10 (interspecies) were used to derive a chronic RfD of 0.5 mg/kg/day.
- Short-, intermediate-, and long-term inhalation exposure scenarios – a NOAEL of 1 mg/m^3 from a six month inhalation study in monkeys. The level of concern is 100 for both occupational and residential exposure scenarios.
- Dermal exposure scenarios – quantification of dermal risk is not required for several reasons described below in Section 5.2, but mainly because LAS are dermal irritants at concentrations greater than about 20% and thus dermal exposure would be self-limiting.

Following is a brief summary of the hazard assessment for LAS:

Absorption, Distribution, Metabolism, Excretion
In animal tests (oral – monkeys, pigs, rats), LAS are readily absorbed from the gastrointestinal tract, are distributed throughout the body, and are extensively metabolized. Excretion is via both the urine and feces. Available dermal absorption data (rats and guinea pigs) indicate that LAS are poorly absorbed from the skin, although prolonged contact may lead to irritation and thus compromise the skin to permit more absorption (WHO, 1996 and HERA, 2004).

Acute Toxicity (Including Irritation, Sensitization)
LAS exhibit a wide range of acute toxicity via the oral route in rats (LD_{50}s of 404 – 1980 mg/kg), with a narrower range in mice (LD_{50}s of 1259-2300 mg/kg). This spans the acute oral toxicity categories of III-IV. LAS are classified as acute toxicity category II for the dermal and inhalation routes of exposure.

LAS is an irritant to the eye (category I), and skin (category II), but is not a skin sensitizer.

Repeated Dose Toxicity (Subchronic and Chronic)
There have been many oral repeated dose studies performed with LAS ranging from a 28-day study in monkeys to nine month studies conducted with rats and mice. There have also been repeated dose dermal (guinea pigs, rabbits, and rats) and inhalation studies (dogs and monkeys). Collectively, the animal data suggest that the liver, kidney and caecum (for oral studies) are the major target organs for toxicity. The liver and kidney effects were dose and duration related in that mild effects (organ weight changes and serum enzyme/clinical chemistry changes indicative of mild organ effects) were seen at lower doses, but increased in severity with both dose and time.

For the purposes of this hazard assessment, several studies were considered collectively to determine a NOAEL of 50 mg/kg/day for the chronic dietary endpoint. The NOAELs in the three studies used to develop the chronic endpoint are 40, 50 and 85 mg/kg/day. The chronic endpoint is based on: increased caecum weight and slight kidney damage (at a LOAEL of 114 mg/kg/d in the six month rat study); reduced body weight in 21-day old pups (at a LOAEL of 250 mg/kg/day in a reproductive toxicity rat study); and significant decreases in renal biochemical parameters (at a LOAEL of 145 mg/kg/day in a nine month drinking water study in rats).

Developmental Toxicity
A number of developmental studies via the oral and dermal routes have been performed with LAS in rats, mice and rabbits; there were also several subcutaneous injection developmental studies reported in mice (WHO, 1996). There is a spectrum of quality in the 20+ studies in terms of dosing (some had only one or two doses), purity of LAS used (some used formulated products that ranged from 1-45% LAS content), and overt toxicity to the pregnant females in the dermal studies due to severe irritating effects. It is concluded that some developmental effects (including some terata) were observed at high doses at which maternal toxicity was observed and

the available information does not suggest any qualitative or quantitative susceptibility differences between pups and pregnant animals.

Reproductive Toxicity
LAS were tested in several multigeneration studies in rats. There were no effects on reproductive parameters in any of these tests at doses up to 250 mg/kg/day.

Carcinogenicity
The available long-term studies that assessed carcinogenicity were older studies (pre-1970) that would not be acceptable under current standards (due to low number of animals used, insufficient number of doses and extent of dosing, and limited histopathological examinations. However, the limited studies provide no evidence of carcinogenicity in animals given LAS orally.

Genotoxicity
The toxicological data show that LAS was not genotoxic in vitro or in vivo.

Neurotoxicity
There's no evidence in the literature to indicate any neurotoxic effects of LAS in humans or laboratory animal.

2.0 REQUIREMENTS

The requirements for an indirect food use for Linear alkylbenzene Sulfonate (LAS) are in Table 1.

Table 1.

Test	Technical	
	Required	Satisfied
870.1100..... Acute Oral Toxicity	yes	yes
870.1200.....Acute Dermal Toxicity	yes	yes
870.1300..... Acute Inhalation Toxicity	yes	yes
870.2400..... Primary Eye Irritation	yes	yes
870.2500.....Primary Dermal Irritation	yes	yes
870.2600.....Dermal Sensitization	yes	yes
870.3100..... Oral Subchronic (rodent)	yes	yes
870.3150..... Oral Subchronic (nonrodent)	no	yes
870.3200.....28-Day Dermal	no	yes
870.3250.....90-Day Dermal	no	--
870.3465..... 90-Day Inhalation	no	no
870.3700a.....Developmental Toxicity (rodent)	Yes	yes
870.3700b.....Developmental Toxicity (nonrodent)	no	yes
870.3800.....Reproduction	no	yes
870.4100a..... Chronic Toxicity (rodent)	No	yes
870.4100b..... Chronic Toxicity (nonrodent)	no	--
870.4200a..... Oncogenicity (rat)	no	yes
870.4200b.....Oncogenicity (mouse)	no	--
870.4300.....Chronic/Oncogenicity	no	--
870.5100.....Mutagenicity—Gene Mutation - bacterial	Yes	yes
870.5300..Mutagenicity—Gene Mutation - mammalian	Yes	yes
870.5375.....Mutagenicity—Structural Chromosomal Aberrations	Yes	yes
870.5xxx..... Mutagenicity—Other Genotoxic Effects	No	--
870.6100a..... Acute Delayed Neurotox. (hen)	No no	- -
870.6100b.....90-Day Neurotoxicity (hen)	no	-
870.6200a..... Acute Neurotox. Screening Battery (rat)	no	-
870.6200b..... 90 Day Neuro. Screening Battery (rat)	no	-
870.6300.....Develop. Neuro	no	-
870.7485.....General Metabolism	No	Yes
870.7600..... Dermal Penetration	No	-
Special Studies for Ocular Effects	No	-
Acute Oral (rat)	no	-
Subchronic Oral (rat)	no	-
Six-month Oral (dog).....	no	-

3.0 DATA GAP(S)

Based on the non-food use of linear alkylbenzene Sulfonate (LAS), as well as the limited use as a house hold detergent, the database appears to be adequate. However, given the uncertainties in the monkey inhalation toxicity study, the Agency requests the registrant to submit a 90-day guideline inhalation toxicity study in the rat, with nose-only exposure to the chemical of concern, not to a mixture of chemicals, so the Agency can determine the specific response to inhalation exposure to that chemical, rather than to a mixture of chemicals.

4.0 HAZARD ASSESSMENT

4.1 Acute Toxicity

Adequacy of data base for acute toxicity: The data base for acute toxicity is considered complete. No additional studies are required at this time. The acute toxicity data on the Linear alkylbenzene Sulfonate (LAS) Technical is summarized below in Table 2.

Table 2. Acute Toxicity Data on Linear alkylbenzene Sulfonate (LAS):

Guideline No./ Study Type	MRID No.	Results	Toxicity Category
870.1100 Acute oral toxicity	Multiple	LD_{50} = range from 404 to over 5000 mg/kg	III-IV
870.1200 Acute dermal toxicity	94032006	LD_{50} = 1200 mg/kg	II
870.1300 Acute inhalation toxicity	Open Literature (HERA 2004)	LC_{50} = 310 mg/m3	II
870.2400 Acute eye irritation	0033443*	Corneal opacity not reversed at 72 hours.	I
870.2500 Acute dermal irritation	003444*	Severe irritation at 72 hours	II
870.2600 Skin sensitization	Open Literature	Non-sensitizer	

* Tox record No.

4.2 Subchronic Toxicity

Adequacy of data base for subchronic toxicity: The data base for subchronic toxicity is considered complete. No additional studies are required at this time. The major reviews by the WHO (1996), and HERA (2004) report and/or summarize many subchronic studies via the oral (gavage, feed, and drinking water), dermal, and inhalation routes. Only the critical studies or ones for which OPP has developed DERs over the years are summarized here.

870.3100 90-Day Oral Toxicity – Rat

(Ikawa et al.1978; as cited in HERA, 2004).
LAS was administered for 2, 4, and 12 weeks to male rats (5/group) at a single dose of 1.5% in the diet (750 mg/kg bw/day). LAS suppressed body weight gain, and the relative liver weight was increased after 2 weeks of LAS administration. Serum biochemical examinations revealed significant increases in ALP and GTP at each observation period and significant decreases in cholesterol and protein in 4 weeks. Enzymatic examinations of the liver revealed decreases in G6Pase and G6PDH and an increase in isocitrate dehydrogenase (IDH) at each observation period. Enzymatic examinations of the renal cortex revealed decreases in G6Pase and 5'-nucleotidase at each observation period, an increase in LDH at 12 weeks, and an increase in IDH at 2 and 4 weeks. Enzymatic examinations in the renal medulla revealed a decrease in Na, K-ATPase, and an increase in LDH at 12 weeks, a decrease in IDH at 2 weeks, and an increase in IDH at 12 weeks.

In another study (MRID No. 43498412; Kay et al. (1965) as cited in HERA, 2004), LAS (87.9% purity) was administered in the diet at dietary levels of 0, 200, 1000, and 5000 ppm for 90 days to weanling Sprague-Dawley Rat (10/sex/dose).

Body weight and food consumption was measured pretest and weekly on all animals and hematology and urine analysis were done on 5/sex/group at days 0, 30, 60, and 90. Clinical chemistry measurements were not performed. All animals were sacrificed by ether inhalation and subject to gross necropsy. Weights of liver, kidneys, spleen, gonads, heart and brain were taken and absolute and relative (both body and brain) organ weights were calculated. Histopathology was performed on 5/sex from control and high dose and 3/sex from low and mid dose animals from 25 organs and tissues. Required tissues not examined were aorta, eyes, cecum, skin, trachea, sciatic nerve, esophagus, rectum, thymus, mammary gland, epididymis, spinal cord, and salivary glands. Two low dose males died early in the study from respiratory illness There was no compound-related effects in body weight, food consumption, hematology, urine analysis, organ weight, and histopathology.

Acceptable/Guideline.

870.3101 90-Day Oral Toxicity - Mouse
This study is not available in the database of this chemical; however, a sub-chronic monkey study is available in the database.

Groups of 3 male and 3 female Rhesus monkeys 18-36 months old and weighing 2.0-4.4 kg, were treated simultaneously with SDDBS (LAS) in distilled water at doses of 0 (controls), 30 mg/kg (oral) + 0.3. mg/kg (subcutaneous), 150 mg/kg (oral) + 0.5 mg/kg (subcutaneous) and 300 mg/kg (oral) + 1 mg/mg (subcutaneous) for 28 days (MRID 43498413). Parameters measured were body weight, ophthalmoscopy, hematology, clinical chemistries, urinalysis, necropsy, organ weights, and histopathology. NOEL is 30 mg/kg (p0) + 0.1mg/kg (sc). Effects seen in the

high dose were emesis (vomiting) and liquid feces. Liquid feces were also seen in the mid dose. All treated animals had fibrosis at the subcutaneous injection site, but this was not included in the determination of a NOEL since this is a common finding for tissue irritants and not an indication of systemic toxicity.

Core Classification: ACCEPTABLE

870.3150 90-Day Oral Toxicity - Dog

This study is not available in the database of this chemical.

870.3200 21/28-Day Dermal Toxicity – Rat

This study is not available in the database of this chemical; however, there were a 28-dermal study in the rabbit (Tox record No. 003441), which was classified as "unacceptable" and an acceptable 30-day study in guinea pigs summarized below.

Mathur et al. (1992). J Toxicol Cutan Ocular Toxicol, 11(1): 3-13. (as cited in WHO 1996). A solution of LAS in distilled water equivalent to 60 mg/kg bw was applied to a 4-cm^2 area of clipped dorsal skin daily of 12 Guinea Pigs for 30 days. The activities of B-glucuronidase, gamma- glutamyl transpeptidase, 5-nucleotidase, and sorbitol dehydrogenase were increased in liver and kidney. Lipid peroxidation was increased in the kidney but not in liver, and the glutathione content was unchanged in both organs. Extensive fatty changes were found in hepatic lobules, with dilation of sinusoids; tubular lesions were found in the kidney, predominantly in the proximal and distal portions.

870.3465 90-Day Inhalation – Rat

This study is not available in the database of this chemical; however, there is an acceptable, non-guideline sub-chronic monkey inhalation study.

In a subchronic inhalation toxicity study in monkeys (MRID 43498403), groups of 5 male and 4 female cynomolgous monkeys, 1.6 to 3.7 kg, were randomly divided into 12 nominal groups (mg/m^3) - control, detergent (D), enzyme (E), or both at levels at 0, l00(D) and (0.001(E), 0.01(E), 0.1(E) and 1(E)) together with [0, 1(D), 10(D), and 100(D)] for 6 hours daily, 5 days a week for 6 month. Particle analysis and gravimetric determinations showed particle size to have a MMD and gravimetric concentrations to be slightly higher than nominal. The detergent formulation contained 13% C_{12} linear alkylbenzene sulfonate (the remaining major ingredients were sodium tripolyphosphate [39%]; sodium sulfate [40%]; and sodium silicate [7%]).

Routine measurements included body weight, toxic signs, clinical evaluation, chest radiograph, tuberculin skin test, pulmonary function tests (3 different tests), hematoloqy, clinical chemistry, urinalysis, intradermal and prick test, necropsy, and histopathology. The NOEL is 1 mg/m^3 detergent dust combined with up to 0.1 mg/m^3 enzyme dust. The detergent dust at 100 mg/m^3 alone and with enzyme dust produced mortality. At least one animal in each group exposed to enzyme dust had precipitating antibodies to the enzyme. There were no effects at any level in total respiratory system flow resistance, diffusion capacity, hematology, clinical chemistry, urinalysis, intradermal or skin-prick challenge test results, and chest X-rays.

In this published study, the detergent was dried and micronized to make it respirable. However, it should be noted that most uses of this detergent are in liquid form.

The detergent dust alone at 100 mg/m^3 (group 2) caused gross signs of respiratory distress, pulmonary histopathological effects, and pulmonary function impairment. This impairment, measured by the nitrogen washout method, was indicative of constricted small airways. Exposure to 10 or 100 mg/m3 together with 0.01 and 0.1 mg/m3 enzyme dust produced the same effects along with weight and decreased weight gain. One animal in the 100 mg/m3 group (group 2) died, and a second was sacrificed in moribund condition during the exposure period. . Their deaths were considered exposure-related according to necropsy and histopathologic observations. Acute effects (pulmonary edema, focal hemorrhaging, bronchiolitis) were also seen in the lungs.

Gross clinical observations of noisy breathing, were consistent, and correlated with subsequent pulmonary function and histopathologic findings. These clinical observations appeared to be related primarily to the level of detergent dust.

Exposure-related histopathological alterations were seen, however, in the lungs from all of the monkeys in Groups 2. They were found in the respiratory bronchioles and proximal alveoli. These alterations were characterized by the infiltration of mononuclear macrophages, lymphocytes, and in some instances, polymorponuclear graculocytes into the walls of the respiratory bronchioles. The walls of the respiratory bronchioles were moderately to markedly fibrosed, and there was a diffuse nonsuppurative alveolities in the proximal alveoli adjacent to respiratory broncioles. The nonsuppurative alveolitis was characterized by an infiltration of mononuclear macrophages and lymphocytes into the alveolar walls and lumen. A moderate to marked fibrosis of the alveolar walls was evident in affected alveoli, as was a moderate pneumocyte hyperplasia. In many monkeys the bronchioles were constricted and there were moderate hypertrophy and hyperplasia of the bronchiolar epithelium. Basal cell hyperplasia and focal squamous metaplasia were seen in the tracheas of monkeys in Groups 2.

Core Classification: ACCEPTABLE, NON-GUIDELINE. This study is considered a data gap.

4.3 Prenatal Developmental Toxicity

Adequacy of data base for Prenatal Developmental Toxicity: The data base for prenatal developmental toxicity is considered complete. There are many developmental studies that have been identified and reviewed in the WHO and HERA documents. No additional studies are required at this time.

870.3700a Prenatal Developmental Toxicity Study – Rat

Teratology - rat, mouse, rabbit, MRID NO. 43498426 (“Palmer Part I”).
Randomized groups of 20 CD-1 pregnant mice, 20 CD rats, and 13 NZW rabbits were housed individually and fed appropriate diets ad libitum. Day 0 of gestation was judged by a vaginal

plug in rats and mice and coitus in rabbits. Dosing began on day 6 and continued daily up to day 15 for mice and rats and day 18 for rabbits. The test material was supplied by Lion fat and Oil Co., Led, Tokyo. Doses were 0, 0.2, 2.0, 300 and 600. mg/kg BW. Animals were observed daily and weighed regularly. At termination (Days 17, 20, and 29 for mice, rats, and rabbits), the uteri were immediately dissected and contents examined to determine implantations, viable young, embryonic deaths (abortion or resorption sites). Ovaries were examined and the number of corpora lutea counted for rats and rabbits. Fetuses were weighed and externally examined for abnormalities. With rabbits, the fetuses were immediately dissected and examined for visceral abnormalities. Sex was determined by gonadal inspection and carcasses preserved in alcohol for subsequent clearing, staining. with alizarin, and skeletal examination. With mice and rats, following weighing and external examination, one third were fixed in Baum's solution for free hand sectioning for visceral abnormalities and the remaining two-thirds fixed in alcohol, cleared, stained with alizarin and examined skeletally.

In assessing results, group means were calculated from the individual litter data in two ways. Mean A: includes all surviving animals showing evidence of implantation, including those with total litter loss. Mean B: includes only animals bearing viable young at termination. Mean B has more meaning when only the occasional animal shows total litter loss and Mean A provides a better index when several animals show total litter loss.

Generally, maternal toxicity ranked rabbits > mice > rats. In all species tested, toxic reactions involved a disturbance of the gastrointestinal tract. Affected rabbits showed diarrhea, anorexia, weight loss and cachexia prior to death. Total litter loss (abortion and/or total resorptions) tended to occur as a result of maternal toxicity. The NOEL for maternal effects is 2.0 mg/kg for rabbits and mice, and 300mg/kg for rats. At doses at or below the NOEL, values for litter size and fetal loss were comparable to controls.

The NOEL for developmental toxicity is 2.0 mg/kg/day in mice, 300 mg/kg/day in rats, and 2.0mg/kg/day in rabbits. Although the identity of the malformations and anomalies was not specified in the report, there was no apparent increase in numbers of malformation at any dose in mice, rats and rabbits. Additionally, mice at the maternally toxic dose of 300 mg/kg/day had increases in the percent of minor visceral and skeletal anomalies. Similarly, in rats, at the maternally toxic dose of 600 mg/kg/day, there was an increase in minor visceral anomalies.

Core Classification: ACCEPTABLE

Dermal Developmental Toxicity — Rat, Rabbit, Mouse MRID: 43511403. (Palmer Part III). The surfactant linear alkylbenzene Sulfonate (LAS) was examined for embryotoxic and teratogenic potential following percutaneous administration (MRID 43511403). Solutions containing, 0.03, 0.3 or 3% LAS were applied to shaved skin during pregnancy days 2-13 in mice, 2-15 in rats and 1-16 in rabbits. Dosages employed were 0.5 mg/rat or mouse/day and 10 mg/rabbit/day. For comparison, further groups of rats and mice were similarly treated with concentrations of 0.3, 3 and 30% of a standard soap solution.

Marked local skin reaction, irritability, weight loss and failure to maintain or establish pregnancy was evident in mice treated with LAS 3% soap, 3 or 30%: marked local reaction and weight loss also occurred in rabbits receiving LAS 3%. Moderate maternal toxicity was observed among mice treated with LAS, 0.3% and mild maternal toxicity in rats receiving LAS 3% or soap 30% and rabbits receiving LAS 0.3%.

Effects on litter parameters were generally restricted to dosages causing marked maternal toxicity in mice, the principal effects being higher fetal loss (with consequent reduction in viable litter size) arising from an increased incidence of total litter losses. Although LAS at 3% was considered to show marked maternal toxicity in the rabbit, the slightly higher fetal loss and lower litter size did not differ significantly from control values.

The moderate maternal toxicity of LAS, 0.3% in the mouse correlated with a higher incidence of embryonic deaths and lower litter size but only the former differed significantly from the corresponding control value.

The incidences of major malformations, minor visceral or skeletal anomalies, and skeletal variants provided no conclusive evidence of specific teratogenicity even at maternally toxic dosages.

The LOEL for maternal toxicity was 0.3% (50.0 mg/kg/day), 3.0% (60.0 mg/kg/day) and 0.3% (9.0 mg/kg/day) LAS in mice, rats and rabbits, respectively. The NOEL for maternal toxicity was 0.03% (5.0 mg/kg/day): 0.3% (6.0 mg/kg/day) and 0.03% (0.9 mg/kg/day) LAS in mice, rats and rabbits, respectively. The LOEL for developmental toxicity was 0.3% (50.0 mg/kg/day), 3.0% (60.0 mg/kg/day) and 3.0% (90.0 mg/kg/day), respectively. The NOEL for developmental toxicity was 0.03% (5.0 mg/kg/day), 0.3% (6.0 mg/kg/day) and 0.3% (9.0 mg/kg/day), respectively.

The study is supplementary and satisfies the guideline requirement for a series 83-3 developmental (dermal) toxicity study.

Mouse-Developmental

In a mouse developmental toxicity study (MRID 43498424 & 43498425), virgin female ICR/Jc1 mice, 9-10 weeks old, and weighing 30-32 grams, were used. Mice were maintained on mouse diet CA-1 and tap water ad libitum. The mice were exposed to light to induce ovulation and were mated with breeder males. The presence of a vaginal plug indicated day 0. On day 0, the mother's hair was plucked from a 2 x 3 cm area of the dorso- thoracic skin and 0.1 ml of 20% aqueous LAS was applied to the skin twice a day from day 0 to day 3. The mice were sacrificed on day 3 and oviducts and uterus removed.

Embryos were flushed from the oviducts and uterus with Whitten medium. After examination, the embryos were then. cultivated at 37^{o}C in medium equilibrated with a 5% carbon dioxide, 5% oxygen, and 90% nitrogen gas mixture.

A 2.0% dermally applied dose of LAS retarded development and interrupted cleavage of eggs. Significantly higher numbers of embryos were found to be deformed in the LAS group in comparison to controls, and most of these embryos were in the morula stage, whereas they were mostly in the late blastocyst stage in controls.

Core Classification: ACCEPTABLE

870.3700b Prenatal Developmental Toxicity Study – Rabbit

This study is included with section 870.3700a.

4.4 Reproductive Toxicity

Adequacy of data base for Reproductive Toxicity: The data base for reproductive toxicity is considered complete. No additional studies are required at this time.

870.3800 Reproduction and Fertility Effects – Rat

In a reproduction study with rats (MRID 43498416), randomized groups of 20/sex/dose weanling Charles River CD rats (the P_0 parental animals) were fed test diets containing 0, 0.02, 0.1, and 0.5% LAS (equivalent to 0, 10, 50, and 250 mg/kg/day) for 84 days (at which time they were 107 - 112 days old). Rats from each dose group were mated (1:1), litters allowed to be delivered, pups counted (F_{1a}), and examined, culled to 8/litter on day 4, and sacrificed at day 21 of lactation. Pups of the F_{1a} and F_{2a} litters were both sacrificed after day 21 of lactation. Ten days later, the rats were again mated to produce the F_{1b} litters. 20/sex/dose of F_{1b} weanlings were selected to generate the P_1 and P_2 parental animals for generating the F_{2a}, $F_{2b,}$ F_{3a} and F_{3b} litters.

Food consumption, body weight, and food efficiency were recorded weekly for the first 8 weeks. Five male and 5 female rats from the F_{1b} and F_{2b} parental groups and F_{3b} pups were selected for necropsy. Body weight, organ weights, hematology, and histology were performed.

General reproduction including fertility, gestation, parturition, neonatal viability, lactation, and post-weanling growth were comparable for control and test groups and no gross abnormalities were found. There were comparable results in body weight, food consumption, hematology and organ weight findings between control and treated animals. The only significant finding in hematology, was in the 0.5% F_{2b} females, whose RBCs count was depressed significantly (15.4%) but was within the range of historical control data. The only histologic lesion of possible significance, for which the data were not presented, was a pancreatic lesion seen in F_{2b} males. This lesion usually consisted of acinar atrophy and degeneration accompanied by a fibrous tissue replacement. There were also indications of mild islet cell hyperplasia. There appeared to be an increased incidence of the general lesion in animals fed 0.5% LAS.

The NOEL is 0.1% or 1000 ppm for reproductive toxicity and 5000 ppm (HDT) for systemic toxicity. Based on the reported findings, the LEL is considered to be 0.5%. due to

histopathology, hematology, and the occasional slightly decreased day 21 body weights in female pups.

Core Classification: ACCEPTABLE

4.5 Chronic Toxicity

Adequacy of data base for chronic toxicity: The data base for chronic toxicity is considered complete. No additional studies are required at this time.

LAS was administered to male/female rats for 9 months in drinking water, at doses of 0.07%, 0.2% and 0.6% (85, 145, 430 mg/kg bw/day) (Yoneyama et al.,1976 as cited in HERA, 2004). Control groups were used. Hematological examination revealed no significant changes in any experimental group and no organ weight changes were observed. Body weight gain was suppressed in the males of the highest dose group and also serum-biochemical and enzymatic parameters of the liver and kidney were affected. A significant decrease in renal Na, K-ATPase was seen in the group given 145 mg/kg bw/day of LAS. The NOAEL is 85 mg/kg bw/day and the LOAEL is 145 mg/kg bw/day.

Groups of 8 or 9 male/females mice were given diets containing LAS at concentrations of 0.6 and 1.8% (corresponding to 500 and 1000 mg/kg bw/day) or drinking water containing LAS at concentrations of 0.07%, 0.2% and 0.6% for 9 months (corresponding to 100, 250, 600 mg/kg bw/day for males and to 100, 250, 900 mg/kg bw/day for females) (Yoneyama et al., 1976 as cited in HERA, 2004). Control groups were used.

In the mice given 500 mg/kg bw/day via the food, body weight gain was not suppressed, but the weight of the liver increased in male and female mice. Enzymatic examinations revealed significant decreases in LDH of the liver and in acid phosphatase of the kidneys in the male mice. Thus, there was no NOAEL in this study since these effects were seen at the lowest dose of 500 mg/kg/d.

In the drinking water study, body weight was depressed at the highest dose for male and females, increase in liver weight in females and significant decreases in renal Na, K-ATPase resulted in a LOAEL of 600 mg/kg/d (males) and 900 mg/kg/d (females) with a NOAEL of 250 mg/kg bw/day.

In a third study by the same authors (Yoneyama et al., 1972 as cited in HERA, 2004), 10 rats/sex/dose were given the following doses of LAS in feed: 0, 0.07%, 0.2%, 0.6%, and 1.8% (equivalent to 0, 40, 115, 340, and 1030 mg/kg/d). The following effects were observed: diarrhea (high dose group only), suppressed growth (340 and 1030 mg/kg/d dose groups), increases cecum weight (all dose groups above 40 mg/kg/d), and renal tubular degeneration (all dose groups above 40 mg/kg/d). Thus, the NOAEL is 40 mg/kg/d with a LOAEL of 115 mg/kg/d for increased cecum weight and slight degeneration of renal tubules.

870.4100b Chronic Toxicity - Dog

This study is not available in the toxicology database of this chemical.

4.6 Carcinogenicity

Adequacy of data base for Carcinogenicity: The data base for carcinogenicity is considered complete. No additional studies are required at this time.

870.4200a Carcinogenicity Study – rat

Takahasi (MRID 43498420) performed an experiment to assess the ability of SDDBS to affect the induction of gastric tumors by 4-NQO in male Wistar rats. Sixty-four male rats of the Motoyania strain and 97 male Wistar rats were used in the study under the following regimen:
Group I (79 rats): 1 mg 4-NQO and 80 mg SDDBS 2-3 times per week for 18 weeks
Group 1' (17 rats): same as Group I, but fasted 12 hours prior to dosing
Group II (37 rats): 4-NQO only as per Group '1
Group III (28 rats): SDDBS only as per Group I

The experiment lasted 560 days and all rats dying on study or terminally sacrificed, were necropsied and examined histologically for gastrointestinal tumors. In Groups I and I', the presence of SDDBS- shifts the incidence of benign papillomas to malignant papillomas of the forestomach and the incidence of adenocarcinoma and sarcoma of the stomach were increased in comparison to Group II with only 4- NQO. The administration of SDDBS by itself has no effect. on gastric tumors (Group III). The study authors concluded .that the increased carcinogenicity produced by SDDBS was due to the better uptake of 4-NQO via LAS'S surfactive/detersive effects on the protective mucous barrier which is normally found in the glandular stomach and other gastric compartments of the rat. The effect of SDDBS was physical rather than chemical in promoting the increased tumorigenicity.

In a similar study by the same investigators, (Takahasi, MRID 43498419) Motoyama male rats were divided into three groups and gavaged with the following regimen;
Group I (37 rats): 1 mg 4-NQO + 80 mg SDDBS + 20 mg ethanol in a 1 ml gavage for 18 weeks.
Group II (13 rats): 4-NQO and ethanol for 18 weeks.
Group III (13 rats): SDDBS + ethanol for 18 weeks.

Again, the experiment lasted 560 days and all rats, dying on study or terminally sacrificed, were necropsied and examined histologically for gastrointestinal tumors.
Survival: Mortality was 59% in Group I, 31% in Group II and 23% in Group III.
Tumors:
Group III - no gastric tumors -
Group II - 9 benign papillomas of forestomach
Group 1 - 8 benign papillomas of forestomach, 2 malignant papillomas of forestomach, 1 hemangiosarcoma of forestomach. In glandular stomach, 2 adenocarcinomas, 1 hemangiosarcoma, 1 hemangioma, 5 squamous cell carcinomas and 2 rats exhibited atrophic gastritis.

The increased toxicity in Group I produced increased mortality and increased numbers of malignant tumors. The role of SDDBS in the tumorigenesis of 4—NQO was to promote increased absorption o 4—NQO through the forestomach and glandular stomach.

Core Classification: ACCEPTABLE

Carcinogenicity Study - rat
MRID No. 43498416
Randomized groups of 50/sex/group weanling Charles River CD rats were fed diets for 24 months containing 0, 0.02, 0.1 and 0.5% LAS (200, 1000, and 5000 ppm, estimated to be 10, 50, and 250 mg/kg/day). Animals were housed individually and observed daily. Body -weight and food consumption was- measured weekly for 12 weeks then- monthly. Interim sacrifices were performed on 5/sex/group at B and 15 months. Hematology was performed (RBCs, differential, WBC, hematocrit). Tail blood was collected from 5/sex/group for hematology at 4, 11, 15, and 21 months. All animals killed at interim sacrifice, died on study, or terminally sacrificed were necropsied -and- representative tissues were fixed in 10% Bouin and processed for H & E. The following tissues were examined: liver, kidney, thyroid, trachea, esophagus, lungs, heart, spleen, pancreas, adrenal, stomach, small-intestine, urinary bladder, gonads, mesenteric lymph nodes, and gross lesions. Liver and kidneys-were weighed and relative organ weights calculated. The carcinogenic aspects of the study are considered negative at 5000 ppm (HDT), which is less than the MTD since no toxicity was observed. However, it should be considered that the HDT is about 25% of the LD_{50} dose for SDDBS.

According to the report, overall survival exceeded 56% with the highest rate (68%) occurring in animals on 0.5% test diet as compared with 53% in controls. There were no treatment—related findings in hematology, histopathology or tumor results. Chronic interstitial nephritis and adrenal telangiectasis were the most commonly observed degenerative conditions. The majority of tumors were subcutaneous fibroadenomas. No data were presented to substantiate these statements.

870.4200b Carcinogenicity (feeding) - Mouse
This study is not available in the toxicology database of this chemical.

4.7 Mutagenicity

Adequacy of data base for Mutagenicity: The data base for Mutagenicity is considered adequate based.

Gene Mutation

Guideline 870.5100 study type: Gene Mutation - bacterial MRID No. 43498429 Classification: Literature, acceptable	Negative at cytotoxic levels or limit concentrations (both with and without S-9 metabolic activation) when tested with Salmonella typhimurium - TA 98 and TA 100 strains.

Cytogenetics

Guideline # 870.5385 study type: Structural Chromosomal Aberrations MRID No. 43498428 Classification: Literature, acceptable	LAS were administered to rats in the diet for 90-days at doses of 0, 280, or 565 mg/kg/d. All test preparations were negative for increased chromosomal damage over controls.

Other Genotoxicity

Guideline # 870.5300 study type: In Vitro cell transformation MRID No. 43498429 Classification,: Literature, acceptable	LAS tested negative in Syrian Hamster Ovary (SHE) cells at up to 50 micrograms/plate.

4.8 Neurotoxicity

Adequacy of data base for Neurotoxicity: These studies are not available or required at this time. However, there's no evidence in the literature to indicate any neurotoxic effects of LAS in humans or laboratory animal.

4.9 Metabolism

Adequacy of data base for metabolism: The data base for metabolism is considered to be complete. No additional studies are required at this time.

Absorption and distribution in major organs and blood were studied. Urine was collected 24 hours after topical application of the test substance. In the guinea pig, the amount of ^{35}S excreted in the urine was about 0.1% of the total administered dose. Organ distribution in the rat was about 5 times greater than in the guinea pig and "relatively large amounts" of ^{35}S were noted in the liver and kidneys.

870.7485 Metabolism – Rat

In a rat metabolism study (MRID 43498431), groups of Charles- River CD male-rats, 150-200g BW, were used in the study. LAS-S^{35} was given orally to fasted rats at doses of 0.6, 1.2, 8, and 40 mg. Urine and feces were collected and analyzed for radioactivity. Tissues were taken for immunoassay at the end of the study. For metabolism studies, urine, bile, or feces were pooled.

The rate and distribution of the excreted dose was independent of concentration. Similar levels of radioactivity were found in urine and feces and within 3 days, 85.2% - 96.6% of the label was recovered in the high dose rats, no detectable radioactivity was found in the carcasses after 3 days. The limit of sensitivity was 0.1% of the dose. Urinary S^{35} was not in inorganic form and no intact LAS-S^{35} was detected. Following methylation, one urinary metabolite was identified as 4-(4'- methylsulfophenyl) pentanoate. LAS-S^{35} in the feces remained un-metabolized.

The absorption in rats with a ligated bile duct by a single gavage dose of 1.2 mg LAS-S^{35} demonstrated that gastrointestinal absorption did not require enterohepatic circulation, since most of the oral dose was found in the urine (74%) and only 9% was found in feces. Recovery was 83%.

Enterohepatic recirculation was found to be not an important factor in LAS—S^{35} excretion by studies in rats with cannulated bile ducts given 1.2 mg/kg of LAS-S^{35} orally. The percent of radioactivity in bile was similar to that in feces and most label was in the urine.

Core Classification: ACCEPTABLE

Metabolism – Monkey
In a Monkey metabolism study (MRID No 43498410), two groups of 2 male and 2 female Rhesus monkeys, 5 kg BW, were used for the oral and subcutaneous metabolism studies (one group for each route of exposure). For the oral studies, each animal, following 2-3 weeks between dose levels, received single oral doses of C^{14}(SDDBS; 25 microcuries.) at levels of 30, 150, and 300 mg/kg. Blood, urine, faces and cage washing samples were taken for mass balance, metabolite identification and plasma kinetics. Following 2-3 weeks after the last single oral dose, each monkey received 7 consecutive daily oral doses of 30 mg/kg/day of C^{14} ALS. Animals were sacrificed after the last dose and tissue samples taken for direct combustion.

For the subcutaneous studies, each- animal, following 2-3 weeks between dose levels, received single subcutaneous doses of C^{14} LAS (SDDBS; 25 microcuries) at levels of 0.1, 0.5 and 1.0 mg/kg. Blood, urine, feces and cage washing samples were taken for mass balance, metabolite identification and plasma kinetics. Following 2-3 weeks after the last, single subcutaneous dose, each monkey received 7 consecutive daily subcutaneous doses of 1.0 mg/kg/day of C^{14} LAS. Animals were sacrificed after the last dose and tissue. samples taken for direct combustion.

After single 30 mg/kg doses the radioactivity was rapidly excreted, mostly during the first 24 hours. Feces and urine contained 23.1% and 71.2%, respectively, in the first 5 days after oral dosing. After subcutaneous injection, 10.9% and 64.1% were found in the urine and feces, respectively, after the same period.

Plasma concentrations were comparable after single oral doses of 30, 150, and 300 mg/kg at 4 hours and averaged 34, 41, and 36 u/ml, respectively. Peak plasma concentrations increased proportional to dose after single subcutaneous injections of 0.1, 0.5, and 1 mg/kg and were 0.16, 0.72, and 1.13 u/ml, respectively.

During the 7 day dosing period, either by oral or subcutaneous injection, there was no accumulation of radioactivity in plasma, since peak concentrations and half-lives were similar after the first and seventh dose. Animals sacrificed after the seventh dose showed no localization in any of the examined tissues. In urine samples analyzed for metabolites, there was no unchanged SDDBS and the 5 metabolites detected were polar, but were not sulphate or glucuronide conjugates.

Core Classification: ACCEPTABLE

870.7600 Dermal Absorption - Rat

No dermal absorption studies are available in the toxicology database.

Studies (Howes, 1975) with isolated human skin preparations as well as in vivo investigations of percutaneous administration of LAS to rats have demonstrated that penetration through skin and subsequent systemic absorption of this surfactant does not occur to any significant extent at 24 to 48 hours. ^{14}C-LAS was applied on the clipped dorsal skin of the rats, which was washed after 15 min. No radioactivity was detected in urine or feces.

4.10 Special/Other Studies: N/A

5.0 TOXICITY ENDPOINT SELECTION

5.1 See Section 9.2 for Endpoint Selection Table.

5.2 Dermal Absorption:

Quantification of dermal risk is not required since: 1) the alkylbenzene sulfonates are surfactants that are dermal irritants at concentrations generally greater than 20% solution. Thus, dermal exposure would be self-limiting to preclude dermal irritation. Additionally, the requirement of the dermal toxicity studies with the end-use product will determine and be used for the personal protective clothing necessary to protect against irritation during product use; 2) no systemic toxicity was seen following repeated dermal applications to rabbits at 200 mg/kg/day (with an end use product), and 3) no developmental toxicity concerns were seen following repeated dermal applications to pregnant mice, rats or rabbits (developmental effects were seen either in the presence of maternal toxicity or at doses higher than those that caused maternal toxicity).

5.3 Classification of Carcinogenic Potential:

There was no Cancer Assessment Review Committee (CARC) for LAS; however, from the available data it doesn't appear that LAS has carcinogenic potential. The WHO (1996) acknowledged that the available studies are inadequate to assess the carcinogenic potential of LAS, but they also concluded that the data show no evidence of carcinogenicity.

6.0 FQPA CONSIDERATIONS

6.1 Special Sensitivity to Infants and Children

Based on the available hazard data, it doesn't appear that LAS exposure in laboratory animal studies results in any special sensitivity to the young. Therefore, the FQPA factor may be reduced to 1X.

Several reproduction and many developmental studies have been performed with LAS in a number of animal species. In the developmental studies, whenever toxicity was observed in adults, it was generally for mild effects (slight body weight changes, intestinal disturbances) except for severe dermal irritation effects in dermal developmental studies. Any developmental

toxicity observed in these same studies included minor increases in visceral/skeletal anomalies and some fetal losses; but only at maternally toxic doses.

In one reproduction study (Buehler et al., 1971), there were slight changes in hematology and histopathology (both within historical control ranges) and slight decreases in body weight in the offspring at the highest dose of 250 mg/kg/d (at which there were no effects on the parental generation). There were no effects in either the parental or offspring in the other two reproductive toxicity studies (see Toxicity Profile Table) – high doses of 70 or 170 mg/kg/d.

There's no evidence in the literature to indicate any neurotoxic effects of LAS in humans or laboratory animal.

There is no need for a special FQPA factor because the mid-dose level of 50 mg/kg/d (NOAEL for offspring effects) in the Buehler study is the basis for the chronic RfD of 50 mg/kg/d. Thus, the chronic hazard value is based on slight pup effects and is protective of laboratory animals of all ages in this hazard assessment.

6.2 Recommendation for a Developmental Neurotoxicity Study

A DNT is not required because there is no evidence of either neurotoxicity or susceptibility to the young following LAS exposure to laboratory animals.

7.0 OTHER ISSUES: N/A

8.0 **REFERENCES** in MRID order

MRID No.	Guideline No./Study Type	Source
Multiple studies	870.1100 Acute oral toxicity	Tox Oneliner
94032006	870.1200 Acute dermal toxicity	Tox Oneliner
Open Literature	870.1300 Acute inhalation toxicity	Open Literature (HERA 2004)
0033443*	870.2400 Acute eye irritation	Tox Oneliner
003444*	870.2500 Acute dermal irritation	Tox Oneliner
N/A	870.2600 Skin sensitization	Open Literature
N/A	870-3100 Subchronic Oral Toxicity – Rat	Ikawa et al.1978. HERA-2004)
N/A	870-3100 Subchronic Oral Toxicity – Rat	Ito, et al. (1978) J. Med. Soc. Toho Univ. 25: 850-875.
43498413	Subchronic Oral Toxicity – Monkey	HERA-2004
N/A	21/28-Day Dermal Toxicity – Guinea Pig	Mathur et al. (1992). J Toxicol Cutan Ocular Toxicol, 11(1): 3-13. (WHO 169).
43498403	Subchronic Inhalation Toxicity – Monkey	HERA-2004
43498426	870.3700a Prenatal Developmental Toxicity Study – Rat, Mouse, Rabbit,	Palmer et al. Part I, HERA-204
43511403	Dermal Developmental Toxicity — Rat, Rabbit, Mouse	Palmer et al. Part III, HERA-2004
43498424 & 43498425	Mouse-Developmental	
43498416	870.3800 Reproduction and Fertility Effects – Rat	
	870.4100a Chronic Toxicity – Rat	Yoneyama et al.,1976 (see tox profile table)
	870.4100b Chronic Toxicity – Mouse	Yoneyama et al.,1976 (see tox profile table)
43498420 & 43498419	870.4200a Carcinogenicity Study – rat	
43498416	870.4200a Carcinogenicity Study – rat	
43498429	870.5100 Gene Mutation - bacterial	
43498428	870.5385 Structural Chromosomal Aberrations	

MRID No.	Guideline No./Study Type	Source
43498427	870.5300 In Vitro cell transformation	
MRID No.	**Guideline No./Study Type**	**Source**
43498431	870.7485 Metabolism – Rat	
43498410	Metabolism – Monkey	
	Isolated human skin preparations	Howes,1975 (see tox profile table)

* Tox record No.

Other Sources:

World Health Organization (WHO). 1996. *Environmental Health Criteria Document for Linear Alkylbenzene Sulfonates and Related Compounds.* (EHC 169, available at http://www.inchem.org/documents/ehc/ehc/ehc169.htm)

Human and Environmental Risk Assessment (HERA). 2004. *LAS – Linear Alkylbenzene Sulfonates (CAS No. 68411-30-3).*

9.0APPENDICES
Tables for Use in Risk Assessment

9.1 Toxicity Profile Summary Tables

9.1.1 Acute Toxicity Table - See Section 4.1

9.1.2 Subchronic, Chronic and Other Toxicity Tables:

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
Subchronic Toxicity			
870.3100 Oral Subchronic (rodent)	Bornmann et al (1963) Study of a Detergent Based on Dodecylbenzene Sulfonate. Fette Seifen Anstrichm, 65 (10): 818-824. (EHC 169) **Open Literature**	0.01% of a preparation containing 51% LAS was administered in the drinking water for 100 weeks Rats (60/sex) Purity: Not Reported	No detrimental effects on body weight and no pathological effects, including tumors, were reported
870.3100 Oral Subchronic (rodent)	Ikawa et al., (1980)/ Ann. Rep. Tokyo Metrop. Res. Lab. Public Health. 29(2): 51-54(Z). 1978 (in Japanese, see WHO, 1996 and HERA, 2004). **Open Literature**	LAS was administered for 2, 4, or 12 weeks at a single dose of 1.5% in the diet (750 mg/kg/d). Male rats (five/group) Purity not reported.	LAS suppressed body weight gain and the relative liver weight was increased after two weeks. Serum biochemical alterations included: significant increases in ALP, GTP (at 2, 4, 12 weeks); significant decreases in cholesterol and protein (4 weeks); decreases in liver enzymes G6Pase and G6PDH and increases in isocitrate DH (all at 2, 4, 12 weeks). The following enzymes associated with kidney function were also altered: decreases in G6Pase, 5'nucleotidase (at 2, 4, 12 weeks) and Na,K-ATPase (12 wks); increase in LDH (12 wks) and IDH (2,4 wks).
870.3100 Oral Subchronic (rodent)	Ito, et al. (1978) Acute, Subacute, and Chronic Toxicity of Magnesium LAS (LAS-Mg). J. Med. Soc. Toho Univ. 25: 850-875. **Open Literature**	Administration by oral gavage at doses of 0, 155, 310, or 620 mg/kg/day (LAS-Mg) and 125, 250, and 500 mg/kg/day (LAS-Na) for one month Sprague-Dawley Rats (12/sex/group) Purity: 99.5%	LAS-Na: Body weight increase was suppressed; feed-efficacy was decreased, and liver weight increased at 500 mg/kg/day. NOAEL: 125 mg/kg bw/d.
870.3100 Oral Subchronic (rodent)	**MRID No. 43498412** Kay et al. (1965) Subacute Oral Toxicity of a Biodegradable, Linear Alkylbenzene Sulfonate. Toxicol Appl. Pharmacol. 7: 812-818 (HERA) **Acceptable** Guideline	SDDBS administered in the diet at dietary levels of 0, 200, 1000, and 5000 ppm for 90 days Weanling Sprague-Dawley Rat (10/sex/dose) Purity: 87.9% a.i.	NOEL: 5000 ppm (HDT) Two low dose males died early in the study from respiratory illness There was no compound-related effects in body weight, food consumption, hematology, urine analysis, organ weight, and histopathology.
870.3100 Oral Subchronic (rodent)	MRID No. 43511401 Mathur et al. (1986) Toxicological Evaluation of a Synthetic Detergent	LAS was administered as a commercial synthetic detergent solution at doses of 0, 50, 100, or 250 mg/kg/day in the feed for 10 weeks	NOEL: < 50 mg/kg/d LOEL: 50 mg/kg/d based on alterations of several enzymes indicative of liver and kidney damage

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
	after Repeated Oral Ingestion in Rats. Industrial Toxicology Research Centre, Mahatma Ganghi Marg, Lucknow Study No. DDBSA JV-RP-013. Acceptable	F Albino Rat (9/group) Purity: Not Reported	
870.3100 Oral Subchronic (rodent)	MRID No. 43498402 Oser et al. (1965) Toxicologic Studies with Branched and Linear Alkyl Benzene Sulfonates in the Rat. Toxicol. Appl. Pharmacol. 7: 819-825. (HERA) Acceptable Guideline	LAS and ABS were administered at dietary levels of 0, 50, or 250 mg/kg/day, adjusted for bw and fc, for 90 days FDRL Strain (Wistar-derived) Rat (15/sex/dose) Purity: Not Reported	NOEL: 50 mg/kg/d LEL: 250 mg/kg/d for increased absolute and relative liver weight in both sexes (21%) and increased relative cecal weight (21%) in males
870.3100 Oral Subchronic (rodent)	Watari et al. (1977) Ultrastructural Observations of the Protective Effect of Glycyrrhizin for Mouse Liver Injury Caused by Oral Administration of Detergent Ingredients (LAS), J. Clin. Electron. Microscopy (Nihon Rinsho Denshikenbikyo Kaishi) 10 (1-2): 121-139. **Open Literature**	Benzenesulfonic acid, C10-13- alkyl derivatives, sodium salt was administered in the drinking water for 6 months at 0 and 100 ppm with 2 months recovery (M: 0 and 17 mg/kg bw, F: 0 and 20 mg/kg bw) M/F ddy Mouse Purity: Not Reported	Liver effects were observed at the only dose tested (17-20 mg/kg/d), but they disappeared following the 2-month recovery period.
870.3100 Oral Subchronic (rodent)	Yoneyama & Hiraga (1977) Effect of Linear Alkylbenzene Sulfonate on Serum Lipid in Rats, J Ann Rep Tokyo Metrop Res Lab, Public Health 28(2): 109-111. (HERA) **Open Literature**	LAS was administered in the diet at concentrations of 180, 360, or 540 mg/kg bw/d for two and four weeks M Wistar Rat (5/group) Purity: 60% a.i.	Body weight gain was suppressed in the group receiving 540 mg/kg bw/d at four weeks, and the relative liver weight was increased at two weeks and thereafter in the groups receiving 360 mg/kg bw/d and 540 mg/kg bw/d. The levels of triglyceride and total lipids in the serum had decreased markedly at two weeks in all the experimental groups, and the levels of phospholipids and cholesterol in the serum had decreased significantly at two weeks in the groups given 360 and 540 mg/kg bw/d. These changes were less apparent at four weeks, but triglyceride, phospholipid, and cholesterol levels in serum were significantly decreased in the group given 540 mg/kg bw. Significant increases in triglyceride levels were seen in the liver after two weeks in the groups receiving 180 and 540 mg/kg bw/d, and in cholesterol levels in the group given 180 mg/kg bw.
870.3100 Oral Subchronic (rodent)	Yoneyama et al. (1978) Effects of LAS on Incorporation of Acetate-1-14C in Liver Lipids in Rats. J Ann Rep Tokyo Metrop Res Lab Public Health, 29 (2): 55-57.	LAS was administered at a concentration of 200 mg/kg bw/d in the diet or in drinking water (560 mg/kg bw/d) for two weeks to determine the effect on the synthesis of lipids in the liver	Uptake of acetate-1-14C by lipids in the liver was increased in both groups; uptake of phospholipids and triglycerides tended to increase, and that of phospholipids increased significantly in rats given LAS in the diet.

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
	Open Literature	M Wistar Rat (5/group) Purity: Not Reported	
870.3100 Oral Subchronic (rodent)	MRID No. 43498413 Heywood et al. (1978) Toxicology Studies of Linear Alkyl Sulfonate (LAS) in Rhesus Monkeys I. Simultaneous Oral and Subcutaneous Administration for 28 Days. Toxicol. Appl. Pharmacol. 11: 245-250. (HERA) Acceptable Guideline	LAS was given to four groups of three males and three females at doses of 30, 150, 300 mg/kg bw/day per gavage (po) and simultaneously with 0.1, 0.5, or 1.0 mg/kg bw/day subcutaneously (sc). Control groups were used. Rhesus Monkey (3/sex/dose), 18-36 months old Purity: Not Reported	At 300 (po) and 1.0 (sc) mg/kg bw/day, the monkeys vomited frequently and usually within 3 hours of administration. An increased frequency of loose or liquid faeces was recorded for animals receiving 150 (po) and 0.5 (sc) mg/kg bw/day. These effects are probably related to the inherent irritative effects of LAS rather than to its systemic toxicity. Fibrosis of the injection sites was found among the entire test group, the incidence and severity being dose related. Ophthalmoscopy, laboratory examination of blood and urine, organ weight analysis and histopathological investigation did not detect any further treatment-related responses. The LOAEL is 150 mg/kg bw/day (po) + 0.5 mg/kg bw/day (sc) based on an increase in liquid feces and the NOAEL is 30 mg/kg/d
870.3200 21-Day Dermal	Mathur et al. (1992) Effect of Dermal Exposure to LAS Detergent and HCH Pesticide in Guinea Pigs: Biochemical and Histopathologic Changes in Liver and Kidney. J Toxicol Cutan Ocular Toxicol, 11(1): 3-13. (WHO 1996) **Open Literature**	A solution of LAS in distilled water equivalent to 60 mg/kg bw was applied to a 4-cm2 area of clipped dorsal skin daily for 30 days 12 Guinea Pigs Purity: Not Reported	The activities of B-glucuronidase, gamma- glutamyl transpeptidase, 5-nucleotidase, and sorbitol dehydrogenase were increased in liver and kidney. Lipid peroxidation was increased in the kidney but not in liver, and the glutathione content was unchanged in both organs. Extensive fatty changes were found in hepatic lobules, with dilation of sinusoids; tubular lesions were found in the kidney, predominantly in the proximal and distal portions.
870.3200 21-Day Dermal	Tox Record No. 003441 Subchronic (28-day) Percutaneous Toxicity (Rabbit) of Compound: B0002.01, (Bio/dynamics Inc., Project No. 4717-77, March 17, 1978, submitted by Procter and Gambel Company, May 10, 1978). **Unacceptable** Core-Minimum Data	SDDBS (end use product Comet Cleanser) was applied to the skin of rabbits for 28 days at 200 mg/kg/d. The hair of each rabbit was clipped from its trunk, so as to expose approximately 25% of the total body surface area and the skin was abraded daily just prior to treatment. 20 M/F Albino New Zealand White Rabbits (5/sex/group) Purity: 10%	NOEL: > 200 mg/kg/d
870.3465 90-Day Inhalation	MRID No. 43498403 Coate et al. (1978) Respiratory Toxicity of Enzyme Detergent Dust. Toxicol. Appl.	SDDBS was administered a SDDBS mixture at levels of 0, 100(detergent), and [.001, .01, 0.1 and 1 (enzyme)] together with [+0, 1, 10, and 100	NOEL: 1 mg/m3 detergent dust combined with up to 0.1 mg/m3 enzyme dust. The detergent dust alone at 100 mg/m^3 caused gross signs of respiratory distress, pulmonary histopathological effects, and pulmonary function

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
	Pharmacol., 45: 477-496. Acceptable Non-Guideline	(detergent)] mg/m3 for 6 hours daily, 5 days a week, for 6 months 12 groups of 5 M/4 F Cynomolgus Monkeys Purity: 13%	impairment indicative of constricted bronchioles. Exposure to 10 or 100 mg/m^3 together with 0.01 and 0.1 mg/m^3 enzyme dust produced the same effects along with weight loss and decreased weight gain.
Developmental Toxicity			
870.3700a Developmental Toxicity (rodent)	Daly et al. (1980) A Teratology Study of Topically Applied LAS in Rats, Fd. Cosmet. Toxicol. 18: 55-58. (HERA) **Open Literature**	LAS was applied to the skin on days 0 through 21 of gestation at doses of 20, 100, and 400 mg/kg bw/d Rat Purity: Not Reported	NOAEL (maternal): 20 mg/kg bw/d NOAEL (fetuses): 400 mg/kg bw/d Maternal toxicity: the dams treated with 400 mg/kg bw/day and 100 mg/kg bw/day showed inhibition of body weight gain and llocal skin effects that compromised the integrity of the skin and caused overt toxicity, like inhibition of the body weight gain. Teratogenicity: there were no findings indicative of effects of LAS on the foetal parameters evaluated. There were no indications of teratogenic or embryotoxic effects.
870.3700a Developmental Toxicity (rodent)	Endo et al. (1980) Studies of the Chronic Toxicity and Teratogenicity of Synthetic Surfactants, Ann. Rep. Tokyo Metrop. Res. Inst. Environ. Prot. (Tokyo Kogai Kenkyujo Nempo), 236-246. (HERA) **Open Literature**	LAS was administered in the drinking water at 0.1%, corresponding to 383 mg/kg bw/d for rats and up to 3030 mg/kg bw/d for rabits from day 6 to 15 (rats) and day 6 to 18 (rabbits) of pregnancy. F Rat and Rabbit Purity: Not Reported	NOAEL (maternal): 383 mg/kg bw/d (rat) LOAEL (maternal): 3030 mg/kg bw/d (rabbit) NOAEL (fetuses): 383 mg/kg bw/d (rat) LOAEL (fetuses): 3030 mg/kg bw/d (rabbit) The effect on the dams was a slight inhibition of body weight gain in the rabbits. The litter parameters of both species did not show any significant differences from those of the controls. Delayed ossification was observed in rabbits, but there was no increase in malformations in either the rabbits or the rats.
870.3700a Developmental Toxicity (rodent)	Imahori et al. (1976) Effects of LAS Applied Dermally to Pregnant Mice on the Pregnant Mice and their Fetuses, J. Jpn. J. Public Health (Nihon Koshueisei Zasshi) 23(2): 68-72. (HERA) **Open Literature**	LAS was applied daily at dermal doses of 15, 150, and 1500 mg/kg bw/d on days 6 through day 15 of pregnancy F Mouse Purity: Not Reported	NOAEL (maternal): 150 mg/kg bw/d NOAEL (fetuses): 1500 mg/kg bw/d The 1500 mg/kg bw/day group showed a clear decrease in the pregnancy rate (67.9%) when compared with a rate of 96.3% in the controls. However, there were no decreases in the litter size, and no changes in the litter parameters with the exception of a slight decrease in foetal body weight. There were no significant increases in the incidence of malformations in the foetuses.
870.3700a Developmental Toxicity (rodent)	**MRID No. 43498423** Masuda et al. (1974) Effects of LAS Applied Dermally to Pregnant Mice on the Development of their Fetuses. 15: 349-355. **Acceptable** Guideline	LAS was applied dermally at a level of 0.5 ml. The ICR-JCL strain received doses of 0, 0.85, 1.7, 2.55, and 3.4% solutions daily from days 1 to 13 of gestation and the ddY strain received doses of 0, 0.017, 0.17, and 1.7% solutions daily from days 2 to 14 of gestation. Mouse (ICR-JCL strain and ddY strain) Purity: Not Reported	NOEL (maternal and developmental toxicity - ddY): 1.7% (HDT) NOEL (maternal toxicity - ICR-JCL): 2.55% NOEL (developmental toxicity - ICR-JCL): 1.7% At 3.4% LAS, maternal body weight and the absolute weight of liver, kidney, spleen were significantly increased over control.. Pregnancy rates were significantly less (33.35) compared to controls (69%). The number of implantations, live fetuses, sex ratio, dead or resorbed fetuses, placenta weight and external malformations were comparable with control. Fetal body weights of 2.55% and 3.4% LAS-treated groups were significantly less than controls.

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
870.3700a Developmental Toxicity (rodent)	**MRID 43498424 and 43498425** Nomura, T et al. (1980) The Synthetic Surfactants AS and LAS Interrupt Pregnancy in Mice. Life Sciences, 26: 49-54. (HERA) Nomura, T. et al. (1987) Killing of Preimplantation Mouse Embryos by AS and LAS. Mutation Research 190: 25-29. (HERA) **Acceptable** Guideline	LAS (0.1 ml) was applied at a concentration of 20% to the dorsal skin of pregnant mice during the pre-implantation period twice a day from day 0 to day 3 of pregnancy Female ICR/Jcl Mouse, 9-10 weeks old Purity: 20%	Development was retarded and cleavage of eggs was interrupted. Significantly higher numbers of embryos were found to be deformed in the LAS group in comparison to controls, and most of these embryos were in the morula stage, whereas they were mostly in the last blastocyst stage in controls. Some dead, deformed, and growth-retarded embryos were observed in the treated group. Although the authors stated that these effects were not due to maternal toxicity since no maternal organs were affected, this statement is probably not correct in view of the high concentration of LAS and its irritation effects. A secondary effect due to maternal toxicity appears much more likely.
870.3700a Developmental Toxicity (rodent)	**MRID 43498426** Palmer et al. (1975) Assessment of the Teratogenic Potential of Surfactants, (Part I), Toxicology 3: 91-106. **Acceptable** Guideline	LAS was administered by gavage on days 6-15 of pregnancy in rats and mice and days 6-18 of pregnancy in rabbits at doses of 0.2, 2, 300, and 600 mg/kg bw/d 20 CD Rats, 20 CD-1 Mice, and 13 New Zealand White Rabbits Purity: 17%	NOAEL (rat - maternal): 300 mg/kg bw/d NOAEL (mouse - maternal): 2.0 mg/kg bw/d (However, there is a large difference between this dose and the next highest dose of 300 mg/kg bw/d, this study does not allow determination of a reliable maternal NOAEL for mice) NOAEL (rabbit - maternal): 2.0 mg/kg b/d (However, the study does not allow determination of reliable NOAELs, given the large difference between the maternal no-effects doses of 2 mg/kg bw/d and the maternal LOAEL dose (300 mg/kg bw/d) that is also the dose for which effects on litters could not be determined due to the high mortality rate in parent animals) NOAEL (rat - developmental): 300 mg/kg bw/d NOAEL (mouse - developmental): 2.0 mg/kg bw/d NOAEL (rabbit - developmental): 2.0 mg/kg bw/d NOAEL (rat - fetal): 600 mg/kg bw/d NOAEL (mouse - fetal): 300 mg/kg bw/d (Due to a high mortality rate of parent animals, no assessment was possible at 600 mg/kg bw/d) NOAEL (rabbit - fetal): could not be determined
870.3700a Developmental Toxicity (rodent)	**MRID 43511403** Palmer, et al. (1975) Assessment of the Teratogenic Potential of Surfactants, (Part III) - Dermal Application of LAS and Soap. Huntingdon Research Centre, Huntingdon, Great Britain. Study No. DDBSA JV-RP4-029. Toxicology 4: 171-181. **Acceptable** Guideline	LAS was administered percutaneously to shaved skin at solutions of 0.03%, 0.3%, and 3% during pregnancy on days 2-13 in mice, 2-15 in rats, and 1-16 in rabbits. Dosages employed were 0.5 ml/rat or mouse/day and 10 ml/rabbit/day CD-1 Mice (20/group), CD Rats (20/group), N2W Rabbits (13/group) Purity: 0.03%, 0.3%, and 3%	LOEL (maternal toxicity, mice): 0.3% (50 mg/kg/d) LOEL (maternal toxicity, rats): 3.0% (60 mg/kg/d) LOEL (maternal toxicity, rabbits): 0.3% (9.0 mg/kg/d) NOEL (maternal toxicity, mice): 0.03% (5.0 mg/kg/d) NOEL (maternal toxicity, rats): 0.3% (6.0 mg/kg/d) NOEL (maternal toxicity, rabbits): 0.03% ((0.9 mg/kg/d) LOEL (developmental toxicity): 0.3% (50 mg/kg/d) LOEL (developmental toxicity): 3.0% (60 mg/kg/d) LOEL (developmental toxicity): 3.0% (90 mg/kg/d) NOEL (developmental toxicity): 0.03% (5.0 mg/kg/d) NOEL (developmental toxicity): 0.3% (6.0 mg/kg/d) NOEL (developmental toxicity): 0.3% (9.0 mg/kg/d)

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			Marked local skin reaction, irritability, weight loss and failure to maintain or establish pregnancy was evident in mice treated with LAS 3% soap, 3 or 30%: marked local reaction and weight loss also occurred in rabbits receiving LAS 3%. Moderate maternal toxicity was observed among mice treated with LAS, 0.3% and mild maternal toxicity in rats receiving LAS 3% or soap 30% and rabbits receiving LAS 0.3%. Effects on litter parameters were dose-dependent, causing marked maternal toxicity in mice, the principal higher fetal loss, reduction in viable litter size. LAS at 3% showed marked maternal toxicity in the rabbit The moderate maternal toxicity of LAS, 0.3% in the mouse correlated with a higher incidence of embryonic deaths and lower litter size but only the former differed significantly from the corresponding control value.
870.3700a Developmental Toxicity (rodent)	Sato et al. (1972) Studies on the Toxicity of Synthetic Detergents: (III), Examination of Teratogenic Effects of Alkylbenzene Sulfonates Spread on the Skin of Mice. Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 24: 441-448. (HERA) **Open Literature**	LAS was applied to the skin of female mice daily on days 0 through 13 of pregnancy with a single LAS dose of 110 mg/kg bw/d. Control group not specified. F Mouse Purity: Not Reported	NOAEL (maternal): 110 mg/kg bw/d No abnormalities were seen in the dam or foetuses.
870.3700a Developmental Toxicity (rodent)	Shiobara S., Imahori A. (1976) Effects of LAS Orally Administered to Pregnant Mice on the Pregnant Mice and their Fetuses. J.Food Hyg. Soc. Jpn. (Shokuhin Eiseigaku Zasshi) 17(4): 295-301. **Open Literature**	LAS was administered by gavage at doses of 10, 100, and 300 mg/kg bw/d at day 6 through 15 of gestation ICR-SLC Mouse (25-33/dose) Purity: Not Reported	LOAEL (maternal): 10 mg/kg bw/d NOAEL (fetuses): 300 mg/kg bw/d 1. Marked maternal and embryonic toxicities, such as maternal death, premature delivery, total litter loss and high fetal death rate, were observed at 300 mg/kg group. 2. Slight suppression of maternal body weight gain and slight body weight suppression of live fetuses were observed in each treated group. 3. External malformations such as cleft palate and exencephaly were observed sporadically both in the control and the treated groups. However, the incidence of these malformations was not significant, and considered to be within the spontaneous incidence of ICR mice.
870.3700a Developmental Toxicity (rodent)	Takahashi et al. (1975) Teratogenicity of Some Synthetic Detergent and LAS. Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 26(2): 67-78. (HERA) **Open Literature**	LAS doses of 40, and 400 mg/kg bw/d were administered daily from day 0 to day 6 of pregnancy or from day 7 to 13 of pregnancy by gavage Mouse (13-14/group) Purity: not reported	NOAEL (maternal): 40 mg/kg bw/d NOAEL (fetuses): 400 mg/kg bw/d At 400 mg/kg bw/day, the pregnancy rate was 46.2% compared to 92.9% in the controls. There was no increase in malformations. Although no information on maternal toxicity is available, it appears likely that maternal toxicity was present at the high dose group.
870.3700a	Tiba et al. (1976) Effects of LAS on Dam,	LAS was administered in	NOAEL (maternal): 780 mg/kg bw/d NOAEL (fetuses): 780 mg/kg bw/d

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
Developmental Toxicity (rodent)	Fetus, and Newborn Rat. J. Food Hyg. Soc. Jpn. (Shokuhin Eiseigaku Zassh) 17(1): 66-71. (HERA) **Open Literature**	the diet at doses of 80 and 780 mg/kg bw/d from day 0 to 20 of gestation F Rat (16/dose) Purity: Not Reported	At 780 mg/kg bw/day there were no abnormalities in the body weight gains of the dams, or in the occurrence and maintenance of pregnancy. The values of the litter parameters did not differ from those of the controls and there was no evidence of teratogenicity. The number of offsprings was rather low in the highest dose group, and the weaning rate of 78.3% was lower than the 100% rate observed in the controls. However, there were no abnormalities in body weight gain, organ weights or functions in the offsprings.
Reproduction Toxicity			
870.3800 Reproduction	**MRID 43498416** Buehler, E., Newmann, E., and King, W. (1971) Two Year Feeding and Reproduction Study in Rats with Linear Alkylbenzene Sulfonate (LAS). Tox. Appl. Pharm. 18: 83-91. (HERA) **Acceptable** Guideline	LAS was administered in the diet at doses of 0, 0.02, 0.1, and 0.5% , equivalent to (0, 10, 50, 250 mg/kg bw/day) for 84 days. Weanling Charles River CD Rat (20/sex/dose) Purity: 98.1%	NOAEL Parental: 250 mg/kg bw/day NOAEL Offspring: 50 mg/kg/d. The LOAEL of 250 mg/kg/day in the offspring is due to slight (non-significant) changes in hematology and histopathology and slight decrease in day 21 body weights.
870.3800 Reproduction	Endo et al. (1980) Studies of the Chronic Toxicity and Teratogenicity of Synthetic Surfactants, Ann. Rep. Tokyo Metrop. Res. Inst. Environ. Prot. (Tokyo Kogai Kenkyujo Nempo), 236-246. (HERA) **Open Literature**	LAS was administered at 70 mg/kg bw/day in the drinking water in a four generation rat study. M/F Wistar Rat Purity: Not Reported	NOAEL: > 70 mg/kg (only dose tested) No effects of LAS administration were observed
870.3800 Reproduction	Palmer et al. (1974) Effect of CLD Reproductive Function of Multiple Generations in the Rat, Report LFO10/731029, Unpublished results. (HERA) **Open Literature**	A commercial light duty liquid detergent of LAS (17%) and alkyl ethoxylate sulphate (7%) was continuously administered in the diet for three generations 60 days prior to mating at concentrations of 0, 40, 200, and 1000 mg/kg bw/d. The corresonding administration of LAS was of 0, 6.8, 34, and 170 mg/kg bw/d. Rat Purity: 17%	NOAEL: 170 mg/kg bw/d Among parental animals over the three generations there were no signs of adverse effects of treatment. Food consumption and bodyweight changes showed no consistent relationship to dosage. Necroscopy revealed no changes due to treatment. The mating performance, the pregnancy rate and the duration of gestation were unaffected. Among litter parameters, organ weight analysis, histopathology and skeletal staining of representative young from the F3b generation revealed no changes that could be conclusively related to treatment.
Chronic Toxicity			
870.4100a Chronic Toxicity	Taniguchi et al. (1978) Results of Studies on Synthetic Detergents. Tokyo, Science and	LAS were applied to the dorsal skin of rats three times per week at doses of 1, 5, or 25 mg/rat for 24	Treatment had no effect on organ weights or histopathological appearance, and there was no evidence of toxicity or carcinogenicity.

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(rodent)	Technology Agency, Research and Coordination Bureau, pp. 18-54. (WHO 1996) **Open Literature**	months. Each application was washed from the skin with warm water after 24 hours. SLC-Wistar Rats Purity: 19.7% a.i.	
870.3100 Chronic Toxicity (rodent)	Yoneyama et al. (1976) Subacute Toxicity of LAS, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health27(2): 105-112, See: IPCS, 1996. (HERA) **Open Literature**	LAS was administered in the diet at concentrations of 500 and 1000 mg/kg bw/d and in drinking water at concentrations of 100, 250, 600 mg/kg bw/d for males and 100, 250, 900 mg/kg bw/d for females for 9 months Mouse (8 or 9/sex/dose) Purity: Not Reported	LOAEL: 500 mg/kg bw/d (in diet) NOAEL: 250 mg/kg bw/d (in water) LAS in diet: in the mice given 500 mg/kg bw/day, body weight gain was not suppressed, but the weight of the liver increased in male and female mice. Enzymatic examinations revealed significant decreases in LDH of the liver and in acid phosphatase of the kidneys in the male mice. LAS in drinking water: body weight was depressed at the highest dose for male and females, increase in liver weight in females, significant decreases in renal Na,K-ATPase.
870.3100 Chronic Toxicity (rodent)	Yoneyama et al. (1976) Subacute Toxicity of LAS, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health27(2): 105-112, See: IPCS, 1996. (HERA) **Open Literature**	LAS was administered for 9 months in the drinking water at doses of 85, 145, 430 mg/kg bw/day M/F Wistar Rat Purity: Not Reported	NOAEL: 85 mg/kg bw/d LOAEL: 145 mg/kg bw/d Haematological examination revealed no significant changes in any experimental group and no organ weight changes were observed. Body weight gain was suppressed in the males of the highest dose group and also serum-biochemical and enzymatic parameters of the liver and kidney were affected. A significant decrease in renal Na,K-ATPase was seen in the group given 145 mg/kg bw/day of LAS.
870.4100a Chronic Toxicity (rodent)	Yoneyama et al. (1972) Studies on the Toxicity of Synthetic Detergents. (II) Subacute Toxicity of Linear and Branched Alkyl Benzene Sulfonates in Rats. Ann Rep Tokyo Metrop Res Lab Public Health, 24: 409-440. **Open Literature**	Technical-grade LAS was administered in the feed for 6 months at a concentration of 0, 0.07, 0.2, 0.6, or 1.8% Wistar SLC Strain Rat (10/sex/dose) Purity: Not Reported	NOAEL: 0.07% (40 mg/kg bw/day) At 1.8%, diarrhea, decrease in body weight gain and tissue damage in caecum liver and kidney were observed. The damage to the kidney was especially remarkable. At 0.6% of the LAS or ABS, the adverse effects observed were a slight decrease of body weight, increase of ceacum weight, increased activity of alkaline phosphatase, decrease of total protein in blood, and the tissue damage in the kidney. At 0.2% of the LAS or ABS, an increase of caecum weight and a slight damage to the kidney were observed.
Carcinogenicity			
870.4200a Oncogenicity (Rat)	**MRID 43498416** Buehler, E., Newmann, E., and King, W. (1971) Two Year Feeding and Reproduction Study in Rats with Linear Alkylbenzene Sulfonate (LAS). Tox. Appl. Pharm. 18: 83-91.	LAS was administered in the diet at doses of 10, 50, and 250 mg/kg/day for 2 years Weanling Charles River CD Rats (50/sex/group) Purity: Not Reported	Negative at 250 mg/kg/day (HDT)

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
	(HERA) **Acceptable** Guideline		
870.4200a Oncogenicity (Rat)	Endo et al. (1980) Studies of the Chronic Toxicity and Teratogenicity of Synthetic Surfactants, Ann. Rep. Tokyo Metrop. Res. Inst. Environ. Prot. (Tokyo Kogai Kenkyujo Nempo), 236-246. (HERA) **Open Literature**	LAS was administered in the drinking water at the dose of 200 mg/kg bw/d 62 M/F Wistar Rat Purity: 38.74% a.i.	The administration of LAS had no effect on the intake of water, mortality, body weight gain, or general condition. In pathological examinations, looseness, atrophy, and fatty change of the hepatic cells in the liver were found in the experimental control group at 6 months, together with significant increases in GOT, GTP and bilirubin. In hematological examinations no effects due to LAS were observed.
870.4200a Oncogenicity (Rat)	Fujii et al. (1977) Pathological Examination of Rats Fed with LAS for their Lifespan, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 28(2): 85-108. (HERA) Yoneyama et al. (1977) Toxicity of LAS by Dietary Administration for Life-Span to Rats, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 28(2): 73-84. (HERA) **Open Literature**	LAS was administered in the feed at a concentration of 0.04, 0.16, and 0.60% for 24 months or lifespan Wistar Weanling Rat (15/sex/dose) Purity: Not Reported	Histopathological examination revealed that there was no evidence of a treatment-related effect on any tissue examined. Whereas a variety of tumors were observed in both linear alkylbenzene sulfonate treated and control rats, none was attributed for the exposure to linear alkylbenzene sulfonate. There was no relationship among the dosage groups, sex, type of tumor, or the site of occurrence.
870.4200a Oncogenicity (Rat)	**MRID 43498420** Takahasi et al. (1969) Effect of Alkylbenzenesulfonate as a Vehicle for 4-Nitroquinoline-1-Oxide on Gastric Carcinogenesis in Rats. GANN: 8, 241-261. **Acceptable** Guideline	For 560 days; Group I (79 rats): 1 mg 4-NQO and 80 mg SDDBS 2-3x per week for 18 weeks; Group I' (17 rats): same as Group 1, but fasted for 12 hours prior to dosing,; Group II (37 rats): 1 mg 4-NQO only; Group III (28 rats): 80 mg SDDBS only 97 M Wistar Rats Purity: Not Reported	In Groups I and I', the presence of SDDBS shifts the incidence of benign papillomas to malignant papillomas of the forestomach and the incidence of adenocarcinoma and sarcoma of the stomach were increased in comparison to Group II with only 4-NQO. The administration of SDDBS by itself has no effect on gastric tumors (Group III). The study authors concluded that the increased carcinogenicity produced by SDDBS was due to the better uptake of 4-NQO via LAS's surfactive/detersive effects on the protective mucous barrier which is normally found in the glandular stomach and other gastric compartments of the rat. The effect of SDDBS was physical rather than chemical in promoting the increased tumorigenicity.
870.4200a Oncogenicity (Rat)	**MRID 43498419** Takahasi et al. (1970) Effect of 4-Nitroquinoline-1-Oxide with Alkylbenzenesulfonate on Gastric Carcinogenesis in Rats. GANN: 61, 27-33. **Acceptable** Guideline	Rats were divided into three groups and gavaged with the following regimen for 560 days: Group I (37 rats) - 1 mg 4-NQO + 80 mg SDDBS + 20 mg ethanol in a 1 ml gavage for 18 weeks; Group II (13 rats) - 4-NQO and ethanol for 18 weeks; Group III (13 rats) - SDDBS + ethanol for 18 weeks	Survival: Mortality was 59% in Group I, 31% in Group II, and 23% in Group III Tumors: Group III - no gastric tumors; Group II - 9 benign papillomas of forestomach; Group I - 8 benign papillomas of forestomach, 2 malignant papillomas of forestomach, 1 hemangiosarcoma of forestomach. In glandular stomach, 2 adenocarcinomas, 1 hemangiosarcoma, 1 hemangioma, 5 squamous cell carcinomas, and 2 rats exhibited atrophic gastritis. The increased toxicity in Group I produced increased

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		64 M Motoyama Strain Rat Purity: Not Reported	mortality and increased numbers of malignant tumors. The role of SDDBS in the tumorigenesis of 4-NQO was to promote increased absorption of 4-NQO through the forestomach and glandular stomach.
870.4200a Oncogenicity (Rat)	**MRID 43498421, -22** Takahasi et al. (1973) Carcinogenic Effect of N-Methyl-N'-Nitro-N-Nitrosoguanidine with Various Kinds of Surfactant in the Glandular Stomach of Rats. **Acceptable** Guideline	SDDBS was administered to 5 groups of rats: (I) 13 rats received 0.1g of MNNG + 4000 mg Tween 60 per L of drinking water for 36 weeks; (II) 16 rats received 0.1 g MNNG + 2000 mg nonipol per L of drinking water for 36 weeks; (III) 15 rats received 0.1 g of MNNG + 1000 mg branched ("hard") SDDBS per L of drinking water for 63 weeks; (IV) 10 rats received 0.1 g MNNG + 1000 mg of linear ("soft") SDDBS per L of drinking water for 63 weeks; (V) 14 rats received o.1 g MNNG per L of drinking water for 63 weeks M Wistar Rats Purity: Not Reported	Survivial was 100% in Groups I, III, and IV, and 93% and 94% in Groups V and II, respectively. The Group I and II rats had more tumors than the controls (Group V), whereas, the rats in Group III, ("hard" SDDBS, and particularly, Group IV (linear "soft" SDDBS) had the fewest tumors in comparison to controls.
870.4200a Oncogenicity (Rat)	Tiba S (1972) Studies on the Acute and Chronic Toxicity of LAS, J. Food Hyg. Soc. Jpn. (Shokuhin Eiseigaku Zasshi) 13(6): 509-516. (HERA) **Open Literature**	LAS was administered in drinking water for 2 years at doses of 20, 100, and 200 mg/kg bw/d M Wistar Rat (20/group) Purity: Not Reported	There were no changes due to the administration of LAS in regard to growth, mortality, the weight of major organs, or histopathological findings
Mutagenicity			
870.5100 Bacterial reverse mutation test	Huls, Report No. AM-93/12, Unpublished data, 1993. (As cited in HERA-2004) **Open Literature**	LAS was tested at 8-5000 ug/plate with and without metabolic activation. The cytotoxicity concentration was >5000 ug/plate. Salmonella typhimurium, strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538 Purity: Not Reported	Negative results
870.5100 Bacterial reverse mutation test	**MRID 43498429** Inoue et al. (1980) Studies of In Vitro Cell Transformation and Mutagenicity by Surfactants and other Compounds, Food. Cosmet. Toxicol 18: 289-296. (HERA)	SDDBS was tested at cytotoxic levels or limit concentrations of 2,000-30,000 ug/plate for 2 days (Salmonella) or 8 days (SHE) Strain: Salmonella typhimurium - TA 98 and TA 100 cells and	Negative (both with and without S-9 metabolic activation)

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
	Acceptable Guideline	Embryonic Syrian Golden Hamster cells (SHE) Purity: Not Reported	
870.5100 Bacterial reverse mutation test	Sunakawa et al. (1981) Studies on the Mutagenicity of Surfactants Following Activation with Various Liver Homogenates (S-9) and Mutagenicity in the Presence of Norharman, Hyg. Chem. (Eisei Kagaku) 27(4): 204-211, See: WHO, 1996. **Open Literature**	LAS was tested at up to 500 ug/plate Salmonella typhimurium Purity: Not Reported	Negative Results
870.5300 In Vitro mammalian cell gene mutation test	Inoue, K. et al. (1977) Osaka-furitsu Koshu Eisei Kenkyusho Kenkyu Hokoku, Shokuhin Eisei Hen 8: 25-8. (HERA) **Open Literature**	Sodium alkylbenzenesulfonate was added to culture at 62.5 ug/ml and 125 ug/l Hamster Lung Cell Purity: Not Reported	At 62.5 ug/ml: induced cell mutation, no effect on sister chromatid exchange At 125 ug/ml: destroyed the cells completely
870.5300 In Vitro cell transformation	**MRID No. 43498427** K. Inoue et al (1980) Food Cosmetic Toxicol. 18:289-296 **Acceptable** **Open Literature,**	Duplicate primary cultures of embryonic SHE and Salmonella typhimurium strain TA 98 and TA 100 cells were exposed to SDDBS and positive and negative controls for 8 days.	SDDBS was negative for transformation up to cytotoxic levels and did not induce mutation in either strains of Salmonalla when allplied up to cytotoxic levels or limit concentration of 2000-3000 ug/plate. SDDBS was tested negative at cytotoxic levels or limit concentrations (both with and without S-9 metabolic activation) of 2,000-30,000 ug/plate for 2 days (Salmonella) or 8 days (SHE)
870.5385 Mammalian bone marrow chomosomal aberration test	Inoue K, et al. (1979) In vivo Cytogenetic Tests of Some Synthetic Detergents in Mice, Ann. Rep. Osaka Perfect. Inst. Public Health 8: 17-24 (in Japanese), See: IPCS, 1996. (HERA) **Open Literature**	LAS was administered at doses of 200, 400, and 800 mg/kg bw/d by gavage for 1 and 5 days M Mouse Purity: Not Reported	There was no significant difference in the incidence of chromosomal aberrations between any of the groups
870.5385 Mammalian bone marrow chomosomal aberration test	Inoue, K. et al. (1977) In Vivo Cytogenetic Tests of Some Synthetic Detergents in Mice. Ann Rep Osaka Prefect Inst Public Health, 8: 17-24. (HERA) **Open Literature**	LAS was administered at a dose of 200, 400, and 800 mg/kg bw/d by gavage for 5 days. One commercial preparation containing 19.0% LAS was also given, at a dose of 800, 1600, or 3200 mg/kg bw, and another containing 17.1% LAS at a dose of 1000, 2000, or 4000 mg/kg bw once only by gavage. M ICR:JCL Mouse Purity: Not Reported	There was no significant difference between any of the groups given LAS and the negative control group in the incidence of chromosomal aberrations

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
870.5385 Mammalian bone marrow chomosomal aberration test	**MRID 43498428** J. Hope (1977) Absence of Chromosome Damage in the Bone Marrow of Rats Fed Detergent Actives for 90 Days. Mutation Research, 56: 47-50. **Acceptable** Guideline	SDDBS was administered in the diet for 90 days at 0, 280, and 565 mg/kg bw/d Colworth/Wistar Weanling Rat (6/sex/dose) Purity: Not Reported	All test preparations were negative for increased chromosomal damage over controls.
870.5385 Mammalian bone marrow chomosomal aberration test	Masabuchi et al. (1976) Cytogenetic Studies and Dominant Lethal Tests with Long Term Administration of Butylated Hydroxytoluene (BHT) and LAS in Mice and Rats, Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 27(2): 100-104. (HERA) **Open Literature**	LAS was administered in the diet for 9 months at a dose of 0.9% in rats (450 mg/kg bw/d) and in mice (1170 mg/kg bw/d) Male Rat and Male Mouse Purity: Not Reported	There were no significant differences in the incidences of chromosomal aberrations between the experimental and control groups
870.5395 Mammalian erthrocyte micronucleus test	Kishi et al. (1984) Effects of Surfactants on Bone Marrow Cells, Bull. Kanagawa Public Health Lab. 14: 57-58. (HERA) **Open Literature**	LAS was administered as a single intraperitoneal injection at a dose of 100 mg/kg bw 3 M ddY Mice Purity: Not Reported	There were no differences in the incidences of polychromatic erythrocytes with micronuclei in the bone marrow cells between the treated group and the control group
870.5395 Mammalian erthrocyte micronucleus test	Koizumi et al. (1985) Implantation Disturbance Studies with LAS in Mice, Arch. Environ. Contam. Toxicol. 14: 73-81. (HERA) **Open Literature**	LAS were administered as a single oral dose of 2 mg to pregnant mice on day 3 of gestation. On day 17 of gestation, each animal received a subcutaneous dose of 1, 2, or 10 mg and were killed 24 h later. Pregnant ICR Mice Purity: Not Reported	There was no difference among treated groups in the incidence of polychromatic erythrocytes with micronuclei in maternal bone marrow or fetal liver or blood. No mutagenetic effect was found in any of the groups.
870.5450 Rodent dominant lethal assay	Masubuchi MA et al. (1976) Cytogenetic Studies and Dominant Lethal Tests with Long Term Administration of Butylated Hydroxytoluene (BHT) and Linear Alkylbenzene Sulfonate (LAS) in Mice and Rats. Ann Rep Tokyo Metrop Res Lab Public Heath,	A diet containing 0.6% LAS at 300 mg/kg bw/d was administered to mice for 9 months. Each of the male mice was then mated with two female mice that had not been given LAS, and 11 of the 14 females became pregnant. The pregnant mice were laparotomized on day 13 of gestation	There were no significant differences in fertility, mortality of ova and embryos, the number of surviving fetuses, or the index of dominant lethal induction (Roehrborn) between the experimental and control groups.

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
	27(2): 100-104. (HERA) **Open Literature**	7 M ICR:JCL Mice Purity: Not Reported	
Metabolism			
870.7485 General Metabolism	**MRID 43498410** Creswell et al. (1978) Toxicology Studies of Linear Alkylbenzene Sulfonate (LAS) in Rhesus Monkeys II. The Disposition of C14-LAS After Oral or Subcutaneous Administration. Toxicology, 11: 5-17. **Acceptable** Guideline	Single oral doses of C14-LAS (SDDBS; 25 ucuries) were administered to each animal, following 2-3 weeks between dose levels, at levels of 30, 150, and 300 mg/kg. Following 2-3 weeks after the last single oral dose, each monkey received 7 consecutive daily oral doses of 30 mg/kg/d of C14-LAS. 2 M/2 F Rhesus Monkeys Purity: Not Reported	After single 30 mg/kg doses the radioactivity was rapidly excreted, mostly during the first 24 hours. Feces and urine contained 23.1% and 71.2%, respectively, in the first 5 days after oral dosing. Plasma concentrations were comparable after the oral doses and averaged 34, 41, and 36 u/ml, respectively. Peak plasma concentrations increased proportional to the dose and were 0.16, 0.72, 1.13 u/ml, respectively. In urine samples analyzed for metabolites, there was no unchanged SDDBS and the 5 metabolites detected were polar, but were not sulphate or glucuronide conjugates.
870.7485 General Metabolism	Lay JP, et al. (1983) Toxicol. Letters 17 (1-2): 187-192 **Open Literature**	(14)C-labeled sodium dodecylbenzenesulfonate was administered daily in the diet at a concentration of 1.4 mg/kg for 5 weeks M Rat Purity: not reported	From a total uptake of 1.213 + or - 0.08 mg/animal of DBS, 81.8% was excreted during the dosing period: 52.4% in feces and 29.4% in urine. Low levels of (14)C-DBS-derived residues were detected in all tissues analyzed on day 35 of the study. Following 1 week on a normal diet, only 7.8% of the nominally stored amount of (14)C was found in the excreta.
870.7485 General Metabolism	Sunakawa et al. (1979) Yakuzaigaku 39 (2): 59-68 **Open Literature**	Sodium-para-dodecylbenzenesulfonate Rat Purity: Not Reported	Blood levels were max at 2 hr, negligible at 48 hr Excretion rate of radioactive label was 99.4% after 48 hr
870.7485 General Metabolism	The Royal Society of Chemistry. (1981) Foreign Compound Metabolism in Mammals. Volume 6: A Review of the Literature Published during 1978 and 1979. London: The Royal Society of Chemistry, p.354. **Open Literature**	(35)S-labeled sodium dodecylbenzenesulfonate was administered as a single oral dose Rat Purity: Not Reported	Rats excreted 64% and 24% of the dose in urine and feces, respectively
870.7485 General Metabolism	The Royal Society of Chemistry. (1981) Foreign Compound Metabolism in Mammals. Volume 6: A Review of the Literature Published during 1978 and 1979. London: The Royal Society of Chemistry, p.354.	Repeated doses of (14)C-labeled alkylbenzenesulfonate were orally administered Rhesus Monkey Purity: Not Reported	Radioactivity did not accumulate in the tissues
870.7485	**MRID 43498431**	LAS-S35 was administered	The rate and distribution of the excreted dose was

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
General Metabolism	W. Michael (1968) Metabolism of Linear Alkylate Sulfonate and Alkyl Benzene Sulfonate. Toxicol. Appl. Pharmacol. 12: 473-485. **Acceptable** Guideline	orally to fasted rats at doses of 0.6, 1.2, 8, and 40 mg Charles River CD M Rat Purity: Not Reported	independent of concentration. Similar levels of radioactivity were found in urine and feces and within 3 days, 85.2% - 96.6% of the label was recovered. In the high dose rats, no detectable radioactivity was found in the carcasses after 3 days. Following methylation, one urinary metabolite was identified as 4-(4'-methylsulfophenyl) pentanoate. LAS-S35 in the feces remained unmetabolized.
Special Studies			
870.3700a Developmental Toxicity (rodent)	Koizumi et al. (1985) Implantation Disturbance Studies with LAS in Mice, Arch. Environ. Contam. Toxicol. 14: 73-81. (HERA) **Open Literature**	LAS was administered as a single oral dose of 350 mg/kg bw on day 3 of gestation Pregnant ICR Mice Purity: Not Reported	LAS was not detected in the uterus
Other	Inoue K, T Sunakawa. (1979) Mutagenicity Tests of Surfactants, Jpn. Fragr. J. 38: 67-75, (in Japanese), See: IPCS, 1996. (HERA) **Open Literature**	LAS tested in a recombination assay at concentrations up to 50 ug/plate Bacillus subtilis Purity: 99.5%	Negative results with and without metabolic activation
Other	Fujise, H. and Aoyama, M. (1984) Nagoya Med J, 28 (3-4): 211-5 **Open Literature**	The proliferation rate of the connective tissue was examined by measuring the activity of proline hydroxylase. The dorsal neck skin of rats was coated with sodium laurylbenzenesulfonate for 4 days, and on the 5th day, the enzyme activity in the skin was measured. Rat Purity: Not Reported	The proline hydroxylase in the part of the skin coated with the irritants showed clearly higher activity than normal skin, although it was still lower than the injured skin region prepared as a positive control.
Other	**MRID 43498430 and 43498408** Kimura et al. (1982) Mechanisms of Toxicities of Some Detergents Added to a Diet and the Ameliorating Effects of Dietary Fiber in the Rat. J. Nutrit. Science and Science and Vitaminology, 28: 483-489. Kimura et al. (1982)	Ringer's bicarbonate (containing sodium lauryl benzene sulfonate) at 0.5 ml/min was used to perfuse a 10 cm length of jejunal segment for 150 minutes; equilibrated for 30 minutes and then the perfusates were collected in 30 minute aliqouts for 120 minutes M Wistar Rat Purity: 0.5%	Alkaline phosphatase was released by an increase of 15-fold in comparison to Ringer's alone (controls without added sodium lauryl benzene sulfonate) and 3-7 times greater than other surfactants tested in Ringer's. The authors conclude that SDDBS has an exfoliative effect on the intestinal brush border

Guideline No./ Study Type	MRID No./ Reference Information/ Study Classification	Dosing and Animal Information	Results
	Toxicity for Detergent Feeding and Effect of the Concurrent Feeding of Dietary Fiber in the Rat. Nutrition Reports International, 26(2): 271-279. **Acceptable** Guideline		
Other	Oba et al. (1968) Biochemical Studies of n-alpha-olefin sulfonates: (II) Acute Toxicity, Skin and Eye Irritation, and Some Other Physiological Properties. J Jpn Oil Chem Soc, 17 (11): 628-634. (EHC 169) **Open Literature**	Solutions of various concentrations of LAS were mixed with red blood cells from rabbits at room temperature for 3 hours Rabbit Red Blood Cell Purity: Not Reported	The 50% haemolytic concentration of LAS was 9 mg/litre
Other	Samejima Y (1991) Effects of Synthetic Surfactants and Natural Soap on the Development of Mouse Embryos In Vitro and the Fertilizing Capacity of Mouse and Human Sperm. J Osaka Univ Med Sch, 3 (12): 675-682. (EHC 169) **Open Literature**	Eggs were fertilized in vitro and incubated in culture medium containing LAS at concentrations between 0.015 and 0.03%. F B6C3F1 Mouse Egg Purity: Not Reported	Concentrations of LAS less than 0.025%: Eggs exposed for 1 hr, washed, and then cultured for 5 days developed normally to the blastocyst stage Concentrations of LAS higher than 0.03%: The eggs did not develop beyond the one-cell stage With continuous exposure to LAS for five days, a concentration of 0.01% slightly impaired development to the blastocyst stage, and 0.025% prevented development to the one-cell stage
Other	Takahashi et al. (1974) Inhibition of Thrombin by Linear Alkylbenzene Sulfonate (LAS). Ann Rep Tokyo Metrop Res Lab Public Health, 25: 637-645. (HERA) **Open Literature**	Purified LAS at various concentrations were added to 10 ul of plasma from rats and prothrombin time was determined M Rat Purity: Not Reported	Prothrombin time was prolonged; the 50% inhibitory concentration was about 0.6 mmol/litre. When LAS at various concentrations were added to a mixture of 1% fibrinogen and thrombin, the time of formation of a mass of fibrin was prolonged by inhibition of thrombin activity. The 50% inhibitory concentration was about 0.05 mmol/litre.
Other	Yanagisawa et al. (1964) Biochemical Studies of Dodecylbenzene Sulfonates; Differences Between Soft and Hard Detergents. Jpn. J Public Health, 11(13): 859-864. (EHC 169) **Open Literature**	The haemolytic action of LAS was investigated by mixing red blood cells from rabbits with solutions of LAS at concentrations of 1-1000 mg/litre at 38 C for 30 min Rabbit Red Blood Cell Purity: Not Reported	Haemolysis occurred at concentrations >= 5 mg/litre.

9.2 Summary of Toxicological Dose and Endpoints for Linear Alkylbenzene Sulfonates

Table 3. Summary of Toxicological Dose and Endpoints for Alkylbenzene Sulfonates			
Exposure Scenario	Dose Used in Risk Assessment, UF	Special FQPA SF*, endpoint and Level of Concern for Risk Assessment	Study and Toxicological Effects
Acute Dietary (All populations)	No endpoint was selected. No effects are attributable to a single dose.		
Chronic Dietary (All populations)	Systemic/ Reproductive NOAEL= 50 mg/kg/day UF = 100 Chronic RfD = 0.5 mg/kg/day	FQPA SF = 1X cPAD = chronic RfD / FQPA SF = 0.5 mg/kg/day	Systemic/Reproductive NOAEL= 50 mg/kg/day; LOAEL = 250 mg/kg/day based on decreased Day 21 female pup body weight (Buehler, E. et al. 1971. Tox. Appl. Pharmacol. 18:83-91) plus NOAEL = 85 mg/kg/day; LOAEL= 145 mg/kg/day from 9 month drinking water rat study based on decreased body weight gain, and serum/ biochemical and enzymatic changes in the liver and kidney (Yoneyama et al. 1976 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 27(2):105-112) plus NOAEL= 40 mg/kg/day (0.07%) LOAEL= 114 mg/kg/day (0.2%) based on increased caecum weight and slight kidney damage in a 6 month rat dietary study (Yoneyama et al 1972 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 24:409-440)

Table 3. Summary of Toxicological Dose and Endpoints for Alkylbenzene Sulfonates			
Exposure Scenario	Dose Used in Risk Assessment, UF	Special FQPA SF*, endpoint and Level of Concern for Risk Assessment	Study and Toxicological Effects
Short-Term Incidental Oral (1-30 days)	Oral NOAEL= 50 mg/kg/day	Residential LOC for MOE = 100	Systemic/Reproductive NOAEL= 50 mg/kg/day; LOAEL = 250 mg/kg/day based on decreased Day 21 female pup body weight (Buehler, E. et al. 1971. Tox. Appl. Pharmacol. 18:83-91) plus NOAEL = 85 mg/kg/day; LOAEL= 145 mg/kg/day from 9 month drinking water rat study based on decreased body weight gain, and serum/ biochemical and enzymatic changes in the liver and kidney (Yoneyama et al. 1976 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 27(2):105-112) plus NOAEL= 40 mg/kg/day (0.07%) LOAEL= 114 mg/kg/day (0.2%) based on increased caecum weight and slight kidney damage in a 6 month rat dietary study (Yoneyama et al 1972 Ann. Rep. Tokyo Metrop. Res. Lab. Public Health 24:409-440)
Short-, intermediate- and Long-Term Inhalation (1 to 30 days, 1-6 months, >6 months)	Inhalation study NOAEL= 1mg/m^3 detergent dust combined with up to 0.1 mg/m^3 enzyme dust Equivalent to approximately 0.14 mg/kg/day (a) (inhalation absorption rate = 100%) purity= 13% active ingredient	**Residential** LOC for MOE = 100 **Occupational** LOC for MOE = 100	Subchronic Inhalation Monkey Study LOAEL = 10 mg/m^3 detergent combined with 0.1 mg/m^3 enzyme dust based on weight loss and decreased weight gain (W. Coates, et al 1978. Tox. Appl. Pharmacol. 45: 477-496) This air concentration is equivalent to approximately 1.4 mg/kg/day (a)

Table 3. Summary of Toxicological Dose and Endpoints for Alkylbenzene Sulfonates			
Exposure Scenario	Dose Used in Risk Assessment, UF	Special FQPA SF*, endpoint and Level of Concern for Risk Assessment	Study and Toxicological Effects
Dermal Endpoint	Quantification of dermal risk is not required since: 1) the alkylbenzene sulfonates are surfactants that are dermal irritants at concentrations generally greater than 20% solution (WHO 1996). Thus, dermal exposure would be self-limiting to preclude dermal irritation. Most pesticide formulations have less than 5% alkylbenzene sulfonates as an inert ingredient, with the vast majority of household products containing approximately 2%. Additionally, the requirement of the dermal toxicity studies with the end-use product will determine whether personal protective clothing would be necessary to protect against irritation during product use; 2) no systemic toxicity was seen following repeated dermal applications to rabbits at 200 mg/kg/day (with an end use product); 3) no developmental toxicity concerns were seen following repeated dermal applications to pregnant mice, rats or rabbits (developmental effects were seen either in the presence of maternal toxicity or at doses higher than those that caused maternal toxicity); and 4) there is no residential exposure to alkylbenzene sulfonates as an active ingredient, however, residential exposure from its use as an inert ingredient in pesticide formulations is expected to be of an intermittent nature (i.e, no continuous, constant contact, multi-day exposure) from household products.		
Cancer (oral, dermal, inhalation)	No evidence of carcinogenicity in reported studies in rats done before 1980 GLPs		

UF = uncertainty factor, FQPA SF = Special FQPA safety factor, NOAEL = no observed adverse effect level, LOAEL = lowest observed adverse effect level, PAD = population adjusted dose (a = acute, c = chronic) RfD = reference dose, MOE = margin of exposure, LOC = level of concern, NA = Not Applicable
NOTE: No Special FQPA Safety Factor recommended because it is assumed that the exposure databases (dietary food, drinking water, and residential) are complete and that the risk assessment for each potential exposure scenario includes all metabolites and/or degradates of concern and does not underestimate the potential risk for infants and children.

(a) Equation used to convert inhalation air concentration to a dose= mg/L* absorption*respiratory volume (L/hr)*duration (hrs) * activity factor / body weight. Thus, 0.001 mg/L * 1*67.94 L/hr (based on default respiratory volumes for a New Zealand Rabbit which is used as a surrogate for a cynomolgus monkey) * 6 hrs * 1 / 2.98 kg (body weight for New Zealand Rabbit used as a surrogate for cynomolgus monkey, study reports monkey body weight ranges from 1.6 to 3.7 kg).

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, DC 20460

OFFICE OF PREVENTION, PESTICIDES, AND TOXIC SUBSTANCES

July 6, 2006

MEMORANDUM

SUBJECT: Environmental Fate Assessment of Alkylbenzene Sulfonates for the Registration Eligibility Document (RED).

TO: Heather Garvie, Chemical Review Manager, Reregistration Team 36
Regulatory Management Branch II
Antimicrobials Division (7510C)

And

Deborah Smegal, Risk Assessor
Reregistration Branch I
Health Effects Division (7509C)

FROM: Talia Milano, Chemist, Team II
Risk Assessment and Science Support Branch (RASSB)
Antimicrobials Division (7510C)

THRU: Norm Cook, Branch Chief
Risk Assessment and Science Support Branch (RASSB)
Antimicrobials Division (7510C)

DP Barcode: 323968

Case No.: 4006

Chemical Names (CAS #)[1]:

Sodium dodecylbenzene sulfonate (#25155-30-0), Benzenesulfonic acid, C10-16-alkyl derivatives (#68584-22-5), and Dodecylbenzene sulfonic acid (#27176-87-0)

1: The CAS # listed reflect the current numbering system. However, dodecylbenzene sulfonic acid is not a pure chemical, and is considered part of the mixture of benzenesulfonic acid. A discussion of this discrepancy can be found in the text and in the Preliminary Risk Assessment.

ENVIRONMENTAL FATE ASSESSMENT OF ALKYYLBENZENE SULFONATES

CASE 4006

PC CODE: 190116

7/6/06

Antimicrobials Division
Office of Pesticide Programs
U.S. Environmental Protection Agency
1200 Pennsylvania Avenue, NW
Washington, DC 20460

Table of Contents

EXECUTIVE SUMMARY

This document is the Environmental Fate Assessment Chapter of the Reregistration Eligibility Decision Document (RED) for the alkylbenzene sulfonates. The currently listed active ingredients that are included under this decision are sodium dodecylbenzene sulfonate (CAS # 25155-30-0), dodecylbenzene sulfonic acid (CAS # 27176-87-0), and benzenesulfonic acid, C10-C16 alkyl derivatives (CAS # 68584-22-5). To date, dodecylbenzene sulfonic acid has been listed separately from benzenesulfonic acid, C10-C16 alkyl derivatives, and identified by the CAS #27176-87-0 on numerous labels and in different databases.

The environmental fate properties of dodecylbenzene sulfonic acid are assumed to be represented by the conclusions made pertaining to benzenesulfonic acid, C10-C16 alkyl derivatives. This is because dodecylbenzene sulfonic acid is not considered to be a pure compound, and is actually included in the mixture of benzenesulfonic acid, C10-16 alkyl derivatives. These two compounds will be addressed as a group, DDBSA, throughout the document. This issue of dodecylbenzene sulfonic acid being a subsidiary of benzenesulfonic acid, C10-16 alkyl derivatives is discussed in more detail in the Preliminary Risk Assessment.

The conclusions presented in this environmental fate chapter are based on the United States Environmental Protection Agency's (USEPA's) Estimation Programs Interface (EPI) Suite and a literature search. EPI Suite provides estimations of physical/chemical properties as well as environmental fate properties.

Based on the output of the model, sodium dodecylbenzene sulfonate is highly unlikely to bioaccumulate in the environment or aquatic organisms (i.e. fish) because the low value for the log Kow (1.96). This also supports that the chemical is soluble in water such that it will exhibit mobility through the soil. In addition, the low log Koc (4.22) further supports the expected soil mobility. The model-calculated linear and non-linear biodegradation probabilities suggest that the linear carbon chain will biodegrade rapidly, whereas the benzene ring is not expected to biodegrade as rapidly. The extremely low vapor pressure along with the short half life of approximately 7.9 hours indicates that if this chemical is present in the soil, it is not likely to be volatile and is expected to degrade rapidly.

Based on the output of the model, DDBSA is expected to behave very similarly as what is projected for sodium dodecylbenzene sulfonate. Based on the low Kow value (3.80), DDBSA is highly unlikely to bioaccumulate in the environment or aquatic organisms (i.e. fish). The chemical is also expected to be soluble in water such that it will exhibit mobility through the soil. In addition, the log Koc (3.69) is low, and this further supports the expected soil mobility. The model-calculated linear and non-linear biodegradation probabilities suggest that the chemical will most likely biodegrade rapidly. The extremely low vapor pressure along with the short half life of approximately 9.48 hours indicates that this chemical is not likely to be volatile and is likely to degrade rapidly in soils.

The output parameters from the EPI Suite model support that potential impacts for both of these chemicals are expected to be very short-lived. This is because they are not likely to persist in

water or microbial soils and sediments. As a result, the environmental fate of alkylbenzene sulfonates is not likely to be of a concern.

1.0 INTRODUCTION

1.1 Purpose

In this document, the Agency presents the results of its review of the potential environmental fate of the alkylbenzene sulfonates, and this information is for use in EPA's development of the Alkylbenzene Sulfonates Reregistration Eligibility Decision Document (RED).

The types of studies indicated by the, "Pesticide Assessment Guidelines, Subdivision N," as being useful for performing environmental fate assessments are degradation studies, metabolism studies, mobility studies, dissipation studies, and accumulation studies. After a search through the USEPA's archives, there are a handful of studies that discuss the environmental behavior of the chemicals addressed in this chapter, however there are no current data evaluation reports (DER's) for the corresponding studies. This absence of documentation is supported by the following memorandum in USEPA's files:

- Memo dated March 2, 1993 (DP Barcodes D185513 and D185394), with the subject: "Phase IV – List D Chemicals; Registration Case #4006," indicates that, "environmental fate assessments can be generated from data available in-house and from information published in the open chemical literature." In addition to this statement, the memo provides a list of the different criteria that need to be met to fulfill the environmental fate requirements. On the list, it is indicated that each criteria has been either satisfied or waived for both sodium dodecylbenzene sulfonate (CAS # 25155-30-0) and dodecylbenzene sulfonic acid (CAS # 68584-22-5).

In addition to the supporting memorandum, the EPI Suite model was run to collect the different environmental properties of the chemicals addressed in this case. These values are provided in Section 3.0, "Model Results**."** The Agency conducted a literature search to further support the output parameters that were provided by the EPI Suite model. The results of the literature search are presented in Section 4.0, "Additional Data From Literature Search."

Minimal or no environmental exposure is expected to occur from the majority of linear alkylbenzene sulfonate uses and it is unlikely that any appreciable exposure to terrestrial or aquatic organisms would occur from limited commercial down-the-drain use because of the very small number of pounds sold for these uses (CBI data). It is conclusive from the chemical properties of the alkylbenzene sulfonates and the published literature that there are most likely no environmental impacts to be concerned with at this time.

1.2 Chemical Identification:

Three chemicals are considered in this document: sodium dodecylbenzene sulfonate, benzene sulfonic acid, C10-16 alkyl derivatives, and dodecylbenzene sulfonic acid. It is important to

reiterate that even though benzene sulfonic acid, C10-16-alkyl derivatives and dodecylbenzene sulfonic acid are listed as separate active ingredients when denoted on labels, dodecylbenzene sulfonic acid is assumed to exhibit the same environmental effects as the benzene sulfonic acid, C10-16-alkyl derivatives. Additionally, these two chemicals will be jointly referred to as DDBSA throughout the document and conclusions will be made based on the properties affiliated with benzene sulfonic acid, C10-16-alkyl derivatives. Table 1 shows chemical information that was used for sodium dodecylbenzene sulfonate and DDBSA. This data in Table 1 was extracted from the Product Chemistry Science Chapter that has been developed for the alkylbenzene sulfonate RED.

Table 1. Chemical Identification Information Alkylbenzene Sulfonates[a]

	Sodium Dodecylbenzene Sulfonate	Benzene Sulfonic Acid, C10-16-alkyl derivatives (DDBSA)
CAS Number	25155-30-0	68584-22-5
Molecular Formula	$C_{18}H_{29}O_3NaS$	$C_{18}H_{30}O_3S$

a: Refer to the product chemistry chapter for a full list of the different chemical and physical properties of each of these compounds.

2.0 USE INFORMATION

2.1 Formulation Types and Percent Active Ingredient

The products containing alkylbenzene sulfonates as the active ingredients (a.i.) are formulated as soluble concentrates, flowable concentrates, ready-to-use solutions, and water soluble packaging. Concentrations of alkylbenzene sulfonates in these products range from 0.036% to 25.6%. In the past registrations, there was a use for acid mine treatments that involved sodium dodecylbenzene sulfonate. The labels that have these uses have been voluntarily cancelled by the registrant. As a result, there are no terrestrial uses of this chemical to be concerned with for this RED.

2.2 Summary of Use Patterns and Formulations

The Agency determines potential exposures to the product by identifying exposure scenarios from the various application methods that are plausible, given the label uses. Based on a review of registered product labels, the use categories for alkylbenzene sulfonates include agricultural premises and equipment, food handling/storage establishment premises and equipment, and commercial /institutional and industrial premises and equipment (Use Site Categories I, II, and III respectively). Examples of registered uses for alkylbenzene sulfonates include, but are not limited to: application to indoor hard surfaces (e.g. urinals, shower stalls, toilet bowls, etc.), food dispensing equipment (e.g. pre-mix and post-mix vending machines), food contact surfaces (glasses, dishes, silverware, countertops, etc.), agricultural tools, and fruits and vegetables (post-harvest). The percentage of alkylbenzene sulfonates in various products can range from 0.036% to 25.6%. Products containing alkylbenzene sulfonates are formulated as

soluble concentrates, flowable concentrates, ready-to-use solutions, or water soluble packaging. All of the scenarios are highly unlikely to produce environmental fate concerns.

3.0 MODEL RESULTS

EPI Suite contains ten models, not all of which were executed for this chapter. EPIWIN, Estimations Programs Interface for Windows, is an interface program that transfers a single SMILES notation to eleven separate structure estimation programs. These programs are useful because they provide chemical properties so that different estimations can be made about the behavior and properties of the particular chemical being discussed. The programs that provided output applicable to this chapter are:

- AOPWIN: This estimates the rate constant for the atmospheric gas-phase reaction between photochemically reduced hydroxyl radicals and organic chemicals. It then uses the calculated rates to estimate the half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals and ozone.
- BIOWIN: Estimates the probability for the rapid aerobic biodegradation of an organic chemical in the presence of mixed populations of environmental microorganisms. Estimates are based upon fragment constants that were developed using multiple linear and non-linear regression analyses.
- HENRYWIN: Estimates Henry's law constant.
- KOWWIN: Estimates the octanol-water partition coefficient
- MPBPWIN: estimates the melting point, boiling point, and vapor pressure
- PCKOCWIN: Estimates the soil sorption coefficient, K_{OC} of organic compounds. The output can be defined as the ratio of the amount of chemical adsorbed per unit weight of organic carbon (oc) in the soil or sediment to the concentration of the chemical in solution at equilibrium. The coefficient provides an indication of the extent to which a chemical partitions between solid and solution phases in soil, or between water and sediment in aquatic ecosystems.
- WSKOWWIN: Estimates the water solubility from the log octanol-water partition coefficient.

The following sections, 3.1 and 3.2 respectively, provide the chemical specific conclusions that are based on model output.

3.1 EPI Suite Output for sodium dodecylbenzene sulfonate (CAS # 25155-30-0)

log Kow: 1.96
Koc: 1.683 E +004 (log Koc: 4.22)
MP: 287.6^{O}C
BP: 660 ^{O}C
VP: 6.02 E-015 mm Hg
Water solubility: 800 mg/L
Henry's Law Constant: 6.02 E-017 atm-m^3/mol
Linear biodegradation probability: 0.5314

Non-linear biodegradation probability: 0.4415
Half life: 7.9 hrs (in the air or atmosphere)

Based on the output of the model, sodium dodecylbenzene sulfonate is highly unlikely to bioaccumulate in the environment or aquatic organisms (i.e. fish) because of the low Kow value. This suggests that the chemical is soluble in water such that it will exhibit mobility through the soil. "In general, the higher its octanol-water partition coefficient Kow, the more likely a chemical is to be bound to organic matter in soils and sediments…Thus, it is chemicals with log Kow values in the 4-7 range that bioconcentrate to the greatest degree" (Barid 303). In addition, the log Koc is low, and this further supports that dodecylbenzene sulfonate will most likely exhibit soil mobility. This is because it is not expected to immediately bind to the soil sediments.

The model-calculated linear and non-linear biodegradation probabilities provide information about the rate of the degradation of the constituents of sodium dodecylbenzene sulfonate in the environment. For numerical comparisons, the BIOWIN model indicates that numbers greater than or equal to 0.5 indicate rapid biodegradation and numbers less than 0.5 do NOT biodegrade quickly. For the sodium dodecylbenzene sulfonate, it is expected that the linear carbon chain will biodegrade rapidly, whereas the benzene ring is not expected to biodegrade as rapidly. The same model also provides an estimation of the behavior of the chemical in the aquatic environment as well as ultimate biodegradation (mineralization). It is estimated that the chemical will biodegrade linearly within days in the aquatic environment, whereas ultimate biodegradation is estimated to take place over the course of weeks.

The extremely low vapor pressure along with the short half life of approximately 8 hours indicates that this chemical is not likely to be volatile, and is likely to degrade rapidly by reaction with photochemically produced hydroxyl radicals in air. The short half-life supports that any potential impacts of the chemical may be very short-lived because the chemical is not likely to persist in water or microbial soils and sediments.

As an aside, insignificant exposure to sodium dodecylbenzene sulfonate, also commonly refeered to as LAS, in the environment is expected for the following reasons: 1.) total LAS usage for these industrial applications is very minor - a very small percentage of the total pounds used in antimicrobials (CBI data); and commercial only use precludes broad environmental exposures that might occur with residential use, 2.) LAS breakdown and degradation in the environment is very rapid, 3.) LAS is significantly reduced by sewage treatment. Industrial water treatment requires a NPDES permit in order to discharge effluents.

3.2 EPI Suite Output for DDBSA (CAS # 68584-22-5)

log Kow: 3.80
Koc: 4.95 E+003 (log Koc: 3.69)
MP: 167.7^{O}C
BP: 437^{O}C
VP: 5.1 E-010 mm Hg
Water solubility: 400g/L (@25^{0}C)

Henry's Law Constant: 2.8 E-011 atm-m3/mol
Linear biodegradation probability: 0.5448
Non-linear biodegradation probability: 0.5407
Half life: 9.48 hrs (in the air or atmosphere)

Based on the output of the model, DDBSA is highly unlikely to bioaccumulate in the environment or aquatic organisms (i.e. fish) because of the low log Kow value. This value suggests that the chemical is soluble in water such that it will exhibit mobility through the soil. Again, the Kow value is low such that the chemical will be highly unlikely to bioconcentrate and is in other words, mobile (Barid 303). In addition, the log Koc is low, and this further supports that dodecylbenzene sulfonate will most likely exhibit soil mobility. This is because it is not expected to immediately bind to the soil sediments.

The model-calculated linear and non-linear biodegradation probabilities provide information about the rate of the degradation of the constituents DDBSA in the environment. For numerical comparisons, the BIOWIN model indicates that numbers greater than or equal to 0.5 indicate rapid biodegradation and numbers less than 0.5 do NOT biodegrade quickly. For the DDBSA, it is expected that overall molecule will most likely biodegrade rapidly. The same model also provides an estimation of the behavior of the chemical in the aquatic environment as well as ultimate biodegradation (mineralization). It is estimated that the chemical will behave similarly to LAS and biodegrade linearly within days in the aquatic environment, and ultimate biodegradation is estimated to take place over the course of weeks.

The extremely low vapor pressure along with the short half life of approximately 9 hours indicates that this chemical is not likely to be volatile and is likely to degrade rapidly by reaction with photochemically produced hydroxyl radicals in air. In addition, the short half-life supports that any potential impacts may be very short-lived because the chemical is not likely to persist in water and microbial soils and sediments.

4.0 ADDITIONAL DATA FROM LITERATURE SERACH

There are minimal studies in house that provide environmental fate data for the two CAS numbers affiliated with this RED. A literature search was conducted for different published articles that could be used as resources for providing information on the chemical behavior of the alkylbenzene sulfonates in the environment. There was a sufficient amount of information available for LAS, but not on DDBSA. Section 4.1 provides a summary of the different published literature that discusses the environmental behavior of LAS. This literature search serves to supplement the conclusions derived from the EPI Suite model output (Section 3.0). Section 4.2 discusses the conclusions for DDBSA. **The excerpts also serve as a foundation for the conclusion that the environmental fate of alkylbenzene sulfonates is not likely to be of a concern.**

4.1 Sodium dodecylbenzene sulfonate (CAS # 25155-30-0)

Several excerpts are included for a discussion of this chemical to provide a well rounded understanding of its behavior in the environment. The location of the full text of where these excerpts were obtained from is fully referenced in the bibliography.

"LAS biodegrades easily and loses its tensioactive properties quickly, as many works of literature testify" (Cavalli 1993).

"Throughout their passage into the environment, LAS are removed by a combination of adsorption and primary and ultimate bio-degradation. LAS are adsorbed onto colloidal surfaces and onto suspended particles…they biodegrade in surface water (half-life 1-2 days), aerobic sediments (1-3 days), and marine and estuarine systems (5-10 days) (WHO 1996).

"For anionic surfactants in general, the most important compartments [where LAS can be found in the environment] are sewage water treatment plants, surface waters, sediment- and sludge-amended soils, and estuarine and marine environments. Both biodegradation (primary and ultimate) and adsorption occur, resulting in decreased environmental concentrations and bioavailability. Reduction in chain length and loss of the parent structure both result in compounds that are less toxic than the parent compound. It is important that these considerations be taken into account when the results of laboratory tests are compared with potential effects on the environment" (WHO 1996).

"The sorption of LAS to soil is a combination of several mechanisms and sorption to both the organic and inorganic fraction of the soil has been demonstrated. The linear alkyl group of LAS is hydrophobic and sorbs to the non-polar fractions of the soil, such as the organic matter. However, the sulfonate group of LAS is negatively charged and hydrophilic and therefore interacts with positively charged soil components or polar groups, such as hydroxyl-groups, minerals, or oxides" (Jacobsen 2004).

"Environmental degradation of LAS homologs in aquatic systems is rapid; the measured half-life in river waters is <2 d[ays]. Degradation processes rapidly reduce chain lengths of LAS in the environment to averages lower than $C_{12,}$" and in addition to this research finding, "[t]oxicity generally decreases with decreasing chain length" (Fairchild 1993). This supports that this chemical has an extremely short-lived presence in the environment, and its degradates are less toxic than the parent compound.

In a published review by Kuhnt (1993), a flow chart is provided to depict the behavior of surfactant in soils. It is conclusive from the flow chart that surfactants that exhibit either low or no adsorption can exhibit enhanced mobility and degradability, which result in low persistence in the environment.

4.2 DDBSA (CAS # 68584-22-5)

There is a deficiency in the availability of literature on DDBSA. The major difference between LAS and DDBSA are the ions on the sulfonate groups which are sodium versus

hydrogen respectively. It is important to also acknowledge that, "[t]he commercial mixture of LAS is composed of a range of homologs with alkyl chain lengths ranging from 10 to 15 carbon units and isomers that vary in phenol position" (Fairchild 1763). This supports that LAS is very similar to DDBSA in terms of the length of the carbon chain, and the empirical formulas provided in Table 1, *Chemical Identification Information for Alkylbenzene Sulfonates* further support this.

5.0 CONCLUSION

As a result of the structural observations and comparisons between LAS and DDBSA along with the similar properties provided by EPI Suite, the literature data that is available for LAS is assumed to be representative of DDBSA. In conclusion, the potential effects of both LAS and DDBSA in the environment are not likely to be of a concern.

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UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, DC 20460

OFFICE OF
PREVENTION, PESTICIDES,
AND TOXIC SUBSTANCES

July 12, 2006

MEMORANDUM:

Subject: Ecological Hazard and Environmental Risk Assessment of alkylbenzene sulfonates for the Registration Eligibility Document (RED). PC Codes: 190116; 079010; 098002

To: Heather A. Garvie, Chemical Review Manager
Antimicrobials Division

From: Richard C. Petrie, Agronomist, Team Leader
Risk Assessment and Science Support Branch (RASSB)
Antimicrobials Division (7510C)

Thru: Norm Cook, Branch Chief
Risk Assessment and Science Support Branch (RASSB)
Antimicrobials Division (7510C)

DP Barcode: 330326
Decision No.: 362579
Case No.: 4006

Chemical Name (s)	**CAS #**
Sodium Dodecylbenzene Sulfonate	25155-30-0
Benzenesulfonic acid, C10-16-alkyl derivatives (DDBSA)	68584-22-5
Dodecylbenzene sulfonic acid (DDBSA)	27176-87-0/68584-22-5

ECOLOGICAL HAZARD AND ENVIRONMENTAL RISK ASSESSMENT ALKYLBENZENE SULFONATES

CASE 4006

PC CODE: 190116

07/12/2006

Richard C. Petrie
Antimicrobials Division
Office of Pesticide Programs
U.S. Environmental Protection Agency
1200 Pennsylvania Avenue, NW
Washington, DC 20460

Table of Contents

Ecological Effects Hazard and Environmental Risk Assessment
alkylbenzene sulfonates

Alkylbenzene sulfonates are used for a variety of indoor antimicrobial uses. Alkylbenzene sulfonates include sodium dodecylbenzene sulfonate, dodecylbenzene sulfonic acid, and benzenesulfonic acid, and are collectively called DDBSA by the DDBSA Joint Venture Task Force. All alkylbenzene sulfonates as pesticides are formulated with phosphoric acid (CAS#s 27276-87-0 and 68584-22-5; mineral acid RED - EPA-738-93-025, December 1993). Alkylbenzene sulfonates through sulfonation and neutralization becomes linear alkylbenzyl sulfonate (LAS).

Currently registered use categories include spray application to agricultural premises and equipment, food handling/storage establishment premises and equipment, commercial-institutional-industrial premises and equipment, medical premises and equipment. Sites include: milking equipment, dairy farms, teat liners, farm utensils, milk claws and inflations, bars, restaurants, dairy equipment, dairy premises, dairy utensils, milk processing plant surfaces-equipment-premises, milk storage, fruit and vegetable wash water, food/milk transport vehicles, food processing plant equipment-handling-storage premises and surfaces, bakery processing equipment, brewery process plant equipment and surfaces, cannery processing equipment, potato washing machines, winery processing equipment, egg processing equipment, beverage processing equipment-premises and surfaces, meat and poultry processing equipment-premises and surfaces, food vending and dispensing machines, soft custard equipment, food stores/markets, seed houses, food service industry pots and pans, research animal facilities, zoo premises, airports, campgrounds, commercial transportation facilities, aircraft, buses, ships, automobiles, railroad trains, shower stalls, urinals, toilet bowls, sickroom premises, and healthcare facilities. There are no home-owner or residential uses currently registered. The only outdoor use, mine acid control, was voluntarily withdrawn by the registrant.

Approximately 300,000 pounds of alkylbenzene sulfonates are used in EPA registered antimicrobial products, which is a small fraction of the approximately 860 million pounds produced each year . The majority of uses of alkylbenzene sulfonates are as household laundry and dish detergents.

I. Ecological Toxicity Data

The toxicity endpoints presented below are based on the results of ecotoxicity studies submitted to EPA to meet the Agency's data requirements for the uses of the alkylbenzene sulfonates. The linear chained alkylbenzene sulfonates (LAS) replaced the highly persistent branched alkylbenzene sulfonates (ABS) in the mid 1960's in laundry detergents. The environmental fate and effects or LAS detergent formulations on aquatic/terrestrial organisms are well studied (see www.inchem.org and www.cler.com for detailed information). Ecotoxicity data available for LAS is assumed to be representative of DDBSA based on available literature.

A. Toxicity to Terrestrial Animals

(1) Birds, Acute and Subacute

In order to establish the toxicity of alkylbenzene sulfonates to avian species for environmental hazard labeling, the Agency requires an acute oral toxicity study using the TGAI for outdoor uses having no environmental exposure of concern. One avian acute test species is required for indoor uses for label hazard purposes. Preferred test species can be either the mallard duck (a waterfowl) or the Northern bobwhite quail (an upland game bird). See Table 1 below for test results.

Table 1. Acute Oral Toxicity of sodium dodecylbenzene sulfonate to Birds

Species	chemical, % Active Ingredient (ai)	Endpoint (mg/kg)	Toxicity Category (TGAI)	Satisfies Guidelines/ Comments	Reference
Northern bobwhite *(Colinus virginianus)*	87.6% Carbon chain not identified. (Nacconal 90G used)	LD_{50} > 1382 NOEL = 279	Slightly toxic	Yes. Acceptable. 14 day test	MRID: 41143901

The results indicate that LAS is slightly toxic to the Northern bobwhite quail on an acute oral basis. The sodium dodecylbenzene sulfonate study MRID 41143901 fulfills guideline requirement 850.2100. The avian acute oral LD50 is > 500 ppm, therefore, an avian environmental hazard statement for birds is not required on manufacturing and end-use product labels.

A subacute dietary study using the TGAI may be required on a case-by-case basis depending on the results of lower-tier ecological studies and pertinent environmental fate characteristics in order to establish the toxicity of a chemical to avian species, however, this testing is not required unless outdoor uses are added to alkylbenzene sulfonate labels.

(2) Mammals, Acute and Chronic Toxicity

In most cases, rat toxicity studies for human health risk assessments are used as surrogates for wild mammal testing. Wild mammal tests are not required for alkylbenzene sulfonates at this time because the currently registered uses are indoor spray applications. Refer to the toxicology section of this RED for mammalian toxicity data.

B. Toxicity to Aquatic Animals

(1) Freshwater Fish, Acute

In order to establish the acute toxicity of pesticides to freshwater fish for environmental hazard labeling, the Agency requires a TGAI study for indoor uses having no environmental exposure of concern. The preferred test species are rainbow trout (a coldwater fish) or bluegill sunfish (a warm water fish). Results of freshwater fish acute testing for LAS are presented in Table 2.

Table 2. Acute Toxicity of LAS to Freshwater Fish

Species	% Active Ingredient (ai)	Endpoints (ppm)	Toxicity Category	Satisfies Guidelines/ Comments	Reference
Fathead Minnow (*Pimephales promelas*)	14.0%*	96hr LC50 = 3.4 mg/L	Moderately toxic	Yes. Supplemental study.	44260002
Rainbow trout (*Oncorhynchus mykiss*)	65.0% C11, C12	96 hr LC50 = 1.68 mg/L	Moderately toxic	Yes. Supplemental study.	44260009

* Carbon chain not identified.

The guideline requirement for a freshwater fish acute test has been fulfilled. In addition the LAS SIAR reports 11 acute freshwater fish studies using commercially relevant LAS and LAB formulations. The LC50 values range from 1.67 to 7.7 mg/L. Data using LAB sulfonic acids in the LAS SAIR report range in toxicity from 3.0 to 10.0 mg/L. Research by Fairchild et al. (1993) indicates that "Degradation processes rapidly reduce chain lengths of LAS in the environment to averages lower than C12. Thus, hazard assessments of LAS to aquatic organisms should focus on environmentally relevant mixtures of average chain lengths of C12 or less." Based on study results above (MRIDs 44260002, 44260009) and studies presented in LAS SIAR, an environmental hazard statement for fish is not required on manufacturing and end-use product labels under consideration in this RED.

(2) Freshwater Invertebrates, Acute

In order to establish the acute toxicity of pesticides to freshwater aquatic invertebrates for environmental hazard labeling, the Agency requires a TGAI study for indoor uses having no environmental exposure of concern. The preferred test species is *Daphnia magna*. See Table 3 below for results of available studies for LAS.

Table 3. Acute Toxicity of LAS to Freshwater Invertebrates

Species	% Active Ingredient (ai)	Endpoints (ppm)	Toxicity Category	Satisfies Guidelines/ Comments	Reference
Waterflea *(Daphnia magna)*	Not reported.	48-hr. EC_{50} = LAS-C10 = 29.5 mg/L, LAS-C12 = 6.84 mg/L, LAS-C14 = 0.80 mg/L, LAS-C16 = 0.20 mg/L.	C-12 = moderately toxic.	Yes. Supplemental study.	47025025

The results of this study indicate that LAS toxicity to Daphnia magna is variable, dependent on the length of the carbon chain. LAS/SIAR (page 37) summarizes 11 *Daphnia* magna studies on commercially relevant LAS that range in EC50 values from 1.62 to 9.3 mg/L. Data on the LAB sulfonic acids give EC50 values for *Daphnia* magna ranging from 2.9 to 12 mg/L. Formulations tested included the C10-C16 b3enzene sulfonic acid and the dodecylbenzene sulfonic acid. Even though the higher carbon chains are more toxic, the CLER (Council for LAB/LAS Environmental Research) ensures that the typical LAS or LAB formulations contain less than 1 - 10% carbon chains C14 or greater. The LAS SIAR report cites 11 *Daphnia magna* studies on commercial LAS formulations with EC50 values ranging from 1.62 to 9.3 mg/L. LAB formulations ranged in toxicity from 2.9 to 12 mg/L. Research by Fairchild et al. (1993) states: "Degradation processes rapidly reduce chain lengths of LAS in the environment to averages lower than C12. Thus, hazard assessments of LAS to aquatic organisms should focus on environmentally relevant mixtures of average chain lengths of C12 or less." Based on study results above (MRID 47025025) and studies presented in LAS SIAR, an environmental hazard statement for aquatic invertebrates is not required on manufacturing and end-use product labels under consideration in this RED.

(3) Estuarine and Marine Organisms, Acute

Acute toxicity testing with estuarine and marine organisms using the TGAI is required when the end-use product is intended for direct application to the marine/estuarine environment or effluent containing the active ingredient is expected to reach this environment. Acute estuarine/marine tests are not required for alkylbenzene sulfonates because the currently registered uses are indoor applications.

(4) Aquatic Organisms, Chronic

Chronic toxicity testing (Fish early life stage, 850.1300/72-4a and aquatic invertebrate life cycle, 850.1400/72-4b) is required for pesticides when certain conditions of use and environmental fate apply. Chronic aquatic organism tests are not required for alkylbenzene sulfonates because the

currently registered uses are indoor applications. The chronic NOAEC toxicity value from the 28 day study for fathead minnow using carbon chain C11.7 was 0.7 mg/L (Fairchild et al, 1993).

C. Toxicity to Plants

Non-target plant phytotoxicity tests are required for pesticides when uses result in exposure to the environment. This testing is not required for alkylbenzene sulfonates because the currently registered uses are indoor applications. Refer to Table 4 below for the summary of a non-target plant phytotoxicity study using green algae.

Table 4. Acute Toxicity of LAS to Green Algae

Species	**% active ingredient (ai)**	**Endpoints (ppm)**	**Toxicity Category**	**Satisfies Guidelines/ Comments**	**Reference MRID:**
Selenastrum capricornutum	Not Reported. Carbon chain not identified.	96 hr. EC50 = 70.27	Slightly Toxic	No. Supplemental.	42439803

II. Risk Assessment and Characterization

Risk assessment integrates the results of the exposure and ecotoxicity data to evaluate the likelihood of adverse ecological effects. One method of integrating the results of exposure and ecotoxicity data is called the quotient method. For this method, risk quotients (RQs) are calculated by dividing exposure estimates by ecotoxicity values, both acute and chronic:

RQ = EXPOSURE/TOXICITY

RQs are then compared to OPP's levels of concern (LOCs). These LOCs are criteria used by OPP to indicate potential risk to nontarget organisms and the need to consider regulatory action. The criteria indicate that a pesticide used as directed has the potential to cause adverse effects on nontarget organisms. LOCs currently address the following risk presumption categories: (1) **acute high** - potential for acute risk is high, and regulatory action may be warranted in addition to restricted use classification; (2) **acute restricted use** - the potential for acute risk is high, but this may be mitigated through restricted use classification; (3) **acute endangered species** - the potential for acute risk to endangered species is high, and regulatory action may be warranted; and (4) **chronic risk** - the potential for chronic risk is high, and regulatory action may be warranted. Currently, AD does not perform assessments for chronic risk to plants, acute or chronic risks to nontarget insects, or chronic risk from granular/bait formulations to mammalian or avian species.

The ecotoxicity test values (i.e., measurement endpoints) used in the acute and chronic risk quotients are derived from the results of required studies. Examples of ecotoxicity values derived from the results of short-term laboratory studies that assess acute effects are: (1) LC_{50} (fish and birds) (2) LD_{50} (birds and mammals) (3) EC_{50} (aquatic plants and aquatic invertebrates) and (4) EC_{25} (terrestrial plants). Examples of toxicity test effect levels derived from the results of long-term laboratory studies that assess chronic effects are: (1) LOEC (birds, fish, and aquatic invertebrates) (2) NOEC (birds, fish and aquatic invertebrates) and (3) MATC (Maximum Allowable Toxic Concentration) (fish and aquatic invertebrates). For birds and mammals, the NOEC value is used as the ecotoxicity test value in assessing chronic effects. Other values may be used when justified. Generally, the MATC (defined as the geometric mean of the NOEC and LOEC) is used as the ecotoxicity test value in assessing chronic effects to fish and aquatic invertebrates. However, the NOEC is used if the measurement endpoint is production of offspring or survival.

Risk presumptions, along with the corresponding RQs and LOCs are tabulated below.

Risk Presumptions for Terrestrial Animals

Risk Presumption	RQ	LOC
Birds and Wild Mammals		
Acute High Risk	EEC[1]/LC_{50} or LD_{50}/sqft[2] or LD_{50}/day[3]	0.5

Acute Restricted Use	EEC/LC_{50} or LD_{50}/sqft or LD_{50}/day (or LD_{50} < 50 mg/kg)	0.2
Acute Endangered Species	EEC/LC_{50} or LD_{50}/sqft or LD_{50}/day	0.1
Chronic Risk	EEC/NOEC	1

[1] abbreviation for Estimated Environmental Concentration (ppm) on avian/mammalian food items

[2] $\frac{mg/ft^2}{LD_{50} * wt. of bird}$ [3] $\frac{mg\ of\ toxicant\ consumed/day}{LD_{50} * wt. of bird}$

Risk Presumptions for Aquatic Animals

Risk Presumption	RQ	LOC
Acute High Risk	EEC[1]/LC_{50} or EC_{50}	0.5
Acute Restricted Use	EEC/LC_{50} or EC_{50}	0.1
Acute Endangered Species	EEC/LC_{50} or EC_{50}	0.05
Chronic Risk	EEC/MATC or NOEC	1

[1] EEC = (ppm or ppb) in water

Risk Presumptions for Plants

Risk Presumption	RQ	LOC
Terrestrial and Semi-Aquatic Plants		
Acute High Risk	EEC[1]/EC_{25}	1
Acute Endangered Species	EEC/EC_{05} or NOEC	1
Aquatic Plants		
Acute High Risk	EEC[2]/EC_{50}	1
Acute Endangered Species	EEC/EC_{05} or NOEC	1

[1] EEC = lbs ai/A

[2] EEC = (ppb/ppm) in water

A. Environmental Fate Assessment Summary (excerpted from the Environmental Fate Science Chapter of this RED document)

No fate studies for DDBSA are available in US EPA's files. It was decided by the agency during Phase IV or reregistration that data in the open literature would be utilized in the DDBSA environmental fate assessment. The EPI Suite model was run to obtain different environmental properties for DDBSA's. These values are provided in Section 3.0, "Model Results**."** The output parameters model support that any potential impacts are expected to be very short-lived. This is because the chemical is not likely to persist in water or microbial soils and sediments. The Agency also conducted a literature search to further support the output parameters that were provided by the EPI Suite model. The results of the literature search are presented in Section 4.0, "Additional Data from Literature Search."

Sodium dodecylbenzene sulfonate is highly unlikely to bioaccumulate in the environment or aquatic organisms (i.e. fish) because the low value for the log Kow (3). The chemical is also expected to be soluble in water such that it will exhibit mobility through the soil. In addition, the low log Koc (4.2261) further supports the expected soil mobility. The model-calculated linear and non-linear biodegradation probabilities suggest that the linear carbon chain will biodegrade rapidly, whereas the benzene ring is not expected to biodegrade as rapidly. The short half life of approximately 7.914 hours indicates that if this chemical is present in the soil, it is not likely to be volatile and is expected to degrade rapidly.

DDBSA is expected to behave very similarly as what is projected for sodium dodecylbenzene sulfonate. Based on the low Kow value (3.80), DDBSA is highly unlikely to bioaccumulate in the environment or aquatic organisms (i.e. fish). The chemical is also expected to be soluble in water such that it will exhibit mobility through the soil. In addition, the log Koc (3.6944) is low, and this further supports the expected soil mobility. The model-calculated linear and non-linear biodegradation probabilities suggest that the chemical will most likely biodegrade rapidly. The short half life of approximately 9.485 hours indicates that this chemical is not likely to be volatile from soils and is expected to degrade rapidly.

As a result of the modular output along with the information gathered from the literature search, the environmental fate of alkylbenzene sulfonates is not likely to be of a concern. Likewise, minimal or no environmental exposure is expected to occur from the majority of alkylbenzene sulfonate antimicrobial pesticide uses because it is unlikely that any appreciable exposure to terrestrial or aquatic organisms would occur. This is assumed based on the information that a very small number of pounds of this chemical are sold for commercial down-the-drain use.

B. Environmental Exposure Assessment

Environmental exposure modeling was not conducted for alkylbenzene sulfonic acids and sulfonates because the currently registered uses are indoor spray applications. Uses such as urinals and toilet bowls could result in minimal exposure to the environment when flushed. However, significant environmental exposure is not expected for the following reasons: 1.) total LAS usage for these industrial applications is very minor - a very small percentage of the total pounds used in

antimicrobials; and commercial only use precludes broad environmental exposures that might occur with residential use, applications are mostly sprayed on and allowed to air dry 2.) LAS breakdown and degradation in the environment is very rapid, 3.) LAS is significantly reduced by sewage treatment. Industrial water treatment requires a NPDES permit in order to discharge effluents.

C. Environmental Risk Assessment

Linear alkyl benzene sulfonates (LAS) have been the principal ingredient in laundry detergent for 30+ years. Volume 12 (10) of the 1993 issue of Environmental Toxicology and Chemistry featured a series of papers on environmental impacts of LAS in a special symposium: Surfactants and Their Environmental Safety - convened by R.A. Kimerle, N.T. De Oude and T.W. La Point. Two papers provide excellent summaries of ecotoxicity endpoints from literature, and feature laboratory vs field analysis of detergent generated LAS impacts on aquatic organisms. An assessment of short and long-term impacts of LAS detergents on the environment was conducted. Monitoring indicates that concentrations of 0.230 mg/L (continuous criterion concentration) and 0.625 mg/L (criterion maximum concentration) are rarely exceeded in aquatic systems protected by activated sludge treatment systems. Ecotoxicity studies indicate that a laboratory derived NOAEC value of 0.40 mg/L LAS is protective of structure and function of experimental streams. Mortality was determined more sensitive than growth as a chronic endpoint in chronic fathead minnow (*Pimephales promelas*) studies. The chronic NOAEC toxicity value from the 28 day study for fathead minnow using carbon chain C11.7 was 0.7 mg/L (Fairchild et al, 1993). In a second symposia study, the in situ toxicity of LAS to natural periphyton communities before and after wastewater treatment was assessed. Upstream and downstream algal communities were evaluated before and after the introduction of LAS into the stream. LAS inhibitory effect levels were higher (3.3 mg/L) than average levels recorded in wastewater treatment plant outflows in the U.S. (0.115 average). Increases and decreases in periphyton community abundance were observed, but determined not to be significant for the three major species evaluated: *Amphora perpusilla, Navicula minima, and Schizothrix calcicola* (Lewis et al, 1993).

No environmental exposure is expected to occur from the majority of linear alkylbenzene sulfonate uses and it is unlikely that any appreciable exposure to terrestrial or aquatic organisms would occur from limited commercial down-the-drain use because of the very small number of pounds sold for these uses as compared to the detergent market and rapid degradation.

D. Endangered Species Considerations

Section 7 of the Endangered Species Act, 16 U.S.C. Section 1536(a)(2), requires all federal agencies to consult with the National Marine Fisheries Service (NMFS) for marine and andronomus listed species, or the United States Fish and Wildlife Services (FWS) for listed wildlife and freshwater organisms, if they are proposing an "action" that may affect listed species or their designated habitat. Each federal agency is required under the Act to insure that any action they

authorize, fund, or carry out is not likely to jeopardize the continued existence of a listed species or result in the destruction or adverse modification of designated critical habitat. To jeopardize the continued existence of a listed species means "to engage in an action that reasonably would be expected, directly or indirectly, to reduce appreciably the likelihood of both the survival and recovery of a listed species in the wild by reducing the reproduction, numbers, or distribution of the species." 50 C.F.R. § 402.02.

To facilitate compliance with the requirements of the Endangered Species Act subsection (a)(2) the Environmental Protection Agency, Office of Pesticide Programs has established procedures to evaluate whether a proposed registration action may directly or indirectly reduce appreciably the likelihood of both the survival and recovery of a listed species in the wild by reducing the reproduction, numbers, or distribution of any listed species (U.S. EPA 2004). After the Agency's screening-level risk assessment is performed, if any of the Agency's Listed Species LOC Criteria are exceeded for either direct or indirect effects, a determination is made to identify if any listed or candidate species may co-occur in the area of the proposed pesticide use. If determined that listed or candidate species may be present in the proposed use areas, further biological assessment is undertaken. The extent to which listed species may be at risk then determines the need for the development of a more comprehensive consultation package as required by the Endangered Species Act.

For certain use categories, the Agency assumes there will be minimal environmental exposure, and only a minimal toxicity data set is required (Overview of the Ecological Risk Assessment Process in the Office of Pesticide Programs U.S. Environmental Protection Agency - Endangered and Threatened Species Effects Determinations, 1/23/04, Appendix A, Section IIB, pg.81). Chemicals in these categories therefore do not undergo a full screening-level risk assessment, and are considered to fall under a "no effect" determination. The active ingredient uses of alkylbenzene sulfonic acids and sulfonates fall into this category for the following reasons:

1. The amount that will actually reach the environment is very small based on usage data for down-the-drain uses.
2. Use for toilets and urinals is limited (no home-owner or residential uses are registered).
3. Breakdown of LAS in the environment and via sewage treatment is rapid and well documented in the literature.

The labeled antimicrobial uses of alkylbenzene sulfonic acids and sulfonates are not expected to result in significant environmental exposure. Therefore, no adverse effects (NE) to listed species are anticipated.

E. Inert Ingredient Use

The alkylbenzene sulfonates are used as "inert" ingredients in agricultural herbicide

formulations. Preplant incorporated and preemergence herbicide treatments are typically applied once per year to the tilled, minimally tilled or no-tilled field before planting or before crop emergence in the spring. Spray applications are primarily via ground spray boom and occasionally by aircraft if a wet spring. Movement of the alkylbenzene sulfonates from the treated field to the aquatic environment can occur at the time of application due to spray drift, or following application via surface water/soil flow or by percolation to groundwater. The FIRST model has predicted a maximum potential concentration of 6.6 ppb alkylbenzene sulfonates in drinking water from inert agricultural uses (memo from K. Leifer, 2006). Available modeling and literature suggest that these chemicals will most likely biodegrade rapidly in soil due to microbial degradation.

The inert agricultural uses of alkylbenzene sulfonates are not expected to adversely affect avian or mammalian species on an acute or chronic basis. Aquatic organisms are also not expected to be adversely affected by inert alkylbenzene sulfonates use acutely or chronically due to the low predicted level of alkylbenzene sulfonates in water by FIRST. A chronic freshwater fish toxicity test NOAEC of 400 ug/L alkylbenzene sulfonates is considered protective of ecosystem structure and function in experimental streams. Therefore, the predicted concentration of 6.6 ug/L in water is well below our chronic Level of Concern (LOC).

III. Confirmatory Data Required – N/A

IV. Label Hazard Statements for Terrestrial and Aquatic Organisms

Manufacturing and end-use products must state:

"Do not discharge effluent containing this product into lakes, streams, ponds, estuaries, oceans, or other waters unless in accordance with the requirements of a National Pollutant Discharge Elimination System (NPDES) permit and the permitting authorities are notified in writing prior to discharge. Do not discharge effluent containing this product to sewer systems without previously notifying the local sewage treatment plant authority. For guidance contact your State Water Board or Regional Office of the EPA."

V. REFERENCES

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INTERNATIONAL PROGRAMME ON CHEMICAL SAFETY

ENVIRONMENTAL HEALTH CRITERIA 169

LINEAR ALKYLBENZENE SULFONATES AND RELATED COMPOUNDS

This report contains the collective views of an international group of experts and does not necessarily represent the decisions or the stated policy of the United Nations Environment Programme, the International Labour Organisation, or the World Health Organization.

First draft prepared at the National Institute of Health Sciences, Tokyo, Japan, and the Institute of Terrestrial Ecology, Monk's Wood, United Kingdom

Published under the joint sponsorship of the United Nations Environment Programme, the International Labour Organisation, and the World Health Organization

World Health Organization
Geneva, 1996

The International Programme on Chemical Safety (IPCS) is a joint venture of the United Nations Environment Programme, the International Labour Organisation, and the World Health Organization. The main objective of the IPCS is to carry out and disseminate evaluations of the effects of chemicals on human health and the quality of the environment. Supporting activities include the development of epidemiological, experimental laboratory, and risk-assessment methods that could produce internationally comparable results, and the development of manpower in the field of toxicology. Other activities carried out by the IPCS include the development of know-how for coping with chemical accidents, coordination of laboratory testing and epidemiological studies, and promotion of research on the mechanisms of the biological action of chemicals.

WHO Library Cataloguing in Publication Data

Linear Alkylbenzene Sulfonates and Related Compounds.

(Environmental health criteria ; 169)
1.Alkane sulfonates - adverse effects 2.Environmental exposure 3.Guidelines I.Series

ISBN 92 4 157169 1 (NLM Classification: QU 98)
ISSN 0250-863X

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NOTE TO READERS OF THE CRITERIA MONOGRAPHS

Every effort has been made to present information in the criteria monographs as accurately as possible without unduly delaying their publication. In the interest of all users of the environmental health criteria monographs, readers are requested to communicate any errors that may have occurred to the Director of the International Programme on Chemical Safety, World Health Organization, Geneva, Switzerland, in order that they may be included in corrigenda, which will appear in subsequent volumes.

* * *

A detailed data profile and a legal file can be obtained from the International Register of Potentially Toxic Chemicals, Case Postale 356, 1219 Châtelaine, Geneva, Switzerland (Telephone no. 979 9111).

* * *

This publication was made possible by financial support from the US Environmental Protection Agency, USA, and from the European Commission.

ENVIRONMENTAL HEALTH CRITERIA FOR LINEAR ALKYLBENZENE SULFONATES AND RELATED COMPOUNDS

A WHO Task Group on Environmental Health Criteria for Linear Alkylbenzene Sulfonates and Related Compounds met at the World Health Organization, Geneva, on 18–22 October 1993. Dr E. Smith, IPCS, welcomed the participants on behalf of Dr M. Mercier, Director of IPCS, and of the three IPCS cooperating organizations (UNEP, ILO, and WHO). The Group reviewed and revised a draft document and evaluated the risks for human health and the environment of exposure to linear alkylbenzene sulfonates, a-olefin sulfonates, and alkyl sulfonates.

The sections of the first draft on toxicology and human health were prepared at the National Institute of Health Sciences (NIHS), Tokyo, Japan, and the sections on the environment at the Institute of Terrestrial Ecology (ITE), Monks Wood, United Kingdom.

Dr E. Smith of the IPCS Central Unit was responsible for the scientific content of the monograph and Mrs E. Heseltine, St Léon-sur-Vézère, France, for the editing.

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The efforts of all who helped in the preparation and finalization of the monograph are gratefully acknowledged.

1. OVERALL SUMMARY, EVALUATION, AND RECOMMENDATIONS

1.1 Identity and analytical methods

Linear alkylbenzene sulfonates (LAS), alpha-olefin sulfonates (AOS), and alkyl sulfates (AS) are anionic surfactants with molecules characterized by a hydrophobic and a hydrophilic (polar) group. Commercial mixtures consist of isomers and homologues of related compounds, which differ in physicochemical properties, resulting in formulations for various applications.

LAS, AOS, and AS can be analysed by nonspecific methods. The assay usually used is one for substances that react with methylene blue, which responds to any compound containing an anionic and hydrophobic group. It thus suffers from analytical interference if used for environmental samples; furthermore, the sensitivity of this method is about 0.02 mg/litre. Although nonspecific alternatives to this method have been developed, they are not commonly used. Specific methods for environmental analysis are available only for LAS and AS. An improved method based on methylene blue reactivity and high-performance liquid chromatography (HPLC) is available for analysis of AOS.

LAS are nonvolatile compounds produced by sulfonation of linear alkylbenzene. Commercial products are always mixtures of homologues of different alkyl chain lengths (C_{10}–C_{13} or C_{14}) and isomers differing in the phenyl ring positions (2 to 5 phenyl). All of the homologues and isomers of LAS can be determined in environmental samples and other matrices by specific analytical methods such as HPLC, gas chromatography, and gas chromatography–mass spectrometry.

AOS are nonvolatile compounds produced by sulfonation of alpha-olefins. They are mixtures of two compounds, sodium alkene sulfonate and hydroxyalkane sulfonate, with alkyl chain lengths of C_{14}–C_{18}.

AS are nonvolatile compounds produced by sulfation of oleochemical or petrochemical alcohols. They are mixtures of homologues with alkyl chain lengths of C_{10}–C_{18}. Specific analytical methods are being developed for environmental monitoring.

1.2 Sources of human and environmental exposure

LAS, AOS, and AS are used as active ingredients in household and personal care products and in specialized applications. After use, such detergent compounds are discharged into the environment in wastewater.

There is occupational exposure to these compounds. The exposure of the general human population and of environmental organisms depends on the application of LAS, AOS, and AS (and other surfactants), on local sewage treatment practices, and on the characteristics of the receiving environment.

In 1990, worldwide consumption figures were about 2 million tonnes of LAS, 86 000 tonnes of AOS, and 289 000 tonnes of AS.

1.3 Environmental concentrations

1.3.1 Linear alkylbenzene sulfonates

Concentrations of LAS have been quantified by means of a specific, sensitive analytical method in almost every environmental compartment in which they might be present. The concentrations decrease progressively in the order wastewater > treated effluent > surface waters > the sea.

In areas where LAS are the predominant surfactants used, the concentrations are usually 1–10 mg/litre in wastewater, 0.05–0.1 mg/litre in effluents treated biologically, 0.05–0.6 mg/litre in effluents treated with a percolating filter, 0.005–0.05 mg/litre in surface waters below sewage outfalls (with concentrations decreasing rapidly to 0.01 mg/litre downstream of the outfall), < 1–10 mg/kg in river sediments ($\leq$ 100 mg/kg in highly polluted sediments near discharge zones), 1–10 g/kg in sewage sludge, and < 1–5 mg/kg in sludge-amended soils (initially 5–10 mg/kg; – 50 mg/kg have been reported after atypically high applications of sludge). The concentrations of LAS in estuarine waters are 0.001–0.01 mg/litre, although higher levels occur where wastewater is discharged directly. The concentrations in offshore marine waters are < 0.001–0.002 mg/litre.

It should be noted that the environmental concentrations of LAS vary widely. This variation is due to differences in analytical methods, in the characteristics of sampling sites (ranging from highly polluted areas with inadequate sewage treatment to areas where sewage undergoes extensive treatment), in season (which can account for a difference of twofold), and in consumption of LAS.

Environmental monitoring shows that there has been no accumulation of LAS in environmental compartments over time. The concentrations in soil do not increase with time but decrease owing to mineralization. As LAS do not degrade under strictly anaerobic conditions (to generate methane), it cannot be concluded that they are mineralized in anaerobic sediments. With current use, the rate of assimilation of LAS in all receiving environmental compartments is equal to the rate of input, implying a steady state.

1.3.2 alpha-Olefin sulfonates and alkyl sulfates

Limited data are available on the concentrations of AOS in the environment owing to the difficulty of analysing them in environmental samples. Nonspecific colorimetric methods (such as that based on methylene blue) allow detection of anionic surfactants in general, but they suffer from analytical interferences and are not suitable for determining specific concentrations of AOS. A specific method is being developed for measuring AS in environmental samples.

Studies conducted in the laboratory indicate that AOS and AS are mineralized rapidly in all environmental compartments and are virtually entirely removed from sewage during treatment. The concentrations in surface water, sediments, soil, estuarine water, and the marine environment are probably low. The levels of AOS in river water have been found to be low.

1.4 Environmental transport, distribution, and transformation

At te mperatures below 5-10°C, the biodegradation kinetics of LAS, AOS, and AS is reduced because of a reduction in microbial activity.

1.4.1 Linear alkylbenzene sulfonates

The routes by which LAS enter the environment vary among countries, but the main route is via discharge from sewage treatment works. When wastewater treatment facilities are absent or inadequate, sewage may be discharged directly into rivers, lakes, and the sea. Another route of entry of LAS to the environment is by the spreading of sewage sludge on agricultural land.

Throughout their passage into the environment, LAS are removed by a combination of adsorption and primary and ultimate bio-degradation. LAS are adsorbed onto colloidal surfaces and onto suspended particles, with measured adsorption coefficients of 40-5200 litres/kg depending on the media and the structure of the LAS. They biodegrade in surface water (half-life, 1-2 days), aerobic sediments (1-3 days), and marine and estuarine systems (5-10 days).

During primary sewage treatment, about 25% of LAS (range, 10-40%) are adsorbed onto and removed with waste sludge. They are not removed during anaerobic sludge digestion but are removed during aerobic treatment of sludge, with a half-life of about 10 days. After application of sludge to soil, 90% of LAS are generally degraded within three months, with a half-life of 5-30 days.

The whole-body concentration factors for LAS range from 100 to 300, for the sum of ^{14}C-LAS and ^{14}C metabolites. Uptake by fish occurs mainly through the gills, with subsequent distribution to the

liver and gall-bladder after biotransformation. LAS are excreted rapidly, and there is therefore no evidence that they undergo biomagnification.

1.4.2 alpha-Olefin sulfonates

Fewer data are available on the environmental transport, distribution, and transformation of AOS than for LAS. It can be inferred that AOS are transported into the environment in a manner similar to that established for LAS, AS and other detergent surfactants, and the environmental fate of AOS is similar to that of LAS and AS. It is readily biodegraded under aerobic conditions, and primary biodegradation is complete within 2-10 days, depending on the temperature. Limited data are available on the bioaccumulation of AOS; no bioaccumulation was observed in fish. There are no data on abiotic degradation.

1.4.3 Alkyl sulfates

AS are transported into the environment by mechanisms similar to those that operate for LAS and AOS. They are readily biodegradable under aerobic and anaerobic conditions in the laboratory and under environmental conditions; primary biodegradation is complete within 2-5 days. The whole-body bioconcentration factor ranges from 2 to 73 and varies with the chain length of alkyl sulfate homologues. AS are taken up, distributed, biotransformed, and excreted by fish in the same way as LAS and are not bioconcentrated in aquatic organisms.

1.5 Kinetics

LAS, AOS, and AS are readily absorbed by the gastrointestinal tract, widely distributed throughout the body, and extensively metabolized. LAS undergo omega- and ß-oxidation. The parent compounds and metabolites are excreted mainly through the kidney, although a proportion of an absorbed dose may be excreted as metabolites in the faeces by biliary excretion. Only minimal amounts of LAS, AOS, and AS appear to be absorbed through intact skin, although prolonged contact may compromise the integrity of the epidermal barrier, thereby permitting greater absorption; high concentrations may reduce the time required for penetration.

1.6 Effects on experimental animals and *in vitro* test systems

The oral LD_{50} values for sodium salts of LAS were 404-1470 mg/kg body weight in rats and 1259-2300 mg/kg body weight in mice, suggesting that rats are more sensitive than mice to the toxicity of LAS. An oral LD_{50} of 3000 mg/kg body weight was measured for a sodium salt of AOS in mice. The oral LD_{50} values of AS in rats were 1000-4120 mg/kg body weight. LAS, AOS, and AS irritate the skin

and eye.

Minimal effects, including biochemical alterations and histo-pathological changes in the liver, have been reported in subchronic studies in which rats were administered LAS in the diet or drinking-water at concentrations equivalent to doses greater than 120 mg/kg body weight per day. Although ultrastructural changes were observed in liver cells at lower doses in one study, the changes appeared to be reversible. Effects were not seen at similar doses in other studies, but the organs may have been examined more closely in the initial study. Reproductive effects, including decreased pregnancy rate and litter loss, have been reported in animals administered doses > 300 mg/kg per day. Histopathological and biochemical changes were observed after long-term dermal application to rats of solutions of > 5% LAS, and after 30 days' application to the skin of guinea-pigs of 60 mg/kg body weight. Repeated dermal application of $\geq$ 0.3% solutions of LAS induced fetotoxic and reproductive effects, but also induced maternal toxicity. Few data are available from studies in experimental animals that allow evaluation of the potential effects of AOS in humans. No effects were observed in rats administered oral doses of 250 mg/kg body weight per day chronically, but fetotoxicity was seen in rabbits administered a maternally toxic dose of 300 mg/kg body weight per day. Application of AOS to the skin and eyes of experimental animals induced local effects.

Although the effects of short- and long-term exposure of animals to AS have been investigated in several studies, most suffered from inadequate histopathological examination or small group sizes; furthermore, the highest doses used in the long-term studies did not produce any toxic effects, so that an NOAEL could not be established. Effects have, however, been reported consistently in rats administered AS in the diet or drinking-water at concentrations equivalent to 200 mg/kg body weight per day or more. Local effects have been observed on the skin and eyes after topical application of concentrations of about 0.5% AS or more. Maternally toxic and fetotoxic effects have been observed at higher concentrations.

Most of the long-term studies are inadequate to evaluate the carcinogenic potential of LAS, AOS, and AS in experimental animals, owing to factors such as small numbers of animals, limited numbers of doses, absence of a maximal tolerated dose, and limited histo-pathological examination in the majority of studies. In those studies in which the pathological findings were adequately reported, maximal tolerated doses were not used, and the doses did not produce toxic effects. Subject to these limitations, however, the studies in which animals were administered LAS, AOS, or AS orally gave no evidence of carcinogenicity; long-term studies in which AOS was applied by skin painting studies also showed no effect.

On the basis of limited data, these compounds do not appear to be genotoxic *in vivo* or *in vitro*.

1.7 Effects on humans

The results of patch tests show that human skin can tolerate contact with solutions containing up to 1% LAS, AOS, or AS for 24 h with only mild irritation reactions. These surfactants caused delipidation of the skin surface, elution of natural moisturizing factor, denaturation of the proteins of the outer epidermal layer, and increased permeability and swelling of the outer layer. Neither LAS, AOS, nor AS induced skin sensitization in volunteers, and there is no conclusive evidence that they induce eczema. No serious injuries or fatalities have been reported following accidental ingestion of these surfactant by humans.

1.8 Environmental effects

1.8.1 Linear alkylbenzene sulfonates

1.8.1.1 Aquatic environment

LAS have been studied extensively both in the laboratory (short- and long-term studies) and under more realistic conditions (micro- and mesocosm and field studies). In general, a decrease in alkyl chain length or greater internalization of the phenyl group is accompanied by a decrease in toxicity. Observations in fish and *Daphnia* indicate that a decrease in chain length of one unit (e.g. C_{12} to C_{11}) results in an approximately twofold decrease in toxicity.

The results of laboratory tests are as follows:

-- *Microorganisms:* The results are highly variable owing to the use of a variety of test systems (e.g. inhibition of activated sludge; mixed cultures and individual species). The EC_{50} values range from 0.5 mg/litre (single species) to > 1000 mg/litre. For microorganisms, there is no linear relationship between chain length and toxicity.

-- *Aquatic plants:* The results are highly species dependent. For freshwater organisms, the EC_{50} values are 10–235 mg/litre (C_{10}–C_{14}) in green algae, 5–56 mg/litre ($C_{11.1}$–C_{13}) in blue algae, 1.4–50 mg/litre ($C_{11.6}$–C_{13}) in diatoms, and 2.7–4.9 mg/litre ($C_{11.8}$) in macrophytes; marine algae appear to be even more sensitive. In algae, there is probably no linear relationship between chain length and toxicity.

-- *Invertebrates:* The acute $L(E)C_{50}$ values for at least 22 freshwater species are 4.6–200 mg/litre (chain length not specified; C_{13}) for molluscs; 0.12–27 mg/litre (not specified; $C_{11.2}$–C_{18})

for crustaceans; 1.7–16 mg/litre (not specified; $C_{11.8}$) for worms, and 1.4–270 mg/litre (C_{10}–C_{15}) for insects. The chronic L(E)C_{50} values are 2.2 mg/litre ($C_{11.8}$) for insects and 1.1–2.3 mg/litre

($C_{11.8}$–C_{13}) for crustaceans. The chronic no-observed-effect concentration (NOEC; based on lethality or reproductive effects) is 0.2–10 mg/litre (not specified; $C_{11.8}$) for crusta-ceans. Marine invertebrates appear to be more sensitive, with LC_{50} values of 1 to >100 mg/litre (almost all C_{12}) for 13 species, and NOECs of 0.025–0.4 mg/litre (not specified for all tests) for seven species tested.

-- *Fish:* The acute LC_{50} values are 0.1–125 mg/litre (C_8–C_{15}) for 21 freshwater species; the chronic L(E)C_{50} values are 2.4 and 11 mg/litre (not specified; $C_{11.7}$) for two species; and the NOECs are 0.11–8.4 to 1.8 mg/litre (not specified; $C_{11.2}$–C_{13}) for two species. Again, marine fish appear to be more sensitive, with acute LC_{50} values of 0.05–7 mg/litre (not specified; $C_{11.7}$) for six species and chronic LC_{50} values of 0.01–1 mg/litre (not specified) for two species. In most of the reports, the chain length was not reported. An NOEC of < 0.02 mg/litre (C_{12}) was reported for marine species.

The average chain length of products commonly used commercially is C_{12}. Compounds of many different chain lengths have been tested in *Daphnia magna* and fish, but the length tested in other freshwater organisms has usually been $C_{11.8}$. The typical acute L(E)C_{50} values for C_{12} LAS are 3–6 mg/litre in *Daphnia magna* and 2–15 mg/litre in freshwater fish, and the typical chronic NOECs are 1.2–3.2 mg/litre for Daphnia and 0.48–0.9 mg/litre for freshwater fish. The typical acute LC_{50} values for LAS of this chain length in marine fish are < 1–6.7 mg/litre.

Saltwater organisms, especially invertebrates, appear to be more sensitive to LAS than freshwater organisms. In invertebrates, the sequestering action of LAS on calcium may affect the availability of this ion for morphogenesis. LAS have a general effect on ion transport. Biodegradation products and by-products of LAS are 10–100 times less toxic than the parent compounds.

The results obtained under more realistic conditions are as follows: LAS have been tested in all freshwater tests at several trophic levels, including enclosures in lakes (lower organisms), model ecosystems (sediment and water systems), rivers below and above the outfall of wastewater treatment plants, and in experimental streams. C_{12} LAS were used in almost all cases. Algae appear to be more sensitive in summer than in winter, as the 3-h EC_{50} values were 0.2–8.1 mg/litre after photosynthesis, whereas in model ecosystems no effects were seen on the relative abundance of algal communities at 0.35 mg/litre. The no-effect levels in these studies were 0.24–5 mg/litre, depending on the organism and parameter tested. These results agree fairly well with those of laboratory tests.

1.8.1.2 Terrestrial environment

Information is available for plants and earthworms. The NOECs for seven plant species tested in nutrient solutions are < 10–20 mg/litre; that for three species tested in soils, based on growth, was 100 mg/kg (C_{10}–C_{13}). The 14-day LC_{50} for earthworms was > 1000 mg/kg.

1.8.1.3 Birds

One study of chickens treated in the diet resulted in an NOEC (based on egg quality) of > 200 mg/kg.

1.8.2 alpha-Olefin sulfonates

There are limited data on the effects of AOS on aquatic and terrestrial organisms.

1.8.2.1 Aquatic environment

Only the results of laboratory tests are available:

-- *Algae:* EC_{50} values of > 20–65 mg/litre (C_{16}–C_{18}) have been reported for green algae.

-- *Invertebrates:* LC_{50} values of 19 and 26 mg/litre (C_{16}–C_{18}) have been reported for Daphnia.

-- *Fish:* The acute LC_{50} values are 0.3–6.8 mg/litre (C_{12}–C_{18}) for nine species of fish. On the basis of short-term studies in brown trout *(Salmo trutta),* golden orfe *(Idus melanotus),* and harlequin fish *(Rasbora heteromorpha),* it can be concluded that the toxicity of C_{14}–C_{16} compounds is about five times lower than that of C_{16}–C_{18}, with LC_{50} values (all measured concentrations) of 0.5–3.1 (C_{16}–C_{18}) and 2.5–5.0 mg/litre (C_{14}–C_{16}). Two long-term studies in rainbow trout showed that growth is the most sensitive parameter, resulting in an EC_{50} of 0.35 mg/litre. In a marine fish, the grey mullet (Mugal cephalus), the 96-h LC_{50} value was 0.70 mg/litre.

1.8.2.2 Terrestrial environment

One study of plants in nutrient solutions showed NOECs of 32–56 mg/litre. In a study of chickens treated in the diet, an NOEC (based on egg quality) of > 200 mg/kg was reported.

1.8.3 Alkyl sulfates

1.8.3.1 Aquatic environment

AS have been studied in short- and long-term studies and in one study under more realistic conditions. Their toxicity is again dependent on the alkyl chain length; no information was available on any difference in toxicity between linear and branched AS.

The results of the laboratory tests are as follows:

-- *Microorganisms:* The EC_{50} values in a marine community were 2.1–4.1 mg/litre (C_{12}). The NOECs in Pseudomonas putida were 35–550 mg/litre (C_{16}–C_{18}).

-- *Aquatic plants:* The EC_{50} values were > 20–65 mg/litre (C_{12}–C_{13}) in green algae and 18–43 mg/litre (C_{12}) in macrophytes. The NOECs were 14–26 mg/litre (C_{12}–C_{16}/C_{18}) in green algae.

-- *Invertebrates:* The LC_{50} and EC_{50} values were 4–140 mg/litre (C_{12}/C_{15}–C_{16}/C_{18}) in freshwater species and 1.7–56 mg/litre (all C_{12}) in marine species. The chronic NOEC in Daphnia magna was 16.5 mg/litre (C_{16}/C_{18}) and those in marine species were 0.29–0.73 mg/litre (chain length not specified).

-- *Fish:* The LC_{50} values were 0.5–5.1 mg/litre (not specified; C_{12}–C_{16}) in freshwater species and 6.4–16 mg/litre (all C_{12}) in marine species. No long-term studies were available.

It should be noted that many of these studies were carried out under static conditions. As AS are readily biodegradable, their toxicity may have been underestimated. In a 48-h study with *Oryzias latipes*, the LC_{50} values were 46, 2.5 and 0.61 mg/litre (measured concentrations) for C_{12}, C_{14}, and C_{16} compounds, respectively. This and other studies indicate that toxicity differs by a factor of five for two units of chain length. In a flow-through biocenosis study with compounds of C_{16}–C_{18}, an NOEC of 0.55 mg/litre was observed.

1.8.3.2 Terrestrial environment

NOEC values of > 1000 mg/kg (C_{16}–C_{18}) were reported for earthworms and turnips.

1.9 Human health risk evaluation

LAS are the most widely used surfactants in detergents and cleaning products; AOS and AS are also used in detergents and personal care products. The primary route of human exposure is, therefore, through dermal contact. Minor amounts of LAS, AOS, and AS may be ingested in drinking-water and as a result of residues on utensils and food. Although limited information is available, the daily intake of LAS via these media can be estimated to be about 5 mg/person. Occupational exposure to LAS, AOS, and AS may occur during the formulation of various products, but no data are available on the effects in humans of chronic exposure to these compounds.

LAS, AOS, and AS can irritate the skin after repeated or prolonged dermal contact with concentrations similar to those found in undiluted products. In guinea-pigs, AOS can induce skin sensitization when the level of gamma-unsaturated sultone exceeds about 10 ppm.

The available long-term studies in experimental animals are inadequate to evaluate the carcinogenic potential of LAS, AOS, and AS, owing to factors such as study design, use of small numbers of animals, testing of insufficient doses, and limited histopathological examination. In the limited studies available in which animals were administered LAS, AOS, or AS orally, there was no evidence of carcinogenicity; the results of long-term studies in which AOS were administered by skin painting were also negative. These compounds do not appear to be genotoxic *in vivo* or *in vitro*, although few studies have been reported.

Minimal effects, including biochemical alterations and histopathological changes in the liver, have been reported in subchronic studies of rats administered LAS in the diet or drinking-water at concentrations equivalent to a dose of about 120 mg/kg body weight per day, although no effects were observed in studies in which animals were exposed to higher doses for longer periods. Dermal application of LAS caused both systemic toxicity and local effects.

The average daily intake of LAS by the general population, on the basis of limited estimates of exposure via drinking-water, utensils, and food, is probably much lower (about three orders of magnitude) than the levels shown to induce minor effects in experimental animals.

The effects of AOS in humans observed in the few studies available are similar to those reported in animals exposed to LAS. As insufficient data are available to estimate the average daily intake of AOS by the general population and on the levels that induce effects in humans and animals, it is not possible to evaluate with confidence whether exposure to AOS in the environment presents a risk to human health. The levels of AOS in media to which humans

may be exposed are likely to be lower than those of LAS, however, as AOS are used less.

Effects have been reported consistently in a few, limited studies in rats administered AS in the diet or drinking-water at concentrations equivalent to doses of 200 mg/kg body weight per day or more. Local effects on the skin and eyes have been observed after repeated or prolonged topical application. The available data are insufficient to estimate the average daily intake of AS by the general population. Since AS surfactants are not used as extensively as those containing LAS, however, intake of AS is likely to be at least three orders of magnitude lower than the doses shown to induce effects in animals.

1.10 Evaluation of effects on the environment

LAS, AS, and AOS are used in large quantities and are released into the environment via wastewater. Risk assessment requires comparison of exposure concentrations with concentrations that cause no adverse effects, and this can be done for several environmental compartments. For anionic surfactants in general, the most important compartments are sewage water treatment plants, surface waters, sediment- and sludge-amended soils, and estuarine and marine environments. Both biodegradation (primary and ultimate) and adsorption occur, resulting in decreased environmental concentrations and bioavailability. Reduction in chain length and loss of the parent structure both result in compounds that are less toxic than the parent compound. It is important that these considerations be taken into account when the results of laboratory tests are compared with potential effects on the environment. Furthermore, in assessing the risk associated with environmental exposure to these three anionic compounds, comparisons should be made with the results of tests for toxicity of compounds of the same chain length.

The effects of LAS on aquatic organisms have been tested extensively. In laboratory tests in freshwater, fish appeared to be the most sensitive species; the NOEC for fathead minnow was about 0.5 mg/litre (C_{12}), and these results were confirmed in tests under more realistic conditions. Differences have been observed among phyto-plankton: in acute 3-h assays on phytoplankton, the EC_{50} values were 0.2-0.1 mg/litre (C_{12}-C_{13}), whereas no effects on relative abundance were found in other tests at 0.24 mg/litre ($C_{11.8}$). Marine species appeared to be slightly more sensitive than most other taxonomic groups.

A broad range of concentrations of all three anionic compounds occurs in the environment, as shown by extensive measurements of LAS. Owing to this broad range, no generally applicable environmental risk assessment can be made for these compounds. A risk assessment must involve appropriate understanding of the exposure and effect concentrations in the ecosystem of interest.

Accurate data on exposure to AS and AOS are needed before an environmental risk assessment can be made. Models are therefore being used to assess exposure concentrations in the receiving environmental compartments. Data on the toxicity of AS and AOS to aquatic organisms, especially after chronic exposure to stable concentrations, are relatively scarce. The available data show that the toxicity of AOS and AS is similar to that of other anionic surfactants.

Saltwater organisms appear to be more sensitive than freshwater organisms to these compounds; however, their concentrations are lower in seawater, except near wastewater outlets. The fate and effects of these compounds in sewage in seawater have not been investigated in detail.

For an evaluation of the environmental safety of surfactants such as LAS, AOS, and AS, actual environmental concentrations must be compared with no-effect concentrations. Research requirements are determined not only by the intrinsic properties of a chemical but also by its pattern or trend of consumption. As these can vary considerably among geographic areas, assessment and evaluation must be carried out regionally.

1.11 Recommendations for protection of human health and the environment

1. As exposure to dusts may occur in the workplace (during processing and formulation), standard occupational hygiene practices should be used to ensure protection of workers' health.

2. The composition of formulations for consumer and industrial use should be designed to avoid hazard, particularly for formulations that are used for cleaning or laundering by hand.

3. Environmental exposure and effects should be appropriately monitored to provide early indications of any overloading of relevant environmental compartments.

1.12 Recommendations for further research

Human health

1. Since the skin is the primary route of human exposure to LAS, AOS, and AS and since no adequate long-term studies of dermal toxicity or carcinogenicity in experimental animals are available, it is recommended that suitably designed long-term studies in which these compounds are applied dermally be conducted.

2. In view of the lack of definitive data on the genotoxicity of

AOS and AS, additional studies should be performed *in vivo* and *in vitro*.

3. In view of the inadequacies of the available studies on reproductive and developmental toxicity, definitive studies should be carried out in laboratory animals to obtain data on the effects and on the effect and no-effect levels of LAS, AOS, and AS.

4. As exposure to LAS, AOS, and AS is not adequately defined, the exposure of the general population should be monitored, particularly when these surfactants are used for cleaning and laundering by hand.

5. Since LAS, AOS, and AS may enhance the transport of other chemicals in environmental media and modulate their bioavailability and toxicity in surface waters, river sediments, and soils to which humans may be exposed, interactions with other environmental chemicals and the consequences for humans should be investigated.

Environmental safety

6. Additional studies should be carried out on the mechanisms of adsorption and desorption of AOS and AS. Studies should also be done on the partitioning of LAS, AOS, and AS between dissolved and suspended colloidal particles in water. Mathematical models of sorption coefficients should be developed and validated on the basis of physical-chemical parameters.

7. Studies of the biodegradation of AOS and AS in sludge-amended soils and river sediments should be carried out when exposure occurs. Studies in river sediments (aerobic and anaerobic zones) should be performed downstream of treated and untreated wastewater and sewage outfalls.

8. Environmental concentrations of LAS, AOS, and AS should be monitored regionally and nationally in order to obtain information on exposure. Analytical methods should be developed for detecting low levels of AOS and AS in relevant environmental compartments.

9. National databases should be developed on the concentrations of LAS, AOS, and AS in wastewater and rivers and on the types, efficiency, and location of wastewater treatment plants, in order to facilitate an assessment of the impact of discharges of these surfactants to the environment.

10. Long-term studies of the toxicity of AOS and AS to fish (freshwater and marine) and aquatic invertebrates should be conducted in order to establish the relative sensitivity of these species.

A. Linear alkylbenzene sulfonates and their salts

A1. SUMMARY

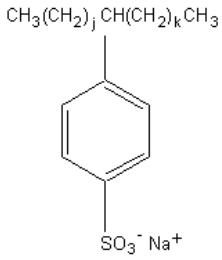
See Overall Summary, Evaluation, and Recommendations (pp. 7-21).

A2. IDENTITY, PHYSICAL AND CHEMICAL PROPERTIES, AND ANALYTICAL METHODS

A2.1 Identity (sodium salt)

Chemical formula: $C_nH_{2n-1}O_3S\ Na$ (*n*: 16-20) (for current commercial products)

Chemical structure:



j,k: integers (*j* + *k* = 7-11)

Common name: Sodium linear alkylbenzenesulfonate

Common synonyms: LAS, LAS sodium salt, linear alkylbenzene-sulfonic acid sodium salt, linear dodecyl-benzenesulfonic acid sodium salt, sodium straight chain alkylbenzenesulfonate

CAS Registry number: 68411-30-3 (LAS sodium salt, C10-13 alkyl)

Common trade names: Ablusol DBC, Agrilan WP, Alkasurf CA, Arylan, Atlas G-3300B, Atlox, Biosoft, Berol, Calsoft, Demelan CB-30, Elecut S-507, Elfan, Emulphor ECB, Emulsogen Brands, Gardilene, Hexaryl, Idet, Kllen, Lutopon SN, Manro, Marlopon, Marlon A, Nacconol 90 F, Nansa HS 80, Nansa Lutersit, Neopelex, Sandozin AM, Sipex, Sulfamin, Sulframin, Surfax 495, Teepol, Tersapol, Tersaryl, Ufaryl DL

80P, Witconate (McCutcheon, 1993)

Abbreviations: LAS, LAS-Na

Specification: LAS are anionic surfactants which were introduced in the 1960s as more biodegradable replacements for highly branched alkyl-benzene sulfonates. LAS are produced by sulfonation of linear alkylbenzene (LAB) with sulfur trioxide (SO_3), usually on a falling film reactor or with oleum in batch reactors. The corresponding sulfonic acid is subsequently neutralized with an alkali such as caustic soda. The hydrocarbon intermediate, LAB, is currently produced mainly by alkylation of benzene with *n*-olefins or *n*-chloroparaffins using hydrogen fluoride (HF) or aluminium chloride ($AlCl_3$) as a catalyst, and the LAS derivatives are thus generally referred to in that context (Cavalli et al., 1993a). Currently, 74% of world production of LAB is via HF and 26% via $AlCl_3$ (Berna et al., 1993a).

LAS are a mixture of homologues and phenyl positional isomers, each containing an aromatic ring sulfonated at the *para* position and attached to a linear alkyl chain of C_{10}-C_{14} (in Europe, predominantly C_{10}-C_{13}) at any position except the terminal one. The product is generally used in detergents in the form of the sodium salt.

Some of the typical characteristics of LAS, including the distribution of alkyl chain lengths and the positions of the phenyl rings in the two types of LAS used in laundry detergents, are shown in the box below. The United States Toxic Substances Control Act inventory lists LAS homologues with chain lengths up to C_{18} (Tables 1 and 2), but these products are not currently used for commercial purposes.

A2.2 Physical and chemical properties

The properties of LAS differ greatly depending on the alkyl chain length. Table 3 shows the Krafft points (temperature at which 1 g of LAS dissolve in 100 ml of water) and the relative critical micelle concentrations of the single homologues.

Typical characteristics of linear alkylbenzene sulfonates used in laundry detergents:

Appearance (commercial product):	White paste (containing water)
Average length of alkyl carbon chain:	11.8
Average relative molecular mass:	342
Unsulfonated matter:	1-2%
Alkyl chain distribution:	
C_{10}	10-15%
C_{11}	25-35%
C_{12}	25-35%
C_{13}	15-30%
C_{14}	0-5%

Phenyl ring position	LAS (LAB-HF[a])	LAS (LAB-$AlCl_3$[b])
2-phenyl	18	28
3-phenyl	16	19
4-phenyl	17	17
5-phenyl	24	18
6-phenyl	25	18

From Cavalli et al. (1993a)
[a] Hydrofluoric acid-catalysed process
[b] Aluminium chloride-catalysed process

Table 1. Mixtures of linear alkylbenzene sulfonates and their salts found in the United States Toxic Substances Control Act inventory

Generic benzene-sulfonic acid groups	CAS number	
	Acid	Salts
(C_{10-13})Alkyl-[a]		68411-30-3 (sodium salt)
(C_{10-16})Alkyl-	68584-22-5	68584-23-6 (calcium salt)
		68584-26-9 (magnesium salt)
		68584-27-0 (potassium salt)
Mono (C_{6-12})alkyl-		68608-87-7 (sodium salt)
Mono(C_{7-17})alkyl-		68953-91-3 (calcium salt)
		68953-94-6 (potassium salt)
Mono(C_{9-12})alkyl-		68953-95-7 (sodium salt)
Mono(C_{10-16})alkyl-		68910-31-6 (ammonium salt)
		68081-81-2 (sodium salt)
Mono(C_{12-18})alkyl-		68648-97-5 (potassium salt)

[a] There may be more than one alkyl substituent per benzene ring (United

States Environmental Protection Agency, 1981).

Table 2. Individual linear alkylbenzene sulfonates (LAS) found in the United States Toxic Substances Control Act inventory

Parent sulfonic acid (abbreviation)	Empirical formula	CAS Registry number		
		Acids	Sodium salts	Other salts
Dodecylbenzene (C_{10} LAS)	$C_{16}H_{26}O_3S$	1322-98-1 (140-60-3)[a]	1322-98-1 (2627-06-7)[a]	
Undecylbenzene (C_{11} LAS)	$C_{17}H_{28}O_3S$	50854-94-9	27636-75-5	NH_4 salt, 61931-75-7
Dodecylbenzene (C_{12} LAS)	$C_{18}H_{30}O_3S$	27176-87-0	25155-30-0 (2211-98-5)[a] (68628-60-4)[b] (18777-54-3)[c]	Al salt, 29756-98-7; NH4 salt, 1331-61-9; Ca salt, 26264-06-2; K salt, 27177-77-1; also numerous salts with alkyl amines
Tridecylbenzene (C_{13} LAS)	$C_{19}H_{32}O_3S$	25496-01-9	26248-24-8	Also salts with alkyl amines
Tetradecylbenzene (C_{14} LAS)	$C_{20}H_{34}O_3S$	30776-59-1 (47377-10-2)a	28348-61-0 (1797-33-7)[a]	
Pentadecylbenzene (C_{15} LAS)	$C_{21}H_{36}O_3S$	61215-89-2		K salt, 64716-02-5
Hexadecylbenzene (C_{16} LAS)	$C_{22}H_{38}O_3S$	(16722-32-0)[a]		K salt, 64716-00-3
Heptadecylbenzene (C_{17} LAS)	$C_{23}H_{40}O_3S$	39735-13-2		

From United States Environmental Protection Agency (1981)
[a] Specifies *para* substitution
[b] Specifies *para* substitution at second position on alkyl chain

Table 3. Relationship between alkyl chain length, Krafft point, and critical micelle concentration (CMC) of linear alkylbenzene sulfonates

Alkyl chain length	Krafft point (°C)	CMC × 10^{-3} (25°C)
10	-1	5.8
12	3	1.1
14	8	0.24
15	-	0.11
16	13	-

From Ohki & Tokiwa (1970)

The solubility of surfactants in water, defined as the concentration of dissolved molecules in equilibrium with a crystalline surfactant phase, increases with rising temperature. For surfactants, a distinct, sharp bend (break point) is observed in the solubility/temperature curve. The steep rise in solubility above the sharp bend is caused by micelle formation. The point of intersection of the solubility and critical micelle curves plotted as a function of temperature is referred to as the Krafft point, which is a triple point at which surfactant molecules coexist as monomers, micelles, and hydrated solids. The temperature corresponding to the Krafft point is called the Krafft temperature. Above the Krafft temperature and critical micelle concentration, a micellar solution is formed and higher than aqueous solubility may be obtained.

As commercial LAS are a mixture of homologues and phenyl-positional isomers, their properties may differ. Even some products with the same alkyl chain distribution (same average carbon number) have different properties, depending on the 2-phenyl isomer content. The solubility in water of commercial LAS used for detergents (average alkyl carbon length, 11.8), for example, which is important for liquid formulations, is typically about 25% at 25°C for LAS (LAB via HF) and about 38% at 25°C for LAS (LAB via $AlCl_3$) (Cavalli et al., 1993a).

As LAS are anionic surfactants, they lower the surface tension of water so that it can wet and penetrate fabrics more easily to loosen and remove soils and stains. Micelles, which are formed at low concentrations, solubilize oil and stains effectively (Ohki & Tokiwa, 1969). Other important properties of LAS are detergency, foaming, sensitivity to Ca and Mg ions, wetting, and surface tension, which reach their optimal values generally when the alkyl chain length is about C_{12} (Yamane et al., 1970).

A physico-chemical property often used in environmental modelling is the octanol-water partition coefficient (K_{ow}). Although it is impossible to measure the K_{ow} for surface-active compounds like LAS, it can be calculated. Roberts (1989) modified the fragment method of Leo & Hansch (1979) in order to take the branching of position into account. He thus defined a function, log (*CP* + 1), where *CP* is found by pairing off carbon atoms along the two branches up to the terminus of the shorter branch. (In the case of LAS, *CP* is the carbon number of the shorter of the integers *j* and *k* noted in section 2.1.) This gave the formula:

$$\log K_{ow} = ALK - 1.44 \log (CP + 1),$$

where *ALK* is log K_{ow} calculated without a branch factor.

In order to calculate log K_{ow} for multicomponent materials like LAS, the calculated K_{ow} for each component is multiplied by the mole fraction of the corresponding component, the products are summed, and the logarithm is calculated to give log *WAK* (*WA,* weighted average).

A2.3 Analysis

A2.3.1 Isolation

A number of analytical methods are available for the determination of LAS in water, but the primary method is assay as methylene blue-active substances (MBAS). The methylene blue reaction responds to any compound containing an anionic centre and a hydrophobic centre, because such compounds tend to form an extractable ion pair when they combine with cationic dyes such as methylene blue; as only the oxidized form is blue, many positive interferences may occur. Negative interference in MBAS analysis is seen in the presence of cationic substances such as proteins and amines (Swisher, 1970, 1987). Therefore, isolation of LAS from a sample is one of the most important aspects of their analysis. Most analytical methods include appropriate procedures for isolation.

A2.3.2 Analytical methods

The analytical methods available for determining LAS in water include nonspecific methods, involving colorimetric, fluorimetric, and atomic adsorption techniques, and specific methods involving techniques such as high-performance liquid chromatography (HPLC), gas chromatography (GC) and GC-mass spectrometry (MS).

A2.3.2.1 Nonspecific methods

The simplest procedure for the determination of LAS in aqueous solution is a two-phase titration method. LAS are titrated in a mixed aqueous chloroform medium with a standard solution of a cationic reagent, such as benzethonium chloride (Hyamine 1622), and a small amount of indicator, such as a mixture of dimidium bromide and acid blue. The end-point is determined by a change in the colour of the organic solvent (ISO 2271, 1972).

The main nonspecific analytical method used is assay for MBAS, described above. Colorimetric techniques are routinely used to determine low concentrations of anionic surfactants, including LAS, in aqueous samples and have been used extensively in testing and environmental monitoring of these materials. The colorimetric methods have the same common analytical basis, that is, formation of solvent extractable compounds between the anionic surfactant and an intensely coloured cationic species. The most commonly used cationic reagent for this purpose is methylene blue (Swisher, 1970, 1987). The same principle has been used as the basis of many other procedures for the determination of anionic surfactants.

It has been shown or predicted that organic sulfates, sulfonates, carboxylates, phenols, and even simple inorganic anions such as cyanide, nitrate, thiocyanate, and sulfate can be methylene blue-reactive (Swisher, 1970, 1987). The negative interferences that can occur as a result of direct competition of other 'cationic' materials are generally considered to be less important than positive interferences, and the entities detected by the analysis are correctly referred to as MBAS.

The procedure developed by Longwell & Maniece (1955) and the improved version of Abbott (1962) are considered to be the best methods for the determination of MBAS in aqueous samples. The sensitivity of these procedures is such that levels of 0.01-0.02 mg/litre MBAS can be determined.

The MBAS response can be used as an acceptable overestimate of the synthetic anionics present in domestic wastewaters, but these materials may comprise only a small proportion of the total MBAS in surface waters (Waters & Garrigan, 1983; Matthijs & De Henau, 1987). Berna et al. (1991) found that LAS contributed 75% of the MBAS in integrated sewage and 50% in treated water. Direct methylene blue analysis of extracts derived from sludge, sediment, and soil invariably leads to highly inflated estimates of LAS (Matthijs & De Henau, 1987). Numerous attempts have been made to improve the specificity of methylene blue analysis, by using a variety of separation steps before the usual colorimetric estimation. Such indirect procedures are usually lengthy, difficult, and still susceptible to interference. A number of analytical methods for the determination of LAS involving extraction and methylene blue are summarized in Table 4.

Table 4. Analytical methods for anionic surfactants in environmental water using methylene blue and extraction

Method	Isolation method/ procedure	Limit of detection (mg/litre)	Interference	Reference
Absorption photometry	Extract LAS in water into chloroform as ion-pair with MB; measure absorption of chloroform solution at 650 nm	50-300	Urea, thiocyanate, chloride	Jones (1945)
	Extract from alkaline solution, wash with	10-100	As above	Longwell & Maniece

	cidic MB			(1955)
	Remove impurities from MBreagent by chloroformextraction	0.1–1	As above	Abbot (1962)
	Remove MBAS by TLC	0.1–1		Oba & Yoshida (1965)
	Remove MBAS on polymer bead column			Takeshita & Yoshida (1975)
	Remove MBAS on ion exchange column	0.02		Yasuda (1980)
UV absorption photometry	Re-extract LAS into water; measure UV absorption at 222 nm	1		Uchiyama (1977)

Table 4 (contd)

Method	Isolation method/ procedure	Limit of detection (mg/litre)	Interference	Reference
Infra-red spectometry	Use to reduce interference from MBAS	1000		Ambe & Hanya (1972)
Gas chromatography	Convert into fluorine derivative; measure by ECD	0.02		Tsukioka & Murakami (1983)
HPLC	Remove MB by cation exchange, HPLC	0.1		Hashimoto et al. (1976)
	Remove MB by anion exchange, HPLC	0.02		Saito et al. (1982)

LAS, linear alkylbenzene sulfonates; MB, methylene blue; MBAS, methylene blue-active substances; TLC, thin-layer chromatography; UV, ultraviolet radiation; ECD, electron capture detection; HPLC, high-performance liquid chromatography

Many other cationic dyes and metal chelates have been used as colorimetric (and fluorimetric) reagents for the determination of anionic surfactants, including LAS. Use of the cationic metal chelates has also led to the development of sensitive atomic absorption methods for indirect determination of anionic surfactants in fresh, estuarine, and marine waters. Although these alternative systems may offer some advantages over the methylene blue cation method, they cannot match the wide experience gained with methylene blue analysis. Some examples of analytical methods based on the use of alternative cationic reagents are shown in Table 5.

A2.3.2.2 Specific methods

Good progress has been made towards developing methods for the specific determination of the many homologues and phenyl-positional isomers of LAS in almost all laboratory and environmental matrices (liquid and solid) at concentrations down to micrograms per litre. High-resolution GC techniques have allowed determination of all the major components of LAS (homologues and phenyl-positional isomers) in environmental samples. Waters & Garrigan (1983) and Osburn (1986) reported improved microdesulfonation-GC procedures for the determination of LAS in both liquid and solid matrices.

Derivatization techniques offer an alternative approach to desulfonation for increasing the volatility of LAS for GC (or GC-MS) analysis (Hon-nami & Hanya, 1980a; McEvoy & Giger, 1986; Trehy et al., 1990. The GC-MS technique was also applied, after ion-pair, supercritical fluid extraction and derivatization, to five sewage sludges, and the LAS were found to occur at 3.83–7.51 g/kg on a daily basis (Field et al., 1992). These GC procedures, however, involve extensive sample pre-treatment and depend on conversion of the isolated LAS into a suitably volatile form for GC determination; they are therefore time-consuming.

HPLC offers a more convenient means for determining homologues of LAS in all types of environmental matrices routinely. Several researchers have reported HPLC procedures for LAS which involve trace enrichment of the surfactant as the first step (Kikuchi et al., 1986; Matthijs & De Henau, 1987; Castles et al., 1989; Di Corcia et al., 1991). Takita & Oba (1985) developed a modified analytical method based on MBAS-HPLC measurement. Further HPLC methods, some requiring no sample preparation, are listed in Table 6.

Table 5. Analytical methods involving reagents other than methylene blue

Method	Isolation method/ procedure	Limit of detection (mg/litre)	Interference	Reference
Absorption photometry	1-Methyl-4-(4-diethyl-aminophenylazo)pyridinium	0.04	Fe[III]	Higuchi et al. (1982)

	iodide; measure chloroform solution at 564 nm			
	Bis[2-(5-chloro-2-pyridylazo)-5-diethyl-aminophenolato]Co [III] chloride; measure benzene solution at 560 nm	0.06		Taguchi et al. (1981); Kobayashi et al. (1986)
	Ethylviolet; measure benzene or toluene solution at 540 nm	0.01		Motomizu et al. (1982); Yamamoto & Motomizu (1987)
Atomic absorption spectrometry	Bis[2-(5-chloro-2-pyridylazo)-5-diethylaminophenolato] Co [III] chloride; measure Co by atomic absorption spectrometry	1×10^{-3}	Hydro-chlorite ion	Adachi & Kobayashi (1982)
	Potassium dibenzo-18-crown-6; measure K	0.05	Alkali, alkaline earth metals	Nakamura et al. (1983)

Table 5 (contd)

Method	Isolation method/ procedure	Limit of detection (mg/litre)	Interference	Reference
Atomic absorption spectrometry	Cu[II] ethylenediamine derivatives; measure Cu	0.03×10^{-3}		Gagnon (1979); Sawada et al. (1983)
Absorption photometry	Bis(ethylenediamine)Cu; determine Cu after addition of 1-(2-pyridylazo)-2-naphthol at 560 nm	5×10^{-3}		Rama Bhat et al. (1980)
GC-MS	Extract solid phase on C_8 column; derivatize LAS with sulfonyl chloride for GC-MS	1×10^{-3}		Trehy et al. (1990)

LAS, linear alkylbenzene sulfonates; GC-MS, gas chromatography-mass spectrometry

Table 6. Analytical methods for linear alkylbenzene sulfonates (LAS) by specific analysees

Extraction method	Analytical conditions	Limit of detection (mg/litre)	Reference
Recover LAS on column chromatograph packed with polymer beads	Column, silica gel, mobile phase hexane:ethanol containing sulfuric acid; UV at 225 nm	0.02-0.03	Takano et al. (1975)
Extract LAS with methylisobutyl ketone	Column, ODS; mobile phase, ethanol:water; UV at 225 nm	0.05	Matsueda et al. (1982)
Recover LAS by ionexchange column chromatography	Column, cyanopropyl-modified silica; mobile phase, ethanol:water; UV at 225 nm	0.04	Saito et al. (1982)
Direct analysis	Column, ODS; mobile phase, methanol: water with sodium perchlorate; fluorescence detector capable of determining alkyl homologue distribution	0.1	Nakae et al. (1980)
Extract LAS using mini-column	Column, ODS; mobile phase, acetonitrile: water with sodium perchlorate; fluorescence detector	0.1×10^{-3}	Kikuchi et al. (1986)
Concentrate LAS using mini-cartridge column connected in sequence with HPLC system	Column, ODS; mobile phase, acetonitrile: water with sodium perchlorate; fluorescence detector	3×10^{-3}	Takami et al. (1987)

Table 6 (contd)

Extraction method	Analytical conditions	Limit of detection (mg/litre)	Reference
Extract LAS with methylisobutyl ketone	Column, ODS; mobile phase, acetonitrile: water (gradient elution to sharpen peak) with sodium perchlorate; UV at 222 nm	NR	Inaba & Amano (1988)
Extract from solids with methanol on Soxhlet	Column, octyl-modified silica; mobile phase, 2-propanol:water: acetonitrile (gradient elution) with sodium perchlorate; fluorescence	0.8 (injected weight)	Marcomini & Giger (1987)

	detector		
Two-step solid phase extraction with C2 and SAX cartridges	Column, C1 Sphesorb; mobile phase, THF:water with sodium perchlorate; fluorescence detector	7×10^{-3}	Castles et al. (1989)
Extract LAS using Carbopack B (graphitized carbon black) cartridge	Column, C8-DB (Supelco); mobile phase, methanol:water with sodium perchlorate; fluorescence detector	0.8×10^{-3}	Di Corcia et al. (1991)
Concentrate LAS on anion-exchange pre-column connected to HPLC system	Column, Wakosil 5C4; mobile phase, acetonitrile:water with sodium perchlorate; UV at 220 nm	10×10^{-3}	Yokoyama & Sato (1991)

Table 6 (contd)

Extraction method	Analytical conditions	Limit of detection (mg/litre)	Reference
Ion-pair extraction under SFE conditions using tetralhyl-ammonium ion pair reagents, coupled with ion-pair derivatization	Column, capillary gas chromatography, 20 m; mass spectrometry with electron impact ionization operating in selected ion mode	NR	Field et al. (1992)
Solid-phase extraction for purification and concentration	HPLC column, Bandapat C_{18} gradient elution water:acetonitrile and 0.15 mol/litre $NaClO_n$	10×10^{-3} (water phase) 0.1 (solid phase)	Matthijs & De Henau (1987)

UV, ultraviolet spectrometry; ODS, octadecyl silica; HPLC, high-performance liquid chromatography; NR, not reported; SFE, supercritical fluid extraction

A3. SOURCES OF HUMAN AND ENVIRONMENTAL EXPOSURE

A3.1 Natural occurrence

LAS do not occur naturally.

A3.2 Anthropogenic sources

LAS are synthetic surfactants that were introduced as prime components of almost all types of household surfactant products in the early 1960s to replace alkylbenzene sulfonates (ABS), which were then in widespread use. The change-over from ABS to LAS took place gradually, starting in the United Kingdom (1960) and then spreading to Germany (1961), the United States of America (1963), Japan (1965) and to other European countries (Brenner, 1968; Husmann, 1968; Waldmeyer, 1968; Tomiyama, 1972).

After use, LAS are discharged into wastewater. As the surfactant components of the detergent products are soluble, they eventually reach raw sewage at concentrations of 1–7 mg/litre (Rapaport et al., 1987). Unlike ABS, which has a branched alkyl chain structure, LAS with a linear, straight alkyl chain structure are readily biodegradable. Their use has alleviated significant environmental hazards such as foaming and residual surfactant in water.

A3.2.1 Production levels and processes

Annual world production of surfactants, excluding soap, in 1990 was estimated to be about 7 million tonnes (Colin A. Houston & Associates, Inc., 1990; Richtler & Knaut, 1991). World consumption of LAS in 1989 was about 2.43 million tonnes, 50% of which was used in North America, western Europe, and Japan (Hewin International Inc., 1992). Worldwide consumption of LAS in 1990 was about 2 million tonnes, with the following geographical distribution: western Europe, 23%; North America, 19%, eastern Asia, 16%, South-east Asia, 12%; eastern Europe, 11%; western Asia, 7%; South America, 7%; and Africa, 5% (CEFIC, 1992). Berna et al. (1993a) reported that, in 1990, 380 000 tonnes were used in western Europe, 180 000 tonnes in eastern Europe, 110 000 in Africa, 100 000 tonnes in western Asia, 305 000 in eastern Asia, 180 000 in South-east Asia, 295 000 in North America, and 140 000 in Latin America. An additional demand of 650 000 tonnes is expected by the year 2000. The estimates for 1990 show an increase over 1987, when LAS production in the United States, Japan, and western Europe was about 1.4 million tonnes, on the basis of global demand for linear alkylbenzene (Painter & Zabel, 1988), and consumption of LAS was about 307 500 tonnes in the United States, 485 000 tonnes in western Europe, and 145 000 tonnes in Japan (Richtler & Knaut, 1988).

LAS are complex mixtures of isomers and homologues in proportions dictated by the starting materials and reaction conditions. LAS are manufactured by reacting the parent alkylbenzenes with sulfuric acid or sulfur trioxide to give the corresponding sulfonic acid, which is then neutralized to the desired salt. This is usually the sodium salt but ammonium, calcium, potassium, and triethanolamine salts are also made. The reactions are smooth and the yields nearly quantitative. Commercial LAS contain linear alkyl chains 10–14 carbons in length, with phenyl groups placed at various internal positions on the alkyl chain, with the exception of 1-phenyl (Painter & Zabel, 1988).

LAS are manufactured in an enclosed process; under normal conditions, therefore, exposure can occur only at the stage of detergent formulation, by inhalation or dermally. Dermal exposure is generally short and accidental, whereas exposure by inhalation can occur continually.

The concentration of surfactants in water from washing machines is 0.2–0.6%. LAS are estimated to represent 5–25% of the total surfactant mixture.

In Germany in 1988, when annual consumption of LAS in the western states was about 85 000 tonnes, daily consumption was 3.8 g per inhabitant per day. As consumption of drinking-water was 190 litres per inhabitant per day, the average LAS concentration in sewage was 20 mg/litre. Consumption of LAS per capita in other countries is shown in Table 7 (Huber, 1989).

A3.2.2 Uses

LAS are the most widely used surfactants in detergent and cleaning products, in both liquid and powder preparations and for household and industrial use. The amount of LAS in a product depends on several factors, including the type of application (washing-up products, light- and heavy-duty powders and liquids) and the formulation, but is usually 5–25%. Small amounts of LAS are used in non-detergent applications, but these represent less than 5% of total world consumption.

Table 7. Specific consumption of linear alkylbenzene sulfonates (LAS) in various countries

Country	Water usage (litres per capita per day)	LAS usage (g per capita per day)	Reference
Germany	–	3.8	Huber (1989)
	185	2.2	Wagner (1978)
United States	560	2.6[a], 2.1[b]	Rapaport et al. (1987)
United Kingdom	208	3.5[c], 2.7[c]	Standing Technical Committee on Synthetic Detergents (1978, 1989)
Spain	–	5.6[a], 2.6[b]	Berna et al. (1989)
Japan	493	2.7	Ministry of Health and Welfare (1992); Hewin International Inc. (1992)

[a] Calculated from sales
[b] Calculated by analysis
[c] Methylene blue-active substances

A4. ENVIRONMENTAL TRANSPORT, DISTRIBUTION, AND TRANSFORMATION

Section summary

The way in which LAS enter the environment varies between countries, but the major route is via discharge from sewage treatment works. Direct discharge of sewage to rivers, lakes, and the sea occurs when wastewater treatment facilities are absent or inadequate. Another route of entry of LAS into the environment is via disposal of sewage sludge on agricultural land.

Throughout their journey into the environment, LAS are removed by a combination of adsorption and primary or ultimate biodegradation. LAS adsorb onto colloidal surfaces and suspended particles, with measured adsorption coefficients of 40–5200 litres/kg, depending on the medium and structure of the LAS. LAS undergo primary biodegradation in all environmentally relevant compartments, such as raw sewage, sewage treatment water, surface waters, sediments, and soils. They are readily and ultimately mineralized under aerobic conditions in the laboratory and the field. They tend not to be biodegraded under methanogenic conditions or if the initial LAS concentration is so high that microbial degradation is inhibited (> 20–30 mg/litre). Typical half-lives for aerobic biodegradation of LAS are 1–8 days in river water, 1–2 days in sediments, and 5–10 days in marine systems. The rate of biodegradation depends on temperature: biodegradation is rapid between 10 and 25°C; at lower temperatures, biodegradation kinetics are reduced, in close association with microbial activity. During primary sewage treatment, LAS are partially adsorbed onto and removed with waste sludge to an extent of about 25% (range, 10–40%). LAS are not removed during anaerobic sludge digestion but are removed during aerobic treatment with a half-life of about 10 days. Application of the sludge to soil generally results in 90% degradation within three months, with a half-life of 5–30 days.

LAS are not bioconcentrated or biomagnified in aquatic organisms. They are readily absorbed through the gills and body surface of fish and are distributed via the blood to the systemic organs. Most LAS-related compounds (parent compound and metabolites) have been detected in the gall-bladder and hepatopancreas of fish. They are usually cleared rapidly, with a half-life of two to three days.

A4.1 Transport and distribution between media

Detergent chemicals such as LAS are normally discharged after use into sewers in communal wastewater. The proportion of wastewater

that is subjected to sewage treatment varies widely between countries. In most advanced countries, 50 to > 90% may be treated, whereas in less developed countries the proportion may be as little as 5–30% (Eurostat, 1991). In countries where there is no or inadequate sewage treatment, LAS are removed from the environment via adsorption and mineralization in the receiving surface waters.

Anionic surfactants such as LAS can adsorb onto the solid substrates associated with sewage, sludge, sediment, and soil; the extent of adsorption is dependent on the composition and physical nature of the solid matrix. Measured values of the adsorption constant (K_d) for LAS on a range of solid substrates were compiled by Painter & Zabel (1989), who reported K_d values of 590–1400 litres/kg for primary sludge, 660–5200 litres/kg for activated sludge, and 40–360 litres/kg for river water sediment.

A4.1.1 Wastewater treatment

Under certain conditions, up to 50% of the LAS present can be biodegraded in sewers before entering sewage treatment (Moreno et al., 1990). In large-volume batch biodegradation tests with acclimatized sludge, the MBAS levels decreased to 10% of the initial concentration within 15 days. During biodegradation, the toxicity of the test solution decreased in parallel with the reduction in MBAS. A relative enrichment of the shorter chain homologues was observed by GC analysis concurrently with the decrease in MBAS levels, indicating preferential removal of the higher homologues (Dolan & Hendricks, 1976).

The distribution and fate of LAS have been established in the course of mass balance studies at sewage treatment plants in Spain (Berna et al., 1989), Italy (Cavalli et al., 1991), Switzerland (Giger et al., 1989), Germany (De Henau et al., 1989), and the United States (Rapaport & Eckhoff, 1990; McAvoy et al., 1993). Efficient, well-operated activated sludge plants generally remove most of the LAS during aerobic treatment, and the overall removal of LAS in primary settlement and secondary aerobic treatment stages can be $\leq$ 98% (Berna et al., 1991). Smaller amounts of LAS were removed (77 ± 15%) in less efficient, trickling filter plants (McAvoy et al., 1993).

The main mechanism for removal of LAS during sewage treatment is biodegradation (Berna et al., 1991), but a significant fraction (on average, 20–30%) of the LAS entering sewage treatment plants may be removed on primary sewage solids and do not undergo aerobic sewage treatment (Giger et al., 1989). Instead, the sludge is digested under anaerobic conditions, and in some countries a high proportion may then be applied raw or digested to agricultural land as a source of plant nutrients (Berna et al., 1991). In Germany and the United Kingdom, 40–45% of sewage sludge is disposed of in this way (Waters et al., 1989). Since LAS do not undergo significant anaerobic biodegradation under methanogenic conditions, concentrations of 3–12 g/kg can be found on dried solids in sludge (see Section 5, Table 10). Any LAS in sludge applied to agricultural soil should then be rapidly biodegraded, since the receiving soil environment is aerobic. In Germany and the United Kingdom a typical application of digested sludge was estimated to add LAS at a rate of 7–16 mg/kg soil (Waters et al., 1989).

Adsorption can account for 15–40% of the removal of LAS from raw sewage during the primary settlement stage of treatment (Berna et al., 1989; Giger et al., 1989). Berna et al. (1989) reported that precipitation and adsorption were particularly important in removing LAS from wastewater containing high concentrations of calcium and magnesium ions.

The percentage adsorption of C_{10}, C_{11}, C_{12}, and C_{13} LAS onto activated sludge, Amazon clay, and various bacteria and algae was directly related to the chain length and phenyl position: longer homologues and more terminal phenyl isomers were adsorbed much more readily than other forms. Adsorption of LAS at a concentration of 23 mg/litre was found to be pH-dependent, with adsorption increasing as the pH decreased from 7 to 3 (Yoshimura et al., 1984a).

A4.1.2 Surface waters, sediments, and soils

The half-life for the removal of LAS by combined sorption and settling < 12 km below a sewage outfall in Rapid Creek, South Dakota, United States, was 0.25 days. The biodegradation half-life was 1.5 days (Rapaport & Eckhoff, 1990). The partition coefficient of LAS between natural water and sediment was reported to increase with increasing chain length and with the position of the phenyl nearer to the end of the chain. Adsorption was increased when either the concentration of suspended solids or fractional organic carbon was increased (Amano & Fukushima, 1993).

Freshwater pearl oysters are cultivated in Lake Nishinoko, Japan, which has an area of 2.8 km^2, an average depth of 1.5 m, and a residence period of 27 days. The water of the lake was found to contain total concentrations of MBAS of 0.01–0.02 mg/litre and LAS concentrations of 0.005–0.018 mg/litre. The partition coefficients of LAS (K_d) were 70 litres/kg for bottom sediment:water and 11 litres/kg for oyster:water (Sueishi et al., 1988). The authors concluded that when a river flows into a semi-enclosed lagoon, the fate of the surfactants is dominated by mass transfer between media and transformation due to degradation rather than spatial transportation.

LAS were present in Swiss soils that had been treated with sludge for 10 years; however, the application rates were six times

higher than normal. The reported half-lives were 5-80 days. The authors noted that it is not entirely correct to use half-life to describe the loss of LAS from soils, because there is competition between biodegradation and sorption on and into soil particulates, and LAS may persist at very low 'threshold' levels. During the 330-day study, the levels of LAS decreased from 45 mg/kg dry soil to a residual level of 5 mg/kg (Giger et al., 1989).

A comparison of the measured concentration of LAS with detailed records on the amount of sludge applied on 51 fields in England indicated that loss of LAS exceeded 98% in fields that had not recently been sprayed with sludge; losses from fields that had been sprayed recently were calculated to be 70-99% of the estimated cumulative load. The calculated half-lives for removal of LAS from soil sprayed with sludge were 7-22 days. Examination of the distribution of homologues suggested that loss of LAS is the result of biodegradation and not leaching (Holt et al., 1989). In a study of the disappearance of LAS from sludge-amended soils at two locations, the average half-lives were 26 days when sludge was applied at a rate of 1.6 kg dry sludge per m^2 (giving a concentration of LAS of 16.4 mg/kg soil) and 33 days when sludge was applied at 5 kg wet sludge per m^2 (concentration, 52.5 mg/kg soil) (Berna et al., 1989). In another study, the half-life for LAS in soil was more than three months; there was no evidence that they accumulate in soil over time (Rapaport & Eckhoff, 1990).

When C_{13} LAS were applied to various soil (surface) types at a concentration of 0.05 mg/kg under laboratory test conditions, the half-lives were 1-5 days, with an average of two days. There was no significant variation with regard to soil type. In a second experiment, the average half-life of C_{12} LAS applied to subsurface soil was 20 days (Larson et al., 1989).

After grass, radishes, and garden beans were grown for 76 days in soil treated with ^{14}C-LAS at a rate of approximately 1.2 g/m^2, 98% of radioactive residues were recovered, with 63.6% released to the atmosphere, 26.8% found in the soil, 6.6% in plant biomass, and 0.9% leached out in percolated water. When potatoes were grown on the soil for 106 days, 97.9% of the radioactivity was recovered, and 72.3% was released to the atmosphere, 18.3% to the soil, 5.9% in plant biomass, and 1.4% leached into percolated water (Figge & Schoberl, 1989).

LAS in a plume of contaminated groundwater on Cape Cod, United States, were degraded rapidly and was found only within 0.6 km of the sewage disposal bed (Thurman et al., 1986).

Effects on the biodegradation of LAS applied at 50 mg/litre of aqueous dispersion were studied in three Japanese soil types inoculated with sewage. The rate of sludge application used in this study was not typical of that found in the environment. Primary degradation, as measured by the presence of MBAS, reached 70% within 16 days. Addition of andosol (allophane) and weathered granite (kaolin and illite) both reduced primary degradation, and 40-50% of the LAS was still present after 30 days, indicating that the rate of microbial degradation of LAS adsorbed onto soils containing large amounts of allophane and/or sesquioxides was reduced. A montmorillonite soil did not affect the rate of degradation (Inoue et al., 1978).

The behaviour of C_{10}-C_{13} LAS and C_{12} LAS at concentrations of 50 and 100 mg/litre was studied by HPLC in perfusion tests on two types of soil, a clay loam and a sandy loam. The sandy loam, with a lower content of humus and clay, adsorbed less LAS with a longer lag. During the first three days of perfusion, only adsorption occurred, 50% being adsorbed; after nine days, decomposition was observed and only 16.6% of the LAS remained; after 15 days, the LAS had almost completely disappeared (Abe & Seno, 1987).

LAS were applied at a rate of 5 g/m^2 to three soil types: loamy orthic luvisol under agricultural land, sandy acidic dystric combisol under a pine forest, and combisol irrigated with wastewater. The half-life in loamy soil was five days; 80% was degraded after 12 days, and none was detectable after 28 days. With 45 mm of precipitation, about 8% of the LAS percolated to a depth of 10-30 cm. The LAS moved significantly more slowly than radioactively labelled water. LAS were less mobile in the sandy soil, with a maximal percolation depth of 5 cm after two weeks, whereas water percolated 15 cm. The half-life in the sandy soil was 10 days, with 80% degradation after 19 days and total degradation after 28 days. The LAS were bound to organic material in the humic litter, which probably slowed degradation and reduced mobility. In combisol irrigated with wastewater, the LAS were bound mainly in the upper 5 cm, with some percolation to 10-30 cm after an application of 180 mm of wastewater. The half-life was 12 days, and 80% was degraded within 21 days; however, there was no further degradation after 28 days, and the remaining LAS were tightly bound. Increasing the application rate to 50 g/m^2 had no effect on percolation; however, the half-life was doubled. Samples collected during the winter showed much slower degradation, with half-lives of 68-117 days. Percolation was also much deeper; the authors suggest this was due to a higher rate of precipitation and extensive evaporation (Litz et al., 1987).

In a study of the adsorption of LAS in aqueous solution onto clay grumusol and sandy regosol soils, a linear adsorption isotherm was obtained. The release of the surfactant was proportional to the initial adsorption and the soil type, suggesting ready desorption. More LAS was adsorbed by the clay soil than by the sandy soil (Acher & Yaron, 1977).

Hydroxy aluminium and iron adsorbed LAS more readily and with a much larger capacity than other soil constituents, such as organic matter, silica gel, layer silicates, and calcium carbonate (Volk & Jackson, 1968).

In a study of the adsorption of LAS applied at a concentration of 2 mg/litre to a variety of Wisconsin (United States) soils, a highly significant correlation was found between adsorption and organic matter content (including the iron and aluminium components), phosphate fixing capacity, and aluminium content. The removal of sesquioxides reduced the adsorption of LAS to zero; however treatment of montmorillonitic soils with H_2O_2 and $Na_2S_2O_4$ increased adsorption by oxidizing and removing the organic matter, indicating that montmorillonite can adsorb LAS. Treatment of soils with H_2O_2 increased adsorption because iron and aluminium were released from organic chelates (Krishna Murti et al., 1966).

Adsorption of LAS to microorganisms was found on the basis of calculated adsorption isotherms to be more important than adsorption to humic substances (Urano et al., 1984; Urano & Saito, 1985).

A4.1.3 Fate models

One model of the fate of LAS predicted the sorption coefficient to within one order of magnitude. The sorption distribution coefficient was consistently underpredicted, so that when the concentrations of LAS in interstitial and overlying water were predicted from concentrations in sediment they were overestimated. The model thus provided conservative estimates for assessing safety in aquatic media (Hand et al., 1990).

The reported concentrations of LAS in Rapid Creek, South Dakota, United States, were compared with expected concentrations generated by the quantitative water–air–sediment interaction fugacity model, which is based on physical, chemical, reactive, and transport properties and emission rates into rivers. In general, close agreement was reached: in both cases, LAS had a residence time of about two days. The authors pointed out that the results might differ if the model were applied in situations that differed hydrodynamically (Holysh et al., 1986).

A model to predict surface water concentrations of LAS in German and American rivers included the following parameters: river flow and velocity, sewage treatment plant location and type, discharge volume, and connected population. The values obtained were in general agreement with those measured. The authors also investigated a septic tank discharge at a Canadian site by applying a groundwater model, which was based on hydrogeological, biodegradation, and sorption data. The predicted and measured concentrations were in good agreement (Hennes & Rapaport, 1989).

A mathematical model was derived to explain a downstream decrease in the concentration of LAS in the Lake Teganuma estuary, Japan. The model included the adsorption coefficient, the biodegradation rate constant, and the rate of transport (diffusive and settling) flux of LAS between water and sediment. The model predictions and laboratory findings were used to confirm that biodegradation is the predominant mechanism for removal of LAS from the estuary (Amano et al., 1991).

A model based on data from the Lake Biwa basin was devised to predict the fate of LAS in Japanese rivers, assuming that complete mixing occurs in any given cross-section of a river. The parameters included the cross-sectional mean concentration of LAS, time elapsed, flow velocity, longitudinal dispersion coefficient, decay due to biodegradation and sedimentation, water depth, and river width (Sueishi et al., 1988).

The measured concentrations of LAS in United States river water under critical flow conditions were mirrored by the predictions of a simple dilution model, which predicts chemical concentrations below the mixing zone of wastewater treatment plants. The model is based on three large databases, which link river flow, treatment type and wastewater discharge volume; the output of the model is a frequency distribution of concentrations just below the mixing zone of treatment plant outfalls. The model predicted that 95% of the river waters below that point would have concentrations of LAS of < 0.35 mg/litre during critical low-flow periods. The sampling sites selected for this study were reported to have a low dilution factor for mixing effluent with surface water, however. The predictions therefore represent a 'worst-case scenario', since the 95 percentile value represents critical low-flow periods, in which the lowest ever recorded flow is used for a consecutive period of seven days within 10 years (McAvoy et al., 1993).

A4.2 Environmental transformation

A4.2.1 Biodegradation

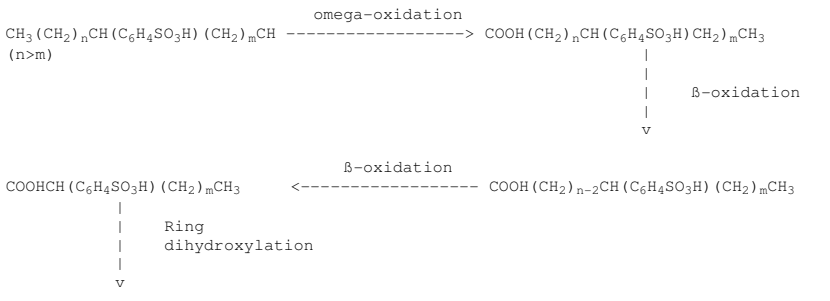
A4.2.1.1 Aerobic degradation

Studies on aerobic biodegradation of LAS can be divided into those of primary degradation and those of ultimate degradation. Primary degradation of LAS occurs during the initial reactions in the metabolic pathway, and the products are often shorter-chain homologues. The ultimate degradation of LAS is that of the entire molecule to its biodegradation end-products, CO_2, H_2O, and NH_4. These products are used in cell synthesis or, in the case of CO_2, excreted. The ultimate degradation of LAS normally requires

the action of several species of bacteria.

The degradation pathway of LAS has been described (Huddleston & Allred, 1963; Swisher, 1963). The steps, shown in Figure 1, are: omega-oxidation of the end of the alkyl chain, rapid ß-oxidation of the chain, and oxidation of the ring.

Figure 1. Postulated metabolic pathway of linear alkylbenzene sulfonates



From Painter (1992)

Swisher (1981) pointed out that ultimate biodegradation (at least 80%) is achievable under the correct conditions, which include:

(i) the presence of mixed bacterial species,
(ii) free access to new bacteria during the test,
(iii) acclimatization,
(iv) enough growth factors and food, and
(v) limitation of the LAS concentration to that found in the environment.

Biodegradation of LAS begins at the terminus of the alkyl chain with an omega-oxidation and is followed by successive cleavage of C_2 fragments (ß-oxidation) (Huddleston & Allred, 1963; Swisher, 1963). The resulting sulfocarboxylic acids have a chain length of four to five carbon atoms (Schöberl, 1989). These intermediates are further biodegraded by oxidative scission of the aromatic ring and cleavage of the sulfonate group (Setzkorn & Huddleston, 1965; Swisher, 1967). Catabolites of further oxidation steps are fed into the central metabolic pathways, i.e. the Krebs cycle and glyoxylate cycle (Schöberl, 1989).

LAS degradation begins at the longest end of the linear alkyl chain, with omega- and ß-oxidation, and proceeds up to the sulfophenylmono-carboxylic acids (one to two CH_2 groups) (Divo & Cardini, 1980). Under mild conditions, as in river water, intermediates such as sulfo-phenylcarboxylic acids are often not degraded, as the greater distance between sulfophenyl groups and the far end of the hydrophobic group increases the speed of primary biodegradation (Swisher, 1976). Once the terminal methyl group has been attacked, primary biodegradation is rapid (Swisher, 1970; Gledhill, 1975). Short-chain sulfophenylmonocarboxylic acids were not degraded by *Pseudomonas* but were degraded by mixed cultures of microorganisms (Leidner et al., 1976). The initial attack that opens the aromatic ring is the rate limiting step for ultimate biodegradation: once the ring is opened, degradation is rapid.

Enzymological methods were used to show that the same sequence of steps occurs when ring degradation proceeds via the catechol derivative. A variety of microorganisms isolated from soil, sewage, and river water showed at least five distinct metabolic routes for the degradation of LAS: omega- and ß-oxidation of the side-chain; oxidation and desulfonation followed by cleavage of the aromatic nucleus; reductive desulfonation of the ring; and metabolic alpha-oxidation of the side-chain, followed by ß-oxidation and desulfonation. Metabolism of alkyl chains shorter than four carbons was initiated through the aromatic nucleus by hydrolytic or reductive desulfonation of the ring (Cain et al., 1971). LAS may also be cleaved by biochemical mechanisms (Schöberl, 1989).

Primary degradation

(i) Low levels of biomass

Measurement of MBAS was compared with measurement of total organic carbon for detecting biodegradation in shake cultures. With the MBAS method, LAS had lost 98% of their activity within five days, whereas 34% of the total carbon had disappeared by that time, and 70% was lost by the end of the 31-day test (Sekiguchi et al., 1975a).

In a modification of the screening test of the Organisation for Economic Co-operation and Development (OECD), accepted by the European Commission, the percentage of dissolved organic carbon was found to have decreased by more than 80% within four weeks. The authors cautioned that the decrease in LAS may not have been due solely to biological degradation, since 40-50% of organic carbon was also removed from abiotic controls, suggesting that adsorption may account for part of the removal of LAS (Canton & Slooff, 1982). When aerobic biodegradation of 10 mg/litre LAS was followed during a

10-day incubation period at 27°C, primary degradation, measured by the MBAS method, was complete within 8-10 days, and the theoretical CO_2 production reached 20-25% within 10 days. At a concentration of 20 mg/litre, no degradation was observed, but this elevated concenration may have inhibited the microbial inoculum (Itoh et al., 1979).

The rate and degree of biodegradation of LAS are dependent on temperature. In an unacclimatized microbial population, no more than 25% biodegradation was achieved at 5°C during a 28-day test,whereas at 15, 25, and 35°C about 90% degradation was achieved within 7-14 days. At 45°C, the microbial population degraded 75% of the LAS within 14 days, but this rate of degradation was not maintained, probably because of loss of the acclimatized seed due to the high temperature. A clearer effect of temperature was observed when the microorganisms were acclimatized to LAS before the test. Under these conditions, the rate of biodegradation increased steadily with increasing temperature from 15 to 35°C (Hollis et al., 1976).

(ii) Wastewater treatment

In the OECD screening test, there was 95% loss of LAS, measured by the MBAS method, and similar losses were measured in OECD confirmatory test No. 1 with 20 mg/litre LAS. In the closed-bottle test with a concentration of LAS of 2 mg/litre, there was 90-95% analytical loss (by the MBAS method) and 60-65% loss of biochemical oxygen demand. Coupled-unit tests with 10 mg/litre LAS and a mean hydraulic retention time of 6 h showed 94% removal of chemical oxygen demand (values > 73% indicate benzene ring opening) (Fischer & Gerike, 1975). In activated sludge, 80-90% of dissolved organic carbon and benzene rings disappeared within 6 h (Swisher, 1972). A bacterium similar to *Klebsiella pneumoniae,* isolated from sewage, degraded 93% of a concentration of LAS reported as 1% (10 g/litre), as measured by the MBAS method (Hong et al., 1984). A direct correlation was found between the rate of primary degradation of 1.5 mg/litre $C_{11.7}$ LAS and the initial bacterial population size (Yediler et al., 1989).

The biodegradation of C_9-C_{13} LAS at concentrations of 25, 50, and 65 mg/litre was monitored in activated sludge at 100 mg/litre over a period of 12 days. Four methods were used: MBAS, chemical oxygen demand, dissolved organic carbon, and ultra-violet spectrophotometry. The results obtained with the MBAS method showed a percentage loss of 94-97% for the three concentrations of LAS, whereas the other methods showed losses of approx. 50% at 25 mg/litre LAS and approx. 70% at 50 and 65 mg/litre. The specific rate of biodegradation was calculated to be 3.6 mg/g per h, on the basis of loss of chemical oxygen demand (Pitter & Fuka, 1979).

The degradation ratio (biochemical oxygen demand:total oxygen demand) for LAS by a synthetic sewage solution after five days was 0.81 for a concentration of 3 mg/litre and 0.14 for 10 mg/litre. Concentrations of 30 and 100 mg/litre LAS were not degraded during the 14-day test. Even after acclimatization to a concentration of 5 mg/litre LAS for one month, the two higher concentrations were not degraded, probably because these levels inhibited the microbial inoculum (Urano & Saito, 1985).

The percentage removal of biochemical oxygen demand and of LAS were found to be significantly correlated in activated sludge and in a trickling filter system under laboratory and field conditions, implying that a well-functioning sewage treatment plant effectively removes LAS (Tang, 1974).

LAS at a concentration of 150 mg/litre were inoculated into sewage water collected from French water treatment plants. In six out of eight experiments, primary degradation was almost complete (90%) within seven days, but in the other two experiments only 45-55% degradation was achieved. The authors concluded that rapid biodegradation of LAS requires the presence of a community of several bacterial species, including *Flavobacterium, Pseudomonas,* and *Acinetobacter* (Gard-Terech & Palla, 1986).

In an extended aeration activated sludge plant, 95-99% of LAS was removed. Degradation of LAS and reduction of biochemical oxygen demand were strongly correlated, in a 1:1 ratio (Knopp et al., 1965). In long-term laboratory tests, 95-97% of LAS was removed by activated sludge (Janicke & Hilge, 1979).

In a wastewater treatment plant where the input water had an MBAS concentration of 6.2-9.4 mg/litre, at least 99% of the LAS present was removed during treatment, biodegradation accounting for 85%. The relative composition of long-chain (C_{12}-C_{13}) homologues adsorbed on the suspended solids was increased in comparison with the relative incidence of short-chain (C_{10}-C_{11}) homologues detected in the aqueous phases. Sulfophenylcarboxylates were identified as intermediates of the biodegradation of LAS but were detected only in the aqueous and not in the adsorbed phases (Cavalli et al., 1993b).

Biodegradation of LAS in field trials with trickling filter sewage was 86-95%, and average biochemical oxygen demand removal was 93.8%. Thus, the LAS appeared to be removed almost as rapidly as the naturally occurring organic material. The linear correlation between degradation and temperature (7.5-17.5°C) was highly significant. Further degradation (94-99%) took place after additional aeration (Mann & Reid, 1971).

MBAS degradation did not correspond to biodegradation of LAS (20-200 mg/litre) in laboratory sludge units, because of the presence of intermediates not accounted for by analysis of MBAS

(Janicke, 1971).

(iii) Surface waters

Primary degradation, measured by HPLC, of 5 mg/litre C_{11} LAS in a static lake microcosm was complete within 18 days. The sulfo-phenylcarboxylic acid intermediates produced were completely degraded within 22 days (Eggert et al., 1979).

Aerobic degradation of 5 mg/litre LAS in river water, measured by MBAS levels, was 100% after seven days at 25°C. Under microaerophilic conditions at 25 and 35°C), no degradation took place within 10 days (Maurer et al., 1971; Cordon et al., 1972).

In die-away tests with water from various sites on the Tama River, Japan, primary biodegradation (measured by the MBAS method) was complete within 7–15 days, but total organic carbon was completely removed within an incubation time of 45 days. In a study of LAS in seawater collected from the mouth of the Tama River, degradation was only 50% complete within 60 days, as measured by total organic carbon (Sekiguchi et al., 1975b). In a study to monitor detergent-degrading bacteria from the Han River, Republic of Korea, the lowest density was found in January and the highest in July; the dominant group throughout the year was *Pseudomonas* (Bae et al., 1982). Mixed and pure isomers of LAS were metabolized readily (97.5%) by bacteria collected during the summer from a sewage lagoon, but bacteria collected from under the ice during the winter were not able to metabolize LAS (Halvorson & Ishaque, 1969).

Primary biodegradation of C_{10}–C_{13} LAS was dependent on incubation temperature in die-away tests with water from the Tama River, Japan: primary biodegradation was complete within two days at 27°C, within six days at 15°C, and within three days at 21°C; at a water temperature of 10°C, however, only 20% of the LAS had been degraded within the nine-day test (Kikuchi, 1985). The optimal temperature for the biodegradation of LAS in a river water die-away test was found to be 25°C (Yoshimura et al., 1984b).

Degradation of 10 mg/litre LAS in a simulated river model was found to be almost complete within 20 days, on the basis of MBAS levels in water and sludge; however, ultra-violet spectrophotometry showed that 40% of the LAS remained in the water and 25% in the sludge. LAS with an alkyl chain length of C_{10} were degraded more slowly than those with a chain length of C_{14}, and LAS compounds with sulfylphenyl groups near the terminal part of the alkyl chains were degraded more easily than those with such groups further from the end (Fujiwara et al., 1975).

In a study of the biodegradation of LAS (10 mg/litre) and a 1:1 LAS:ABS (10 mg/litre) mixture in canal water with an unaerated or aerated system, LAS were rapidly degraded in the unaerated system, by 14.9% within two days and 40.7% within seven days. Biodegradation was more rapid in the aerated tanks, with 40.4% degraded within two days and 74.5% after seven days. Addition of sewage to the test system further increased the rate of degradation in the aerated system: addition of 0.5 ml/litre sewage resulted in degradation of 78.2% after two days and 89.4% after seven days, and addition of 1.0 ml/litre sewage resulted in degradation of 89.7% after two days and 99.8% within three days. No results were reported for the unaerated system. The LAS–ABS mixture was degraded more slowly than pure LAS: after two days, 12.3% was degraded without aeration, 36.4% with aeration, 60.1% with addition of 0.5 ml/litre sewage, and 78.3% after addition of 1.0 ml/litre sewage. The corresponding degradations calculated after seven days were 32.5, 66.0, 80.7, and 87.3%. The authors concluded that degradation of these detergents was increased by aerating the tank and by increasing the number of microflora by adding sewage (Abdel-Shafy et al., 1988).

In the Lake Teganuma estuary (Japan), an average of 66% of LAS is removed, with seasonal variability, ranging from 28% in winter to 100% in summer. Laboratory studies (based on HPLC methods) of estuarine water showed that LAS degraded with a half-life of eight days at 5°C and 0.2 days at 25°C. Model calculations and field monitoring showed that biodegradation is 10 times more important in the removal of LAS from the estuary during summer than is the settling of solids or adsorption to bottom sediments. At lower temperatures, biodegradation and the other removal mechanisms are of equal importance (Amano et al., 1991).

In well water, biodegradation of all LAS homologues (C_{10}–C_{13}) and isomers (maximal concentration, 2.5 mg/litre) after an acclimatization period of one day was reported to follow zero-order kinetics (Yakabe et al., 1992).

In seawater, primary biodegradation of 20 mg/litre LAS was 70% after 10 days; the half-life was six to nine days (Vives-Rego et al., 1987).

(iv) Soil

In soil degradation tests, levels of 2.5 mg/kg MBAS were reached within 15 days of the addition of 20 mg/kg LAS (Cordon et al., 1972). The biodegradation of LAS in soil was studied by measuring the amounts of ferroin reagent-active substance and total organic carbon. At 50 mg/litre LAS, total organic carbon disappeared within 50 days, whereas total ferroin reagent-active substance was completely lost after only 10 days. Both chemical and physical properties of the soils affected the loss of LAS: more LAS was adsorbed onto clay loam than sandy loam, and biodegradation occurred more readily in the clay loam (Abe, 1984). In a further study (initial concentration not given), loss of C_{10}–C_{13} and C_{12} LAS was complete within 15 days when measured as ferroin

reagent-active substances; however, when measured as total organic carbon, residues remained until day 50 in the clay loam and beyond day 60 in the sandy loam (Abe & Seno, 1987).

Ultimate degradation

A number of studies have been conducted of the biodegradation of phenyl-radiolabelled LAS, in which $^{14}CO_2$ production was measured.

(i) Screening tests

In a simple shake-flask system with LAS, CO_2 evolution reached 60% or more of the theoretical value (Gledhill, 1975).

Four gram-negative bacteria synergistically mineralized 10 mg/litre ^{14}C-LAS. After 13 days of incubation, 29% of the ^{14}C-LAS was mineralized to $^{14}CO_2$. Pure cultures were unable to mineralize the LAS, although three of them carried out primary biodegradation, measured by the MBAS method (Jimenez et al., 1991). *Pseudomonas, Alcaligenes, Necromonas,* and *Moraxella* spp. isolated from activated sludge and river water degraded the alkyl chains of C_{12} LAS, while a group of unidentified Gram-negative bacteria cleaved the benzene ring. A mixture of the two groups degraded LAS completely (Yoshimura et al., 1984b).

(ii) Wastewater treatment

Mixed cultures of microorganisms found under natural conditions or in sewage treatment plants can readily degrade LAS, to 95% of MBAS and > 80% of dissolved organic carbon (Schöberl, 1989).

During a 19-day OECD screening test for the biodegradation of ^{14}C-LAS, there was a high degree of ring mineralization, as seen by the evolution of 55% as $^{14}CO_2$. In a continuous system, 80% of the LAS was evolved as CO_2, with a mean retention time of 3 h; 2-3% remained as unaltered surfactant and 15-25% as the sulfophenylcarboxylic acid intermediates (Steber, 1979).

Loss of MBAS (primary biodegradation) and ring cleavage were found to be nearly complete (> 98%) during simulated waste treatment of ^{14}C-LAS. During simulated secondary waste treatment, 62% of alkyl and ring carbon was converted to CO_2, 28-30% was assimilated into biomass, and 8-10% remained as soluble residue. In die-away tests, 85-100% of the substrates of LAS were converted to CO_2 within 91 days (Nielsen et al., 1980; Nielsen & Huddleston, 1981).

Continuous-flow experiments were conducted with mixed bacterial cultures isolated from a detergent plant wastewater containing five species of *Achromobacter* and two species of *Acinetobacter.* All were more efficient at primary degradation than ultimate degradation of LAS at concentrations of 20 and 50 mg/litre. One species of each genus could effect primary degradation even after isolation (Hrsak et al., 1982).

In a semi-continuous activated sludge method, 95% of the phenyl ring of radiolabelled LAS was cleaved, indicating near complete biodegradation of the whole molecule. Complete primary degradation (MBAS method) of C_{10}, C_{12}, and C_{14} LAS was followed by 99-100% ultimate degradation (HPLC and ultra-violet fluorescence). In die-away tests with 10 mg/litre of C_{10}, C_{12}, and C_{14} LAS, primary degradation was rapid and complete; 100% of C_{12} LAS was removed within four days. Almost complete ultimate degradation was observed within the 80-day test, with 90% ring cleavage of C_{10} LAS and C_{11} LAS within 10 days and 70% ring cleavage of C_{14} LAS within 30 days; however, no HPLC analysis was carried out on C_{14} LAS after day 30 (Huddleston & Nielsen, 1979).

The biodegradation of LAS (C_9-C_{14}) by a mixed bacterial culture was studied in river water, forest soil, and wastewater from a detergent plant. The bacteria were acclimatized to 10 mg/litre LAS. Under continuous-flow conditions, LAS at a concentration of 20.8 mg/litre were 96% degraded, and a concentration of 46 mg/litre was 64% degraded. Only 8-10% of the breakdown products were completely mineralized; however, under the flow-through conditions of this test, water-soluble compounds were usually removed via the

aqueous effluent and were not present long enough to allow mineralization. Acclimatization considerably increased the kinetics of mineralization (Hrsak et al., 1981).

(iii) Surface water and sediment

Detritus is a significant site of surfactant removal, and LAS were found to be the most sorptive of the surfactants tested. In wastewater from a pond containing submerged oak leaves, degradation followed first-order kinetics, with a half-life of 12.6 days. LAS were mineralized more slowly by leaves from a control pond, and an S-shaped pattern of degradation was seen (Federle & Ventullo, 1990).

In river water in which the biomass levels were 10-100 times higher below than above a sewage outfall, primary degradation of added $C_{11.6}$ LAS (11 mg/litre) and background LAS (0.37 mg/litre) was rapid in water taken from below the outfall, with a half-life of 0.23 days (based on measurements of MBAS). Mineralization of the benzene ring was rapid in water from below the outfall containing sediment (500 mg/litre), with a half-life of 0.7 days. Water taken above the sewage outfall also underwent ring mineralization, but the rate of degradation was about 25% of that seen for water from below the outfall, with a half-life of 2.7 days. When samples were

incubated in the absence of sediment, ring degradation was much slower, with half-lives of 1.4 days in water taken from below the outfall and approx.14 days in water taken above it. In all cases, degradation was immediate in water taken below the outfall, but occurred after a three-day lag in water taken above (Larson & Payne, 1981).

Degradation of C_{10}-C_{14} homologues of LAS at concentrations of 10 or 100 µg/litre followed first-order kinetics in both river water and river water plus sediment; the half-time for mineralization of the benzene ring was 15-33 h. The length of the alkyl chain and the phenyl position had no significant effect, and there was no effect of suspended sediment or competing homologues (Larson, 1990).

LAS were degraded in leaf litter, creek water, periphyton, and sediment at temperatures as low as 4°C, with half-lives of 6-11 days. Temperature changes altered the dependence of the biodegradation of LAS: the half-lives increased by less than a factor of two over an 18°C temperature range. Under realistic conditions, temperature had less effect than was predicted on the basis of classical thermodynamic studies in the laboratory (Palmisano et al., 1991). The dependence of the biodegradation of LAS follows a classical Arrhenius relationship down to about 12°C, with a tenfold increase in reaction kinetics for every 2°C drop in temperature (Larson, 1990).

Mineralization of LAS in saturated subsurface sediment from a wastewater pond and in a pristine pond was monitored by amending the sediment with ^{14}C-LAS and measuring the evolution of $^{14}CO_2$. Mineralization in both sediments exhibited first-order kinetics. LAS were mineralized without a lag in wastewater sediment, with half-lives of 3.2-16.5 days. In the control pond, LAS were mineralized much more slowly, with half-lives of 5.2-1540 days, and only after a lag of 2-40 days; the lag tended to increase with increasing depth. These findings confirm the assumption that acclimatization considerably increases the kinetics of LAS mineralization (Federle & Pastwa, 1988).

A study was conducted of the biodegradation of LAS by microorganisms associated with the roots of two aquatic plants, duckweed *(Lemna minor)* and cattail *(Typha latifola)*. Microorganisms from the roots of cattail mineralized ^{14}C-LAS without a lag, attaining 17% evolution of $^{14}CO_2$ within the 35-day experiment. Microbiota associated with duckweed roots did not mineralize LAS. The fact that the plants came from a pristine pond or from a wastewater pond had no effect on the ability of the microorganisms to mineralize LAS (Federle & Schwab, 1989).

More than 70% of parent LAS (20 mg/litre) in natural seawater at 22°C was biodegraded within 10 days, with an estimated half-life of 6-9 days (Vives-Rego et al., 1987). In an investigation of the primary biodegradation kinetics of LAS (10 mg/litre) in natural seawater in the presence of sediments (250 g/litre), 60% remained after 20 days at 15°C and almost 100% of LAS at 5°C; however, at 20 and 25°C, only a small percentage of the original concentration remained (Sales et al., 1987). In another study in seawater, 97% of parent LAS (10 mg/litre) was biodegraded within two weeks (von Bock & Mann, 1971).

More than 85% of LAS ($C_{11.8}$) in estuarine water underwent primary biodegradation, measured as MBAS removal, after 11 days (Arthur D. Little Inc., 1991). In water from Chesapeake Bay, United States, 75% of MBAS were removed within three days (Cook & Goldman, 1974). In a study of effluent-exposed estuarine waters, with phenyl-radiolabelled C_{13} LAS, production of $^{14}CO_2$ represented 42% of the added label. Addition of sediment from the site (1 g/litre) increased the $^{14}CO_2$ yield to 60%. In both tests, the half-life for mineralization of LAS was about seven days. Up to 54% of a radiolabelled control chemical, glucose, was mineralized. Thus, mineralization of LAS occurs rapidly in pre-exposed estuarine systems, with half-lives shorter than the typical hydraulic residence times of such estuaries (Shimp, 1989).

(iv) Soils and groundwater

A simple shake-flask system was used to determine CO_2 evolution in a test to assess the ultimate biodegradability of LAS by microorganisms in soil and sewage. At 30 mg/litre, high relative-molecular-mass LAS were biodegraded more slowly than those with a low relative molecular mass. Ultimate biodegradation could not be assessed precisely within the 28-day test period, but CO_2 removal was 37-77% and dissolved organic carbon removal was 59-84%. Ultimate biodegradation of the entire molecule (total CO_2) occurred concomitantly with biodegradation of the benzene ring ($^{14}CO_2$). Ring desulfonation, measured as ^{35}S-LAS, was rapid and occurred mainly after primary biodegradation (MBAS method) (Gledhill, 1975).

The kinetics of the ultimate biodegradation of C_{10}-C_{14} LAS to CO_2 was studied in a sludge-amended soil at 0.1-10 times environmental concentrations. All four homologues underwent rapid degradation, with half-lives for the breakdown of the benzene ring of 18-26 days (Ward & Larson, 1989).

Microbial mineralization of 50 µg/kg ^{14}C-LAS was examined in soil types ranging from a loamy sand impacted with sewage effluent to a highly organic alpine soil, by monitoring the evolution of $^{14}CO_2$. LAS were mineralized without a lag in all soils; mineralization exhibited first-order kinetics in nine of the 11 soil types. Asymptotic yields of CO_2 ranged from 16 to 70%; the

half-lives were 1.1-3.7 days. The degradation rates were not correlated with microbial activity, pH, total organic content, or previous exposure (Knaebel et al., 1990).

After ^{14}C calcium and sodium salts of LAS were applied to two silty loam soils, the distribution of ^{14}C was similar. After 60 days, 31-47% of the applied ^{14}C had evolved as $^{14}CO_2$ and 31-40% was present as soil residue, possibly as a combination of parent and metabolized surfactant (Kawashima & Takeno, 1982).

A4.2.1.2 Anaerobic degradation

Degradation of LAS (measured as MBAS) was much slower under anaerobic conditions in activated sludge than under aerobic conditions. No degradation had taken place after one day; up to 20% had been degraded between days 3 and 21, and 36% after 28 days. When soil and wastewater were used, only 20% of the MBAS had disappeared within 28 days (Oba et al., 1967). No significant removal of LAS was reported in an anaerobic sludge digester at a Swiss sewage treatment plant (Giger at al., 1989).

In a review of the fate of LAS in anaerobic and aerobic sewage treatment plants, it was concluded that drying anaerobic sludge on open beds considerably reduces the LAS content. Anaerobic degradation of LAS is, however, limited, as the addition of LAS at 15 g/kg raw sewage (about 15 g/litre raw sewage) may inhibit anaerobic degradation. In the laboratory, digestion of LAS was impaired at concentrations of > 15-20 g/kg, and a concentration of 20 g/kg seriously inhibited gas production, especially when other potentially inhibitory compounds were present. The concentration of LAS normally found in sewage (5-10 g/kg) is, however, unlikely to inhibit anaerobic degradation (Painter & Zabel, 1989). About 15-35% of LAS in raw sewage is physically removed in primary settlers in sewage treatment plants, accounting for most of the LAS found in anaerobic sludge. Precipitation of LAS is correlated with water hardness, since the solubilities of the calcium and magnesium salts of LAS are very low; the solubility products ranged from 2.2×10^{-10} for C_{10} LAS to 6.2×10^{-13} for C_{13} LAS (Berna et al., 1989). The effect of water hardness was confirmed by mass balance analysis of Na^+, Ca^{2+}, and Mg^{2+} (Berna et al., 1993b). The content of total calcium and magnesium in anaerobically digested sludge was 43 times higher than that in water. High contents of LAS in the sludge (up to 30 g/kg) did not inhibit the anaerobic digestion process (Painter & Mobey, 1992), probably because LAS were present as calcium and magnesium salts and therefore had reduced bioavailability.

LAS were not degraded in an anaerobic sediment from a pond receiving wastewater from a laundromat. Despite an exposure period of 25 years, no anaerobic degradation was reported (Federle & Schwab, 1992).

Pre-aerobic treatment of LAS may cause changes in the molecule that permit subsequent degradation under anaerobic conditions (Ward, 1986).

A4.2.2 Abiotic degradation

The mechanisms of abiotic degradation of LAS reported below are not of environmental significance, since biodegradation and sorption are rapid, effective removal mechanisms.

A4.2.2.1 Photodegradation

In a study of the kinetics of the photodecomposition of C_{12} LAS, using a continuous-flow reactor, the initial concentrations were 60-182 mg/litre and the radiation wavelength was 200-450 nm. Conversion of LAS to intermediate products occurred within 1 min, yielding 7 mol CO_2 per mol LAS, and was complete within 20 min. The reaction rate was increased by two orders of magnitude by ferric perchlorate (Matsuura & Smith, 1970).

Rapid photodegradation of LAS (50 mg/litre) occurred within 1-2 h in an aqueous, aerated titanium dioxide suspension without noble metal catalysts. There was rapid decomposition of the aromatic ring and slower oxidation of the aliphatic ring. Photodegradation was dependent on the simultaneous presence of titanium dioxide, oxygen, and light (Hidaka et al., 1985).

A4.2.2.2 Cobalt-60 irradiation

The decomposition of LAS was studied in distilled water irradiated with cobalt-60 gamma rays, which react with water to produce oxygen, peroxide, hydrogen peroxide, and other strong oxidizing agents. A concentration of 10 mg/litre LAS was reduced to 7.8 mg/litre by absorption of 10 Gy and to 0.9 mg/litre by absorption of 100 Gy. The rate of irradiation was found to be less important than the total absorbed energy (Rohrer & Woodbridge, 1975).

A4.2.3 Bioaccumulation and biomagnification

Studies of the bioaccumulation potential of LAS have all been carried out with LAS labelled with ^{14}C or ^{35}S. It should be noted that as these techniques do not usually allow consideration of metabolic transformation the actual bioaccumulation of the parent compound may be overestimated. Toxic concentrations of the breakdown products of LAS are discussed in section A9.3.7.

A4.2.3.1 Aquatic organisms

Bioaccumulation has been studied in daphnids and fish (Table 8).

LAS are readily absorbed through the gills and body surface of fish and are subsequently distributed via the blood to the organs and tissues; most LAS accumulate in the gall-bladder and hepatopancreas. Clearance is usually rapid, with a half-life of two to three days. Short-chain LAS are accumulated to a lesser degree than long-chain LAS.

Only 1% of 0.5 mg/litre LAS added to water was retained in *Daphnia magna* within three or four days after transfer to 'clean' water. Almost all of the chemical was in the form of intact LAS. In fathead minnows *(Pimephales promelas)*, metabolic transformation occurred. All tissues monitored showed some uptake, with concentration factors ranging from 79–372 in muscle to 21 000–70 000 in gall-bladder. Within four days of transfer to 'clean' water, 85% of the LAS had been lost, and almost 100% was lost within 10 days (Comotto et al., 1979).

Table 8. Bioconcentration factors for linear alkylbenzene sulfonates in aquatic invertebrates and fish

Organism	Static/flow	Exposure concentration (mg/litre)	Duration of test (days)	Chain length	Steady state	Bioconcentration factor	Tissue	Reference
Daphnia magna	Flow	0.07	3	C_{12}	?	490		Comotto et al. (1979)
		0.11				560		
		044				720		
		0.09	3	C_{13}	Yes	1250		
		0.11				1050		
		0.41				1325		
Cyprinus carpio	Static	61.1	1	C_{12}	Yes	4.1	Skin surface	Kikuchi et al. (1978)
						1000	Gall-bladder	
	Flow	0.5	4	C_{12}	Yes	20	Whole body	Wakabayashi et al. (1978)
						30	Hepatopancreas	
						9000	Gall-bladder	
		0.0091	5	C_{12}	Yes	16	Whole body	Wakabayashi et al. (1981)
		0.3				400		
		1.0				300		
Pimephales promelas	Flow	0.1	11	C_{12}	Yes	551	Whole body	Comotto et al. (1979)
				C_{13}		1223		
				C_{12}, C_{13}		269		

Table 8 (contd)

Organism	Static/flow	Exposure concentration (mg/litre)	Duration of test (days)	Chain length	Steady state	Bioconcentration factor	Tissue	Reference
Lepomis macrochinus	Flow	0.063	28	C_{12}	Yes	260	Whole body	Bishop & Maki (1980)
		0.064				120		
	Flow	0.5	35	$C_{11.7}$	Yes	107	Whole body	Kimerle et al. (1981)
						5000	Gall-bladder	

Static, water unchanged for the duration of the test; flow, concentration in water maintained continuously

In an experiment in which the aqueous concentrations of an initial concentration of 1.1 mg/litre LAS decreased by 20% during the test, the compounds were concentrated in the gills of carp *(Cyprinus carpio)* within 2 h of exposure, with a concentration factor of 40. Skin surface, muscle, brain, kidney, hepatopancreas, and gall-bladder showed more gradual uptake of LAS over the 24 h of exposure, with concentration factors ranging from 4.1 for skin surface to 1000 for gall-bladder. Blood, gonads, and spleen also took up LAS but were not monitored throughout the period of exposure. LAS was lost rapidly from all tissues except the gall-bladder during 48 h in 'clean' water (Kikuchi et al., 1978).

In the bluegill *(Lepomis macrochirus)*, a steady state was reached within 120–168 h. The bioconcentration factor was calculated by a kinetic method to be 286 for a concentration of LAS of 0.8 mg/litre and 132 for 0.08 mg/litre. LAS were cleared rapidly after the fish were transferred to 'clean' water, with 99% eliminated within 336 h; the time for clearance was 29–30 h (Bishop & Maki, 1980). In another study, a steady state was reached within seven days; the bioconcentration factor in whole body using a kinetic method was reported to be 104; and the half-time for clearance was two to five days during a depuration period of 14 days. The authors postulated that fish excrete LAS in the urine and excrete shorter-chain carboxylates with the benzene ring intact across the gill membranes. Both forms may also be excreted in the faeces (Kimerle et al., 1981).

A4.2.3.2 Terrestrial plants

Foliar uptake of the calcium and sodium salts of ^{14}C-LAS (chain length not specified) by peanuts was studied seven and 30 days after application. No movement of LAS was detected: 70–80% remained within the same leaf to which the compound was applied, and no LAS were detected in other parts of the plant (Kawashima & Takeno, 1982).

Aqueous solutions of ^{14}C-LAS (chain length not specified) were

applied to soil (orthic luvisol), and ryegrass *(Lolium perenne)* was grown under laboratory conditions for up to seven days. Uptake of LAS after three days was 80 mg/kg at an application rate of 1 mg/kg dry weight, 370 mg/kg at a rate of 5 mg/kg, and 18 900 mg/kg at 50 mg/kg. After seven days, levels of 600, 5000, and 19 300 mg/kg were measured at the three dose levels, respectively (Litz et al., 1987).

^{14}C-LAS (chain length not specified) were applied under field conditions to both loamy orthic luvisol and sandy dystric cambisol soils irrigated with wastewater at rates of 5 and 50 g/m^2. After 49 days, rye grass grown in the loamy soil contained residues of 130 and 1000 mg/kg dry weight at the two exposure rates, respectively.

Plants grown in the sandy soil contained 230 and 470 mg/kg, respectively, after 54 days (Litz et al., 1987).

Two plant-soil microcosms were exposed to ^{14}C-LAS (chain length not specified), and LAS degradation and percolation were followed for up to 109 days. The initial soil concentrations were 16.2 µg/g dry soil in potato soil (sandy) and 27.2 µg/g in grass, bean, and radish soil (clay-like). The concentrations of radiolabelled compounds in the plants decreased rapidly: at the end of exposure, 39.1-65.8 µg LAS equivalents per g fresh weight of plant were found in potatoes (study duration, 76 days) and 62.1-213.3 µg/g in grass, radishes, and beans (study duration, 109 days) (Figge & Schoberl, 1989).

A5. ENVIRONMENTAL LEVELS AND HUMAN EXPOSURE

Section summary

The concentrations of LAS have been quantified by means of a specific, sensitive analytical method in almost every environmental compartment in which they might be present. The concentrations decrease progressively from wastewater to treated effluent and surface waters, and low concentrations are found in the sea.

The environmental concentrations of LAS are directly dependent on use patterns, the type and efficiency of sewage treatment, and the characteristics of the receiving environment. In areas where LAS are the predominant surfactants used, typical concentrations are 1-10 mg/litre in wastewater, 0.05-0.1 mg/litre in effluents that have undergone biological treatment, 0.05-0.6 mg/litre in effluents passed through a percolating filter, 0.005-0.050 mg/litre in surface waters below sewage outfalls (with concentrations decreasing rapidly to 0.01 mg/litre downstream from the outfall), < 1-10 mg/kg in river sediments (up to 100 mg/kg in highly polluted sediments near discharge zones), 1-10 g/kg in sewage sludge, and < 1-5 mg/kg in sludge-amended soils. The initial concentration of LAS in sludge-amended soils is 5-10 mg/kg, but up to 50 mg/kg have been reported after atypically heavy appli-cations. The concentration of LAS in estuarine waters is 0.001-0.010 mg/litre but is higher where wastewater is discharged directly. The concentrations in offshore marine waters are < 0.001-0.002 mg/litre.

A wide range of environmental concentrations has been reported, owing to use of different analytical methods; differences in characteristics of sampling sites, which range from highly polluted areas with inadequate sewage treatment to areas where sewage undergoes extensive treatment; seasonal differences, which can account for a twofold variation; and differences in the use of LAS.

Monitoring has shown no accumulation of LAS in environmental compartments over time. The concentrations in soil do not increase with time but are diminished due to mineralization. As LAS are not degraded under strictly anaerobic condition, they are not mineralized in anaerobic sediments. With current use of LAS, the rates of their assimilation in all receiving environmental compartments is equal to their rate of input, implying a steady state.

A5.1 Environmental levels

LAS have been measured in most environmental compartments, including discharge (raw sewage), sewers, sewage treatment plants, sludge-amended soils and land fill, river water, river sediments, subsurface soils, groundwater, and estuaries (Berna et al., 1991).

A decline in the concentrations of anionic surfactants in the environment, as assessed by measurement of MBAS, was seen in Europe, Japan, and the United States after ABS was replaced by LAS (Sullivan & Evans, 1968; Sullivan & Swisher, 1969; Gerike et al., 1989). Similar declines have been observed more recently in countries such as Thailand, where the change to LAS detergents is also more recent (Berna et al., 1991).

A5.1.1 Wastewater, sewage effluent, and sludge

The concentrations of LAS in sewage influent and effluent at sewage treatment plants are shown in Table 9; those in sewage sludge are given in Table 10.

The efficiency of wastewater treatment plants in removing LAS is reported to exceed that of removal of biochemical oxygen demand. Activated sludge removed an average of 98% LAS, trickling filters removed 80%, and primary clarification, 27%. The average concentration in raw sewage was 3.5 mg/litre, and those in effluent were 2.1 mg/litre after primary treatment and 0.06 mg/litre in activated sludge. The average chain length of LAS was $C_{12.5}$ in sewage sludge and C_{12} in influent sewage (Rapaport & Eckhoff, 1990).

The amount of LAS removed in a sewage treatment plant was 93% on the basis of total organic carbon and 98.1% on the basis of a specific method. The contribution of LAS to the total organic carbon was estimated to be 0.93% in treated water and 3.0% in digested sludge; 75.9% of LAS present in the raw sewage was mineralized during treatment and 7% was in the form of sulfoxyphenyl-carboxylates, a product of the biodegradation of LAS, suggesting that biodegradation of LAS had reached a steady state. These figures were obtained by analysis for sulfoxyphenylcarboxylates (Berna et al., 1993b).

In another study, 40% of LAS was removed in a wastewater treatment plant. The half-life for removal from the sewer pipe was calculated to be 11 h (Moreno et al., 1990).

A5.1.2 Sediment

The concentrations of LAS in sediment are shown in Table 11, and those in sediment samples collected at various distances from sites of effluent outfall are shown in Table 12.

Table 9. Concentrations of methylene blue-active substances (MBAS) and linear alkylbenzene sulfonates (LAS) in sewage influent and effluent

Location	Year	Material	Concentration (mg/litre)		Reference
			MBAS	LAS	
Switzerland (29 sites, 1 sampling)	1986	Raw sewage		0.95–3.9	Brunner et al. (1988)
		Effluent		0.007–0.33	
Germany (11 sites, 1 sampling)	1985	Influent (activated sludge)	5.1 (1–13.3)	4 (0.54–12.4)	Matthijs & De Henau (1987)
		Influent (trickling filter)	8.8 (8.1–9.9)	7.4 (6.8–8.4)	
		Effluent (activated sludge)	0.19 (0.09–0.28)	0.07 (0.05–0.11)	
		Effluent (trickling filter)	1.1 (0.84–1.5)	0.76 (0.61–0.94)	
United Kingdom (several samples)	1982	Effluent	0.69 (0.58–0.81)	0.31 (0.21–0.42)	Gilbert & Pettigrew (1984)
River Thames area (5 sites, several samples)	1987	Sludge		15.1–341	Holt et al. (1989)
Israel (4 sites)	1983	Influent	9.6–10.6[a]		Zoller (1985)
		Effluent	0.3–11.0[a]		
United States (4 sites, 45 samples	1979	Effluent		0.078–0.303	Eganhouse et al. (1983)
	1976–86	Influent		3.7 ± 1.1	Rapaport & Eckhoff (1990)
		Effluent (activated sludge)		0.05 ± 0.04	
		Effluent (trickling filter)		0.6 ± 0.3	
		Effluent (primary)		2.2 ± 0.4	

Table 9 (contd)

Location	Year	Material	Concentration (mg/litre)		Reference
			MBAS	LAS	
United States		Influent	5.9–6.5	5.7–6.5	Osburn (1986)
(1 sampling)		Influent	3.7–5.2	3.8–4.9	
		Effluent	0.39–1.02	0.14–0.60	
(2 sites, 9 samples)	1983	Raw influent	4.17	3.73	Sedlak & Booman (1986)
		Primary influent	3.18	2.97	
		Primary effluent	1.66–2.82	1.73–2.51	
		Final effluent	0.03–0.06	0.02–0.05	
Canada (4 sites, 45 samples yearly)	1976–86	Influent		2.0 ± 0.6	Rapaport & Eckhoff (1990)
		Effluent (activated sludge)	0.09 ± 0.05		
		Effluent (primary)		1.7–2.3	
Japan (5 sites, 60 samples)	1972–73	Influent	5.1–14.0		Oba et al. (1976)
		Effluent	0.3–4.7		
(6 sites, 1–2 samples)	1984	Influent (suspended particles)		0.236–1.504	Takada & Ishiwatari (1987)
		Effluent (suspended particles)		0.0001–0.001	

[a] Total anionic surfactants (mainly LAS)

Table 10. Concentrations of methylene blue-active substances (MBAS) and linear alkylbenzene sulfonates (LAS) in sewage sludge

Location	Year	Material	Concentration (mg/litre)		Reference
			MBAS	LAS	
Switzerland (8 and 12 sites, 1 sampling)		Digested sludge		2900–11 900	McEvoy & Giger (1985, 1986)
(29 sites, 1 sampling)	1986			50–13 800[a]	Brunner et al. (1988)
Spain (5 sites, several samplings)		Activated sludge (anaerobic digestion)		7000–30 200[a]	Berna et al. (1989)

		Aerated, settling system		400-700[a]	
Finland (12 sites, 1 sampling)		Digested sludge		3400-6300[a]	McEvoy & Giger (1986)
Belgium (11 sites, 1 sampling)	1985	Aerobic sludge Digested sludge	5399 (3042-8133) 9017 (3632-17 006)	281 (182-432) 4917 (1327-9927)	Matthiijs & De Henau (1987)
Germany (4 sites, 45 samples yearly)	1981-86			4920 (1330-9930)	Rapaport & Eckhoff (1990)

Table 10 (contd.)

Location	Year	Material	Concentration (mg/litre)		Reference
			MBAS	LAS	
United States					
(4 sites, 45 samples yearly)	1981-86			4660 ± 1540	Rapaport & Eckhoff (1990)
12 sites, NY, (1 sampling)		Digested sludge		6900[a]	McEvoy & Giger (1986)
(12 sites, CA, 1 sampling)		Digested sludge		5200[a]	
(1 sampling)		Primary sludge	110-126	107-127	Osburn (1986)
(2 sites, OK, 9 samples)	1983	Primary sludge	4610-6120	5340-6310	Sedlak & Booman (1986)
		Secondary sludge	520-990	410-860	
		Anaerobic digester	6860	6660	
		Aerobic digester	3820	4250	
		Drying bed (anaerobic)	170	160	
		Drying bed (aerobic)	230	150	
Southern California (marine)	1981	Effluent particulates		1342	Eganhouse et al. (1983)

[a] Dry weight

Table 11. Concentrations of methylene blue-active substances (MBAS) and linear alkylbenzene sulfonates (LAS) in sediments in the United States and Japan

Location	Year	Concentration (mg/kg)		Reference
		MBAS	LAS	
United States				
Rivers (activated sludge)			0.3-3.8	McAvoy et al. (1993)
Rivers (trickling filter)			0.2-340	
Mississippi River	1991-92		< 0.01-5	Tabor et al. (1993)
Japan				
Tokyo Bay (1 sampling, few samples)	1969	35 (33-37)		Ambe (1973)
River (1 sampling, few samples)		61 (55-65)		
River Sagami estuary (16 sites, 1 sampling)		7.9-39[a]	ND-17	Utsunomiya et al. (1980)
Sagami Bay (16 sites, 1 sampling)		5.1-15	ND	
Rivers	1977		< 1-260	Environment Agency Japan (1978)
Lake Suwa (1 site, 3 samples)	1977		1.0-7.0	
Rivers (9 sites, 7 samples, 1 year); (1 site 52 samples)	1982-83		107 (ND-567)	Takada & Ishiwatari (1987); Takada et al. (1992b)
Estuaries (1 site, 52 samples)	1983-84		4.82 (0.12-36.6)	Takada et al. (1992b)
Tokyo Bay (9 sites, 7 samples, 1 year)	1980		71.0	Takada & Ishiwatari (1987)
Tokyo Bay	1984		0.02 (ND-0.06)	Takada et al. (1992a)
Sumida River (12 sites, 1 sampling)	1982		0.069	Kikuchi et al. (1986)
Tama River (3 sites, 8 samples)	1977		3.5-86.3	Hon-Nami & Hanya (1980b)
Tama River (10-12 sites)	1982		0.141	Kikuchi et al. (1986)
Tokyo Bay (10-12 sites)	1982		< 0.001-0.002	

Table 11 (contd)

Location	Year	Concentration (mg/kg)		Reference
		MBAS	LAS	
Japan (contd).				
Tsurumi River (7 sites, 12 samples)	1984		17-45[a]	Yoshikawa et al. (1985)
Tama River	1981		2.79-10.72	Yoshimura et al. (1984b)
Ports and coast	1977		< 1-2.9	Environment Agency Japan (1978)

ND, not determined
[a] Dry weight

Table 12. Concentrations of methylene blue-active substances (MBAS) and linear alkylbenzene sulfonates (LAS) in sediment of rivers in Germany and the United States at various distances from effluent outfalls

Location	Year	Sampling site (distance from effluent outfall)	Concentration (mg/litre)		Reference
			MBAS	LAS	
German rivers (14 sites, several	1978-82	Below outfall		1.5-174[a]	De Henau et al.

samples)					(1986)
United States					
Rivers (4 sites, 45 samples) yearly	1978-82	Below outfall		190	Rapaport & Eckhoff (1990)
		< 5 miles (8.0 km)		11.9	
		> 5 miles (8.0 km)		5.3	
(1 sampling)		0.5 miles (0.8 km)	118-317	100-322	Osburn (1986)
		4.4 miles (7.1 km)	4.1-19	2.0-5.1	
		7.4 miles (11.9 km)	7.5-10.6	1.3-4.4	
Rapid Creek, South Dakota	1979-80	0.8 km		44.6-275	Games (1983)
		7 km		3.2-9.1	
		11.7 km		2.1-8.4	
		25.3 km		2.7-10.1	
		48 km		1.4	
		87.2 km		1.5	
Little Miami River, Ohio (4 sites, 1 sampling)		Downstream from sewage treatment plants		ND-1.2 24.7-290[b]	Hand et al. (1990)
Rivers (4 sites, 45 samples)	1978-82	Below outfall		190	Rapaport & Eckhoff (1990); McAvoy et al. (1993)
		Above outfall[c]		1.0-1.2	
		Below outfall (left)[c]		0.3-1.6	
		Below outfall (middle)[c]		0.6-3.8	

Table 12 (contd)

Location	Year	Sampling site (distance from effluent outfall)	Concentration (mg/litre)		Reference
			MBAS	LAS	
United States (contd)					
Rivers (4 sites, 45 samples) (contd).	1978-82	Below outfall (right)[c]		0.8-3.4	
		Above outfall[d]		0.2-0.9	
		Below outfall (left)[d]		0.2-130	
		Below outfall (middle)[d]		0.6-124	
		Below outfall (right)[d]		9-340	

[a] 13 of the 14 samples contained < 25 mg/kg and 10 contained < 10 mg/kg
[b] Suspended solids
[c] Activated sludge
[d] Trickling filter

Concentrations of LAS > 10 mg/kg were measured in sediments from the upper estuaries near Tokyo Bay and < 1 mg/kg in the lower estuaries. The concentrations of LAS in sediments decreased offshore, falling below 0.01 mg/kg in sediments sampled 10 km from the mouths of the rivers. The authors suggested that loss of LAS was due to rapid degradation in the coastal zone (Takada et al., 1992a).

It was reported in one study that C_{13} was the most abundant homologue of LAS in river sediment (Yoshikawa et al., 1985); another group found that C_{12} was the most abundant of the LAS in estuarine sediments and that no C_{10} were present (Utsunomiya et al., 1980). C_{12} and C_{13} LAS predominated in sediment and C_{10} and C_{11} homologues were the most abundant in water (Hon-Nami & Hanya, 1980b). The average chain length of LAS in Japanese river sediments was $C_{11.8}$-$C_{12.2}$ (Hon-Nami & Hanya, 1980b; Yoshimura et al., 1984a).

In a study of marine sediments from an area adjacent to the point of discharge from a submarine sewer, LAS were detected only in the vicinity of the discharge, at a concentration of 0.1 mg/kg, and not in sediment sampled 50 m outside this area. The average chain length was $C_{11.7}$. In a comparison of the chain lengths of LAS detected in various environmental compartments and those used in detergent products, the LAS detected in sludge and sediment were relatively higher homologues and those in the water phase were lighter (Prats et al., 1993).

The average concentration of LAS in river sediments sampled upstream of an activated sludge treatment plant outfall was 1.1 mg/kg, and those in sediments downstream of the plant were 0.3-3.8 mg/kg (McAvoy et al., 1993).

A5.1.3 Surface water

The concentrations of LAS in water are shown in Table 13 and those in samples taken at various distances from sites of effluent outfall in Table 14.

After replacement of branched-chain ABS, which are only sparingly biodegradable, with the straight-chain LAS, the concentrations of MBAS decreased in many rivers. ABS were replaced by LAS in Japan in the late 1960s; the ratio of LAS to total ABS in river water rose from 20 to 70% in 1967-70 and had reached 90% by 1973 (Miura et al., 1968; Ihara et al., 1970; Oba et al., 1975). The levels of MBAS were monitored in the Illinois River, United States, from 1959 to 1966; those in 1965 and 1966 reflected the change in surfactant usage (Sullivan & Evans, 1968), and this trend continued in 1967 and 1968 (Sullivan & Swisher, 1969). In the River Rhine, the level of anionic detergents, measured as MBAS, fell steadily between 1971 and 1977 (Hellmann, 1978). In water samples from 140 sites on

Table 13. Concentrations of methylene blue-active substances (MBAS) and linear alkylbenzene sulfonates (LAS) in water

Location	Year	Water sample	Concentration (mg/litre)		Reference
			MBAS	LAS	

Freshwater

Location	Year	Water sample	Concentration (mg/litre) MBAS	Concentration (mg/litre) LAS	Reference
United States					
Rivers (4 sites, 45 samples yearly)	1978-86			0.041-0.115	Rapaport & Eckhoff (1990)
Little Miami River, Ohio (4 sites, one sampling)		Interstitial		< 0.05 ND-0.08	Hand et al. (1990)
Illinois River (one sampling)[a]	1959-65 1965-66 1968		0.54 0.22 0.05-0.06		Sullivan & Swisher (1969)
Rapid Creek, South Dakota	1979-80			0.01-0.270	Games (1983)
Mississippi River (36 sites)	1991-92			< 0.01-0.3	McAvoy et al. (1993)
(350 samples)			< 0.01-0.046	< 0.005	Tabor et al. (1993)
Japan					
Rivers (23 sites, 51 samples)	1977			< 0.01-2.9	Environment Agency Japan (1978)
Rivers (1 sampling)				0.018-0.59	Tsukioka & Murakami (1983)
Oohori River (6 sites monthly)	1987-88			approx. 0.5-1.6	Amano et al. (1991)
Lake Teganuma (6 sites monthly)	1987-88			ND-approx. 0.7	
Tama River (3 sites, 8 samples)	1977-78		0.24-1.24	0.108-0.491	Hon-Nami & Hanya (1980a)

Table 13 (contd.)

Location	Year	Water sample	Concentration (mg/litre) MBAS	Concentration (mg/litre) LAS	Reference
Japan (contd)					
Rivers, Hyogo Prefecture (70 sites)				0.004-2.5	Kobuke (1985)
Tama River (3 sites, 1 sampling)				0.035-0.219	Yoshikawa et al. (1984)
Tama River (10-12 sites)	1982			0.128	Kikuchi et al. (1986)
Sumida River (10-12 sites)	1982			0.005-0.01	Kikuchi et al. (1986)
Rivers (1 sampling)			0.06-0.12		Saito & Hagiwara (1982)
Rivers, Niigata Prefecture (6 sites, 1 sampling)	(1981)		0.02-2.63	0.18 (max)	Motoyama & Mukai
Rivers, coastal area, Hiroshima Prefecture (20 sites)				0.019 (0.001-0.06)	Okamoto & Shirane (1982)
Inland Sea, Eastern Seto (4 sites, 1 sampling)	1975		0.016-0.077		Yoshida & Takeshita (1978)
(17 sites, 1 sampling)	1976		0.01-0.048		
Tsurumi River, Kanagawa (7 sites once)	1984-76	Surface	0-0.8	0.01-0.29	Yoshikawa et al. (1985)
Yodo River, Osaka (several sites)	1989	Surface		0.043-0.089	Nonaka et al. (1990)
Tama River, Tokyo (2 sites, 4 samples)	1981	Surface		0.2	Yoshimura et al. (1984b)
Sumidogawa River (2 samples)	1983	Suspended		0.0048-0.054	Takada & Ishiwatari
Tomogawa River (5 samples)		particles		0.0005-0.0025	(1987)
Teshiro River, Nagoya (4 sites, 4 samples)	1989	Surface		0.01-0.27	Kojima (1989)

Table 13 (contd)

Location	Year	Water sample	Concentration (mg/litre) MBAS	Concentration (mg/litre) LAS	Reference
Japan (contd)					
Lake Biwa, Shiga	1988	Surface		0.00	Shiga Prefecture (1988)
Teganuma, Chiba (1 site, 12 samples)	1988	Surface		ND-0.423	Amano et al. (1989)
River (several sites)	1988	Surface		0.019-1.4	Nonaka et al. (1989)
Nagoya Bay	1989	Surface		0.00	Kojima (1989)
Rivers, Fukuoka City				ND-1.6	Ohkuma (1981)
Europe					
River Rhine (several sites)	1971-72	0.08-0.24			Hellmann (1978)
Saar River (11 sites, 1 sampling)	1985		0.13 (0.03-0.25)	0.04 (0.01-0.09)	Matthijs & De Henau (1987)
German rivers (several sites)	1976-79		0.075-0.5		Fischer (1980)
Dutch river (Amsterdam drinking-water supply) (8 sites)			0.004-0.141	0.003-0.037	Waters (1976)
Florence, Italy (several samples)	1983	Aqueduct	0 .01-0.1		Mancini et al. (1984)
(several sites)	1982	Well water	0.00-0.01		
United Kigdom					
Rivers	1982		0.04-0.26	0.012-0.08	Gilbert & Pettigrew (1984)
Rivers (8 sites)			0.035-0.217	0.009-0.097	Waters (1976)
Rivers (4 sites)	1977-78		0.022-0.473	0.007-0.173	Waters & Garrigan (1983)

Table 13 (contd)

Location	Year	Water sample	Concentration (mg/litre) MBAS	Concentration (mg/litre) LAS	Reference

Groundwater	1992			< 0.01–0.02	Field et al. (1992)
Estuarine and marine water					
North Sea (19 sites)	1989			< 0.0005–0.0012	Stalmans et al. (1991)
Krka River estuary, Croatia (below 50 m > 50 m)	1990	Wastewater Estuarine water	0.003–0.007 0.001–0.002	0.42–0.78	Terzic & Ahel (1993)
Tokyo Bay, Japan (8 samples)	1978		0.03–0.07	< 0.003–0.014	Hon-Nami & Hanya (1980a)
Tokyo Bay, Japan (10–12 samples)	1982			0.001–0.03	Kikuchi et al. (1986)
Osaka Bay, Japan (several sites)	1988	Surface		ND–0.0072	Nonaka et al. (1989)

ND, not detected
[a] 10–20% of MBAS were LAS

Table 14. Concentrations of methylene blue-active substances (MBAS) and linear alkylbenzene sulfonates (LAS) in water at various distances from effluent outfalls

Location	Year	Sampling site (distance from effluent outfall)	Concentration (mg/litre)		Reference
			MBAS	LAS	
United States					
Rivers (4 sites, 45 samples yearly)	1978–86	Below outfall		0.115	Rapaport & Eckhoff (1990)
		< 5 miles (8 km)		0.079	
		> 5 miles (8 km)		0.041	
(1 sampling)		0.5 miles (0.8 km)	0.400	0.270	Osburn (1986)
		4.4 miles (7.1 km)	0.300	0.150	
		7.4 miles (11.9 km)	0.250	0.120	
		15.8 miles (25.4 km)	0.240	0.100	
		30.0 miles (48.3 km)	0.130	0.040	
		55.0 miles (88.5 km)	0.100	0.010	
Rapid Creek, South Dakota	1979–80	0.8 km		0.270	Games (1983)
		7 km		0.150–0.190	
		11.7 km		0.120	
		25.3 km		0.080	
		48 km		0.040	
		87.2 km		0.010	
Rivers		Above outfall		< 0.01–0.9	McAvoy et al. (1993)
		Below outfall (left)		< 0.01–0.33	
		Below outfall (middle)		< 0.01–0.3	
		Below outfall (right)		< 0.01–0.3	

Table 14 (contd)

Location	Year	Sampling site (distance from effluent outfall)	Concentration (mg/litre)		Reference
			MBAS	LAS	
Canadian rivers (4 sites, 45 samples yearly)	1978–86	Below outfall		0.053	Rapaport & Eckhoff (1990)
Rio Grande, Brazil (1 sampling, 50 samples)	1979	90 m	0.05–4.5		Kantin et al. (1981)
German rivers (several sites)	1976–79	Unpolluted	0.075		Fischer (1980)
		Polluted	0.2–0.5		
(4 sites, 45 samples yearly)	1978–86	Below outfall		0.01–0.09	Rapaport & Eckhoff (1990)
United Kingdom					
Rivers (several samples)	1982	Above discharge	0.04 (0.02–0.07)	0.012 (0.008–0.019)	Gilbert & Pettigrew (1984)
		Close to discharge	0.26 (0.11–0.47)	0.08 (0.01–0.17)	
		5–16 km	0.16 (0.08–0.23)	0.04 (0.008–0.095)	
Avon River (4 sites)	1977–78	Head water	0.03–0.039	0.009–0.015	Waters & Garrigan (1983)
		0.5 km	0.21–0.371	0.056–0.173	
		6 km	0.095–0.22	0.011–0.095	
Tean River (4 sites)	1977–78	Head water	0.035–0.073	0.008–0.019	
		Directly below sewage treatment	0.208–0.473	0.067–0.144	
		5 km	0.145–0.234	0.019–0.07	

Table 14 (contd.)

Location	Year	Sampling site (distance from effluent outfall)	Concentration (mg/litre)		Reference
			MBAS	LAS	
United Kingdom (contd)					
Trent River (4 sites)	1977–78	Head water	0.022–0.052	0.01–0.011	
		20–35 km below head water	0.08–0.227	0.007–0.072	
Nene River tributary (4 sites)	1978		0.104	0.011	
		In the vicinity of sewage effluent disharge	0.206–0.216	0.035–0.037	
		3.5 km	0.184	0.035	
		13.5 km	0.06	0.007	

four German rivers, MBAS concentrations fell by 90% between 1964 and

1987 (Gerike et al., 1989).

The mean level of MBAS in rivers in the United Kingdom was 0.15 mg/litre. On average, only 26% was attributable to LAS (by microdesulfonation and gas–liquid chromatography), but the levels of LAS and their contribution to the total MBAS concentration varied according to the sampling site, with a higher proportion of LAS in samples from sites near sewage effluent discharge points (Waters & Garrigan, 1983). Similar findings were reported by Gilbert & Pettigrew (1984), who found that LAS represented 45% of total MBAS in actual sewage. Sites immediately below sewage outfalls were found to have higher MBAS:LAS ratios than sites further downstream (Osburn, 1986).

In Lake Biwa basin, Japan, during the summer months of 1983, LAS were found in a wide range of concentrations. The highest, measured as MBAS, were > 0.2 mg/litre at river mouths. The levels in rivers flowing from densely populated areas were 0.05–0.2 mg/litre MBAS and those flowing from less populated areas were < 0.05 mg/litre. The middle stream zone of the River Isasa, in a densely populated area, contained levels of 0.36–1.91 mg/litre, and surfactant levels in residential areas showed daily fluctuations related to discharge (Sueishi et al., 1988). Several observations apply to these studies. Firstly, the fact that daily fluctuations were observed indicates that the samples may have been taken from the actual discharge plume, so that the wastewater effluent may not have been completely mixed with the recipient surface water. Secondly, in several Japanese studies of heavy discharge zones, anionic surfactants could not be detected in surface waters, although the analytical detection limit of MBAS in the mid-1980s was 0.05–0.1 mg/litre. Thirdly, sewage treatment at several of the sites has improved considerably over the last decade.

Seasonal trends in the concentrations of LAS were observed in the Oohori River and Lake Teganuma, Japan, in 1987 and 1988, with low levels in summer and high levels in winter (Amano et al., 1991).

The concentrations of LAS were measured in the Tamagawa River, Japan, at two-week intervals for two years, by sampling water from the boundary between freshwater and brackish zones. The concentrations measured in winter were about five times higher than those measured in summer, when long-chain homologues tended to be depleted. The distribution of isomers also showed a clear seasonal trend, with a greater loss of external isomers in summer. The seasonal changes are thought to be the result of differences in water temperature and microbial activity. The flux of LAS in the river was estimated to be 320 tons/year (293 tonnes/year), which exceeds the total amount of LAS accumulated in the bay sediment, indicating that > 99.9% of LAS in the estuary and the bay was degraded (Takada et al., 1992b).

The concentrations of LAS in suspended particles from tributaries of Tokyo Bay, Japan, were 0.5–53.8 µg/litre. Those in suspended particles from a wastewater influent were 297–504 µg/litre and those in the effluent, 0.1–1.22 µg/litre (Takada & Ishiwatari, 1987).

The concentrations of LAS in the estuary of the Krka River, Croatia, were 420–780 µg/litre near municipal wastewater outlets; 50 m from the wastewater outlets, the concentrations were 7.2 µg/litre at a depth of 0.5 m and 3.2 µg/litre at a depth of 6 m. The concentrations in water sampled more than 50 m from the input area were 1–2 µg/litre. The Krka River estuary was reported to be highly stratified, with vertical transport of pollutants reduced by the freshwater–saline boundary. The concentrations of LAS were negatively correlated with salinity; the maximum concentration, 24 µg/litre, was detected in the surface monolayer. An increase in the relative abundance of lower homologues of LAS (C_{10} and C_{11}) was reported in comparison with the original distribution of homologues in the wastewater, indicating more rapid depletion of higher homologues, possibly by biodegradation and fast settling with particles from sewage (Terzic & Ahel, 1993).

In a comparison of the distribution of homologues of LAS in the Tama River, Japan, with those established for active substances used in commercial detergents, the levels of C_{12} and C_{13} LAS were found to decrease over time and those of C_{10} and C_{11} to increase (Hon-Nami & Hanya, 1980a). C_{11} was the commonest LAS homologue in river water (Kobuke, 1985; Yoshikawa et al., 1985), and no C_{13} LAS were present (Utsunomiya et al., 1980). The average chain length of LAS in Japanese rivers was $C_{10.9}$–$C_{11.2}$ (Nakae et al., 1980; Yoshimura et al., 1984a; Kobuke, 1985).

Several research groups have confirmed that such changes in chain length occur during the environmental passage of LAS. In a study in which the concentration of homologues of LAS was measured quantitatively by HPLC during activated sludge treatment and lagoon treatment of wastewater in Spain, the average chain length decreased from $C_{11.7}$ in raw material, to $C_{11.3}$ in the dissolved phase of raw wastewater, and to $C_{10.3}$ in the dissolved phase of treated effluent. A slight increase in average chain length was reported for the solids compartment in each of these systems, adding to laboratory findings that the longest homologues adsorb most strongly to sediment. The reduction in average chain length in the water compartments was environmentally significant, since shorter homologues of LAS are less toxic to aquatic organisms. Thus, the LC_{50} values for daphnia were higher for shorter homologues (> 20 mg/litre for C_{11} and 10 mg/litre for $C_{11.7}$) (Prats et al., 1993).

The Japanese Soap & Detergent Association (1992) reported a

decrease in LAS concentrations in the Tama River near Tokyo, Japan, from 2.3 mg/litre in 1967 to 0.2 mg/litre in 1991. The decrease was attributed to the development of sewage systems along the river: sewage coverage was 26% in 1974 and 89% in 1990. This information can be used to estimate concentrations of LAS in developing countries with inadequate sewage systems but where detergent use is increasing.

Low levels of LAS were reported in water from the Scheldt River estuary and in a series of samples from the North Sea (see Table 13). The concentrations in the estuary decreased rapidly from about 0.010–0.012 mg/litre to values below the limit of analytical detection (0.5 µg/litre) concurrently with an increase in salinity. The concentrations decreased more rapidly than on the basis of dilution alone, indicating that removal occurred rapidly. The authors did not report whether the removal of LAS was related to adsorption onto settling solids, to biodegradation, or to a combination of the two. The concentration of LAS in samples taken offshore was consistently below the limit of detection (Stalmans et al., 1991).

A5.1.4 Soil and groundwater

The levels of LAS in sludge-amended soil were 0.9–1.3 mg/kg in German soils used for agriculture. A level of 2.2 mg/kg was found in the United Kingdom in soil that was used only for the disposal of sludge (De Henau et al., 1986). MBAS were found at a level of 24.7 mg/kg (14.4–37.5 mg/kg) and LAS at 1.4 mg/kg (0.9–2.2 mg/kg) in German agricultural soils that had been amended with sludge (Matthijs & De Henau, 1987). The levels of LAS in soils near the River Thames, United Kingdom, in 1987 to which sludge had been applied previously were < 0.2–2.5 mg/kg. Soils that had received an application of sludge during 1987 had levels of LAS of < 0.2–19.8 mg/kg (Holt et al., 1989).

Levels of 13–47 mg/kg were found on the surface of sludge-amended soil in the United States in 1979; < 5 mg/kg were found at a depth of 15–90 cm (Rapaport & Eckhoff, 1990).

A concentration of 22.4 mg/kg LAS was measured in agricultural soil that had recently been amended with anaerobically digested sludge. The concentration was 3.1 mg/kg six months after application of the sludge and 0.7 mg/kg after 12 months (Prats et al., 1993). HPLC, fluorescence detection, and mass spectrometry were used to analyse samples of a groundwater plume which originated from an underground discharge of sewage. It was found that 96% of the LAS was removed from the aqueous phase during sewage treatment and an additional 3% during infiltration with groundwater. The concentrations in ground-water were below the detection limit of 0.01–0.02 mg/litre. The disappearance of LAS during groundwater infiltration was calculated to follow first-order kinetics. LAS were detected (by mass spectrometry) at only trace levels in groundwater sampled 20–500 m down the gradient from the infiltration zone (Field et al., 1992).

A5.1.5 Drinking-water

The concentration of LAS reported in Dutch tap-water was 0.003 mg/litre; MBAS levels were about three times higher. In tap-water in the United Kingdom, the concentration of LAS was 0.007 mg/litre; that of MBAS was again three times higher (Waters, 1976). The concentrations of LAS in Italian well-water were below the analytical limit of detection of 0.0084 mg/litre (Mancini et al., 1984). LAS were not detected in Japanese drinking-water in the 1970s at a limit of detection of 0.001 mg/litre (Yushi, 1978).

A5.1.6 Biota

The concentrations of LAS in biota are shown in Table 15.

A5.2 Environmental processes that influence concentrations of linear alkylbenzene sulfonates

A shift towards LAS of lower chain lengths has been reported in environmental samples in comparison with the distribution of chain lengths in raw materials. It has also been reported that about 50% of the total LAS in samples of water is associated with either suspended particles or dissolved organic matter. Reductions in both the chain length and the concentration of dissolved LAS will result in decreased aquatic toxicity (see also section 9).

A5.2.1 Changes in chain length distribution during environmental removal of linear alkylbenzene sulfonates

The concentrations of LAS and related compounds were measured in 350 samples of water and sediment from the Mississippi River, United States. Those in surface water were < 0.005 mg/litre. LAS in sediment had longer chains than those in the overlying water column (Tabor et al., 1993).

A gradual reduction in the average chain length of homologues was observed as they passed through a wastewater treatment plant: untreated wastewater, $C_{12.1}$; treated effluent, C_{12}; surface water below a sewage outfall, $C_{11.7}$ (Castles et al., 1989). Isomers of C_{13} LAS have partition coefficients that are typically one order of magnitude higher than those of the corresponding isomers of the C_{12} LAS homologues (Amano et al., 1991).

Table 15. Total body concentrations of linear alkylbenzene sulfonates in biota in Japan

Organism	Year	Location	Concentration (mg/kg dry weight)	Reference
Algae	1980–81	River	< 1–368	Katsuno et al. (1983)
Pond snail (Sinotaia quadratus histrica)	1979	River	0.4–1.81	Tanaka & Nakanishi (1981)
Gizzard shad (Konosirus punctatus)	1982 1983	Bay	< 1 or < 2 < 0.1–0.3	Tokai et al. (1990)

A5.2.2 Specification of linear alkylbenzene sulfonates in surface waters

In most programmes for monitoring LAS in the environment, the total sample of waste or surface water is analysed, and separate concentrations of LAS in the fractions of dissolved and suspended solids are not determined. In a study in which these concentrations were reported, the mean levels of dissolved LAS were 8.4 mg/litre in raw wastewater (range, 5.6–11.4 mg/litre) and 5.5 mg/litre in the suspended solid fraction. In the seven wastewaters studied, an average of about 65% was present in the filtered (filtration, < 1 µm) 'dissolved' fraction and 35% in the 'solids-associated' fraction. In treated effluent, 85% of LAS was in the dissolved fraction and 15% in the solids-associated fraction (Berna et al., 1993b). In wastewater treatment works, 49–63% of the LAS was in the dissolved phase and 37–51% in the solids-associated phase (Berna et al., 1989). In filtered (0.7 µm) wastewater containing LAS at 2.55–2.95 mg/litre, 25–30% LAS was dissolved, and the remaining 70–75% was associated with the solid phase (Cavalli et al., 1991).

The average chain length of homologues of LAS in raw wastewater was lower in the dissolved phase ($C_{11.2}$–$C_{11.4}$) than in the solids-associated phase ($C_{11.9}$–$C_{12.0}$). The authors reported that 39–43% of LAS was present in the dissolved phase and 57–61% in the solids phase (Prats et al., 1993).

Humic acids extracted from sediments and soils formed strong association complexes with LAS under environmental conditions, as observed with fluorescence quenching techniques. The bioavailabilty of LAS to aquatic organisms is reduced as a result of these complexes (McAvoy et al., 1993).

A5.3 Estimation of human intake

Human daily intake has been estimated on the assumption that LAS are taken up from drinking-water and from washing food, vegetables, dishes, and the skin. The estimates vary from 4.5 to 14.5 mg/day (Ikeda, 1965; Tokyo Metropolitan Government, 1974; Sterzel, 1992). The higher figure is based on dubious assumptions about the concentrations of LAS on vegetables, and the lower value is probably a more realistic estimate.

The human intake of all anionic surfactants is estimated to be 0.044–0.944 mg/kg per day (Sterzel, 1992), and the maximum daily intake of ABS, 0.14 mg/kg per day (Ikeda, 1965).

A6. KINETICS

Section summary

LAS are readily absorbed by experimental animals in the gastrointestinal tract, are distributed throughout the body, and are extensively metabolized. The parent compound and metabolites are excreted primarily via the urine and faeces, although there are marked differences between the isomers in the route of excretion. The main urinary metabolites identified in rats are sulfophenylbutanoic acid and sulfophenylpentanoic acid, which are probably formed through omega-oxidation followed by ß-oxidation of LAS, although the metabolic pathways in primates may differ. Although few data are available, it would appear that dermally applied LAS are not readily absorbed through the skin, although prolonged contact may compromise the epidermal barrier and permit more extensive absorption.

A6.1 Absorption, distribution, and excretion

After oral administration of 2 mg/animal of the calcium or sodium salt of ^{14}C-LAS (chain length, C_{12}) to Wistar rats, radiolabel was detected in plasma after 0.25 h, reaching maxima at 2 h (0.86 and 1.00 µg/g of the two salts, respectively), and then decreasing gradually with time; the mean biological half-lives were calculated to be 10.9 and 10.8 h, respectively. Four hours after oral administration of the calcium or sodium salt, the concentration of radiolabel was high in the digestive tract (especially in the stomach: 22.56 and 31.67 µg/g as the parent compound or metabolites; and large intestine: 43.24 and 27.26 µg/g) and in the urinary bladder (34.89 and 16.58 µg/g). The concentrations were also high in the liver (2.73 and 2.13 µg/g), kidney (1.19 and 1.35 µg/g), testis (0.08 and 0.11 µg/g), spleen (1.63 and 0.16 µg/g), and lung (0.49 and 0.44 µg/g). At 48 and 168 h, there was little further change. During the 168-h period after administration, 50% of the radiolabel on the calcium salt was excreted in urine and 51% in faeces, and 47% of that on the sodium salt was excreted in urine and 50% in the faeces (Sunakawa et al., 1979).

Doses of 1 mg per 200 g body weight of two radiolabelled LAS isomers (chain length, C_{12}) with the benzene sulfonate moieties at the 2 and 6 positions were administered orally and intravenously to rats; the same dose was also administered to anaesthetized rats with bile-duct cannulas by intravenous or intraduodenal injection. Forty-eight hours after oral or intravenous administration, there were marked differences in the disposition of the isomers in the urine and faeces: most of the radiolabel associated with the 2 isomer (75.3%) was in the urine, whereas most of that on the 6 isomer (77.9%) was present in the faeces. After intravenous administration to bile duct-cannulated rats, 88.6% of the 2 isomer was recovered in the urine, whereas 83.1% of the 6 isomer was in the bile. Studies of absorption after intraduodenal administration showed that both isomers were extensively absorbed within 6 h (Rennison et al., 1987).

After a dose of 1.2 mg ^{35}S-LAS in aqueous solution was administered by gavage to bile duct-ligated rats, 89% was absorbed from the gastro-intestinal tract, as seen by the presence of radiolabel recovered in urine. Absorption probably occurred mainly via portal venous blood, since only 1.6% was recovered in the lymphatic system. When the same dose was administered to bile duct-cannulated rats, 46% of the radiolabel was recovered in urine, 29% in faeces, and 25% in bile after 90 h. Enterohepatic circulation was determined in a study in which the bile from one rat was transmitted to the intestine of another through a cannula; all of the radioactive LAS excreted in the bile was reabsorbed. In a separate study, 40–58% of single oral doses of ^{35}S-LAS ranging from 0.6 to 40.0 mg was excreted in the urine and 39–56% in the faeces within 72 h of administration (Michael, 1968).

The excretory pattern of ^{14}C-sodium dodecylbenzene sulfonate was examined in male rats administered a concentration of 1.4 mg/kg of diet daily for five weeks. The total intake was 1213 µg/rat, of which 81.8% was excreted during the dosing period, with 52.4% in the faeces and 29.4% in the urine. After a further week on a normal diet, however, only 7.8% of the estimated residual amount was found in excreta. Of a single intraperitoneal injection of 0.385 mg ^{14}C-sodium dodecylbenzene sulfonate/rat (2.26 mg/kg body weight), 84.7% was eliminated within the first 24 h and 94.5% within 10 days (Lay et al., 1983).

LAS were not detected in the uterus of pregnant ICR mice administered a single oral dose of 350 mg/kg body weight on day 3 of gestation (Koizumi et al., 1985).

^{14}C-LAS (chain length, C_{10}–C_{14}, predominantly C_{11}, C_{12}, and C_{13}) were applied at 250 µg/7.5 cm^2 in water to clipped dorsal skin of rats; the treated area was washed after 15 min, and the animals were restrained from grooming. Most of the radiolabel was rinsed off, but some of the ^{14}C-LAS (11 ± 4 µg/cm^2) were detected on the treated area; none were detected in urine or faeces 24 h after the application. In an accompanying study in vitro, there was no measurable penetration of ^{14}C-LAS (chain length, C_{12}) through isolated human epidermis or rat skin 24 or 48 h after application (Howes, 1975).

A mixture of ^{35}S-LAS and white petrolatum (29 mg/0.3 ml) was applied to a 4-cm^2 area of the dorsal skin of guinea-pigs, and 24 h after the application about 0.1% of the applied dose was found in urine and about 0.01% in blood and the main organs. After dermal application of the same dose to rats and guinea-pigs, the concentration of ^{35}S in the liver was 9.7 µg/g equivalent of LAS in rats and about 0.4 µg/g in guinea-pigs (Hasegawa & Sato, 1978).

After a single oral administration of 150 mg/kg ^{14}C-LAS (mean relative molecular mass, 349) in aqueous solution to rhesus monkeys (Macaca mulatta), plasma concentrations of radiolabel reached a maximum equivalent to 41.2 µg/ml at 4 h and then declined over 6–24 h, with a biological half-life of about 6.5 h. The observed peak plasma concentration of radioactivity (33.6 µg/ml) and the biological half-life (about 5 h) after seven consecutive daily oral administrations of 30 mg/kg body weight were similar to those found after a single administration. The highest concentration of ^{14}C (238.6 µg/g) was found in the stomach 2 h after the last dose. Concentrations were also high in the intestinal tract (108 µg/g), kidney (135.6 µg/g), and liver (64.8 µg/g) and were moderately high in the lung (19.8 µg/g), pancreas (17.7 µg/g), adrenal glands (20.6 µg/g), and pituitary gland (17 µg/g). At 24 h, the concentrations were higher in the intestinal tract (255.4 µg/g) and liver (10.5 µg/g) than in plasma (2.4 µg/g), whereas those in most tissues were lower than those in plasma, indicating that there is no specific accumulation or localization of LAS and their metabolites in these tissues. After seven subcutaneous doses of 1 mg/kg per day of ^{14}C-LAS, most of the radiolabel remained in the skin; the concentration was generally highest at the injection site (113.96 µg/g). The levels of radiolabel were also high in the intestinal tract (2.41 µg/g), kidney (1.83 µg/g), lung (2.45 µg/g), spleen (2.43 µg/g), thyroid (1.24 µg/g), and pituitary (1.00 µg/g) at 2 h. The concentration in most tissues was generally lower at 4 h, except in the intestinal tract (3.50 µg/g), liver (1.74 µg/g), and kidney (1.92 µg/g). The high level of radiolabel in the intestinal tract probably indicates biliary excretion. The average rates of excretion of radiolabel in urine and faeces during 120 h after administration of single oral or subcutaneous doses of ^{14}C-LAS to male and female rhesus monkeys are shown in Table 16. In animals of each sex, radiolabel was excreted primarily in the urine after either route of administration (Cresswell et al., 1978).

When sodium ^{35}S-dodecylbenzenesulfonate (3.3 mmol/kg body

weight) was administered in the diet to young pigs, at least 35% of the dose was absorbed through the intestinal tract. After 40 h, 30–40% of the dose had been excreted in urine and > 60% in faeces. The concentration of radiolabel after 200 h was relatively high in bristles and bones and low in liver, kidney, and spleen (quantitative data not presented). After 10 weeks, traceable amounts of ^{35}S (0.05% of the administered dose) were found in bristles, bones, skin, lung, and brain (Havermann & Menke, 1959).

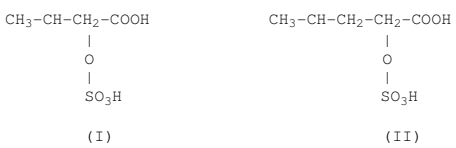
Table 16. Excretion of ^{14}C-linear alkyl benzene sulfonates in rhesus monkeys

Route of administration	Sex	Concentration (%)	
		Urine	Faeces
Oral (30 mg/kg body weight)	Male	68.3	25.9
	Female	74.0	20.3
Subcutaneous (1 mg/kg)	Male	63.8	12.5
	Female	64.3	9.2

From Cresswell et al. (1978); values are average rates of excreted radioactivity during the 120-h period after a single dose.

A6.2 Biotransformation

The main metabolites isolated from the urine of rats administered ^{35}S-LAS orally were probably a mixture of sulfophenyl butanoic (I) and sulfophenyl pentanoic acids (II):



(I) (II)

The material used in the experiment was a mixture of C_{10}–C_{14} LAS (mainly C_{11}, C_{12}, and C_{13}). The compounds in this mixture are probably degraded by omega-oxidation, followed by catabolism through a ß-oxidation mechanism to form the above metabolites, with excretion of four or five carbons in the urine (Michael, 1968).

After oral administration of the calcium or sodium salt of ^{14}C-LAS to rats, two metabolites were detected in urine and four in faeces by thin-layer chromatography. The two urinary and two of the faecal metabolites were believed to be compounds similar to metabolites (I) and (II) previously identified by Michael (1968) (Sunakawa et al., 1979).

Thin-layer chromatography of urine extracts after oral or sub-cutaneous administration of ^{14}C-LAS to rhesus monkeys showed only trace amounts of the unchanged compound, and five metabolites more polar than LAS were detected. These metabolites have not been identified. Incubation of urine samples with ß-glucuronidase or sulfatase did not affect the components, which were therefore probably not present as the corresponding conjugates (Cresswell et al., 1978).

A7. EFFECTS ON LABORATORY MAMMALS AND *IN VITRO* TEST SYSTEMS

Section summary

The oral LD_{50} values for sodium salts of LAS are 404–1470 mg/kg body weight in rats and 1259–2300 mg/kg body weight in mice. LAS irritate skin and eyes.

Minimal effects, including biochemical alterations and histopathological changes in the liver, were reported in subchronic studies in rats administered LAS in the diet or drinking-water at concentrations equivalent to a dose of about 120 mg/kg body weight per day. Although ultrastructural changes in liver cells were observed at lower doses in one study, these changes appeared to be reversible. Effects have not been seen at similar doses in other studies, but the organs may have been examined more closely in this study. Reproductive effects, including decreased pregnancy rate and litter loss, have been reported in animals administered doses > 300 mg/kg body weight per day. Histopathological and biochemical changes have been observed following long-term dermal application on rats of solutions of LAS at concentrations > 5% and after 30 days' dermal application on guinea-pigs of 60 mg/kg body weight. Repeated dermal application of solutions containing $\geq$ 0.3% LAS induced fetotoxic and reproductive effects, although these doses also induced maternal toxicity.

The available long-term studies are inadequate to evaluate the carcinogenic potential of LAS in experimental animals, owing to the small number of animals used, low or insufficient doses tested, the absence of a maximal tolerated dose, and limited histopathological examination. The limited studies available in which animals were administered LAS orally, however, provide no evidence of carcinogenicity.

Limited data also indicate that LAS are not genotoxic *in vivo* or *in vitro*.

A7.1 Single exposures

The LD_{50} values for the sodium and magnesium salts of LAS given orally, subcutaneously, or intravenously are summarized in Table 17. Rats appear to be more sensitive than mice to LAS, regardless of the route of exposure. The LD_{50} values for LAS given orally were 1259–3400 mg/kg body weight in mice and 404–1900 mg/kg body weight in rats. Differences were seen according to the sex, strain, and age of the animals and the test material.

Table 17. Acute toxicity of linear alkylbenzene sulfonates

Species/ strain	Sex	Route	LD_{50}[a] (mg/kg body weight)	Test material[b]	Reference
Mouse					
NR	NR	Oral	2170	60% active ingredient	Yanagisawa et al. (1964)
DD	M	Oral	2300	34.55% solution	Tiba (1972)
ddY	M	Oral	1665	Purified	Kobayashi et al. (1972)
ICR-JCL	F	Oral	1950	Purified	
	M	Oral	1250	Commercial soln, 19.0%	Kuwano et al. (1976)
	F	Oral	1540	Commercial soln, 19.0%	
	M	Oral	1370	Commercial soln, 17.1%	
	F	Oral	1560	Commercial soln, 17.1%	
	M	Oral	2160	99.5% active ingredient of C_{10}-C_{13}	Ito et al. (1978)
	F	Oral	2250	99.5% active ingredient of C_{10}-C_{13}	
	M	Oral	2600	Magnesium salt of above	
	F	Oral	3400	Magnesium salt of above	
	M	s.c.	1250	99% active ingredient of C_{10}-C_{13}	Ito et al. (1978)
	F	s.c.	1400	99% active ingredient of C_{10}-C_{13}	
	M	s.c.	1529	Magnesium salt of above	
	F	s.c.	1550	Magnesium salt of above	

Table 17 (contd)

Species/ strain	Sex	Route	LD_{50}[a] (mg/kg body weight)	Test material[b]	Reference
ICR-JCL (contd)	M	i.v.	207	99% active ingredient of C_{10}-C_{13}	
	F	i.v.	298	99% active ingredient of C_{10}-C_{13}	
	M	i.v.	98	Magnesium salt of above	
	F	i.v.	151	Magnesium salt of above	
NR	NR	i.v.	120		Yanagisawa et al. (1964)
Rat					
FDRL	M,F	Oral	650	Nominal chain length, C_{12} (range C_9-C_{15})	Oser & Morgareidge (1965)
Wistar					
6 w	M	Oral	873	Purified	Kobayashi et al. (1972)
6 w	F	Oral	760		
10 w	M	Oral	404		
10 w	F	Oral	409		
	M	Oral	1460	99.5% active ingredient of C_{10}-C_{13}	Ito et al. (1978)
	F	Oral	1470	99.5% active ingredient of C_{10}-C_{13}	
	M	Oral	1900	Magnesium salt of above	
	F	Oral	1840	Magnesium salt of above	

Table 17 (contd)

Species/ strain	Sex	Route	LD_{50}[a] (mg/kg body weight)	Test material[b]	Reference
CRJ-SD	M	s.c.	840	99.5% active ingredient of C_{10}-C_{13}	
	F	s.c.	810	99.5% active ingredient of C_{10}-C_{13}	
	M	s.c.	710	Magnesium salt of above	
	F	s.c.	730	Magnesium salt of above	
	M	i.v.	119	99.5% active ingredient of C_{10}-C_{13}	
	F	i.v.	126	99.5% active ingredient of C_{10}-C_{13}	
	M	i.v.	27.2	Magnesium salt of above	
	F	i.v.	35.0	Magnesium salt of above	

NR, not reported; M, male; F, female; s.c., subcutaneous; i.v., intravenous; w, weeks
[a] As active ingredient
[b] Sodium salt, unless specifically indicated

The main clinical signs observed after oral administration of doses near or greater than the LD_{50} consisted of reduced voluntary activity, piloerection, diarrhoea, and weakness. Diarrhoea was more severe in rats than mice (Kobayashi et al., 1972). Convulsions, torsion, and paralysis of the hind limbs were also observed in some of mice (Kobayashi et al., 1972; Kuwano et al., 1976). Death usually occurred within 24 h of administration. Transient cardiac arrest, dyspnoea, cyanosis, respiratory collapse, and death occurred during intravenous injection (Ito et al., 1978).

At autopsy, hyperaemia and haemorrhage of the stomach and intestine, bloating of the intestine with thinning of its wall, and congestion of some internal organs were the main macroscopic findings; histological examination showed congestion and epithelial degeneration of the gastrointestinal mucosa (Kobayashi et al., 1972; Kuwano et al., 1976; Ito et al., 1978).

A7.2 Short-term exposure

A7.2.1 Mouse

In a study of the toxicity of a commercial preparation of LAS (17.1% active ingredient), 44 male and 16 female C57Bl TW mice were given subcutaneous injections according to the following schedule: 0.02 ml of 1% of the preparation for 10 consecutive days from the day of birth, 0.04 ml of the same solution for the following 10 days, 0.02 ml of a 10% solution five times over the next 10 days, and 0.04 ml of the same solution every other day for a further 30 or 60 days. Eight males and six females served as untreated controls. Epilation and dermatitis usually occurred in animals given continuous injections of the test material. Adhesions between some organs, most frequently between the spleen and kidney, were observed in those receiving injections from the day of birth. Neither the growth nor the survival of the animals was affected. Although the weights of the liver, kidney, and spleen were significantly increased in animals receiving treatment for 60 days, histopathological examination of the liver, kidney, adrenal glands, and thyroid by light and electron microscopy showed no evidence of toxicity (Kikuchi, 1978).

A7.2.2 Rat

A7.2.2.1 Administration in the diet

Groups of five male Wistar rats were fed diets containing LAS (60% active ingredient; chain length distribution: 10.6% C_{10}, 34.1% C_{11}, 27.7% C_{12}, 19.0% C_{13}, 8.7% C_{14}) at a concentration of 0, 0.6, 1.2, or 1.8% (equivalent to 180, 360, or 540 mg/kg body weight per day) for two and four weeks, and lipids in serum and liver were analysed. Body weight gain was suppressed in the group receiving 1.8% at four weeks, and the relative liver weight was

increased at two weeks and thereafter in the groups receiving 1.2 and 1.8%. The levels of triglyceride and total lipids in the serum had decreased markedly at two weeks in all the experimental groups, and the levels of phospholipids and cholesterol in the serum had decreased significantly at two weeks in the groups given 1.2 and 1.8%. These changes were less apparent at four weeks, but triglyceride, phospholipid, and cholesterol levels in serum were significantly decreased in the group given 1.8%. Significant increases in triglyceride levels were seen in the liver after two weeks in the groups receiving 0.6 and 1.8%, and in cholesterol levels in the group given 0.6% (Yoneyama & Hiraga, 1977).

Technical-grade sodium LAS (87.9% active ingredient; chain length distribution: 1.8% C_{10}, 43.2% C_{11}, 32.2% C_{12}, 5.3% C_{14}, 1.5% C_{15}) were fed to five groups of 10 weanling Sprague–Dawley rats of each sex at a dietary level of 0, 0.02, 0.1, or 0.5% (equivalent to 8.8, 44, or 220 mg/kg body weight per day) for 90 days. No adverse effects were found on survival, growth, food conversion efficiency, haematological values, urinary analytical values, or absolute or relative organ weights. There were no gross or microscopic histological changes attributable to ingestion of the test material (Kay et al., 1965).

Technical-grade LAS (normal chain length, C_{12}; range, C_9–C_{15}; mean relative molecular mass, 346) were fed to three groups of weanling FDRL rats, each consisting of 15 males and 15 females, at a dose of 0, 0.05, or 0.25 g/kg body weight per day for 12 weeks. No adverse effects were noted on survival, behaviour, growth, food conversion efficiency, haematological measurements, blood chemistry, urine analytical values, organ weights, or gross or microscopic appearance, except for a slight increase in liver weight in females given 0.25 g/kg body weight per day (Oser & Morgareidge, 1965).

A diet containing LAS at a concentration of 1.5% (equivalent to 750 mg/kg body weight per day) or a control diet was given to groups of five male Wistar rats for 2, 4, or 12 weeks. LAS depressed body weight gain, and the relative liver weight was significantly increased after two weeks of treatment. The activities of alkaline phosphatase and glutamate–pyruvate transaminase in serum were significantly increased at each observation period, and cholesterol and protein levels were significantly decreased by four weeks. In the liver, the activities of glucose-6-phosphatase and glucose-6-phosphate dehydrogenase were decreased, and the activity of isocitrate dehydrogenase was increased at each observation point.

Enzymatic examination of the renal cortex showed decreased activities of glucose-6-phosphatase and 5'-nucleotidase at each observation period, an increase in the activity of lactate dehydrogenase at 12 weeks, and increased activity of isocitrate dehydrogenase at 2 and 4 weeks. In the renal medulla, the activity of Na,K-ATPase was decreased, that of lactate dehydrogenase was

increased at 12 weeks, and that of isocitrate dehydrogenase was decreased at 2 weeks but increased at 12 weeks (Ikawa et al., 1978).

Groups of five male Wistar rats were given a diet or drinking-water containing LAS at a concentration of 0.4% (diet: 200 mg/kg body weight per day; drinking-water: 560 mg/kg per day) for two weeks in order to determine the effects of LAS on the synthesis of lipids in the liver. Lipids were thus measured in the liver, and uptake of acetate-1-^{14}C by the lipids was examined. Decreases in the levels of total lipids and triglyceride were seen in both groups, but there were no significant changes in phospholipid or cholesterol levels. Uptake of acetate-1-^{14}C by lipids in the liver was increased in both groups; uptake of phospholipids and triglycerides tended to increase, and that of phospholipids increased significantly in rats given LAS in the diet (Yoneyama et al., 1978).

A7.2.2.2 Administration by gavage

Groups of 12 male and 12 female Sprague-Dawley rats were given the magnesium salt of LAS by gavage at a dose of 0, 155, 310, or 620 mg/kg body weight for one month. Body weight gain was depressed in males and females at 620 mg/kg body weight; one male and two females at this dose also had diarrhoea and loss of appetite and subsequently died. Haematological examination revealed significant decreases in haemoglobin concentration and haematocrit in males at 620 mg/kg body weight. A significant increase in the activity of alkaline phosphatase and a significant decrease in calcium levels were seen in males at 310 or 620 mg/kg body weight; and a significant increase was seen in the activity of glutamate-oxalate transminase and a significant decrease in protein levels in females at those doses. Females at all doses had a significant decrease in calcium levels. At the highest dose, females had a significant increase in the activity of alkaline phosphatase, a significant decrease in cholesterol level, and increased weight of the liver, but the weight of the thymus decreased. The weight of the heart decreased in females at 310 and 620 mg/kg body weight. Histological examination of the liver revealed no abnormalities (Ito et al., 1978).

Groups of 12 male and 12 female Sprague-Dawley rats were given the sodium salt of LAS (chain length distribution: < 0.1% C_9, 10.1% C_{10}, 33.7% C_{11}, 31.0% C_{12}, 25.1% C_{13}) at a dose of 0, 125, 250, or 500 mg/kg body weight by gavage once a day. Diarrhoea was observed in the group receiving 500 mg/kg, and soft faeces were observed in the other two groups. Body weight gain was depressed in males of all groups and in females at 500 mg/kg. Haematological examination revealed no abnormalities. Serum analysis revealed a significant increase in the activity of alkaline phosphatase in males at 500 mg/kg, a significant decrease in calcium levels in males of all groups, significant increases in the activity of

gluatamate-oxalate transaminase and in blood-urea nitrogen in females at 500 mg/kg, a significant decrease in calcium level in females at 250 or 500 mg/kg, and significantly decreased protein and albumin levels in females of all groups. At 500 mg/kg, the weights of spleen and heart were significantly decreased in males; in females, liver weights were increased but the weights of the heart and thymus were decreased. No histological abnormalities were seen in the liver (Ito et al., 1978).

A7.2.2.3 Dermal application

Continued, repeated, or extremely high doses of LAS, like other detergents, compromise the integrity of the skin so that penetration occurs, causing a variety of anomalies. As the design of the following two studies was not adequate, the observations are not considered to be relevant to human risk assessment.

Application of 2 ml of a commercial preparation of LAS (23.4% active ingredient) to the thoracic skin of six male Wistar rats resulted in redness and wrinkling of the skin after 24 h. The redness then increased, the corium was lacerated, and bleeding occurred. These effects were most severe after five to seven days, but after a further 10 days the skin began to recover. Six rats died after 19 days, probably because of the extremely high dose used. The livers of three rats were examined by electron microscopy after three and 30 days and the findings compared with those in the control group. At three days, marked changes were seen in the components of the liver parenchymal cells, such as separation of the intracellular space, appearance of dark cells with high electron density, dysmorphia of mitochondria, extracellular prolapse of mitochondria, proliferation of rough-surfaced endoplasmic reticulum, lysosome proliferation, and a decrease in the prevalence of fatty droplets. At 30 days, many liver parenchymal cells were filled with abnormally divided and proliferated mitochondria, and an abnormal increase in smooth-surfaced endoplasmic reticula was noted. There were no granules of glycogen or fatty droplets. Structures resembling necrotic cells were also observed (Sakashita et al., 1974).

A commercial preparation of LAS (23.4% active ingredient) was applied dermally to male rats (number not given) at a dose of 5 mg/kg body weight active ingredient once a day for 30 days, and the liver was examined by electron microscopy. Degeneration was seen

in part of the liver, in the form of atrophy and high density. Intra-mitochondrial deposits and deformation of the Golgi apparatus were also noted (Sakashita, 1979).

A7.2.2.4 Subcutaneous injection

A commercial preparation of LAS (27% active ingredient) was given subcutaneously to groups of five male and five female Wistar rats at a dose of 2 ml/kg body weight per day of a 0, 0.02, 0.2, or 2% solution of the preparation for 25 or 50 days. Rats receiving the 2% solution had reduced body weight gain, increased weights of liver, kidney, and spleen, a low serum albumin:globulin ratio, low serum protein, and reduced ornithine aminotransferase activity in the liver (Hayashi, 1980).

A7.2.3 Guinea-pig

Twelve guinea-pigs were treated daily for 30 days with a solution of LAS in distilled water equivalent to 60 mg/kg body weight, which was applied to a 4-cm^2 area of clipped dorsal skin. Twelve controls received acetone at 0.5 ml. The animals were sacrificed after 30 days, and samples were taken from liver and kidney and homogenized for determination of enzymes, lipid peroxidation, glutathione, and protein. The activities of ß-glucuronidase, gamma-glutamyl transpeptidase, 5-nucleotidase, and sorbitol dehydrogenase were increased in liver and kidney. Lipid peroxidation was increased in kidney but not in liver, and the glutathione content was unchanged in both organs. Extensive fatty changes were found in hepatic lobules, with dilation of sinusoids; tubular lesions were found in the kidney, predominantly in the proximal and distal portions (Mathur et al., 1992).

A7.2.4 Monkey

LAS (chain length, C_{10}–C_{13}) were given to four groups of three male and three female rhesus monkeys at a daily dose of 0, 30, 150, or 300 mg/kg body weight orally simultaneously with a dose of 0, 0.1, 0.5, or 1.0 mg/kg per day subcutaneously, for 28 days. Monkeys that received 300 mg/kg orally and 1.0 mg/kg subcutaneously vomited frequently, usually within 3 h of administration; these animals and those given 150 mg/kg orally and 0.5 mg/kg subcutaneously also had an increased frequency of loose or liquid faeces. Fibrosis at the injection sites was reported in all test animals, and the incidence and severity were related to dose. Treatment had no effect on ophthalmoscopic, haematological, or urinary parameters, on organ weight, or on histopathological appearance (Heywood et al., 1978).

The studies of short-term exposure to LAS are summarized in Table 18.

Table 18. Summary of studies of short-term exposure to linear alkylbenzene sulfonates (LAS)

Species, strain, numbers per group	Test material (specification)	Route	Dosage	Results	Reference
Mouse, C57Bl TW 44 M, 16	LAS (a.i. 17.1%)	s.c.	63 or 76 mg/kg bw/day, 60–90 days	Abdominal adhesions, increased weights of liver, kidney, and spleen after 60-day treatment; no histopathological changes in liver, kidney, adrenal or thyroid glands	Kikuchi (1978)
Rat, Wistar 5 M	LAS, C_{10}–C_{14} (a.i. 60%)	Diet	0, 0.6, 1.2, 1.8%, 4 weeks	Decreased serum triglyceride, total lipids, phospholipids, and cholesterol; increased relative liver weight at 1.2 and 1.8%; suppression of body weight gain at 1.8%	Yoneyama & Hiraga (1977)
Rat, SD 10 M, 10 F	LAS, C_{10}–C_{15} (a.i. 8–9%)	Diet	0, 0.02, 0.1, 0.5%, 90 days	No adverse effects	Kay et al. (1965)
Rat, FDRL 15 M, 15 F	LAS, C_9–C_{15} (a.i. 39.5%)	Diet	0, 0.05, 0.25 g/kg bw per day, 12 weeks	Slight increase in liver weight in females at high dose	Oser & Morgareidge (1965)
Rat, Wistar 4 M	LAS (NS)	Diet	1.5%, 24 weeks	Increased activities of serum, hepatic, and renal enzymes; depressed body weight gain; increased relative liver weight	Ikawa et al. (1978)

Table 18 (contd)

Species, strain, numbers per group	Test material (specification)	Route	Dosage	Results	Reference
Rat, CRJ-SD 12 M, 12 F	LAS, Na, C_{10}–C_{13} (a.i. 99.5%)	Gavage	125, 250, 500 mg/kg bw per day, 1 month	Altered serum enzyme activity and calcium levels at high doses; decreased serum protein and albumin levels in all treated females; decreased spleen and heart weights in males at highest dose; increased liver weight and decreased heart and thymus weights in females at highest dose;	Ito et al. (1978)

				no histopathological abnormalities in liver	
Rat, CRJ-SD 12 M, 12 F	LAS Mg, C_{10}-C_{13} (a.i. 96.9%)	Gavage	155, 310, 620 mg/kg bw per day, 1 month	Altered haemoglobin, haematocrit, serum enzyme activities, calcium level at high doses; depressed body weight gain at highest dose; increased liver weight and decreased heart and thymus weights in females at highest dose; no histopathological abnormalities in liver	Ito et al. (1978)
Rat, Wistar 6 M	LAS detergent (a.i. 23.4%)	Dermal	2 ml/animal 3.5 × 4.5 cm, 30 days	Skin irritation; liver parenchymal changes with necrotic cells; no glycogen granules or fat droplets	Sakashita et al. (1974)
Rat, Wistar 6 M	LAS detergent (a.i. 23.4%)	Dermal	5 mg/kg bw, once/day, 30 days	Degenerative changes in liver	Sakashita (1979)

Table 18 (contd)

Species, strain, numbers per group	Test material (specification)	Route	Dosage	Results	Reference
Rat, Wistar 5 M, 5 F	LAS detergent (a.i. 27%)	s.c.	0, 0.02, 0.2, 2%, 2 ml/kg bw per day, 50 days	Depressed body weight gain; increased weights of liver, kidney, and spleen; and altered hepatic enzyme activities at highest dose	Hayashi (1980)
Rat, Wistar 8 M, 8 F	LAS (a.i. 60.2%)	Drinking-water	0.4%, 2 weeks	Decreased hepatic total lipids and triglycerides; increased uptake of acetate-1-^{14}C, phospholipids, and triglycerides	Yoneyama et al. (1978)
Guinea-pig 12 M, 12 F	LAS (NS)	Dermal	60 mg/kg bw, 30 days on 4 cm^2	Altered hepatic and renal enzyme activities; fatty degeneration in liver; renal tubular lesions	Mathur et al. (1992)
Rhesus monkey 3M, 3F	LAS C_{10}-C_{13} (a.i. 20.5%)	Gavage s.c.	0.30, 150, 300 mg/kg 0, 0.1, 0.5, 1.0 mg/kg bw per day, 28 days	Vomiting and diarrhoea; no ophthalmic, haematological or urinary changes; no effect on organ weights; no histopathological changes	Heywood et al. (1978)

M, male; F, female; a.i., active ingredient; s.c., subcutaneous

A7.3 Long-term exposure; carcinogenicity

A7.3.1 Mouse

A7.3.1.1 Administration in the diet

Groups of eight or nine ICR mice were given diets containing LAS at a concentration of 0.6 or 1.8% for nine months (corresponding to intakes of 500 and 1000 mg/kg body weight per day). There was no reduction in body weight gain at either dose, but the weight of the liver was increased in both males and females. Significant decreases were seen in the activities of hepatic lactate dehydrogenase and renal acid phosphatase in male mice (Yoneyama et al., 1976).

A7.3.1.2 Administration in the drinking-water

Drinking-water containing 100 ppm LAS (corresponding to 20 mg/kg body weight per day) was supplied to ddy mice (sex and number not stated) for six months, and they were then allowed to recover for two months. Mice were killed for electron microscopy of the liver at one, two, three, and six months and after the two-month recovery period. Hepatic damage was observed at one and six months, consisting of the disappearance of the nucleolus, atrophy of the Golgi apparatus, degranulation of rough-surfaced endoplasmic reticulum, degeneration of mitochondria, and increased numbers of primary and secondary lysosomes including autophagic vacuoles with a myelinated core. In mice examined after the two-month recovery period, some hepatic damage was seen, which was characterized by changes in mitochondrial structure and the presence of numerous fat droplets. Other cellular effects had reversed, indicating that the liver cells had recovered (Watari et al., 1977). Because an extremely high dose was used in this study, the observations have little relevance to human risk.

Groups of eight or nine ICR mice were given water containing LAS at a concentration of 0.07, 0.2, or 0.6% for nine months, corresponding to intakes of about 0.1, 0.25, or 0.6 g/kg body weight per day for males and 0.1, 0.25, or 0.9 g/kg body weight per day for females. Body weight gain was depressed in males and females at 0.6%, and there were dose-related increases in liver weight in females in all dose groups. In the group given 0.6% LAS, the activity of hepatic glutamate-oxalate transaminase was significantly decreased in males and the activity of renal glucose-6-phosphatase was decreased in animals of each sex (Yoneyama et al., 1976).

A7.3.2 Rat

A7.3.2.1 Administration in the diet

LAS (98.1% active ingredient; chain length distribution, C_{10}-C_{14}) were fed to four groups of Charles River weanling rats,

each consisting of 50 males and 50 females, at a dietary level of 0, 0.02, 0.1, or 0.5% (corresponding to 10, 50, or 250 mg/kg body weight per day) for two years. No adverse effects on growth or feed conversion efficiency were observed. Five males and females from each group were killed at 8 and 15 months, and all survivors at 24 months; all animals were necropsied, haematological values were determined, and tissues were taken for histological examination. No consistent change was seen that could be considered a toxic response. Animals that showed significant loss of weight, development of tumours, or other evidence of abnormalities were also sacrificed and their tissues preserved for study. The incidences of tumours and of common incidental diseases were similar in all dietary groups (Buehler et al., 1971).

Diets containing technical-grade LAS (chain length distribution: 10.6% C_{10}, 34.1% C_{11}, 27.7% C_{12}, 19.0% C_{13}, 8.7% C_{14}; mean relative molecular mass, 345.8) at a concentration of 0, 0.07, 0.2, 0.6, or 1.8% were given to groups of 10 Wistar rats of each sex for six months. The group given 1.8% had diarrhoea, markedly depressed growth, increased caecal weight, and marked degeneration of renal tubules. The group given 0.6% had slightly depressed growth, increased caecal weight, increased serum alkaline phosphatase activity, decreased serum protein, and degeneration of renal tubules. The group given 0.2% had increased caecal weight and slight degeneration of renal tubules. The group given 0.07%, corresponding to about 40 mg/kg body weight per day, showed no effects attributable to treatment (Yoneyama et al., 1972).

Groups of eight male and eight female Wistar rats were given diets containing LAS at a concentration of 0, 0.6, or 1.8% for nine months, corresponding to intakes of 230 or 750 mg/kg body weight per day for males and 290 or 1900 mg/kg body weight per day for females. In rats given 1.8% LAS, body weight gain was reduced in both males and females. Haematological examination revealed a significant decrease in leukocytes in males at 0.6% and significant decreases in mean corpuscular volume and mean corpuscular haemoglobin in females at 1.8%. The activity of glutamate-oxalate transferase and the levels of cholesterol and albumin in serum were significantly decreased and the activity of alkaline phosphatase and the levels of blood-urea nitrogen and cholinesterase were significant increased in males at 1.8%; females at that dose had a significant decrease in cholesterol level and a significant increase in alkaline phosphatase activity. At 0.6%, males had a significant decrease in glucose level, and females had a significant decrease in the activity of glutamate-pyruvate transaminase. The caecal weight of male rats and

the liver and caecal weights of female rats at 1.8% were significantly increased. Enzymatic examination of the liver revealed dose-related decreases in the activities of glucose-6-phosphate dehydrogenase and lactate dehydrogenase in male rats. At 1.8%, males had significantly decreased activities of glucose-6-phosphatase, glutamate-pyruvate transaminase, and glutamate-oxalate transaminase and a dose-related decrease in the activity of glucose-6-phosphate dehydrogenase; females had significantly decreased activities of glucose-6-phosphatase and glutamate-oxalate transaminase. Enzymatic examination of the kidneys of females at 1.8% showed significantly decreased activities of glucose-6-phosphatase, Na,K-ATPase, and lactate dehydrogenase (Yoneyama et al., 1976).

Groups of 50 male and 50 female Wistar weanling rats were given diets containing LAS (10.6% C_{10}, 34.1% C_{11}, 27.7% C_{12}, 19.0% C_{13}, 8.7% C_{14}; mean relative molecular mass, 345.8) at a concentration of 0, 0.04, 0.16, or 0.6%. In each group, five rats of each sex were fed for one, three, six, or 12 months, and groups of 15 rats of each sex were fed for 24 months or more. The group fed 0.6% had slightly increased liver and caecal weights, and increased activity of glutamate-pyruvate transaminase and alkaline phosphatase in serum. The treatment had no adverse effect on the intake of food, body weight gain, general condition, mortality, or mean survival. On the basis of these results, it was concluded that a diet containing LAS at a concentration of 0.6% (300 mg/kg body weight per day) had no adverse effects on the rats (Yoneyama et al., 1977).

Groups of 50 male and 50 female Wistar rats were fed LAS (C_{10}-C_{14}) in the diet at a concentration of 0, 0.04, 0.16, or 0.6% and were then submitted to a detailed histopathological examination. After one month, proliferation of hepatic cells in the liver, slight swelling of the renal tubules, and narrowing of the tubular lumen were found in treated animals. Since these alterations later disappeared, they were considered to represent adaptation to the administration of LAS. No histological lesions were seen in the organs of rats that were fed for 24 months or more that could be attributed to treatment. Various types of tumour were observed in both treated and control rats but did not appear to be due to LAS (Fujii et al., 1977).

A7.3.2.2 Administration in the drinking-water

Groups of eight to nine male and eight to nine female Wistar rats were given LAS at a concentration of 0, 0.07, 0.2, or 0.6% in drinking-water for nine months. Body weight gain was suppressed in males given 0.6%. Haematological examination revealed no significant change in any of the experimental groups, but a dose-related decrease in cholesterol level was seen in males. No change in organ weight was seen that was due to administration of LAS. Significant decreases in the activities of glutamate-oxalate transaminase and lactate dehydrogenase were seen in males at 0.2% and a dose-related

increase in the activity of glutamate-oxalate transaminase in females. A significant decrease in renal Na,K-ATPase was seen in the group given 0.2%. The dose of 0.07% corresponded to intakes of LAS of 50 and 120 mg/kg body weight per day in males and females, and

the dose of 0.2% to intakes of 120 and 170 mg/kg body weight per day, respectively (Yoneyama et al., 1976).

A commercial preparation of LAS (27% active ingredient) was given to groups of five male Wistar rats in drinking-water at a concentration of 0, 0.3, 3, 30, or 300 ppm (corresponding to 0.007, 0.07, 0.7, or 7 mg/kg body weight per day) for 60, 124, or 181 days. Although a reduction in body weight gain, changes in blood biochemistry, and increased ornithine aminotransferase activity in the liver were noted in some animals, they were not proportional to dose or feeding period (Hayashi, 1980).

Groups of 20 male Wistar rats were given water containing LAS (34.55% commercial solution) at a concentration of 0, 0.01, 0.05, or 0.1% for two years, the highest dose corresponding to an intake of about 200 mg/kg body weight per day. No changes attributable to the administration of LAS were seen in terms of growth, mortality, the weights of major organs, or histopathological appearance (Tiba, 1972).

A group consisting of 62 male and 62 female Wistar rats was given drinking-water containing LAS (mean relative molecular mass, 348; 38.74% active ingredient) at a concentration of 0.1% (corresponding to 140 mg/kg body weight per day), and a control group of 37 male and 37 females was given normal drinking-water. Five to 12 rats in the experimental group and three to 12 rats in the control group were killed at 3, 6, 12, and 18 months, and all surviving animals were killed at 24-26 months. Administration of LAS had no effect on the intake of water, mortality, body weight gain, or general condition. Histopathological examination revealed atrophy; fatty changes were found in hepatic cells in treated animals at six months, when there were also significant increases in the activities of glutamate-oxalate and glutamate-pyruvate transaminases and in the level of bilirubin. LAS had no effect on haematological parameters (Endo et al., 1980).

A group of 60 male and 60 female rats (strain not specified) received drinking-water containing 0.01% of a preparation containing 51% LAS for 100 weeks; a similar group was untreated. No detrimental effects on body weight and no pathological effects, including tumours, were reported (Bornmann et al., 1963).

A7.3.2.3 Administration by gavage

Groups of 20 male and 20 female Sprague-Dawley rats were given a solution of a magnesium salt of LAS at doses of 10, 75, 150, or 300 mg/kg body weight per day by gavage for six months. Body weight gain was suppressed, and slight decreases were observed in serum protein, albumin, and calcium ion level, but the changes were within the physiological range (Ito et al., 1978).

A7.3.2.4 Dermal application

A dose of 0.1 ml/kg body weight of a 0.5, 1.0, or 5.0% solution of magnesium LAS (in 3% polyethylene glycol) was applied to the backs of 20 male and 20 female Sprague-Dawley rats six times a week for six months. Slight redness at the application site was observed transiently in males and occasionally in females at 5%. Body weight was slightly suppressed in males at that dose, and one male in the control group and one at 5.0% died of unknown causes. Treatment had no definite effect in terms of food conversion efficiency, urinary, haematological, serum biochemistry, or histopathological findings, or organ weights (Ito et al., 1978). No systemic toxicity was reported in this study. Sakashita et al. (1974) and Sakashita (1979) (see section 7.2.2.3) may have obtained positive results because they used a shorter period of exposure, during which skin integrity may have been compromised, resulting in absorption of the preparation of LAS through the skin to produce systemic effects.

LAS (19.7% active ingredient) were applied to the dorsal skin of SLC-Wistar rats three times per week at a dose of 0.005, 0.025, or 0.125 ml/rat (equivalent to 1, 5, or 25 mg/rat) for 24 months. A dose of 0.025 ml of an LAS-based detergent containing 19.9% LAS (equivalent to 5 mg LAS per rat) and distilled water was given to controls. Each application was washed from the skin with warm water after 24 h. Treatment had no effect on organ weights or histopathological appearance, and there was no evidence of toxicity or carcinogenicity (Taniguchi et al., 1978).

Long-term studies of exposure to and the carcinogenicity of LAS are summarized in Table 19.

A7.4 Skin and eye irritation; sensitization

The potential of LAS to irritate the skin depends on the concentration applied. On the basis of the criteria of the European Commission and the OECD test guideline, LAS were classified as irritating to the skin at concentrations above 20% (European Committee of Organic Surfactants and Their Intermediates, 1990).

Table 19. Summary of studies of long-term exposure to linear alkylbenzene sulfonates (LAS)

Species, strain, numbers per group	Test material (specification)	Route	Dosage	Results	Reference
Mouse, SLC-ICR 8-9 M, 8-9 F	LAS (a.i. 60%)	Diet	0, 0.6, 1.8%, 9 months	Increased liver weight; decreased hepatic and renal enzyme activities in males	Yoneyama et al. (1976)
Mouse, ddy (NR)	LAS (NS)	Drinking-	20 mg/kg bw per	Degenerative changes in liver,	Watari et al. (1977)

		water	day, 6 months end of treatment	with partial recovery after	
Mouse, ICR 8-9 M, 8-9 F	LAS (a.i. 60%)	Drinking-water	0, 0.07, 0.2, 0.6, 1.8%, 9 months	Depressed body weight gain at high dose; dose-related increase in liver weight in all treated females; changes in hepatic enzyme activities at high dose	Yoneyama et al. (1976)
Rat, Wistar 10 M, 10 F	LAS, C_{10}-C_{14}	Diet	0, 0.07, 0.2, 0.6, 1.8%, 6 months	Dose-related depression of growth, caecal enlargement, and renal tubular degeneration at > 0.07%	Yoneyama et al. (1972)
Rat, Wistar 8 M, 8 F	LAS (a.i. 60%)	Diet	0, 0.6, 1.8%, 9 months	Depressed body weight gain at high dose; changes in haematological parameters, in serum and hepatic enzyme activities, and in cholesterol levels at both doses; changes in renal enzyme activities in females at high dose	Yoneyama et al. (1976)

Table 19 (contd)

Species, strain, numbers per group	Test material (specification)	Route	Dosage	Results	Reference
Rat, Wistar 8-9 M, 8-9 F	LAS (a.i. 60%)	Drinking-water	0, 0.07, 0.2, 0.6%, 9 months	Depressed body weight gain in males at high dose; no changes in haematological parameters or organ weight; changes in serum and renal enzyme activities at 0.2%	Yoneyama et al. (1976)
Rat, Wistar 50 M, 50 F	LAS, C_{10}-C_{14} (a.i. 60%)	Diet	0, 0.04, 0.16, 0.6%, 24 months	Slight increase in liver and caecal weights and changes in serum enzym activities at high dose; no effect on body weight gain	Yoneyama et al. (1977)
Rat, Charles River 50 M, 50 F	LAS, C_{10}-C_{14} (a.i98.1%)	Diet	0, 0.02, 0.1, 0.5%, 2 years	No treatment-related effects	Buehler et al. (1971)
Rat, Wistar 50 M, 50 F	LAS, C_{10}-C_{14} (a.i. 60%)	Diet	0, 0.04, 0.16, 0.6%, 2 years	Transient changes in liver and kidney; no treatment-related histopathological abnormalities at end of study	Fujii et al. (1977)
Rat, SD 20 M, 20 F	LAS Mg, C_{10}-C_{13} (a.i. 96.9%)	Gavage	75, 150, 300 mg/kg bw per day, 6 months	Depressed body weight gain; no significant adverse effects	Ito et al. (1978)
Rat, Wistar, 5 M	LAS detergent (a.i. 27%)	Drinking-water	0, 0.3, 3, 30, 300 ppm, 181 days	Depressed body weight gain and changes in blood biochemistry and liver enzyme activity considered not to be related to treatment	Hayashi (1980)

Table 19 (contd)

Species, strain, numbers per group	Test material (specification)	Route	Dosage	Results	Reference
Rat, Wistar, 20 M	LAS (a.i. 34.55%)	Drinking-water	0, 0.01, 0.05, 0.1%, 2 years	No adverse effects	Tiba (1972)
Rat, Wistar 62 M, 62 F	LAS (a.i. 38.74%)	Drinking-water	0, 0.1%, 26 months	Fatty changes and atrophy in liver; changes in hepatic enzyme activities; no effect on body weight gain	Endo et al. (1980)
Rat 60 M, 60 F	LAS (Marlon BW 2043)	Drinking-water	0, 0.01%, 100 weeks	No adverse effects	Bornmann et al. (1963)
Rat, SD 20 M, 20 F	LAS Mg, C_{10}-C_{13} (a.i. 96.9%)	Dermal	0.5, 1.0, 5% in polyethylene glycol, 6 months	Slight reduction in body weight gain of males at high dose; no other adverse effects	Ito et al. (1978)
Rat, SLC-Wistar 25 M, 25 F	LAS (a.i. 19.7%)	Dermal	0, 6.7, 33.3, 167.0 mg/kg bw, 3 × per week, 2 years	No adverse effects	Taniguchi et al. (1978)
Rat, SLC-Wistar 25 M, 25 F	LAS detergent (a.i. 19.9%)	Dermal	0, 33.3 mg/kg bw 3 × per week, 2 years	No adverse effects	Taniguchi et al. (1978)

M, male; F, female; NS, not specified; a.i., active ingredient; SD, Sprague-Dawley

A7.4.1 Studies of skin

Solutions of LAS (chain length distribution, C_{10}-C_{13}; purity, 99.9%) were applied to the backs of groups of three male Wistar rats at a rate of 0.5 g of a 20 or 30% solution once a day for 15 days. On the sixteenth day of the experiment, the skin at the application site and the tissues of the tongue and oral mucosa (to examine the effects of licking) of the rats that received 30% were examined histologically. Body weight gain was reduced in the group

exposed to 20%, and body weight was decreased in animals exposed to 30%. An infiltrating, yellow-red brown crust was observed after two to three days at 20% and after one to two days at 30%; at four to six days, the crust was abraded, and erosion was observed. Histological examination of the application site revealed severe necrosis of the region, from the epidermis cuticle to the upper layer of the dermis, severe infiltration of leukocytes in the necrotic site, diffuse inflammatory cell infiltration of all of the layers of the corium, and swelling of collagenous fibres in the dermis. Histological examination of the tongue showed no changes, but examination of the oral mucosa revealed atrophy and slight degeneration of the epithelium (Sadai & Mizuno, 1972).

Some batches of a paste of LAS (volume not stated) induced weak to moderate sensitization in guinea-pig skin at induction concentrations of 2–100% and challenge concentrations of 1–2%. A prototype liquid laundry detergent (10% LAS) induced sensitization at a challenge concentration of 1% (0.1% as LAS) (Nusair et al., 1988).

The biochemical and pathomorphological effects of LAS on the skin of four female albino CDRI guinea-pigs were investigated by shaving the abdominal skin and immersing the animals up to the neck in a 1% aqueous solution of neutralized LAS for 90 min daily for seven consecutive days. A control group was immersed in water according to the same schedule. After each immersion, the animals were washed and their skin dried. The animals were killed after seven days, and skin samples were taken. The skin of guinea-pigs exposed to the solution of LAS had increased activity of histidine decarboxylase, decreased sulfhydryl groups and histamine, and decreased activity of lactic dehydrogenase. It appeared to be shrunken, with thinner layers of dermis and epidermis than controls. There were also areas of scarring in the epidermis and ridging of epidermis and dermis (Misra et al., 1989a).

A7.4.2 Studies of the eye

A volume of 0.1 ml of a solution of LAS (relative molecular mass, 346.5) at five concentrations ranging from 0.01 to 1.0% was instilled into the eyes of rabbits (13 per group). The rabbits were observed for 24 h after application. The group receiving 0.01% had no abnormalities, but that given 0.05% had slight congestion.

Concentrations of 0.5% and more induced marked reactions, such as severe congestion and oedema, increased secretion, opacity of the cornea, and disappearance of the corneal reflex (Oba et al., 1968a).

Solutions of LAS (chain length distribution, C_{10}–C_{14}; 80.9% C_{11}–C_{13}) at six concentrations ranging from 0.01 to 5.0% were instilled into the eyes of rabbits (three per group). The rabbits were observed for 168 h after application. The group given 0.01% had no reaction, but within 2 h those given 0.05% had slight congestion and those at 0.1% had considerable congestion or oedema, which had disappeared by 24 h. Animals given 0.5% or more had marked reactions, such as severe congestion and oedema, increased secretion, opacity of the cornea, and disappearance of the corneal reflex, for 24 h but then tended to recover; the signs had disappeared completely within 120 h (Iimori et al., 1972).

A7.5 Reproductive toxicity, embryotoxicity, and teratogenicity

The reproductive toxicity of LAS and formulations of LAS has been evaluated in studies by oral (gavage, diet, drinking-water), dermal (skin painting), and parenteral (subcutaneous) administration. Similar effects were seen, regardless of the route of application. The studies had a number of deficiencies, however, which are summarized below.

In some studies, widely separated dose levels were used (Palmer et al., 1975a; Takahashi et al., 1975; Tiba et al., 1976; Hamano et al., 1976), so that it is difficult to assess dose-response relationships and to interpret the results. Some of the studies included only one dose (Bornmann et al., 1963; Sato et al., 1972; Endo et al., 1980) and some two (Iimori et al., 1973; Nolen et al., 1975; Takahashi et al., 1975; Hamano et al., 1976; Tiba et al., 1976). The studies done on formulations are difficult to interpret, as the effects seen may have been due to another component. In some cases, the details of the formulation are not given, so that the dose of LAS is also unknown. Certain studies of dermal exposure (Sato et al., 1972; Masuda et al., 1973, 1974; Palmer et al., 1975a; Nishimura, 1976; Daly et al., 1980) involved levels that compromised the integrity of the skin and caused overt toxicity.

The teratogenic effects of some commercial formulations of LAS reported by Mikami and co-workers (1969), mainly in mice, were not reproduced in other studies. A number of studies indicated that LAS have some reproductive toxicity, but the effects were seen only at doses that caused maternal toxicity. No teratogenic effects were observed. These studies are summarized in Tables 20–22.

Table 20. Studies of the reproductive toxicity and teratogenicity of linear alkylbenzene sulfonates (LAS) and formulations of LAS, administered orally

Route	Species (no. of animals/group)	Dose (mg/kg bw per day)	Length of treatment (days)	Comments and results	Reference
LAS					
Diet	Charles River rats (20)	14, 70, 350 (0.02, 0.1, 0.5%)	84	Combined study of reproduction and teratogenicity (three generations);	Buehler et al. (1971)

				no effects attributable to LAS	
Diet	SD rats (16)	78, 780 (0.1, 1.0%)	0–20	No abnormalities at either dose; few offspring at high dose	Tiba et al. (1976)
Gavage	ICR mice (NS)	300, 600	6,8,10	High incidence of cleft palate and exencephaly in fetuses at high dose	Mikami et al. (1969)
Gavage	ICR mice (14)	40, 400 (0.4, 4.0%)	0–6 7–13	No effects at low dose; reduced weight gain and pregnancy rate at high dose	Takahashi et al. (1975)
Gavage	ICR mice (25–33)	10, 100, 300	6–15	Reduced weight gain at all levels, particularly at highest dose; two dams died at highest dose; all fetuses of one dam died *in utero;* decreased body weight and delayed ossification in living fetuses but no increase in incidence of malformations	Shiobara & Imahori (1976)

Table 20 (contd)

Route	Species (no. of animals/group)	Dose (mg/kg bw per day)	Length of treatment (days)	Comments and results	Reference
LAS (contd).					
Gavage	ICR mice	14, 20, 350	1–3	No effect on implantation rate at any dose	Koizumi et al. (1985)
Gavage	CD rats (20) CD-1 mice (20) NZW rabbits (13)	0.2, 2.0, 300, 600	6–15, rats and mice 6–18, rabbits	No effects on any species at two lower doses Rats: reduced weight gain and one death at highest dose Mice: reduced weight gain, seven deaths, and four litter losses at 300 mg/kg bw per day; 18 deaths, one litter loss and one non-pregnancy at 600 mg/kg bw per day Rabbits: reduced weight gain, 11 deaths, two litter losses at 300 mg/kg bw per day; all animals died at highest dose	Palmer et al. (1975a)
Gavage	CD rats (30)	125, 500, 2000	6–15	Two-generation study of reproductive and developmental toxicity; delayed ossification significant at highest dose, slight at middle dose; no reproductive or developmental toxicity	Robinson & Schroeder (1992)

Table 20 (contd)

Route	Species (no. of animals/group)	Dose (mg/kg bw per day)	Length of treatment (days)	Comments and results	Reference
LAS (contd).					
Drinking-water	Charles River rats (10)	7 (0.01%)		Three-generation study of fertility; no teratogenic effects	Bornmann et al. (1963)
Drinking-water	Wistar rats (20)	70 (0.1%)		Four-generation study of reproductive toxicity; no effects attributable to LAS	Endo et al. (1980)
Drinking-water	Wistar rats (20) NZW rabbit (11)	383 mg/rat (0.1%) 3030 mg/rabbit (0.1%)	6–15 6–18	No effects in rats; rabbits had reduced weight gain and delayed ossification but no malformations	Endo et al. (1980)
17% LAS, 7% alcohol ethoxylate sulfate					
Gavage	CD rats (20) CD-1 mice (20) NZW rabbits (13)	0.8, 8, 1,200, 2400 1.064, 10.64, 1600, 320 0.8, 8, 1200, 2400	6–15 6–15 6–18	No increase in major malformations or significant changes in anomalies	Palmer et al. (1975a)
45% LAS					
Diet	CD rats (25)	80, 400, 800 (0.1, 0.5, 1.0%)	6–15	No treatment-related effects on reproduction or embryonic development	Nolen et al. (1975)

Table 20 (contd)

Route	Species (no. of animals/group)	Dose (mg/kg bw per day)	Length of treatment (days)	Comments and results	Reference
1% LAS					
Gavage	ICR mice (18–23)	800, 1200, 1500, 3000	6–15	No increase in fetal malformations; decreased body weight and delayed ossification at 1200 mg/kg bw	Yamamoto et al. (1976)
19% LAS					
Gavage	IRC mice (9–13)	125, 4000	6	No effect on fetal viability or development	Hamano et al. (1976)

NS, not specified

Table 21. Studies of the reproductive toxicity and teratogenicity of linear alkylbenzene sulfonates (LAS) and formulations of LAS, administered dermally

Species (no. of animals/group)	Dose (mg/kg bw per day)	Length of treatment (days)	Comments and results	Reference
LAS				
CD rats (20)	0.6, 6.0, 60 (0.03, 0.3, 3.0%)	1–15	Slight reduction in body weight gain at highest dose; no effect on litter parameters at any dose; no evidence of malformations	Palmer et al. (1975a)
CD-1 mice (20)	5, 50 , 500 (0.03, 0.3, 3.0%)	2–13	Reduced body weight gain, fewer pregnancies, and total litter loss at highest dose; no malformations	
NZW rabbits (13)	0.9, 9, 90 (0.03, 0.3, 3.0%)	1–16	Marked reduction in body weight gain, fewer pregnancies, and two litter losses at highest dose; reduced body weight gain at 9 mg/kg bw per day; no malformations	
Wistar rats (20)	20, 100, 400 (1, 5, 20%)	0–20	Reduced body weight gain, decreased pregnancy rates and delayed ossification at highest dose; no effects at lower doses	Nishimura (1976)
Wistar rats (20)	20, 100, 400 (1, 5, 20%); rinse-off	0–20	Irritation at site and reduced body weight gain at two higher doses; no change in fetal parameters at any level	Daly et al. (1980)

Table 21 (contd)

Species (no. of animals/group)	Dose (mg/kg bw per day)	Length of treatment (days)	Comments and results	Reference
Wistar rats (contd)				
	0.1, 2, 10 (0.05, 0.1, 0.5%); leave on	0–20	No change in fetal parameters at any level	
ddy/s mice (16)	110 (2.22%)	0–13	No abnormalities in dams or fetuses	Sato et al. (1972)
ddy mice (4–10)	0.084, 0.84, 8.4 (0.017, 0.17, 1.7%)	2–14	No fetal or reproductive effects	Masuda et al. (1973, 1974)
ICR mice (25–30)	4.2, 8.4, 12.0, 16.5 (0.85, 1.7, 2.55, 3.4%)	1–13	Delayed ossification at two highest doses	
ICR mice (27–28)	15, 150, 1500 (0.03, 0.3, 3.0%)	6–15	Clear decrease in pregnancy rate and decrease in fetal weight at highest dose; no increase in malformations in fetus	Imahori et al. (1976)
17% LAS, 7% ethanol, 15% urea				
ICR mice (11–20)	2.5, 25, 75 (0.5, 5, 15%)	1–13	Decrease in pregnancy rate at highest dose; no other effects	Inoue & Masuda (1976)

Table 21 (contd)

Species (no. of animals/group)	Dose (mg/kg bw per day)	Length of treatment (days)	Comments and results	Reference
16.3% LAS				
ICR mice (17–50)	25, 50, 100 (5, 10, 20%)	0–13	Reduced pregnancy rate and some total litter losses at highest dose	Nakahara et al. (1976)
Unknown formulation				
ddy/s mice (21)	65 (15%)	0–13	Decreased body weight gain, decreased pregnancy rate, decreased fetal weight, and delayed ossification	Sato et al. (1972)
Unknown formulation				
IRC mice (27–39)	75, 100 (15, 20%)	0–12	Decreased pregnancy rates at both levels	Iimori et al. (1973)
Unknown formulation				
IRC mice (15–19)	30, 65, 85, 100, 125 (13.0, 17.0, 20.0, 25.0%)	0–13	Decreased pregnancy rates at all doses; decreased fetal body weight; delayed ossification at all doses except 65 mg/kg bw per day	Takahashi et al. (1975)

Table 22. Studies of the reproductive toxicity and teratogenicity of linear alkylbenzene sulfonates (LAS) and LAS formulations, administered subcutaneously

Species (no. of animals/group)	Dose (mg/kg bw per day)	Length of treatment (days)	Comments and results	Reference
LAS				

ICR mice (21-24)	0.4, 2.0, 10%	7-13	No significant effects on dams; high incidence of skeletal variations and delayed ossification, not dose-related; no abnormalities	Masuda & Inoue (1974)
ICR mice (12-19)	20, 200 (0.35, 1.00%)	0-3 8-11	Irritation at injection site and reduced pregnancy rate at highest dose; no malformations or anomalies	Takahashi et al. (1975)
17% LAS, 7% ethanol, 15% urea				
CR mice (16-17)	30, 150	7-13 0-13	No increase in major malformations or minor anomalies; increase in implantations at high dose given on days 0-13	Inoue & Masuda (1976)

A7.6 Mutagenicity and related end-points

A7.6.1 Studies in vitro

Assays for mutagenicity were performed *in vitro* with two commercial products containing 17.1 and 19% LAS, either undiluted or diluted 10 and 100 times (Oda et al., 1977), 99.5% pure LAS (Fujita et al., 1977), 95.5% pure sodium salt, or 96.2% pure calcium salt (Inoue & Sunakawa, 1979), using *Bacillus subtilis* H17 (*rec*$^+$) and M45 (*rec*$^-$), *Salmonella typhimurium* TA98 and TA100 (including a metabolic activation system), and *Escherichia coli WP2 uvrA*. All of the assays gave negative results. LAS 99.5% pure (Fujita et al., 1977) were also tested in *S. typhimurium* TA1535 and TA1537, again with negative results. Thesodium and calcium salts in the presence of various liver homogenates (Sunakawa et al., 1981) and a 22.2% solution of LAS (C_{10}-C_{14}, 10-200 µg/plate) (Inoue et al., 1980) were tested in *S. typhimurium* TA98 and TA100. No mutagenicity was seen.

A7.6.2 Studies in vivo

Groups of male ICR:JCL mice were given LAS at a dose of 200, 400, and 800 mg/kg body weight per day by gavage for five days and were killed 6 h after the final administration for examination of chromosomal aberrations in bone-marrow cells. One commercial preparation containing 19.0% LAS was also given, at a dose of 800, 1600, or 3200 mg/kg body weight, and another containing 17.1% LAS at a dose of 1000, 2000, or 4000 mg/kg body weight once only by gavage. The highest doses were 50% of the respective LD_{50} values. Bone marrow was examined 6, 24 and 48 h after administration. There was no significant difference between any of the groups given LAS and the negative control group in the incidence of chromosomal aberrations. Mitomycin C, used as a positive control at 5 mg/kg body weight, induced severe chromosomal aberrations (Inoue et al., 1977).

Groups of five male Wistar rats, Sprague-Dawley rats, and ICR mice were given a diet containing 0.9% LAS for nine months. The equivalent doses were 450 mg/kg body weight per day in rats and 1170 mg/kg body weight per day in mice. There were no significant differences in the incidence of chromosomal aberrations between the experimental and control groups (Masubuchi et al., 1976).

After LAS (C_{10}-C_{15}) were fed to groups of six male and six female Colworth/Wistar rats in the diet at concentrations of 0.56 or 1.13%, equivalent to 280 or 565 mg/kg body weight per day, for 90 days, no alteratuons were seen in chromosomes in bone marrow (Hope, 1977).

In three male ddY mice given LAS at 100 mg/kg body weight by intraperitoneal injection, there was no differences between the treated animals and a control group in the incidence of polychromatic erythrocytes with micronuclei in bone-marrow cells (Kishi et al., 1984).

An assay to detect dominant lethal mutations was performed in seven male ICR:JCL mice given a diet containing 0.6% LAS at 300 mg/kg body weight per day for nine months. Each of the male mice was then mated with two female mice that had not been given LAS, and 11 of the 14 females became pregnant. The pregnant mice were laparotomized on day 13 of gestation to determine the numbers of luteal bodies, implantations, surviving fetuses, and dead fetuses. There were no significant differences in fertility, mortality of ova and embryos, the number of surviving fetuses, or the index of dominant lethal induction (Roehrborn) between the experimental and control groups (Masubuchi et al., 1976).

LAS were administered as a single oral dose of 2 mg to pregnant ICR mice on day 3 of gestation; on day 17 of gestation, each animal received a subcutaneous dose of 1, 2, or 10 mg/mouse and was killed 24 h later. There was no difference among treated groups in the incidence of polychromatic erythrocytes with micronuclei in maternal bone marrow or fetal liver or blood. No mutagenic effect was found in any of the groups (Koizumi et al., 1985).

A7.7 Special studies

A7.7.1 Studies in vitro

The haemolytic action of LAS was investigated by mixing red blood cells from rabbits with solutions of LAS at concentrations of 1-1000 mg/litre at 38°C for 30 min. Haemolysis occurred at concentrations $\geq$ 5 mg/litre (Yanagisawa et al., 1964). Red blood cells from rabbits were mixed with solutions of various concentrations of LAS (relative molecular mass, 346.5) at room temperature for 3 h. The 50% haemolytic concentration of LAS was 9 mg/litre (Oba et al., 1968a).

Purified LAS at various concentrations were added to 10 µl of normal plasma obtained from male rats, and prothrombin time was determined. Prothrombin time was prolonged; the 50% inhibitory concentration was about 0.6 mmol/litre. When LAS at various concentrations were added to a mixture of 1% fibrinogen and thrombin, the time of formation of a mass of fibrin was prolonged by inhibition of thrombin activity. The 50% inhibitory concentration was about 0.05 mmol/litre (Takahashi et al., 1974).

LAS influenced the thermal denaturation and decreased the fluorescence profile of bovine serum albumin *in vitro,* indicating protein-LAS interaction (Javed et al., 1988).

Eggs from female B6C3F1 mice were fertilized *in vitro* and incubated in culture medium containing LAS at concentrations between 0.015 and 0.03%; eggs grown in culture medium without LAS served as controls. Eggs exposed for 1 h, washed, and then cultured for five days developed normally to the blastocyst stage when the concentration of LAS was less than 0.025%; at concentrations higher than 0.03%, the eggs did not develop beyond the one-cell stage. With continuous exposure to LAS for five days, a concentration of 0.01% slightly impaired development to the blastocyst stage, and 0.025% prevented development to the one-cell stage (Samejima, 1991).

LAS with a chain length distribution of C_{10}-C_{14} did not induce transformation of cryopreserved primary cultures of Syrian golden hamster embryo cells *in vitro* (Inoue et al., 1979, 1980).

A7.7.2 Biochemical effects

The levels of amylase, alkaline phosphatase, glutamate-oxalate transaminase, and glutamate-pyruvate transaminase and of the electrolytes Ca, P, and Mg in serum were determined up to 24 h after a single oral administration of 2, 5, 50, or 100 mg/kg body weight of LAS (60% active ingredient) or dermal application of 5 ml of a 1, 5, 10, or 20% solution of LAS to rabbits (number not stated). The levels of total Ca, Ca^{2+}, Mg, and P were generally lower after either type of administration than before. Although there was no definite trend, the activities of the enzymes tended to decrease regardless of the route of the administration or the dose (Yanagisawa et al., 1964).

Groups of three male mice were given an intraperitoneal injection of 0.3 g/kg body weight of LAS (C_{14}) in order to study the effects on the formation of methaemoglobin, determined 0.5, 1, and 2 h afterinjection of LAS. The level of methaemoglobin in the experimental groups was not significantly greater than that in the control group at any time (Tamura & Ogura, 1969).

The effects of LAS (sodium dodecylbenzenesulfonate) on fasting blood glucose level and glucose tolerance curves were investigated in 40 male and 50 female albino rats pretreated with 0.25 g/kg body weight per day of LAS for three months. At the end of this period, the rats were divided into four groups and given distilled water, 6.1 g/kg body weight of glucose, 0.94 g/kg body weight of LAS, or 6.1 g/kg body weight of glucose plus 0.94 g/kg body weight of LAS by gavage. Blood glucose was then estimated at 30-min intervals. Administration of LAS in conjunction with glucose resulted in higher initial levels of blood glucose in male rats and persistently higher levels in females than did administration of glucose alone. Females in control and pretreated groups generally had higher blood glucose levels in response to administration of glucose or LAS plus glucose than did male rats (Antal, 1972).

A8. EFFECTS ON HUMANS

Section summary

Human skin can tolerate contact with solutions of up to 1% LAS for 24 h with only mild irritation. Like other surfactants, LAS can delipidate the skin surface, elute natural moisturizing factor, denature the proteins of the outer epidermal layer, and increase permeability and swelling of the outer layer. LAS do not induce skin sensitization in humans, and there is no conclusive evidence that they induce eczema. No serious injuries or fatalities have been reported following accidental ingestion of LAS-containing surfactant preparations.

A8.1 Exposure of the general population

Surface-active agents are used in shampoos, dish-washing products, household cleaners, laundry detergents, and other applications such as industrial cleaners. LAS are major components of such products. In general, the concentration of nonionic and ionic surfactants is 10-20%.

A8.2 Clinical studies

A8.2.1 Skin irritation and sensitization

LAS are mildly to moderately irritating to human skin, depending on the concentration. There is no evidence that they sensitize the skin in humans.

The relative intensity of skin roughness induced on the surface of the forearms of volunteers (a circulation method) due to contact with LAS of different alkyl chain lengths (C_8, C_{10}, C_{11}-C_{16}) was characterized mainly by gross visible changes. C_{12} LAS produced more skin roughening than LAS with longer or shorter alkyl chains. The degree of skin roughening *in vivo* correlated with the extent of protein denaturation measured *in vitro* (Imokawa et al., 1975a).

Primary skin irritation induced by an LAS formulation (average chain length, C_{12}; relative molecular mass, 346.5), by alpha-olefin sulfonates (AOS) (27% C_{15}, 25% C_{16}, 28% C_{17}, 8% C_{18}; relative molecular mass, 338.5), and by alkyl sulfates (AS) (C_{12}; relative molecular mass, 346.5) was compared in a 24-h closed-patch test on the forearms of seven male volunteers. A 1% aqueous solution (pH 6.8) of each substance was used, and the relative intensity of skin irritation was scored by grading erythema, fissuring, and scales. The average score for LAS was similar to that for AOS but significantly lower than that for AS ($p < 0.05$) (Oba et al., 1968a).

In another comparison, the intensity of skin irritation induced by 1% aqueous solutions of LAS (C_{10}–C_{13}), AOS (C_{14}, C_{16}, C_{18}), and the sodium salt of AS (C_{12}–C_{15}) was studied in a 24-h closed-patch test on the forearm and in a test in which the substance was dripped onto the interdigital surface for 40 min once daily for two consecutive days at a rate of 1.2–1.5 ml/min. Skin reactions were scored by grading erythema in the patch test and by grading scaling in the drip test. In the patch test, the score for LAS was similar to that for AOS but significantly lower than that for AS. In the drip test, the score for LAS was similar to that for AS but higher than that for AOS (Sadai et al., 1979).

Repeated patch tests with LAS at aqueous concentrations of 0.05 and 0.2% produced mild to moderate primary irritation. In a study on the sensitization potential of LAS for human skin, a 0.1% aqueous preparation caused no sensitization in 86 subjects (Procter & Gamble Co., unpublished data).

No skin sensitization was seen in 2294 volunteers exposed to LAS or in 17 887 exposed to formulations of LAS (Nusair et al., 1988).

A8.2.2 Effects on the epidermis

The main effects of surface-active agents on the epidermal (stratum corneum) are:

-- delipidation of the skin surface or outer layer;

-- elution of natural moisturizing factor, which maintains the water content of the outer layer;

-- denaturation of stratum corneum protein; and

-- increased permeability, swelling of the outer layer, and inhibition of enzyme activities in the epidermis.

These effects and some others present a hazard to the skin; they are described below.

In an investigation of the relationship between the irritating potential of LAS *in vivo* and its ability to remove lipid from the stratum corneum *in vitro,* LAS removed detectable levels of lipids only at levels above the critical micelle concentration (0.04%). LAS removed only small amounts of cholesterol, free fatty acids, the esters of those materials, and possibly squalene. At concentrations below that level, LAS can bind to and irritate the stratum corneum. The clinical irritation produced by LAS is therefore unlikely to be directly linked to extraction of lipid, and milder forms of irritation may involve binding of LAS to and denaturation of keratin as well as disruption of lipid (Froebe et al., 1990).

The results of the human arm immersion test with measurement of eluted amino acids and protein, the skin permeation test, freeing of sulfhydryl groups, and the patch test were compared for nine kinds of surfactant, including LAS, ABS, AS, alcohol ethoxylate sulfate, soap, nonionic surfactant, and amphoteric surfactant. LAS gave intermediate reactions in the patch test and the permeation test and showed a high level of sulfhydryl group freeing activity. The results of the tests for evaluating surfactants did not agree with those for the immersion test, which the author considered to provide the best simulation of actual use (Polano, 1968).

In a number of studies, denaturation of outer layer proteins was observed *in vitro* (Van Scott & Lyon, 1953; Harrold, 1959; Wood & Bettley, 1971; Imokawa et al., 1974; Okamoto, 1974; Imokawa et al., 1975b; Imokawa & Katsumi, 1976). Sodium dodecylbenzenesulfonate stimulated penetration of sodium ions through isolated human epidermis, partly because the detergent can denature proteins of the epidermal stratum corneum (Wood & Bettley, 1971). Sodium laurate and sodium lauryl sulfate were the most effective of several surfactants in inducing swelling of the horny layer (Putterman et al., 1977). The lysosome labilizing effects of surfactants, measured as the release of enzyme from lysosomes, were shown to diminish in the order cationic > anionic > nonionic surfactants (Imokawa & Mishima, 1979). When ovalbumin was used as a simulated epidermis protein, sodium lauryl sulfate was found to denature skin protein extensively by exposing concealed sulfhydryl groups in LAS of alkyl chain length C_8–C_{16} (Blohm, 1957).

In immersion tests of the hand and the forearm up to 5 cm above the wrist, falling off of skin scales diminished in the order: *sec*-alkane sulfonate > LAS > AOS, alcohol ethoxylate sulfate (Okamoto, 1974), but the distribution of carbon chain lengths among the samples was not described. In a comparison of skin roughening by a circulation method, the effects diminished in the order C_{12} AS > C_{12} AOS > C_{12} *sec*-alkane sulfonate > C_{12} LAS (Imokawa et al., 1974, 1975a,b). Skin roughening caused by several surfactants that are components of commercial products was studied

by the method of Ito & Kakegawa (1972), in which various concentrations are dripped onto the fingers. The effects diminished in the order C_{10}–C_{13} LAS = C_{12}–C_{15} AS > C_{11}, C_{13}, C_{15} alcohol ethoxylate sulfate (n = 0–3) > C_{14}, C_{16}, C_{18} AOS > C_{11}–C_{15} polyoxyethylene alkylether (Sadai et al., 1979).

A8.2.3 Hand eczema

The skin reaction to 0.04, 0.4, and 4.0% aqueous solutions of LAS (10.0% C_{10}, 34.3% C_{11}, 31.5% C_{12}, 24.7% C_{13}) was tested in a 24-h closed-patch test on the lower backs of 10 healthy volunteers and 11 patients with hand eczema (progressive keratosis palmaris). The incidence and intensity of skin reactions were

greater in the group with hand eczema, but the difference was not statistically significant (Okamoto & Takase, 1976a,b).

In order to assess the possible etiological correlation between exposure to LAS and hand eczema, 0.04, 0.4, and 4% aqueous solutions of LAS were applied in 48-h closed-patch tests on the lower backs of 20 women with hand eczema and 42 with other skin diseases. The skin reaction was scored grossly from 0 to 5 on the basis of the occurrence or intensity of erythema, papules, and vesicles. The average score appeared to increase in parallel with the concentration of LAS but did not differ between the groups with hand eczema and other skin diseases (Sasagawa et al., 1978).

Nine proprietary household detergents were tested in 24-h closed-patch tests on the lower backs of 160 women with hand eczema. The surfactant concentrations in five of the products were: (i) 2% ABS-Na, 15% LAS-Na; (ii) 2% ABS-Na, 14% LAS-Na; (iii) 17% LAS-Na, 12% alcohol ethoxylate sulfate; (iv) 11% ABS-Na, 11% LAS-Na; (v) 19% LAS-Na. When the detergents were applied daily (for an unspecified period) at an aqueous concentration of 0.175–0.8%, positive responses were observed in 3.1% of the women, but they were considered not to be allergic because the redness of the skin disappeared completely within two days (Kawamura et al., 1970).

Three proprietary household detergents containing LAS were tested in 24-h closed-patch tests on the forearms of 13 women with 'housewives' dermatitis' and 13 with other skin diseases. The detergent was applied either undiluted or in a 0.2% aqueous solution. Undiluted solutions of all three detergents caused mild to moderate skin reactions, at incidences of 38.5, 48.1, and 73.1%, which did not differ between the groups with housewives' dermatitis and other skin diseases. The 0.2% aqueous solutions did not induce skin reactions (Ishihara & Kinebuchi, 1967).

Two series of field tests were conducted to estimate if exposure to a variety of synthetic detergent formulations was associated with causation or aggravation of hand eczema in women. In the first series, 162 female volunteers were divided into two groups and instructed to wear a rubber glove on either the left or the right hand while using the detergents. The test was conducted for one month, and the gross appearance of hands before and after the test period was compared. The relative intensity of noninflammatory keratosis of the hands was increased in individuals in both groups on hands that were covered and to a slightly greater extent on hands that were uncovered. In the second series of tests, 881 housewives were divided into three groups and instructed to use only one brand of household detergent, containing LAS, AOS, or ABS during the test period and to wear rubber gloves on both hands while using the detergent. The test was conducted for 1.5 months, and the gross appearance of hands before and after the test period was compared.

Skin roughness was not worsened in any of the three groups (Watanabe et al., 1968).

A8.2.4 Occupational exposure

Sixty workers exposed at work to an atmosphere containing LAS at 8.64 mg/m^3 were tested for serum lipid and sugar content and for the activities of selected serum enzymes. The levels of total plasma lipids and plasma cholesterol were slightly lower in the exposed group than in controls, but no differences were noted for blood sugar, plasma phospholipid, plasma lipoprotein, alpha-amylase, leucine aminopeptidase, or pseudocholinesterase. The duration of exposure before testing was not indicated (Rosner et al., 1973).

In an investigation of the asthmagenic properties of sodium isononanoyl oxybenzene sulfonate, detergent industry workers were also tested with LAS. Three workers previously exposed to sodium isononanoyl oxybenzene sulfonate, three unexposed controls without asthma, and three controls with asthma were challenged with 0.01–100 µg of LAS. No changes were seen after inhalation of LAS in any of the subjects; but sodium isononanoyl oxybenzene sulfonate induced asthmatic symptoms in the previously exposed workers and not in the control groups (Stenton et al., 1990).

A8.2.5 Accidental or suicidal ingestion

No symptoms were seen in four cases of accidental ingestion of unknown amounts of a household synthetic detergent containing LAS as the main component (Hironaga, 1979).

A 32-year-old woman who had ingested 160 ml of a 21% aqueous solution of LAS with suicidal intent showed transient, slight mental confusion, vomiting, pharyngeal pain, hypotension, decreased plasma cholinesterase activity, and increased urinary urobilinogen, but all of these symptoms disappeared rapidly (Ichihara et al., 1967).

In a review of 1 581 540 cases of human exposure to a wide range

of chemicals reported by the United States Poison Control Centers in 1989, 7983 people had been exposed to household automatic dishwasher preparations (alkali, anionic or nonionic, other or unknown) and 506 had required treatment in a health facility; 8950 had been exposed to household cleansers, with 894 requiring treatment; 12 876 had been exposed to laundry preparations, with 1542 treated; and 621 had been exposed to industrial detergents (anionic, cationic, nonionic), with 321 cases requiring treatment. There were no deaths, and only 12 of the treated cases were classified as 'major outcome'. Virtually all the reports involved accidental exposure. The compositions of the cleaning preparations, routes of exposure, and clinical descriptions were not provided (Litovitz et al., 1990).

A9. EFFECTS ON OTHER ORGANISMS IN THE LABORATORY AND THE FIELD

Section summary

LAS have been tested extensively, both in the laboratory and under field conditions, but the following aspects must be considered in interpreting test results. Comparison of the results of tests carried out on either mixtures of homologues of LAS or LAS of specified chain length is restricted, because the toxicity of LAS is influenced by the chain length, and homologues of lower chain length are less toxic than those with longer chains; furthermore, chain length was rarely specified in older studies. Studies of the effects of formulations of LAS on environmental biota are not included in this section.

Organisms are not exposed to a constant concentration of LAS in water, owing to the high adsorptivity and biodegradability of LAS. As LAS are adsorbed on suspended solids or food particles, they have reduced bioavailability. The adsorption kinetics of LAS also depend on the chain length of the homologues. Studies of aquatic toxicity involving flow-through or static renewal (at least daily) should therefore be given more prominence than studies based on static conditions, although flow-through and static renewal cannot be used in (semi-) chronic studies of lower organisms, such as daphnia. Studies in which the actual concentration was measured should likewise be given more consideration than those that rely on nominal concentrations.

The effects of LAS on the aquatic environment have been studied in short- and long-term studies in the laboratory and under more realistic conditions: micro- and mesocosm and field studies. In general, a decrease in alkyl chain length or a more internal position of the phenyl group is accompanied by a decrease in toxicity. Data on fish and daphnia indicate that a decrease in chain length of one unit (e.g. C_{12} to C_{11}) is accompanied by an approximately 50% decrease in toxicity, but there is no linear relationship between chain length and toxicity. In aquatic microorganisms, the effects are strongly related to variables such as the type of test system and use of mixed cultures as opposed to individual species. EC_{50} values range from 0.5 mg/litre (single species) to > 1000 mg/litre.

In freshwater fish, the acute LC_{50} values of C_{8}–C_{15} LAS are 0.1–125 mg/litre. The chronic L(E)C50 values of LAS ($C_{11.7}$ and not specified) in two species tested were 2.4 and 11 mg/litre, and NOECs ranging from 0.11 to 8.4 mg/litre have been reported for $C_{11.2}$–C_{13} (or not specified). Marine fish appear to be more sensitive, with acute LC_{50} values for $C_{11.7}$ (or not specified) in six species of 0.05–7 mg/litre, chronic LC_{50} values for LAS of unspecified chain length in two species of 0.01–1 mg/litre, and an NOEC for C_{12} in one species of < 0.02 mg/litre.

Results in aquatic plants are also species dependent. In freshwater plants, the EC_{50} values for LAS (with chain lengths shown in parentheses) were 10–235 mg/litre for green algae (C_{10}–C_{14}), 5–56 mg/litre for blue algae ($C_{11.1}$–C_{13}), 1.4–50 mg/litre for diatoms ($C_{11.6}$–C_{13}), and 2.7–4.9 mg/litre for macrophytes ($C_{11.8}$). Marine algae appear to be even more sensitive. There is probably no linear relationship between chain length and toxicity to algae.

The effects of LAS on freshwater algae have also been tested under realistic conditions in systems with various trophic levels, comprising enclosures in lakes (lower organisms), model ecosystems (sediment: water systems), a river below and above a wastewater treatment plant outfall, and experimental streams. In general, C_{12} LAS were used. Algae were more sensitive in summer, when the 3-h EC_{50} values with regard to photosynthesis were 0.2–8.1 mg/litre, whereas studies of model ecosystems showed no effects on the relative abundance of algal communities at 0.35 mg/litre. No effects were seen in these studies at 0.24–5 mg/litre, depending on the organism and parameter tested.

In aquatic invertebrates, the acute $L(E)C_{50}$ values were 4.6–200 mg/litre for molluscs (either C_{13} or not specified), 0.12–27 mg/litre for crustaceans ($C_{11.2}$–C_{18} or not specified), 1.7–16 mg/litre for worms ($C_{11.8}$ or not specified), and 1.4–270 mg/litre for insects (C_{10}–C_{15}). The chronic $L(E)C_{50}$ values were 2.2 mg/litre for insects ($C_{11.8}$) and 1.1–2.3 mg/litre for crustaceans ($C_{11.8}$–C_{13}). The chronic NOEC for crustaceans, on the basis of lethality or reproduction, was 0.2–10 mg/litre ($C_{11.8}$ or not specified). Marine invertebrates are more sensitive, with LC_{50} values of 1 to >100 mg/litre (almost all C_{12}) and NOEC values of 0.025–0.4 mg/litre (chain lengths not specified).

Biodegradation products and by-products of LAS are 10–100 times less toxic than the parent compound.

Fewer data are available on the effects of LAS in the terrestrial environment. For the plant species tested, the NOEC values were < 10–20 mg/litre in nutrient solutions and 100 mg/kg (C_{10}–C_{13}) for growth of plants in soils. The 14-day LC_{50} for earthworms was > 1000 mg/kg.

One study in which chickens were treated in the diet resulted in an NOEC based on egg quality of > 200 mg/kg.

A9.1 Effect of chain length on the toxicity of linear alkylbenzene sulfonates

The ecotoxicity of homologues of LAS varies according to the length of the alkyl chain and the position of the benzene ring on this chain. In general, homologues with longer chains are more ecotoxic than shorter ones, and ecotoxicity increases with the proximity of the benzene ring to the end of the chain. The results of studies on the effect of LAS chain length on acute toxicity to fish are presented in Table 23.

The effect of chain length can also be seen on the basis of quantitative structure-activity relationships (Roberts, 1989, 1991) calculated from the octanol-water partition coefficients of homologues of LAS. The slope of the relationship varied from 0.64 to 0.78; therefore, using an average slope of 0.70, it was calculated that a decrease in chain length from C_{12} to C_{11} reduced the aquatic toxicity of LAS by a factor of 2.4, with a corresponding decrease in the octanol-water partition coefficient of 0.54.

Table 23. Effect of the chain length of linear alkylbenzene sulfonates (LAS) on their acute toxicity to freshwater fish

Homologue of LAS	Fathead minnow Pimephales promelas 48-h LC_{50} (mg/litre)[a]	Goldfish Carassius auratus 6-h LC_{50} (mg/litre)[b]	Guppy Lebistes reticulatus LC_{50} (mg/litre)[c]	Golden orfe Idus idus melanotus 96-h LC_{50} (mg/litre)[d]
C10	43.0	61.0	50	16.6
C11	16.0	22.5		6.5
C12	4.7	8.5	5	2.6
C13	0.4	3.3		0.57
C14	0.4		1	0.26
C16		0.087	1	0.68
C18		0.38		15

[a] From Kimerle & Swisher (1977)
[b] From Gafa (1974)
[c] From Borstlap (1967)
[d] From Hirsch (1963)

A9.2 Microorganisms

No adverse effects were seen on the performance of laboratory-scale activated sludge units after addition of ≤ 20 mg/litre LAS. At 50 mg/litre, nitrification was decreased in extended aeration units that were treating synthetic sewage (Janicke & Niemitz, 1973). A bacterium similar to *Klebsiella pneumoniae* isolated from sewage degraded LAS at a concentration of 10 ml/litre, but a concentration of 20 ml/litre inhibited the growth of the bacterium by 39% (Hong et al., 1984).

The toxicity of microorganisms in activated sludge increases with the length of the alkyl chain up to approximately C_{12} and then decreases (Table 24), presumably because of decreased bioavailability (e.g. greater sorption of these higher chain lengths) (Verge et al., 1993).

Table 24. Results of tests for the inhibition of activated sludge by the sodium salt of linear alkylbenzene sulfonates (LAS)

LAS	Chain length	3-h EC_{50} (mg/litre)
Pure homologues	C_{10}	1042–1200
	C_{11}	740–782
	C_{12}	500–723
	C_{13}	700–795
	C_{14}	900–1045
Commercial formulations	C_{11}	760
	$C_{11.6}$	550
	C_{13}	650

From Verge et al. (1993)

A mixed bacterial culture was acclimatized to 10 mg/litre LAS (C_9–C_{14}) and was then maintained in either river water, forest soil, or wastewater from a detergent plant, the concentration of LAS being increased every five days. At 20.8 and 46 mg/litre, no effect was reported on the specific growth rate of the bacteria; however, at 70 mg/litre, the growth rate was inhibited by 18%, and at

95 mg/litre growth was almost zero. Concentrations of 186 and 465 mg/litre LAS inhibited growth completely (Hrsak et al., 1981).

The acute toxicity of LAS (C_9-C_{14}) in naturally occurring bacteria was studied in freshwater and seawater samples by measuring ^{3}H-thymidine incorporation. The EC_{50} values were 0.5–1.66 mg/litre for all samples. Toxicity was found to increase with an increasing relative abundance of longer carbon chains (Martinez et al., 1989).

For bacteria collected from the Rhone River plume (an estuarine area) and exposed to LAS, the EC_{50}, based on ^{3}H-thymidine incorporation, was 11.9 mg/litre (Martinez et al., 1991).

The 8-h EC_{50}, based on specific growth rate, of *Pseudomonas fluorescens* in solutions of $C_{11.1}$ LAS under static conditions was 3200–5600 mg/litre (Canton & Slooff, 1982).

The effect of $C_{11.6}$ LAS on the structure and function of microbial communities was studied in a flow-through model ecosystem containing several trophic levels at concentrations of 0.5 or 5 mg/litre. LAS had no effect on microbial structure at either dose level, but at 5 mg/litre it inhibited the degradation of both glucose and LAS. In an experiment in which LAS were supplied in sewage, neither microbial structure nor function was affected (Larson & Maki, 1982).

The effects of LAS on the microbial activity of soils were studied on the basis of Fe[III] reduction. The no-effect-level was found to be 250 mg/kg; the EC_{50} was about 500 mg/kg in a strongly adsorbing soil and 33–55 mg/kg in a poorly adsorbing soil (Welp & Brummer, 1985).

LAS at concentrations of 0.8–50 g/m^2 had no effect on respiration of loamy soil, sandy soil, or sandy soil irrigated with wastewater for one or 14 days (Litz et al., 1987).

A9.3 Aquatic organisms

A9.3.1 Aquatic plants

A9.3.1.1 Freshwater algae and cyanobacteria

The 96-h EC_{50} values for C_{13} LAS on population growth were 116 mg/litre for the green alga *Selenastrum capricornutum*, 5 mg/litre for the blue-green alga *Microcystis aeruginosa*, and 1.4 mg/litre for the diatom *Navicula pelliculosa*. The EC_{50} values for C_{12} LAS were 29 mg/litre for *Selenastrum* and 0.9 mg/litre for *Microcystis* (Lewis & Hamm, 1986). The EC_{50} for $C_{11.7}$ LAS on growth of *Selenastrum* was reported to be 83 mg/litre (Konno & Wakabayashi, 1987). The EC_{50} values for $C_{11.6}$ LAS were found to be 50–100 mg/litre for *Selenastrum*, 10–20 mg/litre for *Mycrocystis*, and 20–50 mg/litre for the diatom *Nitzschia fonticola* (Yamane et al., 1984). The seven-day EC_{50} for C_{12} LAS in the green alga *Chlorella pyrenoidosa*, based on growth, was 10 mg/litre (Kondo et al., 1983).

The 96-h EC_{50} values in algae grown in solutions of $C_{11.1}$ LAS under static conditions, measured as biomass, were 32–56 mg/litre for *Microcystis aeruginosa* and 18–32 mg/litre for *Chlorella vulgaris* (Canton & Slooff, 1982).

A study of the toxicity of various formulations of LAS to the algae *Scenedesmus subspicatus* and *Selenastrum capricornutum* (Table 25) indicated that commercial mixtures are as or slightly less toxic than homologues. This finding may be due to a difference in the sensitivity of the two algae, since those tested with the homologues were of a different origin than those tested with commercial LAS (Verge et al., 1993).

Table 25. Results of tests for the toxicity of the sodium salt of linear alkylbenzene sulfonates (LAS) in algae

LAS	Chain length	72-h EC_{50} (mg/litre)
Pure homologues	C_{10}	235
	C_{11}	118
	C_{12}	62
	C_{13}	33
	C_{14}	18
Commercial formulations	C_{11}	80
	$C_{11.6}$	80
	C_{13}	62

From Verge et al. (1993)

LAS (chain length not specified) significantly reduced the growth of the green alga *Selenastrum capricornutum* at a concentration of 40 mg/litre or more. A significant decrease in growth was also noted at 10 mg/litre, but no significant effect was observed at 20 or 30 mg/litre (Nyberg, 1988).

A9.3.1.2 Marine algae

Growth of Gymnodinium breve was reduced by 69% rafter nine days' exposure to C_{12} LAS (Kutt & Martin, 1977). These results were

confirmed in a study in which C_{13} LAS were introduced at the bottom or surface of a water column: Exposure to LAS at concentrations > 0.025 mg/litre inhibited growth completely within two days (Hitchcock & Martin, 1977). These results suggest that *Gymnodinium breve* is more sensitive to the effects of LAS than other algae.

For $C_{11.7}$ LAS, the seven-day EC_{50} for growth and the two-day EC_{50} for ATP activity on the marine diatom *Thalassiosira pseudonana* were both 10 mg/litre (Kondo et al., 1983).

Exposure of the alga *Porhyra yezoensis,* a standard test species in Japan, to LAS (C_{10}-C_{14}) under semi-static conditions gave a 10-day E_{50} (based on growth) of 0.56 mg/litre (Takita, 1985).

A9.3.1.3 Macrophytes

The seven-day EC_{50} values for $C_{11.8}$ LAS on the duckweed Lemna minor under flow-through conditions were 2.7 mg/litre for frond count, 3.6 mg/litre for dry weight, and 4.9 mg/litre for root length. The time-independent EC_{50} for growth rate and doubling time was 4.8 mg/litre (Bishop & Perry, 1981).

A9.3.2 Aquatic invertebrates

A9.3.2.1 Acute toxicity

The acute toxicity of LAS to aquatic invertebrates is summarized in Tables 26 and 27. For marine invertebrates, the 96-h LC_{50} values for C_{12} LAS range from 3 mg/litre for barnacles to > 100 mg/litre for several other species (Table 26). Freshwater invertebrates show a range of 48-h LC_{50} values from 0.11 mg/litre (C_{16}) for a daphnid to 270 mg/litre ($C_{11.8}$) for an isopod (Table 27). Several marine invertebrate species are more sensitivite to LAS at the larval stage than as adults (Table 26).

Freshwater mussels *(Anodonta cygnea)* were more sensitive to LAS during the reproductive period than during the non-reproductive period, the 96-h LC_{50} being reduced from 200 to 50 mg/litre (Bressan et al., 1989).

Studies with *Daphnia magna* revealed a correlation between chain length and toxicity. The acute toxicity (24-h and 48-h LC_{50}) of LAS to *Daphnia magna* increased with chain length between C_{10} and C_{14} (Kimerle & Swisher, 1977) and with chain lengths between C_{10} and C_{16} (Maki & Bishop, 1979), although similar values were obtained for C_{16} and C_{18} homologues. No significant difference in sensitivity was seen between *Daphnia magna* and *Daphnia pulex.* A similar result was obtained with homologue mixtures (Martinez et al., 1989): toxicity was correlated with the homologues in which long chains were the most abundant.

Partial biodegradation of LAS significantly reduces the specific toxicity (by unit weight) of the remaining LAS to *Daphnia magna.* For example, LAS with a high relative molecular mass and a 48-h LC_{50} of 2 mg/litre had an LC_{50} of 30-40 mg/litre after 80-85% degradation (Kimerle & Swisher, 1977); the longer homologues and more terminal isomers, which are the most toxic, are therefore also the more readily biodegraded. Shorter carboxylates formed during the degradation of LAS were three to four orders of magnitude less toxic than LAS (Swisher et al., 1978). Other workers also found a

Table 26. Acute toxicity of linear alkylbenzene sulfonates (LAS) to estuarine and marine invertebrates

Organism	Size or age	Static or flow	Temp. (°C)	Salinity (%)	LAS chain length	End-point	Concentration (mg/litre)[a]	Reference
Sea squirt (Ciona intestinalis)	Larva	Static	20		NS	6-h LC_{50}	1	Renzoni (1974)
Common mussel (Mytilus edulis)		Static	6-8	32-34	C_{12}	96-h LC_{50}	> 100	Swedmark et al. (1971)
		Static	15-17	32-34	C_{12}	96-h LC_{50}	50	
Mussel (Mytilus galloprovincialis)		Staticr	18	35	NS	48-h LC_{50}	39.8	Bressan et al. (1989)
	Adult		18	35	NS	96-h LC_{50}	1.66	
Cockle (Cardium edule)		Static	6-8	32-34	C_{12}	96-h LC_{50}	5	Swedmark et al. (1971)
	Juvenile	Static	15-17	32-34	C_{12}	96-h LC_{50}	5	
Clam (Mya arenaria)		Static	6-8	32-34	C_{12}	96-h LC_{50}	70	
		Static	15-17	32-34	C_{12}	96-h LC_{50}	< 25	
Scallop (Pecten maximus)		Static	6-8	32-34	C_{12}	96-h LC_{50}	< 5	
Scallop		Static	15-17	32-34	C_{12}	96-h LC_{50}	< 5	
Decapod (Leander adspersus)		Static	15-17	32-34	C_{12}	96-h LC_{50}	50	
	Intermoult	Static	6-8	32-34	C_{12}	96-h LC_{50}	50	
	Postmoult	Static	6-8	32-34	C_{12}	96-h LC_{50}	25	
Hermit crab (Eupagurus bernhardus)		Static	6-8	32-34	C_{12}	96-h LC_{50}	> 100	

Table 26 (contd)

Organism	Size or age	Static or flow	Temp. (°C)	Salinity (‰)	LAS chain length	End-point	Concentration (mg/litre)[a]	Reference
Spider crab	Larva	Static	6-8	32-34	C_{12}	96-h LC_{50}	9	
(Hyas araneus)	Adult	Static	6-8	32-34	C_{12}	96-h LC_{50}	> 100	
Shore crab (Carcinus maenus)		Static	6-8	32-34	C_{12}	96-h LC_{50}	> 100	
Barnacle	Larva	Static	6-8	32-34	C_{12}	96-h LC_{50}	3	
(Balanus balanoides)	Adult	Static	6-8	32-34	C_{12}	96-h LC_{50}	50	
Brine shrimp (Artemia salina)		Static	25		C_{11}-C_{13}	24-h LC_{50}	33	Price et al. (1974)

Static: water unchanged for duration of test; NS, not specified; static[r], static renewal: water changed every 12 h; flow, flow-through conditions: LAS concentration in water maintained continuously
[a] Based on nominal concentration

Table 27. Acute toxicity of linear alkylbenzene sulfonates (LAS) to freshwater invertebrates

Organism	Size or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	LAS chain length	End-point	Concn (mg/litre)	Reference
Bivalve mollusc	11 cm	Static[r]	18		8.0	NS	96-h LC_{50}	200[b]	Bressan et al.
(Anodonta cygnea)			18		8.0	NS	96-h LC_{50}	50[b,c]	(1989)
Bivalve mollusc (Unio elongatulus)	9 cm	Static[r]	18		8.0	NS	96-h LC_{50}	182.5[b]	
Snail (Gonobasis sp.)		Static	21	62	7.3	av. C_{13}	24-h LC_{50}	4.6[b]	Dolan & Hendricks (1976)
Snail (Physa integra)		Flow	15	41-47	7.5-7.7	NS	96-h LC_{50}	9[b]	Arthur (1970)
Amphipod (Gammarus pseudolimnaeus)		Flow	15	41-47	7.5-7.7	NS	96-h LC_{50}	7[b]	
Amphipod (Gammarus sp.)	4.3 mm	Static	22	165	7.9-8.4	$C_{11.8}$	48-h LC_{50}	3.3[b]	Lewis & Suprenant (1983)
Campeloma decisum		Flow	15	41-47	7.5-7.7	NS	96-h LC_{50}	27[b]	Arthur (1970)
Water flea (Daphnia magna)	< 24 h	Static	20	25		$C_{11.7}$	24-h LC_{50}	17	Wakabayashi et al. (1988)
	< 24 h	Static	21	120	7.4	C_{10}	48-h LC_{50}	9.55[d]	Maki & Bishop (1979)

Table 27 (contd)

Organism	Size or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	LAS chain length	End-point	Concn (mg/litre)	Reference
Water flea (contd)	< 24 h	Static	21	120	7.4	C_{11}	48-h LC_{50}	1.15[d]	
(Daphnia magna)	< 24 h	Static	21	120	7.4	C_{12}	48-h LC_{50}	5.88-6.84[d]	
	< 24 h	Static	21	120	7.4	C_{13}	48-h LC_{50}	2.63[d]	
	< 24 h	Static	21	120	7.4	C_{14}	48-h LC_{50}	0.68-0.8[d]	
	< 24 h	Static	21	120	7.4	C_{16}	48-h LC_{50}	0.11-0.2[d]	
	< 24 h	Static	21	120	7.4	C_{18}	48-h LC_{50}	0.12[d]	
	< 18 h	Static				$C_{13.3}$	48-h LC_{50}	2.3[b]	Kimerle &
	< 18 h	Static				C_{10}	48-h LC_{50}	12.3[b]	Swisher (1977)
	< 18 h	Static				C_{11}	48-h LC_{50}	5.7[b]	
	< 18 h	Static				C_{12}	48-h LC_{50}	3.5[b]	
	< 18 h	Static				C_{13}	48-h LC_{50}	2.0[b]	
	< 18 h	Static				C_{14}	48-h LC_{50}	0.7[b]	
	< 24 h	Static	19			$C_{11.2}$	48-h LC_{50}	18-32[b]	Canton & Slooff (1982)
	< 24 h	Static	21	131	7.4-7.8	$C_{11.8}$	48-h LC_{50}	4.8[d]	Lewis (1983)
	< 24 h	Static	22	165	7.9-8.4	$C_{11.8}$	48-h LC_{50}	1.8-5.6[b]	Lewis & Suprenant (1983)
	< 24 h	Static	21	295-310	7.3-8.4	$C_{11.8}$	48-h LC_{50}	3.6-4.7[b]	Taylor (1985)
	< 48 h	Static	22	241	7.8	C_{11}	48-h EC_{50}	2.2[b,e]	Barera & Adams (1983)
		Flow				$C_{11.8}$	48-h LC_{50}	4.4[d]	Bishop & Perry (1981)
	< 12 h	Flow	21	120	7.4	$C_{11.8}$	96-h LC_{50}	23.94[d]	Maki (1979a)
	< 12 h	Flow	21	120	7.4	C_{13}	48-h LC50	2.19[d]	

Table 27 (contd)

Organism	Size or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	LAS chain length	End-point	Concn (mg/litre)	Reference
Water flea (Daphnia pulex)	< 24 h	Static	20	25		$C_{11.7}$	24-h LC_{50}	18	Wakabayashi et al. (1988)

	< 24 h	Static	21	120	7.4	C_{12}	48-h LC_{50}	8.62[d]	Maki & Bishop (1979)
	< 24 h	Static	21	120	7.4	C_{14}	48-h LC_{50}	0.59[d]	
	< 24 h	Static	21	120	7.4	C_{16}	48-h LC_{50}	0.15[d]	
Oligochaete (Dero sp.)	6.0 mm	Static	22	165	7.9-8.4	$C_{11.8}$	48-h LC_{50}	1.7[b]	Lewis & Suprenant (1983)
Roundworm (nematode) (Rhabditis sp.)	0.3 mm	Static	22	165	7.9-8.4	$C_{11.8}$	48-h LC_{50}	1.7[b]	
Flatworm (Dugesia sp.)	3.4 mm	Static	22	165	7.9-8.4	$C_{11.8}$	48-h LC_{50}	1.8[b]	
Branchiura sowerbyi		Staticr	10	25	8.0	NS	96-h LC_{50}	10.8[b,f]	Bressan et al. (1989)
			10	25	8.0	NS	96-h LC_{50}	4.4[b]	
Worm (Limnodrilus hoffmeisteri)		Staticr	10	25	8.0	NS	96-h LC_{50}	7.8[b,f]	
			10	25	8.0	NS	96-h LC_{50}	2.0[b]	
Isopod (Asellus sp.)	5.3 mm	Static	22	165	7.9-8.4	$C_{11.8}$	48-h LC_{50}	1.8[b]	Lewis & Suprenant (1983)

Table 27 (contd)

Organism	Size or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	LAS chain length	End-point	Concn (mg/litre)	Reference
Midge (Chironomus riparius)	Larva	Flow	22	150	7.8-8.4	$C_{11.8}$	72-h LC^{50}	2.2[d]	Pittinger et al. (1989)
Midge (Paratanytarsus parthenogenica)	3.6 mm	Static	2	165	7.9-8.4	$C_{11.8}$	48-h LC_{50}	1.8[d]	Lewis & Suprenant (1983)
Mosquito (Aedes aegypti)	Larva	Static				C_{10-13}	24-h LC_{50}	6[b]	Van Emden et al. (1974)
	Larva	Static				C_{10-15}	24-h LC_{50}	2[b]	
	3-4 d	Static	23			$C_{11.1}$	48-h LC_{50}	56-100[b]	Canton & Slooff (1982)
Mayfly (Isonychia sp.)	Larva	Static	10	53	7.5-7.8	$C_{11.6}$	24-h LC_{50}	13.6[b]	Dolan et al. (1974)
	Larva	Static	10	53	7.5-7.8	$C_{11.6}$	48-h LC_{50}	10.4[b]	
	Larva	Static	10	53	7.5-7.8	$C_{11.6}$	96-h LC_{50}	5.33[b]	
	Larva	Static	10	53	7.5-7.8	$C_{13.1}$	24-h LC_{50}	4.19[b]	
	Larva	Static	10	53	7.5-7.8	$C_{11.6}$	48-h LC_{50}	12.47[b]	
	Larva	Static	10	53	7.5-7.8	$C_{11.6}$	96-h LC_{50}	1.36[b]	

Static[r], static renewal: water changed every 12 h; NS, not specified; flow, flow-through conditions: LAS concentration in water maintained continuously; static: water unchanged for duration of test

[a] mg/litre $CaCO_3$

[b] Based on nominal concentration

[c] Test performed during the reproductive period

[d] Based on measured concentrations

[e] Based on immobilization

[f] Organism exposed in the presence of sediment

reduction in the acute toxicity of LAS to *Daphnia magna* during primary degradation (Gard-Terech & Palla, 1986).

Increasing hardness also increased the acute toxicity (48-h LC_{50}) of $C_{11.8}$ LAS from a nominal concentration of 7.1 mg/litre at 25 mg/litre $CaCO_3$ to 4.0 mg/litre at 350 mg/litre $CaCO_3$; however, significant additional physiological stress was induced if the hardness of the culture water was significantly different from that of the test water. Pre-exposure to 0.4 mg/litre LAS (one-tenth of the 48-h LC_{50}) for up to seven generations (14 weeks) had no significant effect on the susceptibility of daphnids to acute exposures (Maki & Bishop, 1979).

Loading density, ranging from 10 daphnids per 20 ml to 20 daphnids per 1000 ml, had no significant effect on the acute toxicity of $C_{11.8}$ LAS for *Daphnia magna* (Lewis, 1983). Daphnids fed a diet containing Selenastrum had a significant, twofold decrease in acute toxicity due to $C_{11.8}$ LAS in comparison with unfed daphnids (Taylor, 1985). The presence of sediment reduced the acute toxicity of LAS to the oligochaete worms *Branchiura sowerbyi* and *Limnodrilus hoffmeisteri*. The NOEC and LOEC for *B. sowerbyi* were 2.5 times higher in the presence of sediment, and those for *L. hoffmeisteri* were 4-4.5 times higher (Bressan et al., 1989; see also Table 27).

The 96-h EC_{50} values for duplicate studies of the effect of LAS on attachment of the podia of the sea urchin Hemicentrotus pulcherrimus were 3.7 and 3.8 mg/litre (Lee & Park, 1984).

The data from other studies (Lal et al., 1983, 1984a,b; Misra et al., 1984; Chattopadhyay & Konar, 1985; Misra et al., 1985; Devi & Devi, 1986; Misra et al., 1987, 1989a,b, 1991) could not be adequately interpreted because of deficiencies in the data or method, including inadequate characterization of the test material with regard to chain-length distribution and use of test material in an acidified form. The range of values for toxicity reported in these studies was 10-100 times greater than that in numerous studies of the same or similar species, and the high values have not been verified by these or other researchers. As the toxic effects

reported are not considered to be representative of those of commercial LAS, the data were not used in evaluating the environmental effects of LAS.

A 72-h LC_{50} of 2.2 mg/litre was reported for $C_{11.8}$ LAS in newly hatched larvae of the midge *(Chironomus riparius)* (Pittinger et al., 1989).

A9.3.2.2 Short-term and long-term toxicity

The 21-day LC_{50} for the water flea *(Daphnia magna)* was 18 mg/litre, and the NOEC, based on survival, was 10 mg/litre under static renewal conditions. The 21-day EC_{50}, based on reproduction, was estimated to be > 10 mg/litre (Canton & Slooff, 1982). The 14-day EC_{50} for C_{12} LAS in *Daphnia carinata,* based on reproduction, was 16.8 mg/litre (Hattori et al., 1984).

Diet had a significant effect on the sensitivity of *Daphnia magna* to the chronic toxicity of $C_{11.8}$ LAS. The NOEC values showed a threefold variation of 1.2-3.2 mg/litre and the 21-day LC_{50} values a twofold variation of 2.2-4.7 mg/litre with diet. A threefold variation in toxicity in tests in *Daphnia* is not, however, unusual (Taylor, 1985).

Under continuous-flow conditions, a 21-day LC_{50} value of 1.67 mg/litre was found for daphnids *(Daphnia magna)* exposed to $C_{11.8}$ LAS and 1.17 mg/litre for those exposed to C_{13} LAS. The EC_{50} values for reproductive toxicity were 1.5 mg/litre for $C_{11.8}$ LAS and 11.1 mg/litre for C_{13} with respect to total young production, 2.3 mg/litre for $C_{11.8}$ and 1.4.1 mg/litre for C_{13} for average brood size, and 2.31 mg/litre for $C_{11.8}$ and 1.29 mg/litre for C_{13} for percentage of days on which reproduction occurred (Maki, 1979a).

Campeloma decisum, Gammarus pseudolimnaeus, and *Physa integra* were exposed to LAS at concentrations of 0.2-4.4 mg/litre for six weeks; amphipods were exposed for a further 15 weeks. Survival, growth, reproduction, feeding, and mobility were studied. The maximum acceptable concentrations of LAS were found to be 0.2-0.4 mg/litre for Gammarus and 0.4-1.0 mg/litre for *Campeloma; P. integra* were not significantly affected (Arthur, 1970).

Fertilized eggs of sea urchins *(Paracentrotus lividus)* were treated with LAS at concentrations of 0-0.5 mg/litre for 40 days. The pattern of embryonic development was unaffected, but the mean length of the somatic rods of the echinoplutei were reduced successively with increasing LAS concentrations. A significant reduction in growth occurred at doses between 0.35 and 0.4 mg/litre; above 0.45 mg/litre, alterations in skeletal development were induced (Bressan et al., 1989).

Oligochaete worms *(B. sowerbyi)* were maintained in LAS at a concentration of 0.5, 2.5, or 5.0 mg/litre for up to 140 days in the presence of sediment. Exposed worms laid fewer cocoons and eggs, but the worms exposed to 5 mg/litre were the least affected. The percentage of degenerated cocoons, the percentage of worms hatching, the mean number of eggs per cocoon, and the mean embryonic development time were all unaffected by treatment. Worms exposed via the sediment only were not affected (Bressan et al., 1989).

Growth of mussels *(Mytilus galloprovincialis)* exposed to LAS at a concentration of 0.25 or 0.5 mg/litre for 220 days, expressed as mean length of the major axis of the shell, was significantly slowed ($p < 0.001$). The mean (± SE) increments in growth were: control, 3.11 ± 0.34; 0.25 mg/litre, 1.71 ± 0.15; 0.5 mg/litre, 1.48 ± 0.16 (Bressan et al., 1989).

Eggs of the common mussel, *M. edulis,* were exposed from the time of fertilization for 240 h. Fertility was decreased at the lowest concentration of 0.05 mg/litre and fertilization did not take place at concentrations in excess of 1 mg/litre. LAS at concentrations > 0.3 mg/litre inhibited the development of mussel larvae by delaying the transitory stages of larval development. Reduced growth rates were observed at concentrations > 0.1 mg/litre (Granmo, 1972).

Newly fertilized eggs of American oysters *(Crassostrea virginica)* were exposed to LAS (chain length not specified, but likely to be C_{13}) for 48 h. The percentage of eggs that developed normally was significantly reduced at concentrations greater than 0.025 mg/litre. The percentage survival of oyster larvae hatched in 'clean' water and exposed to LAS at a concentration of 1 mg/litre for 10 days was significantly decreased, and growth (mean length) was significantly reduced at 0.5 mg/litre (Calabrese & Davis, 1967).

Embryos of sea urchins *(P. lividus)* were exposed to LAS at concentrations of 0.25-0.5 mg/litre from the time of fertilization for 40 h. At concentrations > 0.45 mg/litre, skeletal development was totally inhibited; a significant decrease was observed at 0.3 mg/litre. The effect of LAS was found to be maximal at the end of gastrulation when calcium uptake is high (Bressan et al., 1991).

The effects of LAS were studied on the eggs and sperm of the sea squirt *Ciona intestinalis.* Fertility and hatchability were markedly reduced at 0.1 mg/litre when eggs and sperm were exposed for the entire developmental period; however, if they were exposed only before fertilization, fertility and hatchability were slightly reduced at 0.1 mg/litre but markedly at 1 mg/litre. Male gametes appeared to be particularly sensitive to the toxic effects of LAS (Renzoni, 1974).

Two marine benthic filter feeders, the sea squirts *Botryllus schlosseri* and *Botrylloides leachi* were exposed at different periods of development to LAS. When larvae were exposed from spawning for 6 h, the incidence of abnormal metamorphosis was significantly increased at 1 mg/litre LAS for *Botryllus* and 2 mg/litre for *Botrylloides*. The frequency of spontaneously settled larvae of both species also increased with exposure to LAS and seemed to be a selective effect of LAS. The frequency was significantly different from controls at 1 and 3 mg/litre for the two species, respectively. In a second experiment, young colonies

were exposed to LAS for 15 days immediately after discharge by the parental colony. Growth rates were significantly decreased at 0.5 mg/litre for *Botryllus* and at 0.25 mg/litre for *Botrylloides*. When colonies were exposed from the end of metamorphosis, their growth rates were similarly affected, but the mortality rate was significantly lower. The effects of LAS thus appear to be exerted mainly on the pelagic phase of the life cycle (Marin et al., 1991).

No significant reduction in egg hatching of midges *(Chironomus riparius)* was seen at the highest concentration of $C_{11.8}$ LAS tested (18.9 mg/litre), but newly hatched larvae were more sensitive, with a 72-h LC_{50} of 2.2 mg/litre. In bioassays of part of the life cycle in a sediment and water system, the percentages of winged adults emerging were monitored after continuous exposure of larvae and pupae. The NOEC for sediment containing LAS was 319 mg/kg (dry weight). In the absence of sediment, the NOEC was 2.40 mg/litre. Both tests were conducted for about 20 days (Pittinger et al., 1989).

A9.3.2.3 Biochemical and physiological effects

Juvenile mussels *(M. galloprovincialis)* were exposed to LAS at a concentration of 0.25 or 0.5 mg/litre for 220 days. Oxygen uptake and the retention rate of neutral red (a measure of filtration rate) were significantly decreased, but no effect was detected on nitrogen excretion (measured as ammonia). When the experiment was repeated over a seven-day period at a concentration of LAS of 1 or 1.5 mg/litre, no significant effect was seen on nitrogen metabolism and the results for oxygen uptake were inconclusive. The filtration rate was again significantly reduced when compared with that in control mussels (Bressan et al., 1989).

The 48-h LC_{50} for lugworms *(Arenicola marina)* exposed to LAS was calculated to be 12.5 mg/litre (95% confidence interval, 8.6-18.2). When tissues from a lugworm exposed to a concentration close to that of the LC_{50} were examined for changes in morphology by both light and electron microscopy, serious damage was reported in the caudal epidermis, epidermic receptors, and gills; no effect was reported in the thoracic epidermis or the intestine. In the caudal epidermis, LAS destroyed the papillae, disrupting the internal structure, occasionally displacing the musculature below the papillae and thus giving it direct contact with seawater. Deciliation of the epidermic receptors was also reported. These effects were considered to indicate that the physiological response of damaged epidermic receptors was reduced or blocked by exposure to LAS. Changes in the morphology of the gills included destruction of the epithelium and blood vessels, causing complete solubilization of branch apexes, and development of holes at the base of the gills (Conti, 1987).

A9.3.3 Fish

A9.3.3.1 Acute toxicity

The acute toxicity of LAS to fish is summarized in Tables 28 and 29. Only a few studies were available on marine fish, providing two 96-h LC_{50} values, 1 and 1.5 mg/litre LAS. Tests in various species of freshwater fish gave a wide range of LC_{50} values: the 48-h values ranged from 0.2 mg/litre for brown trout *(Salmo trutta)* to 125 mg/litre for the golden orfe *(Idus idus memanotus)*, and the 96-h values ranged from 0.1 mg/litre for brown trout to 23 mg/litre for white tilapia *(Tilapia melanopleura)*.

The acute toxicity tended to increase with increasing carbon chain length. Thus, C_{14} LAS were more acutely toxic to bluegill *(Lepomis macrochirus)* than C_{12} compounds (Swisher et al., 1964); the acute toxicity of LAS to the golden orfe increased with chain length from C_8 to C_{15} but decreased at C_{16} (Hirsch, 1963).; and a similar trend was found for fathead minnows *(Pimephalus promelas)* exposed to LAS with chain lengths of C_{10} to C_{14} (Kimerle & Swisher, 1977).

The 96-h LC_{50} values in bluegill (Lepomis macrochirus) were 0.64 mg/litre for C_{14} and 3 mg/litre for C_{12} LAS but 75 mg/litre for the intermediate degradation product, sulfophenylundecanoic acid disodium salt (Swisher et al., 1964). Biodegradation of LAS with a high relative molecular mass progressively shifted the homologue distribution in favour of shorter chain lengths and reduced the acute toxicity of the compound to bluegill (Dolan & Hendricks, 1976). Similar findings were reported for fathead minnow (Swisher et al., 1978), goldfish *(Carassius auratus)* (Divo & Cardini, 1980) and zebra fish *(Brachydanio rerio)* (Gard-Terech & Palla, 1986).

In rainbow trout *(Oncorhynchus mykissi)*, addition of LAS (C_{10}-C_{15}) to activated sludge plant effluent increased the nominal 96-h LC_{50} from 0.36 to 29.5 mg/litre (Brown et al., 1978). No deaths were observed among bluegill exposed for 4-11 days to effluent from continuous-flow activated sludge units fed 100 mg/litre LAS (Swisher et al., 1964).

Water hardness was found to be the most significant environmental factor in the acute toxicity of LAS to bluegill, increasing with the level of hardness. At a water hardness of 15 mg/litre $CaCO_3$, the mean LC_{50} was 4.25 mg/litre; at 290 mg/litre $CaCO_3$, the LC_{50} was reduced to 2.85 mg/litre (Hokanson & Smith, 1971). Similarly, when water hardness was increased from 0 to 500 mg/litre $CaCO_3$, the LC_{50} for C_{18} LAS in goldfish was reduced from 15 to 5.7 mg/litre (Gafa, 1974). Exposure of the freshwater bleeker *(Puntius gonionotus)* to LAS gave 96-h LC_{50} values of 13.6 mg/litre at a water hardness of

50 mg/litre $CaCO_3$, 11.8 mg/litre at 110 mg/litre $CaCO_3$, and 11.4 mg/litre at 260 mg/litre $CaCO_3$ (Eyanoer et al., 1985).

The toxicity of $C_{11.7}$ LAS to the medaka *(Oryzias latipes)* increased with increasing salinity, but the effect was less pronounced than that of water hardness (Wakabayashi & Onizuka, 1986).

Temperature was reported to have no significant effect on the acute toxicity of LAS (Hokanson & Smith, 1971), but in another study increasing the water temperature from 28 to 35°C marginally decreased the 96-h LC_{50} for the bleeker, from 11.8 to 11.5 mg/litre (Eyanoer et al., 1985).

A reduction in the dissolved oxygen concentration from 7.5 to 1.9 mg/litre reduced the 24-h LC_{50} in bluegill from 2.2 to 0.2 mg/litre. When the fish were first acclimatized to reduced oxygen levels, the effect was less pronounced (Hokanson & Smith, 1971).

No significant effect on the acute toxicity of LAS to bluegill was observed after a bentonite suspension was added to water at concentrations of 0, 50, or 200 mg/litre (Hokanson & Smith, 1971). Addition of gluten, however, reduced the 24-h and 48-h acute toxicity of LAS to both himedaka *(Oryzias latipes)* and cobalt suzume *(Chrysiptera hollisi)* (Iimori & Takita, 1979).

A9.3.3.2 Chronic toxicity

Exposure of the eggs of fathead minnows (Pimephales promelas) to LAS from laying until all surviving eggs had hatched under flow-through conditions gave a nine-day LC_{50} of 2.4 mg/litre, which would result in an LC_{50} of 3.4 mg/litre after 24 h of exposure (Pickering, 1966).

Eggs of cod *(Gadus morhua)* were exposed to LAS at a concentration of 0.005, 0.02, 0.05, or 0.1 mg/litre from fertilization until hatching under flow-through conditions. There were no significant effects at 0.005 mg/litre. At a concentration of 0.02 mg/litre, only 42% of the embryos completely developed into larvae, and there was an increased occurrence of tail malformations in comparison with controls. At 0.05 mg/litre, few eggs developed to embryos. No eggs developed to the blastula stage at a concentration of 0.1 mg/litre. In a repetition of the test at 0.05 mg/litre, fewer eggs and larvae died, but there was an increased frequency of abnormal embryos and inactive and crippled larvae (Swedmark & Granmo, 1981).

Eggs, larvae, and immature adult fathead minnows *(Pimephales promelas)* were exposed to LAS at a concentration of 0.34, 0.63, 1.2, or 2.7 mg/litre for up to four months. No significant effect was observed on the number of spawnings, the total number of eggs produced, the mean number of spawnings per female, the mean number of eggs per spawning, or the percentage hatchability; however, the two highest concentrations significantly reduced the survival of fry (Pickering & Thatcher, 1970).

The effects of $C_{11.8}$ and C_{13} LAS on the number of females, the number of spawnings, total number of eggs produced, and number of eggs per female were also studied in the fathead minnow over a period of one year. As $C_{11.8}$ LAS had no significant effect on these parameters at a concentration of 1.09 mg/litre and a water hardness of 120 mg/litre $CaCO_3$, the NOEC was 0.9 mg/litre; C_{13} LAS were more toxic, and the NOEC was 0.15 mg/litre. At a lower water hardness (39 mg/litre), however, survival of larvae was impaired at 0.74 mg/litre (Maki, 1979a). NOECs in the fathead minnow in life-cycle and embryo-larval tests were dependent on mean alkyl chain length: 5.1–8.4 mg/litre for $C_{11.2}$, 0.48 mg/litre for $C_{11.7}$, and 0.11–0.25 mg/litre for $C_{13.3}$ (Holman & Macek, 1980).

The LC_{50} value of LAS in the eggs of carp *(Cyprinus carpio)* exposed from spawning to hatching was 11 mg/litre. In determinations of the sensitivity of eggs at different stages of development after spawning, the 24-h LC_{50} values were 15 mg/litre for eggs exposed between 2 and 26 h, 25 mg/litre for exposure between 26 and 50 h, and 32 mg/litre for exposure between 50 h and hatching (Kikuchi et al., 1976).

Bluegill *(Lepomis macrochirus)* were exposed to LAS from fertilization to yolk-sac resorption at a concentration of 1.8, 3.5, 4.6, or 5.5 mg/litre. The lowest concentrations did not affect hatchability or survival. Survival among those exposed to 3.5 mg/litre which hatched successfully was significantly reduced within two days of hatching, and 95% were dead by the end of the experiment. Eggs exposed to 4.6 or 5.5 mg/litre failed to hatch (Hokanson & Smith, 1971).

The NOEC of LAS in guppies *(Poecilia reticulata)*, based on

mortality, behaviour, and growth over 28 days, was 3.2 mg/litre (Canton & Slooff, 1982).

Studies of the short- and long-term toxicity of LAS to freshwater and marine fish are summarized in Tables 28 and 29.

A9.3.3.3 Biochemical and physiological effects

The main injury to the gills of catfish *(Heteropneustes fossilis)* exposed to LAS at 1 or 2.5 mg/litre was progressive separation of the lamellae from their vascular components.

Table 28. Toxicity of linear alkylbenzene sulfonates (LAS) to freshwater fish

Organism	Size or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	LAS chain length	End-point	Concn (mg/litre)	Reference
Brown trout (Salmo trutta)		Flow	15	26-30		NS	48-h LC_{50}	5.3	Reiff et al. (1979)
		Flow	15	26-30		NS	96-h LC_{50}	4.6	
		Flow	15	26-30		NS	48-h LC_{50}	2.3	
		Flow	15	26-30		NS	96-h LC_{50}	1.4	
		Flow	15	26-30		NS	48-h LC_{50}	0.4	
		Flow	15	26-30		NS	96-h LC_{50}	0.4	
		Flow	15	250		NS	48-h LC_{50}	2	
		Flow	15	250		NS	96-h LC_{50}	0.9	
		Flow	15	250		NS	48-h LC_{50}	0.7-0.9	
		Flow	15	250		C_{10-C15}	48-h LC_{50}	0.2	
		Flow	15	250		C_{10-C15}	96-h LC_{50}	0.1	
Masu trout (Oncorhynchus masou)	2 mo	Static[r]	8.5-9.6	30		$C_{11.7}$	96-h LC_{50}	4.4	Wakabayashi et al. (1984)
Rainbow trout (Oncorhynchus mykiss)		Flow	15	250		$C_{12.6}$	96-h LC_{50}	0.36[b]	Brown et al. (1978)
	40 d	Static[r]	8.8-10.9	25		$C_{11.7}$	96-h LC_{50}	4.7	Wakabayashi et al. (1984)
	4 d	Static[r]	10	25		$C_{11.7}$	96-h LC_{50}	2.1	Wakabayashi & Onizuka (1986)
	19 d	Static[r]	10	25		$C_{11.7}$	96-h LC_{50}	3.4	
Goldfish (Carassius auratus)		Static	20			C_{16}	6-h LC_{50}	61	Gafa (1974)
		Static	20			C_{17}	6-h LC_{50}	22.5	
		Static	20			C_{18}	6-h LC_{50}	8.5	

Table 28 (contd)

Organism	Size or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	LAS chain length	End-point	Concn (mg/litre)	Reference
Goldfish (contd) (Carassius auratus)		Static	20			C_{19}	6-h LC_{50}	3.3	
		Static	20			C_{16-C19}	6-h LC_{50}	7.6	
		Static	20			C_{16-C19}	6-h LC_{50}	10	
		Static	20			C_{16-C19}	6-h LC_{50}	12.2	
		Static	20	100		NS	6-h LC_{50}	8.2	Reiff et al. (1979)
		Static	20	100		NS	6-h LC_{50}	7	
		Static	20	100		NS	6-h LC_{50}	4.3	
	3.1-6.0 cm	Flow	20-23	45-96	7.1-9.3		24-h LC_{50}	7.6	Tsai & McKee (1978)
		Flow	20-23	45-96	7.1-9.3		48-h LC_{50}	7.5	
		Flow	20-23	45-96	7.1-9.3		72-h LC_{50}	7.0	
		Flow	20-23	45-96	7.1-9.3		96-h LC_{50}	6.2	
Bluegill sunfish (Lepomis macrochirus)	1.6 g	Static	23	76	7.5	av. C_{13}	48-h LC_{50}	0.72[b]	Dolan & Hendricks (1976)
	1.6 g	Static	23	76	7.5	av. C_{13}	96-h LC_{50}	0.72[b]	
		Flow	23	50	7.5	av. C_{13}	96-h LC_{50}	4[c]	Thatcher & Santner (1967)
	Finger	Static	25	15		$C_{11.2}$	48-h LC_{50}	4.0-4.5[b]	Hokanson & Smith (1971)
	Finger	Static	25	290		$C_{11.2}$	48-h LC_{50}	2.8-2.9[b]	
		Flow				$C_{11.8}$	96-h LC_{50}	1.7[c]	Bishop & Perry (1981)
Fathead minnow (Pimephales promelas)		Static				$C_{13.3}$	48-h LC_{50}	1.7[b]	Kimerle & Swisher (1977)
		Static				C_{10}	48-h LC_{50}	43[b]	
		Static				C_{11}	48-h LC_{50}	16[b]	

Table 28 (contd)

Organism	Size or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	LAS chain length	End-point	Concn (mg/litre)	Reference
Fathead minnow (contd)		Static				C_{12}	48-h LC_{50}	4.7[b]	
		Static				C_{14}	48-h LC_{50}	0.4[b]	
	2-3 mo	Static		40		$C_{11.2}$	96-h LC_{50}	12.3[c]	Holman & Macek (1980)
	2-3 mo	Static		40		$C_{11.7}$	96-h LC_{50}	4.1[c]	
	2-3 mo	Static		40		$C_{13.3}$	96-h LC_{50}	0.86	
		Static	25				48-h LC_{50}	4.6	Pickering & Thatcher (1970)
		Static	25				96-h LC_{50}	5.0	
		Flow	15	43	7.2-7.9		96-h LC_{50}	3.4	McKim et al. (1975)

		Flow	23	50	7.5		96-h LC_{50}	4.2	Thatcher & Santner (1967)
		Flow	25				96-h LC_{50}	4.2-4.5	Pickering & Thatcher (1970)
	2.5 cm	Flow	18	116	7.9	C_{12}	96-h LC_{50}	3.5	Solon et al. (1969)
Harlequin fish		Flow	20	20		NS	48-h LC_{50}	7.6	Reiff et al.
(Rasbora heteromorpha)		Flow	20	20		NS	96-h LC_{50}	6.1	(1979)
		Flow	20	20		NS	48-h LC_{50}	5.1	
		Flow	20	20		NS	96-h LC_{50}	4.6	
		Flow	20	20		C_{10}-C_{15}	48-h LC_{50}	0.9	
		Flow	20	20		NS	96-h LC_{50}	0.7	
Carp (Cyprinus carpio)	4.4 mg	Static	22	25	7	$C_{11.7}$	12-h LC_{50}	5.6	Kikuchi et al.
		Static	22	25	7	$C_{11.7}$	48-h LC_{50}	5.6	(1976)

Table 28 (contd)

Organism	Size or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	LAS chain length	End-point	Concn (mg/litre)	Reference
Carp (contd)	3.5-5.5	Static	21		7.5-7.8	NS	48-h LC_{50}	6.8	Lopez-Zavala
	cm	Static	21		7.5-7.8	NS	96-h LC_{50}	5.0	et al. (1975)
	7 d	Static[r]	22	25	7.0	$C_{11.7}$	48-h LC_{50}	5.6	Arima et al.
	6 mo	Static[r]	22	25	6.5-7.1	$C_{11.7}$	48-h LC_{50}	10	(1981)
	50 d	Static[r]	21	75		$C_{11.7}$	96-h LC_{50}	4.4	Wakabayashi et al. (1984)
	2 d	Static[r]	20	25		$C_{11.7}$	96-h LC_{50}	4.6	Wakabayashi &
	15 d	Static[r]	20	25		$C_{11.7}$	96-h LC_{50}	2.6	Onizuka (1986)
White tilapia	5-7 cm	Static	21		7.5-7.8	NS	48-h LC_{50}	26	Lopez-Zavala
(Tilapia melanopleura)	5-7 cm	Static	21		7.5-7.8	NS	96-h LC_{50}	23	et al. (1975)
Guppy (Poecilia reticulata)	3-4 wk	Static[r]	23			C_8-C_{14}	96-h LC_{50}	5.6-10	Canton & Slooff (1982)
Northern pike (Esox lucius)		Flow	15	43	7.2-7.9		96-h LC_{50}	3.7	McKim et al. (1975)
White sucker (Catostomus commersoni)		Flow	15	43	7.2-7.9		96-h LC_{50}	4	McKim et al. (1975)
Golden orfe		Static	18-20			C_8	48-h LC50	125	Hirsch (1963)
(Idus idus melanotus)		Static	18-20			C_9	48-h LC50	88	
		Static	18-20			C_{10}	48-h LC50	16.6	

Table 28 (contd)

Organism	Size or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	LAS chain length	End-point	Concn (mg/litre)	Reference
Golden orfe (contd)		Static	18-20			C_{11}	48-h LC_{50}	6.6	
		Static	18-20			C_{12}	48-h LC_{50}	2.6	
		Static	18-20			C_{13}	48-h LC_{50}	0.57	
		Static	18-20			C_{15}	48-h LC_{50}	0.23	
		Static	18-20			C_{16}	48-h LC_{50}	0.68	
	1.2-1.8 g	Static	20			NS	48-h LC_{50}	3.94	Mann (1976)
		Static	20			NS	48-h LC_{50}	1.85	
		Static	20			NS	48-h LC_{50}	1.24	
		Flow	20	150		NS	48-h LC_{50}	4.9	Reiff et al. (1979)
		Flow	20	150		NS	48-h LC_{50}	2.4	
		Flow	20	150		NS	48-h LC_{50}	1.2	
		Flow	20	268		NS	48-h LC_{50}	2.1-2.9	
		Flow	20	268		NS	96-h LC_{50}	1.9-2.9	
		Flow	20	268		NS	48-h LC_{50}	1.3-1.7	
		Flow	20	268		NS	96-h LC_{50}	1.2-1.3	
		Flow	20	268		NS	48-h LC_{50}	0.8-0.9	
		Flow	20	268		NS	96-h LC_{50}	0.4-0.6	
Himedaka (killifish) (Oryzias latipes)	4-5 wk	Static[r]	23			C_8-C_{14}	96-h LC_{50}	10-18	Canton & Slooff (1982)
	323 mg	Static[r]	23-24		5.6-6.1	$C_{11.7}$	48-h LC_{50}	15	Kikuchi et al.
	323 mg	Static[r]	23-24		5.6-6.1	$C_{11.7}$	48-h LC_{50}	10	(1976)
	approx. 262 mg	Static[r]	21-22		6.7-7.1	C_{12}	48-h LC_{50}	12	Kikuchi &
	approx. 262 mg	Static[r]	21-22		6.7-7.1	NS	48-h LC_{50}	10	Wakabayashi (1984)

Table 28 (contd)

Organism	Size or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	LAS chain length	End-point	Concn (mg/litre)	Reference
Himedaka (contd)						C_{161}	48-h LC_{50}	> 50	Tomiyama (1974)
						C_6	48-h LC_{50}	> 50	
						C_8	48-h LC_{50}	> 50	
						C_{10}	48-h LC_{50}	> 50	

					C_{12}	48-h LC_{50}	4	
					C_{14}	48-h LC_{50}	4	Iimori & Takita (1979)
			25		7.2–7.9	48-h LC_{50}	7.6	Hidaka et al. (1984)
			25		7.2–7.9	96-h LC_{50}	7.3	
	Adult	Static[r]	20	5	$C_{11.7}$	96-h LC_{50}	13	Wakabayashi & Onizuka (1986)
	Adult	Static[r]	20	25	$C_{11.7}$	96-h LC_{50}	8.8	
	Adult	Static[r]	20	125	$C_{11.7}$	96-h LC_{50}	4.8	
	Adult	Static[r]	20	625	$C_{11.7}$	96-h LC_{50}	3.2	
	Adult	Static[r]	20	0	$C_{11.7}$	48-h LC_{50}	6.7	Wakabayashi & Onizuka (1986)
	Adult	Static[r]	20	1	$C_{11.7}$	48-h LC_{50}	4.8	
	Adult	Static[r]	20	5	$C_{11.7}$	48-h LC_{50}	4.7	
	Adult	Static[r]	20	10	$C_{11.7}$	48-h LC_{50}	3.5	
	Adult	Static[r]	20	15	$C_{11.7}$	48-h LC_{50}	3.8	
	Adult	Static[r]	20	20	$C_{11.7}$	48-h LC_{50}	2.5	
	Adult	Static[r]	20	25	$C_{11.7}$	48-h LC_{50}	1.9	
	Adult	Static[r]	20	30	$C_{11.7}$	48-h LC_{50}	1.6	
	Adult	Static[r]	20	35	$C_{11.7}$	48-h LC_{50}	1.4	

Table 28 (contd)

Organism	Size or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	LAS chain length	End-point	Concn (mg/litre)	Reference
Cobalt suzume (Chrysiptera hollisi)							48-h LC_{50}	1.3	Iimori & Takita (1979)
Smallmouth bass (Micropterus dolomieu)		Flow	15	43	7.2–7.9	NS	96-h LC_{50}	3.7	McKim et al. (1975)
Black bullhead (Ictalurus melas)		Flow	23	50	7.5	NS	96-h LC_{50}	6.4	Thatcher & Santner (1967)
Common shiner (Notropis cornutus)		Flow	23	50	7.5	NS	96-h LC_{50}	4.9	Thatcher & Santner (1967)
Emerald shiner (Notropis atherinoides)		Flow	23	50	7.5	NS	96-h LC_{50}	3.3	Thatcher & Santner (1967)
Bleeker	0.3 g	Static	28			NS	96-h LC_{50}	11.8	Eyanoer et al. (1985)
(Puntius gonionotus)	0.3 g	Static	35			NS	96-h LC_{50}	11.5	
	0.3 g	Static		50		NS	96-h LC_{50}	13.6	
	0.3 g	Static		110		NS	96-h LC_{50}	11.8	
	0.3 g	Static		260		NS	96-h LC_{50}	11.4	

Table 28 (contd)

Organism	Size or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	LAS chain length	End-point	Concn (mg/litre)	Reference
Ayu	0.26 mg		1			NS	48-h LC_{50}	0.86	Sueishi et al. (1988)
(Plecoglossus altivelis)	0.29 g		1			NS	48-h LC_{50}	0.53	
	1.24 g		1			NS	48-h LC_{50}	0.77	
	6.51 g		1			NS	48-h LC_{50}	1.45	
	27.98 g		1			NS	48-h LC_{50}	1.17	

Flow, flow-through conditions: LAS concentration in water maintained continuously; NS, not specified; staticr, static renewal: water changed periodically; static, water unchanged for the duration of test; finger, fingerling

[a] mg/litre $CaCO_3$

[b] Based on nominal concentration

[c] Based on measured concentrations

Table 29. Toxicity of linear alkylbenzene sulfonates (LAS) to marine fish

Organism	Size or age	Static or flow	Temp. (°C)	Salinity (‰)	LAS chain length	End-point	Concn (mg/litre)	Reference
Cod (Gadus morhua)	30 cm	Static	6–8	32–34	C_{12}	96-h LC_{50}	1[a]	Swedmark et al. (1971)
	30 cm	Static	15–17	32–34	C_{12}	96-h LC_{50}	< 1[a]	
Flounder		Static	6–8	32–34	C_{12}	96-h LC_{50}	1.5[a]	
(Pleuronectes flesus)		Static	15–17	32–34	C_{12}	96-h LC_{50}	< 1[a]	
Plaice (Pleuronectes platessa)		Static	6–8	32–34	C_{12}	96-h LC_{50}	> 1 -< 5[a]	
Mosbled sole	Newly hatched				NS	48-h LC_{50}	0.5–1	Yasunaga (1976)
(Limanda yokohamae)	10 days				NS	48-h LC_{50}	0.1–0.5	
	30 days				NS	48-h LC_{50}	0.5–1	
	40 days				NS	48-h LC_{50}	< 0.1	
	Newly hatched				NS	48-h LC_{50}	0.05–0.1	
Olive flounder	5 days				NS	48-h LC_{50}	< 0.1	

(Paralichtys olivaceus)	10 days				NS	48-h LC_{50}	0.1-0.5	
	30 days				NS	48-h LC_{50}	0.1-0.5	
Himedaka (killifish)	Adult	Static[r]	20	0	$C_{11.7}$	48-h LC_{50}	6.7	Wakabayashi &
(Oryzias latipes)	Adult	Static[r]	20	1	$C_{11.7}$	48-h LC_{50}	4.8	Onizuka (1986)
	Adult	Static[r]	20	5	$C_{11.7}$	48-h LC_{50}	4.7	

Table 29 (contd)

Organism	Size or age	Static or flow	Temp. (°C)	Salinity (%)	LAS chain length	End-point	Concn (mg/litre)	Reference
Himedaka (contd)	Adult	Staticr	20	10	$C_{11.7}$	48-h LC_{50}	3.5	
	Adult	Staticr	20	15	$C_{11.7}$	48-h LC_{50}	3.8	
	Adult	Staticr	20	20	$C_{11.7}$	48-h LC_{50}	2.5	
	Adult	Staticr	20	25	$C_{11.7}$	48-h LC_{50}	1.9	
	Adult	Staticr	20	30	$C_{11.7}$	48-h LC_{50}	1.6	
	Adult	Staticr	20	35	$C_{11.7}$	48-h LC_{50}	1.2	

Static: water unchanged for duration of test; static[r], static renewal: water changed periodically; NS, not specified
[a] Based on nominal concentration

The activity of the enzymes of aerobic metabolism was decreased, and that of lactate dehydrogenase was strongly increased (Zaccone et al., 1985). Concentrations of 2.19 mg/litre $C_{11.8}$ LAS and 0.39 mg/litre C_{13} LAS significantly increased the 24-h mean ventilation rate (number of opercular closures per minute) of bluegill *(Lepomis macrochirus)* (Maki, 1979b).

A concentration of 36 mg/litre LAS severely affected the viability of the perfused gills of rainbow trout *(Oncorhynchus mykissi)*. Vascular resistance increased gradually during perfusion, with a concomitant decrease in oxygen transfer. LAS at 0.05 mg/litre more than doubled cadmium transfer (0.8 µg/litre) through the perfused gills; and at concentrations of 36 mg/litre LAS and 0.9 mg/litre cadmium, there was a marked reduction in cadmium transfer (Pärt et al., 1985).

A9.3.3.4 Behavioural effects

Hidaka and co-workers have reported several studies of the avoidance of surfactants by fish (Hidaka et al., 1984; Hidaka & Tatsukawa, 1989; Tatsukawa & Hidaka, 1978). The results should be interpreted with caution, since the environmental relevance and the reproducibility and sensitivity of these tests is unclear; furthermore, no effect was seen after removal of the olfactory organs. Another study (Maki, 1979a) showed no adverse toxicological effects at concentrations two times greater than those reported to cause avoidance reactions.

Hidaka et al. (1984) found that the minimal avoidance concentration of LAS, i.e. the concentration at which fish spent 65% of a 5-min period in clean water in order to avoid LAS, was 13.5 µg/litre for medakas *(Oryzias latipes)*. Medakas exposed to LAS at concentrations of 5–50 µg/litre for 10 min showed significant avoidance to 10, 20, and 30 µg/litre. No significant avoidance of concentrations of 10–50 µg/litre LAS was found after removal of the olfactory organs (Hidaka & Tatsukawa, 1989).

The threshold concentrations for avoidance of LAS by ayu *(Plecoglossus altivelis)* were 0.11 µg/litre of a formulation and 1.5 µg/litre of pure reagant LAS (Tatsukawa & Hidaka, 1978).

A9.3.3.5 Interactive effects with other chemicals

The chronic toxicity of *para, para*-DDT (50 mg/litre) to goldfish *(Carassius auratus)* was increased by prior exposure to LAS at 4 mg/litre for 37 days (Dugan, 1967).

The toxicity of 1 mg/litre LAS solution to mosquito fish exposed under static conditions was not affected by allowing the LAS solution to react with excess chlorine (Katz & Cohen, 1976).

A concentration of 1 mg/litre LAS significantly increased the toxicity of fuel oil to bluegill *(Lepomis macrochirus)*, reducing the 24-h LC_{50} from 91 to 51 mg/litre. The authors concluded that sublethal concentrations of LAS increased the toxicity of fuel oil by increasing its penetration (Hokanson & Smith, 1971). The toxicity of No. 2 and No. 4 fuel oils in six species of freshwater fish was increased in the presence of 1–5 mg/litre LAS (Rehwoldt et al., 1974).

The uptake of cadmium by freshwater trout *(Salmo gairdneri)* exposed to 0.14 µmol/litre LAS was more than two times greater than in controls. Reduced cadmium uptake was reported in fish exposed to 100 µmol/litre LAS. The authors reported that trout exposed to low levels of both LAS and cadmium could take up lethal cadmium concentrations. LAS were reported to interact with the gill proteins involved in cadmium transport, resulting in increased permeability to cadmium (Pärt et al., 1985).

Fathead minnows *(Pimepheles promelas)* were exposed to various pesticides in the presence and absence of 1 mg/litre LAS. Parathion acted synergistically with LAS, reducing the 96-h LC_{50} from 1410 to 720 µg/litre. Endrin and LAS showed no synergism, and no consistent results were obtained for DDT (Solon et al., 1969). Methyl parathion, ronnel, trithion, and trichloronat were also found

to act synergistically with LAS, but neither *ortho-ethyl-ortho-4-*nitrophenyl phenylphos-phonothioate nor dicapthon exhibited synergism. The synergistic relationship does not appear to be exclusive to a general structural group (Solon & Nair, 1970).

Goldfish *(Carassius auratus)* were exposed to mixtures of LAS and chloramines and LAS and copper at ratios of 1:1, 2:1, and 1:2, and toxicity curves and 24-h and 96-h LC_{50} values were compared. LAS and chloramines had an additive effect at a ratio of 1:1, but at 2:1 and 1:2 synergistic effects were seen. LAS and copper at ratios of 1:1 and 2:1 had additive effects; however, at 1:2, high concentrations and longer exposure times had additive effects, and low concentrations and shorter exposure times had synergistic effects (Tsai & McKee, 1978).

When eggs of cod *(Gadus morhua)* were exposed to mixtures of LAS and zinc or copper from fertilization to hatching, zinc had a weak synergistic affect on the toxicity of LAS, but LAS had a strong synergistic affect on the toxicity of copper (Swedmark & Granmo, 1981).

In a study of the effect of polyoxyethylene (20) on the acute toxicity of C_{12} LAS, red killifish *(Oryzias latipes)* and carp *(Cyprinus carpio)* were exposed to the 48-h LC_{50} of LAS for the respective species and to 5–40 mg/litre of either a polyoxyethylene sorbitan ester, a polyethylene glycol, a polypropylene glycol, or a protein (albumin, kaolin, or bentonite). Addition of most of these substances decreased mortality. No mortality was observed in carp exposed to LAS and 14 or 28 mg/litre polyoxyethylene (20) sorbitan monooleate (SMOE20) or to other nonionic surfactants with a similar polyoxyethylene sorbitan ester structure-polyoxyethylene (6) sorbitan monolaurate, polyoxy-ethylene (6) sorbitan monooleate, polyoxyethylene (20) sorbitan monolaurate, and polyoxyethylene (20) sorbitan monostearate-or to albumin. No significant effect on mortality induced by LAS was reported after simultaneous exposure to polyoxyethylene (6) sorbitan monostearate, polyethylene glycol, polypropylene glycol, kaolin, or bentonite. The authors also examined the histological effects of these chemicals on the gills of carp exposed to high concentrations of LAS, including the 48-h LC_{50} of 3.5 mg/litre and the LC_{100} of 7 mg/litre. Histological changes in fish exposed only to 3.5 mg/litre LAS included the appearance of mucous cells and agglutination of the secondary lamellae; carp exposed to a mixture of LAS and SMOE20 showed only slight swelling of the secondary lamellae and slight proliferation of the gill epidermal cells. Exposure only to LAS at 7 mg/litre resulted in marked proliferation of the epidermal cells and agglutination of secondary lamellae; exposure to both LAS and SMOE20 induced only swelling of the secondary lamellae. No effects were reported on the gills of control fish or on other organs of the exposed fish; and no significant differences from controls were reported in haematological or serum biochemical parameters for fish exposed to either LAS or the LAS:SMOE20 mixture. When the distribution of LAS in the tissues and organs of carp was examined, higher levels were found in the blood and most organs after exposure to LAS only than after exposure to the mixture; the differences were statistically significant in blood, muscle, and gill but not in spleen or gall-bladder. Adsorption of the 5- and 6-phenyl isomers of LAS was similar when they were given alone or in conjunction with SMOE20, but more of the 4- and (especially) the 2-phenyl isomers was adsorbed by fish receiving LAS alone, indicating that SMOE20 decreases the acute toxicity of LAS to fish by decreasing the adsorption on the gills of the more toxic isomer (Toshima et al., 1992).

A9.3.4 Amphibia

No reliable data were available.

A9.3.5 Studies of the mesocosm and communities

Diversity and similarity indices were used in many studies to assess the effects of LAS on phytoplankton communities, usually on the basis of taxonomy, mean number of species, and density. Mean density and similarity indices were then compared with those of controls. In general, these indices are not sensitive to change, as the densities of some species may decrease while the indices do not.

The effects of C_{12} and C_{13} LAS on short-term photosynthetic activity were studied in plankton sampled from Acton Lake, Ohio, United States, during May–October in the laboratory and *in situ*. Toxicity increased with the temperature of the water, the most sensitive period being June–August, and LAS were less toxic during periods of diatom dominance and low phytoplankton density. Thus the density of diatoms decreased during June–August, and that of green and blue algae increased. The comparison of the results of laboratory and field tests was highly dependent on species and the *in-situ* end-point. Short-term tests for photosynthetic activity in situ gave 3-h EC_{50} values of 0.2–8.1 mg/litre (mean, 1.9 mg/litre) for C_{13} LAS and 0.5–8.0 mg/litre (mean, 3.4 mg/litre) for C_{12} LAS (Lewis & Hamm, 1986). (See also section 9.3.1.1.)

In another study of the effect of LAS on phytoplankton communities in Acton Lake, Ohio (Lewis, 1986), phytoplankton were exposed *in situ* to LAS at a concentration of 0.01, 0.02, 0.24, 0.80, 27, or 108 mg/litre for 10 days. The LOEL for LAS, based on community similarity indices and the mean number of species, was 108 mg/litre. The similarity index (coefficient of community) decreased as the concentration of LAS increased, with calculated values of 0.62 at 0.01 mg/litre and 0.43 at 108 mg/litre. No significant effects were seen on the community diversity index or phytoplankton density. Green algae were the species least affected,

on the basis of abundance, followed in order of decreasing tolerance by blue-green algae and diatom species. *Chlorophyta* species were the most abundant at higher concentrations of LAS, comprising 74% of the total cell volume at 108 mg/litre; their abundance tended to increase to a maximum at this concentration and then decrease to values similar to those of the controls. *Chlorophyta* species of the genera *Chlamydomonas, Oocystis,* and *Sphaerocystis* were not found after exposure to higher concentrations of LAS. *Chlamydomonas* was found only in waters with a concentration of LAS $\leq$ 0.8 mg/litre, and Oocystis and Sphaerocystis were found only at concentrations $\leq$ 27 mg/litre. The peak density of blue-green phytoplankton (56% of cell volume) was achieved at 0.24 mg/litre LAS, declining to 17% at 108 mg/litre. The density of the major species, Schizothrix calcicola, was greatest at 27 mg/litre LAS but declined to a level below that of controls at 108 mg/litre LAS. The abundance of diatoms was low at all concentrations of LAS. At concentrations $\leq$ 0.24 mg/litre, the average density of diatoms was 23% of the total cell volume, similar to that of controls; at concentrations of 0.24–0.8 mg/litre, the diatom density was 10% of the cell volume. The mean densities of the major diatom species, such as *Cyclotella glomerata, Cyclotella pseudostelligera,* and *Nitzschia frustulum v. perminuta,* followed the overall trend for diatoms, reaching a peak at low LAS concentrations and declining to control values at higher concentrations.

In the same study, the laboratory-based 96-h EC_{50} values for exposure to $C_{11.8}$ LAS were calculated to be 29.0 mg/litre for *Selenastrum* and 0.0096 mg/litre for Microcystis, on the basis of population growth. The lowest concentration of LAS that produced a significant effect on algal growth in the laboratory was 0.05–1.0 mg/litre, which is considerably lower than the 27–108 mg/litre value found to be the lowest that altered the structure of a natural phytoplankton community. The differences between the results of laboratory and field tests were smaller for a laboratory-based EC_{50} than for an LOEL. Calculations based on the EC_{50} give a 30-fold difference for Microcystis but essentially no difference for *Selenastrum* (Lewis, 1986).

The toxic effects of LAS were also examined on periphyton communities above and below the outfall of a wastewater treatment plant on Little Miami River, Ohio, United States. The dominant species at both test sites were diatoms, *Amphora perpusilla* and *Navicula minima* accounting for at least 80% of the total cell volume. The tests were conducted *in situ,* with 21-day continous-flow exposure to LAS (average chain length, $C_{11.9}$) in river water entering submerged exposure tubes at a concentration of 0.2, 1.1, 9.8, or 28.1 mg/litre, after a four-week colonization period. The delivery rate of LAS was adjusted daily according to measurements of river flow in order to maintain the desired test concentrations. The periphyton at the site below the treatment plant outfall were exposed to LAS in the presence of 20–30% treated municipal effluent. No effects on the structure or function of the periphyton community above the outfall were reported after exposure to an average concentration of LAS $\leq$ 1 mg/litre. The lowest concentration that had an effect on the upstream periphyton community was 9.8 mg/litre, which reduced photosynthesis by 16%; a concentration of 28.1 mg/litre reduced photosynthesis by 64%, with a noticeable reduction in chlorophyll a. No effects on community similarity or diversity were reported in comparison with control communities. Mean cell densities were increased by 26% after exposure to 0.2 mg/litre LAS and by 17% after exposure to 1.1 mg/litre; exposure to 28.1 mg/litre reduced mean cell density by 28%. Exposure to LAS had no significant effects on the abundance of the three main species in the upstream community. Increased photosynthesis (by 12–39%) and chlorophyll *a* (50–51%), were reported after exposure to 1.1 or 9.8 mg/litre LAS, but exposure to 28.1 mg/litre resulted in a 52% decrease in photosynthesis and a 71% decrease in chlorophyll *a.* No effects on the similarity or diversity of the periphyton community were reported at any concentration of LAS tested. Cell densities of periphyton were increased by 34% after exposure to 9.8 mg/litre LAS and by 13% after exposure to 28.1 mg/litre. The abundance of the three main species in the downstream periphyton community was not affected. The lowest concentration of LAS that induced an effect was 3.3 mg/litre for the upstream periphyton community and 16.6 mg/litre for the downstream community. The authors suggested that the difference between the two values was due to the presence of 20–30% sewage downstream, which reduced the bioavailability of LAS (Lewis et al., in press).

When an aquatic ecosystem was exposed to LAS at concentrations of 0.25–1.1 mg/litre for 90 days, the numbers of phytoplankton were unaffected but primary productivity was significantly reduced at all concentrations. The zooplankton population showed a more variable response: the number of rotifers was reduced at all concentrations, and those of *Diaptomus* and *Cyclops* were reduced at $\geq$ 0.51 mg/litre. The number of ostracods was decreased at 0.38 mg/litre but was increased at 0.51 and 1.1 mg/litre. The chironomid population was significantly reduced at concentrations $\geq$ 0.38 mg/litre (Chattopadhyay & Konar, 1985). Exposure of an aquatic ecosystem consisting of phytoplankton, zooplankton, and benthic organisms to 1 mg/litre of a preparation of LAS for 90 days significantly reduced the numbers of phytoplankton and zooplankton per litre but did not significantly affect the numbers of chironomid larvae (Panigrahi & Konar (1986).

The effect of C_{12} LAS on microbial communities was studied in a model ecosystem consisting of a 19-litre glass tank containing sediment from Winton Lake, Ohio, United States, and several trophic levels, comprising bacteria, algae, macrophytes *(Elodea canadensis, Lemna minor),* macroinvertebrates *(Daphnia magna, Parantanytarsus parthenogenica),* and blugill sunfish *(Lepomis macrochirus).*

After a four-week equilibrium period, LAS were added at 0.5 or 5.0 mg/litre to a flow-through system with six to 10 replacements per day for 26 days. The structure of the microbial communities was not affected, and no differences were reported in mean biomass or number of colony-forming units between the microorganisms exposed at the two levels. The function of the microbial communities, assayed by measuring the degradation of both LAS and D-glucose, was reduced only at 5.0 mg/litre. In a similar system, in which the same concentrations of LAS were added in the form of sewage effluent, no effect was seen on the structure of the microbial community or on their function, measured only as the degradation of LAS (Larson & Maki, 1982).

Addition of LAS (average chain length, $C_{11.8}$) at a measured, relatively uniform concentration of 0.36 ± 0.05 mg/litre to 50-m outdoor experimental streams had no effect on total density, species richness, percentage similarity, or dominance of macroinvertebrates or periphyton or on the processing of organic matter of leaf discs. Fathead minnows *(Pimephales promelas)* and amphipods *(Hyallela azteca)* were exposed in groups of 10 and 20 per box placed in the streams at three locations. The mortality rates of the amphipods were 17–25% after exposure to LAS and 47% among controls; no effects were seen on the survival or weights of the fish, although minor effects were found on length (Fairchild et al., 1993).

A study of the fate and effects of surfactants in outdoor artificial streams addressed the effect of LAS on drift and population densities of macroinverebrates, the reproductive behaviour of an amphipod, the scud *(Gammarus pulex)*, the survival of a fish, the three-spined stickleback *(Gasterosteus aculeatus)*, and photosynthesis by the community. The concentration of LAS in sediment was reported to increase with increasing water concentration, and selective adsorption of longer-chain LAS homologues to sediment was reported. The microbial populations of both the water and the sediment adapted to LAS, resulting in a reduction in its half-life during the test. LAS at concentrations < 1.5 mg/litre did not affect macroinverebrate drift, population density, or community photosynthesis. Survival of the fish and reproduction by the amphipod were affected at concentrations of 1.5–3.0 mg/litre (Mitchell & Holt, 1993).

A9.3.6 Field studies

The effect of LAS downstream of a sewage outflow was studied by monitoring sediment, water, and the distribution of invertebrates at an upstream control site, a site near the discharge point, and a site 200 m downstream of the outflow. The concentrations of LAS in sediment were 1–40 mg/kg dry weight, with concentrations < 2 mg/kg at the control site and 200 m downstream. No effect of LAS in the effluent or in the streambed sediments could be discerned on the invertebrate populations (Ladle et al., 1989).

A9.3.7 Toxicity of biodegradation intermediates and impurities of linear alkylbenzene sulfonates

Tests of degradation products and impurities of LAS show that they are less toxic than LAS themselves.

A9.3.7.1 Individual compounds

The 48-h LC_{50} values in Daphnia magna were 208 ± 85 mg/litre for sulfophenylundecanoic acid, disodium salt (mixed isomers, 6–10 phenyl); about 6000 mg/litre for 3-(sulfophenyl) butyric acid, disodium salt; and about 5000 mg/litre for 4-(sulfophenyl) valeric acid, disodium salt. The equivalent 48-h LC_{50} values in the fathead minnow *(Pimephales promelas)* were 77 ± 12, about 10 000, and about 10 000 mg/litre, respectively (Kimerle & Swisher, 1977).

The 24-h LC_{50} values in Daphnia were about 22 000 mg/litre for 3-sulfophenylbutyric acid, disodium salt; about 12 000 mg/litre for 3-sulfophenylheptanoic acid, disodium salt; > 22 000 mg/litre for 3-sulfophenylbutyric acid, disodium salt; and 2 000 mg/litre for sulfophenylundecanoic acid, disodium salt. Other tests were carried out with the last two compounds, giving 96-h LC_{50} values of about 28 000 and 1200 mg/litre in fathead minnows *(Pimephales promelas)*;

28-day NOELs of > 2000 and > 200 mg/litre for survival and reproduction of *Daphnia*; and 30-day NOECs of > 1400 and > 52 mg/litre for survival of the fry of fathead minnows (egg hatchability and fry growth were less sensitive) (Swisher et al., 1978).

The 96-h LC_{50} for mixed isomers of sulfophenylundecanoic acid disodium salt in bluegill *(Leponis macrochirus)* was 75 mg/litre (Swisher et al., 1964). The 24-96-h LC_{50} values in fathead minnows were 1000–1500 mg/litre for sulfophenylundecanoic acid (C_{11}) and 25 000–32 000 mg/litre for sulfophenyl butyrate (C_4) (Swisher et al., 1978).

The 48-h LC_{50} for the alkanoic acid derivatives of 2-sulfophenyl C_{13} LAS and 4-sulfophenyl C_{13} LAS in nearly pure form was > 800 mg/litre in goldfish *(Carassius auratus)* (Divo & Cardini, 1980).

The 24-h LC_{50} values for *Daphnia magna* exposed to dialkyltetralin sulfonates, which are trace contaminants of LAS, were 420, 195, 110, 50, and 27 mg/litre for tetralin sodium sulfonates of chain lengths C_{10}, C_{11}, C_{12}, and C_{13}, respectively (Arthur D. Little Inc., 1991).

A9.3.7.2 Effluents

Interpretation of tests on effluents must take into account the following:

-- As concentrations arwe often reported as MBAS, testing of effluent from a sewage treatment plant may result in overestimation of the actual concentrations of LAS, owing to interference (see section 2.3).

-- The bioavailability of LAS is decreased by the presence of high concentrations of suspended solids; thus, as effluents are diluted in the environment, availability is usually increased, although biodegradation occurs.

Addition of LAS (C_{10}-C_{15}) to detergent-free activated sludge plant effluent (95% was removed as MBAS) gave a nominal 96-h LC_{50} in rainbow trout *(Oncorhynchus mykiss)* of 0.36 mg/litre. After treatment, the 96-h LC_{50} was 29.5 mg/litre, expressed in terms of the concentration of the surfactant in the influent (Brown et al., 1978).

When bluegill were exposed to effluent from continuous-flow activated sludge units fed 100 mg/litre LAS, none died during 4-11-day exposure (Swisher et al., 1964).

A9.4 Terrestrial organisms

A9.4.1 Terrestrial plants

Young seedlings of tomato, lettuce, radish, pea, cucumber, and barley were grown in a soil-based compost and were watered and given a foliar spray of a preparation of LAS. No effects were noted at concentrations up to 100 mg/litre (Gilbert & Pettigrew, 1984). In another study, barley, tomato, and bean plants were grown from seed and watered with a solution containing LAS at a concentration of 10, 25, or 40 mg/litre. Plants that received the lowest dose germinated at the same time as controls, but plants watered at 25 or 40 mg/litre germinated three days later. The growth of barley plants was inhibited at all three concentrations; however, the dose of 25 mg/litre increased the growth rate of beans, and the highest dose increased the growth rate of both tomatoes and beans (Lopez-Zavala et al., 1975).

The 21-day EC_{50} values for LAS (C_{10}-C_{13}), based on the emergence of seedlings and early stages of growth, were 167 mg/litre in sorghum, 289 mg/litre in sunflower, and 316 mg/kg in mung bean. The highest concentration that caused no significant reduction in the growth of any of the three species was 100 mg/kg (Holt et al., 1989; Mieure et al., 1990). In a second study, 407 mg/kg $C_{11.36}$ or 393 mg/kg $C_{13.13}$ LAS were mixed with sewage sludge, and nine common plant species, including five crop plants, were exposed as seed either at the same time or two weeks after application of the sludge to soil at a rate of 9000 kg/ha. There was no significant effect on seed germination and no significant inhibition of growth (Mieure et al., 1990).

Orchid seedlings *(Phalaenopsis* or *Epidendrum* sp.) were grown in culture media containing either the sodium or the ammonium salt of LAS at a concentration of 10, 100, or 1000 mg/litre. The lowest dose had no effect on growth, and that of ammonium LAS had no effect on germination. At 100 mg/litre, survival was halved and germination completely inhibited (Ernst et al., 1971). A concentration of 1000 mg/litre caused drastic changes in morphology, loss of membranes, swelling of thylakoids, and the appearance of dense osmophilic granules in chloroplasts (Healey et al., 1971).

The growth of pea seedlings grown for 26 days in quartz sand to which 0.005% (50 mg/kg) LAS had been added was significantly reduced, as measured by the fresh weight of roots and the length and fresh weight of pea greens (Lichtenstein et al., 1967).

LAS were not toxic with respect to growth at the early life stages of radish, Chinese cabbage, and rice when added in hydroponic culture at concentrations of 10, 20, and 20 mg/litre, respectively; concentrations of 20, 35, and 35 mg/litre were toxic (Takita, 1982).

When seeds of *Pisum sativum* and *Crotolaria juncea* were exposed to LAS for 24 h before sowing, the percentage germination was reduced at concentrations of 1 ml/litre for *P. sativum* and 10 ml/litre for C. juncea, although no statistical analysis was presented. No germination occurred after exposure to LAS at concentrations of 20 ml/litre for *P. sativum* and 40 ml/litre for *C. juncea*. Radicle length was reduced at $\geq$ 0.1 ml/litre in both species (Sharma et al., 1985).

Application of LAS at 50 g/m^2 under field conditions to loamy and sandy soils (corresponding to 0.47-1 mg/kg dry weight, respectively) led to considerable physiological damage, including leaf necrosis, chlorosis, and turgescence, to ryegrass *(Lolium perenne)* after 14 days; however, there was no difference in the fresh weight yield after harvesting at 45-54 days (Litz et al., 1987).

A9.4.2 Terrestrial invertebrates

When the earthworm *Eisenia foetida* was exposed to $C_{11.36}$ LAS incorporated into soil at nominal concentrations of 63-1000 mg/kg dry weight, the 14-day LC_{50} was > 1000 mg/kg. On the basis of a statistical analysis of body weights, the no-effect concentration was 250 mg/kg; this was confirmed by HPLC to be 235 mg/kg. In a second study, $C_{11.36}$ and C_{13}.13 LAS were incorporated into

sludge and applied to soil, and the earthworm *Lumbricus terrestris* was exposed to the subsequent mixture, which contained LAS at concentrations of 84–1333 mg/kg. The 14-day LC_{50} was again found to be greater than the highest concentration (> 1333 mg/kg). The no-effect concentration, based on weight and burrowing behaviour, was the nominal concentration of 667 mg/kg, measured by HPLC as 613 mg/kg. The worms were exposed, however, to LAS under conditions of continuous light, which would inhibit them from surfacing to feed and thus increase their exposure to and the toxicity of the test over that of the same concentration in the field (Mieure et al., 1990).

Topical application to house flies *(Musca domestica)* of LAS at the same time as parathion, diazinon, or dieldrin in ratios of 1:1 and 1:10 had no effect on the toxicity of the insecticides. When LAS were added to soil treated with parathion or diazinon, however, a significant synergistic effect was observed on the toxicity of the insecticides to the fruit fly *Drosophila melanogaster*. The optimal concentration of LAS that resulted in synergy was 23 mg/kg (Lichtenstein, 1966).

A9.4.3 Birds

No significant effect on egg quality was found after Leghorn chickens were fed a diet containing 200 mg/kg LAS for 45 days (Lopez-Zavala et al., 1975).

B. alpha-Olefin sulfonates

B1. SUMMARY

See Overall Summary, Evaluation, and Recommendations (pp. 7–21).

B2. IDENTITY, PHYSICAL AND CHEMICAL PROPERTIES, AND ANALYTICAL METHODS

B2.1 Identity

Chemical formula: $C_nH_{2n}O_3S$ Na, $C_nH_{2n+1}O_4S$ Na (n = 14–18)

Chemical structure:

$CH_3(CH_2)_jCH{:}CH(CH_2)_kSO_3^-\ Na^+$

$CH_3(CH_2)mCH(CH_2)_nSO_3^-\ Na^+$

OH (m,n, integers)

Common names: Sodium alpha-olefinsulfonate, alpha-olefin-sulfonic acid sodium salt, AOS sodium salt

Common trade names: Bioterge AS 40 F, Elfan OS 46, Geropon MLS/A, Hostapur OS Brands, Lipolan, Lipomix G, Lipon PB-800, Lutensit A-PS, Nansa LSS38/AS, Sawaclean, Sermul EA 214, Sulframin AOS, Witconate (McCutcheon, 1989)

Abbreviations: AOS, AOS-Na

CAS Registry numbers:
29963-33-5 Sodium 1-tetradecenesulfonate
29734-60-9: Sodium hexadecenesulfonate

13513-23-0: Sodium 3-hydroxyhexadecyl-1-sulfonate
26446-92-4: Octadecene-1-sulfonic acid sodium salt
13513-42-3: 3-Hydroxy-1-octadecanesulfonic acid, sodium salt

Specifications: AOS are mixtures consisting of about 60–65% alkene sulfonates, 30–35% hydroxylalkane sulfonates, and 5–10% disulfonates. Various positional isomers of alkene sulfonates and hydroxyalkane sulfonates have been reported (Gentempo et al., 1985; Williamson, 1993). Sodium C_{14}–C_{16} AOS are typically shipped as solutions containing 35–40% active matter in water. Sodium C_{16}–C_{18} AOS are typically slurries containing 28–30% active matter in water at ambient temperature.

B2.2 Physical and chemical properties

AOS are white crystalline solids consisting of various chemical compounds and their isomers, with different properties. Typical properties of AOS are given in Table 30. Two ranges are usually offered; the commonest are based on C_{14}–C_{16} olefin and the other

on C_{16}–C_{18} olefin. Detergency is maximal with alkyl chain lengths of C_{15}–C_{18}. Maximal detergency is also obtained with the same range of alkyl chain lengths in a detergent formulation that includes alkali builders and chelating agents (Yamane et al., 1970). AOS are stable, even in hot acidic media.

Table 30. Relationship between alkyl chain length, Krafft point, critical micelle concentration (CMC), and surface tension of alpha-olefin sulfonates

Alkyl chain length	Krafft point[a] (°C)	CMC[a] (g/litre)	Surface tension (dyne/cm)

12	-	4.0	-
14	-	1.0	30
16	10	0.3	33
18	30	0.1	35
20	40	-	-
		(25°C)	(25°C)

From Ohki & Tokiwa (1970)

[a] The solubility of surfactants in water, defined as the concentration of dissolved molecules in equilibrium with a crystalline surfactant phase, increases with rising temperature. For surfactants, there is a distinct, sharp bend (break-point) in the solubility-temperature curve. The steep increase in solubility above the sharp bend is caused by micelle formation. The point of intersection of the solubility and critical micelle curves, plotted as a function of temperature, is referred to as the Krafft point. This is a triple point at which surfactant molecules coexist as monomers, micelles, and hydrated solids. The temperature corresponding to the Krafft point is called the Krafft temperature. At above the Krafft temperature and critical micelle concentration, a micellar solution is formed. Under these conditions, higher levels than the aqueous solubility may be obtained.

B2.3 Analytical methods

There is no officially recognized specific procedure for the analysis of AOS in environmental samples. The methods commonly used to analyse anionic surfactants are also used for AOS, except those involving high-performance liquid chromatography (HPLC), which has limited use in environmental analyses for AOS, because they do not absorb ultra-violet radiation as effectively as do linear alkylbenzene sulfonates (LAS). A modified version of the methylene blue-active substance (MBAS)-HPLC method described in the monograph on LAS has been developed (Takita & Oba, 1985).

Nonspecific methods used in the analysis of anionic surfactants in general, such as the MBAS method, can be used to analyse materials for AOS (see section 2.3 of the monograph on LAS).

B3. SOURCES OF HUMAN AND ENVIRONMENTAL EXPOSURE

B3.1 Natural occurrence

AOS do not occur naturally.

B3.2 Anthropogenic sources

B3.2.1 Production levels and processes

AOS are synthesized industrially. Although they have been available since the 1930s, production for use in commercial surfactant formulations was somewhat limited until recently owing to a lack of suitable feedstock. Development of continuous and short-contact sulfur trioxide sulfonation processes and the increased availability of highly pure Ziegler-derived alpha-olefin feedstock has recently made AOS surfactants competitive with other surfactants on the market (Arthur D. Little Inc., 1977, 1981).

The estimated world consumption of AOS in 1988 was 50 200 tonnes (Colin A. Houston & Associates Inc., 1990). In 1990, that group estimated that world consumption would be 51 900 tonnes; an alternative estimate (Hewin International Inc. 1992) was 76 000 tonnes (Table 31).

Table 31. Estimated worldwide consumption of alpha-olefin sulfonates (tonnes)

Region	Household products	Personal care products	Industrial and institutional use	All uses
North America	3 000	7 000	4 000	14 000
Western Europe	2 000	3 000	3 000	8 000
Japan	24 000	7 000	2 000	33 000
Rest of the world	18 000	3 000	-	21 000
Total	57 000	20 000	9 000	76 000

From Hewin International Inc. (1992)

AOS are prepared commercially by direct sulfonation of linear alpha-olefins with a dilute stream of vaporized sulfur trioxide in a continuous thin-film reactor. The olefin is obtained by wax cracking or ethylene polymerization with a Ziegler-type catalyst (Tomiyama, 1970). The reaction is complex and follows several paths, forming large amounts of various sultones as intermediates which hydrolyse during subsequent quenching and neutralization. Commercial AOS products contain a mixture of two major components, alkene sulfonate and hydroxyalkane sulfonate, with smaller amounts of alkene disulfonates, hydroxyalkane disulfonates, and saturated sultones.

B3.2.2 Uses

AOS are good detergents, have good foaming characteristics in hard water and are used in heavy-duty laundry detergents, light-duty dishwashing detergents, shampoos, and cosmetics. Table 31 indicates

the use patterns for AOS.

B4. ENVIRONMENTAL TRANSPORT, DISTRIBUTION, AND TRANSFORMATION

Section summary

It can be inferred that AOS are transported into the environment in a similar manner to that established for LAS, alkyl sulfates, and other detergent surfactants. Fewer data are available on the environmental transport, distribution, and transformation of AOS than for LAS. The environmental fate of AOS is similar to that of LAS and alkyl sulfates: it is readily biodegraded under aerobic conditions, and primary biodegradation is complete within 2–10 days, depending on the temperature. At temperatures below 5–10°C, biodegradation kinetics are reduced, owing to a reduction in microbial activity. No data were available on abiotic degradation. There was no evidence of bioaccumulation or bioconcentration in a study of fish in which the uptake and distribution of AOS were examined.

B4.1 Transport and distribution between media

In the same manner as other detergent compounds, AOS are discharged into the environment in wastewater. The wastewater may undergo sewage treatment if such facilities are available. In countries where there are no adequate wastewater treatment facilities, AOS released to the environment are removed by biodegradation and adsorption mechanisms (see section 4.2 of the monograph on LAS).

Limited studies of the adsorption of AOS are available. In a study of the adsorption of C_{12} AOS on river sediments, the equilibrium quantities adsorbed were proportional to the organic carbon content of the sediments, with a sorption coefficient K_{oc} (dimensionless; normalized for the level of organic matter) of 0.65. This indicates that adsorption of C_{12} AOS is slightly weaker, than, for example, that of C_{12} LAS or C_{12} alkyl sulfonates (Urano et al., 1984). Like other detergent chemicals, AOS are adsorbed onto sewage sludge and river sediments in the environment.

B4.2 Biotransformation

B4.2.1 Biodegradation

B4.2.1.1 Aerobic biodegradation

Primary biodegradation of AOS, studied in die-away tests in water from various sites on the Tama River, Japan, was complete within three to five days when measured by the MBAS method; however, total organic carbon was completely removed after an incubation time of 20 days. In a study of AOS in seawater collected from the mouth of the Tama River, 99% of MBAS was removed within one day, and 90% of organic carbon was removed within five days (Sekiguchi et al., 1975b).

In a comparison of the MBAS and total organic carbon methods for measuring biodegradation with the shake-culture method, AOS lost 99% of their activity as measured by the MBAS method and 90% of total carbon within one day; 100% was lost within five days (Sekiguchi et al., 1975a). In another study, complete loss of parent AOS (initial concentration, 100 mg/litre) as determined by the MBAS method was seen within 15 days, and 90% of total organic carbon was removed within eight days (Miura et al., 1979). In a static die-away test system, 90% biodegradation of three commercial AOS products, comprising 100% C_{14}–C_{16} AOS and > 95% C_{15}–C_{18} AOS (determined as MBAS), was reported within four days (Gafa & Lattanzi, 1974).

In a shake-culture test in Bunch-Cambers medium, C_{15}–C_{18} AOS were degraded by 99% (determined as MBAS) or 90% (removal of total organic carbon) within one day; 100% total organic carbon was removed within five days. The authors did not verify whether the removal was the result of adsorption or mineralization (Sekiguchi et al., 1972). The biodegradation of C_{15} AOS and three C_{15}–C_{18} compounds with disulfonate contents of < 4, 15, and 50% in a shake-flask culture system was reported to be 96% (determined as MBAS), with no significant difference between compounds (Oba et al., 1968b).

In a modified OECD screening test, 85% of C_{14}–C_{18} AOS (measured as chemical oxygen demand) was removed. Measurement of MBAS in the same test indicated 99% removal (Gerike, 1987).

The aerobic biodegradation of 20 mg/litre AOS at 27°C was followed during a 10-day incubation period. Primary degradation, measured by the MBAS method, was complete within 10 days. The theoretical CO_2 production had reached 30–40% within that time (Itoh et al., 1979).

The oxygen uptake of C_{14}–C_{18} AOS was reported to be 85% of the theoretical oxygen demand in a closed-bottle test (Gerike, 1987). The average biochemical oxygen demand for C_{12}–C_{18} AOS containing up to 40% hydroxylalkane sulfonates was 51.6% at five days, while glucose under the same conditions had a biochemical oxygen demand of 69.6% (Procter & Gamble Co, unpublished data).

The primary and ultimate biodegradability of a series of pure AOS homologues (C_{12}, C_{14}, C_{16}, and C_{18}) was determined by measuing CO_2 production. Primary biodegradation was 98–99% within three days, the rate of degradation varying with chain length. Degradation of C_{12} and C_{14} AOS occurred at a similar rate (65%

within 30 days), but C_{18} AOS degraded more slowly. Mineralization of all AOS samples was reported to be at least 50% within two weeks,

whereas mineralization of glucose during that time was 75–80% (Kravetz et al., 1982). In a study of the biodegradation of the two major breakdown products of AOS, alkene sulfonate and hydroxyalkane sulfonate, AOS homologues (C_{15}, C_{16}, C17, C_{18}) were degraded to about 50%, and in each case the alkene sulfonate was degraded at least twice as fast as the hydroxyalkane sulfonate (Sekiguchi et al., 1975c).

The biodegradation of C_{18} AOS at a concentration of 28 mg/litre was studied in activated sludge (concentration, 100 mg dry matter per litre) over 12 days: 90% was lost within eight days, as measured by removal of chemical oxygen demand. The specific rate of biodegradation was calculated to be 5.3 mg/g per h (Pitter & Fuka, 1979).

In the OECD confirmatory test with activated sludge, 20 mg/litre AOS were degraded, as follows: 97% C_{14} AOS within 17 days, 98% C_{16} AOS within seven days, and 94% C_{14}–C_{18} AOS within eight days (Maag et al., 1975).

Primary biodegradation of C_{15}–C_{18} AOS was dependent on incubation temperature in die-away tests with water from the Tama River, Japan. Primary biodegradation was complete within two days at 27°C, within five days at 15°C, and within two days at 21°C; however, at a water temperature of 10°C about 20% of the AOS had still not been degraded within the nine-day test (Kikuchi, 1985).

When C_{15}–C_{18} AOS were added to seawater, no MBAS activity was present after five days (Marquis et al., 1966).

B4.2.1.2 Anaerobic degradation

The primary anaerobic biodegradation of C_{15}–C_{18} AOS (measured as MBAS) by bacteria on sludge sampled from a sewage treatment plant was 19% within 14 days and 31% within 28 days. More parent AOS were degraded by bacteria from the bottom of a private cesspool, with 34% lost within 14 days and 43% within 28 days. The anaerobic degradation reported may have been due to the presence of hydroxyalkane sulfonate compounds (Oba et al., 1967). AOS and LAS were reported to be the two surfactants that were least degraded anaerobically (Itoh et al., 1987).

B4.2.2 Abiotic degradation

No information was available.

B4.2.3 Bioaccumulation and biomagnification

Rapid, significant absorption of ^{14}C-AOS by the gills of goldfish *(Carassius auratus)* was seen after exposure to AOS at a concentration of 10 mg/litre. The concentration of AOS in the gills

increased from 0.3 mg/kg after 0.5 h of exposure to 48.3 mg/kg after 3 h. AOS were not detected in the alimentary canal (Tomiyama, 1975). Three hours is a relatively short exposure, and the authors did not determine whether a steady state of adsorption had been achieved. Tomiyama (1978) reported that AOS accumulated to the greatest extent in the gills of exposed fish, with additional accumulation in the gall-bladder. Only limited conclusions can be drawn from this study, however, owing to the short exposure period.

B4.3 Interaction with other physical, chemical, and biological factors

No information was available.

B5. ENVIRONMENTAL LEVELS AND HUMAN EXPOSURE

Few data are available on environmental concentrations of AOS because of the lack of an accepted analytical method for this purpose. A modified analytical method based on MBAS-HPLC measurement has been used to measure AOS (Takita & Oba, 1985). The concentration in the Tama River, Japan, was calculated to be < 0.0016–0.002 mg/litre.

The annual average concentration of AOS in wastewater was 0.160–0.164 mg/litre on the basis of total MBAS concentrations of 8.4 and 8.2 mg/litre. AOS was not detected in the effluent from a treatment plant outfall (Oba et al., 1976).

AOS can be expected to mineralize rapidly in all environmental compartments and to be removed to a large extent during sewage treatment. Environmental concentrations in receiving surface waters, sediments, soils, estuaries, and the marine environment can also be expected to be low.

B6. KINETICS

Section summary

AOS administered orally are readily absorbed by the gastrointestinal tract of rats and are distributed throughout the body; they are eliminated primarily in the urine and, to a lesser extent, in the faeces within 24 h of administration. AOS applied dermally are absorbed only minimally by intact skin. Several metabolites have been isolated, but their chemical structures have not been identified.

B6.1 Absorption, distribution, and excretion

^{14}C-AOS were synthesized by sulfonation and hydrolysis of tetradecene-1-^{14}C. The labelled compound was composed of a mixture of about 55% sodium 3-hydroxyalkane sulfonate [$C_{11}H_{23}CH(OH)-CH_2SO_3Na$] and about 45% sodium 2-^{14}C alkenyl sulfonate [$C_{11}H_{23}CH_2CH_2{}^{14}CH_2SO_3Na$]. After oral administration of 100 mg/kg ^{14}C-AOS (50 µCi/kg) in water to rats, the level of radiolabel in blood reached a peak at 3 h (0.08% of the dose/ml) and then rapidly decreased, since little radioactivity was detected 24 h after the administration. At 4 h after administration, 0.45% of the dose per gram of tissue was detected in liver and 0.65% in kidney, but the levels in tissues other than the gastrointestinal tract were < 0.1%. Thereafter, the radiolabel in organs and tissues decreased rapidly, and 24 h after administration, about 0.8% was detected in the caecal contents and < 0.02% in other tissues. No specific accumulation was observed in any tissue. Within 24 h of administration, 72% of the dose was excreted in urine and 22% in faeces. At the end of the experiment, after four days, no ^{14}C residue (< 0.1% of the dose) was detected in urine or faeces. Cumulative excretion in the bile within 12 h after administration was about 4.3% of the radioactivity administered (Inoue et al., 1982).

The biological half-lives of AOS and their metabolites in blood after intravenous administration of 10 mg/kg ^{14}C-AOS in rats were 15 and 1 h, respectively. The marked difference in half-life can be accounted for by the fact that the binding of AOS to plasma proteins, especially serum albumin, increased in proportion to its concentration while that of the metabolites did not increase to any appreciable extent. The volume of distribution of AOS was 8 litres/kg, and that of the metabolites was 0.5 litres/kg (Inoue et al., 1982).

A dose of 0.5 ml of a 0.2% aqueous solution of ^{14}C-AOS was applied to the dorsal skin (4 × 3 cm) of rats with bile-duct and bladder cannulae. The total amount absorbed through the skin was estimated to be about 0.6% on the basis of the recoveries of ^{14}C in urine, bile, and the main organs over 24 h. At that time, the level of radiolabel was higher in the liver (0.123% of dose) than in the kidney (0.059%), spleen (0.004%), brain (0.01%), or lung (0.012%). A total of about 0.24% of the applied dose was recovered in these organs. After 24 h, 0.33% of the radiolabel was excreted in the urine and 0.08% in the bile. When the solution was painted on skin damaged by 20 applications of cellophane adhesive tape to remove the stratum corneum, the rates of excretion were 36.3% in the urine and 1.8% in the bile (Minegishi et al., 1977).

B6.2 Biotransformation

AOS and its metabolites were investigated in tissues and excrement after oral administration of 100 mg/kg ^{14}C-AOS to rats. AOS and a metabolite more polar than AOS were detected in blood, liver, kidney, bile, and urine by thin-layer chromatography. As most of the ^{14}C-labelled compounds in urine were alcoholic, unsaturated, and of sulfonic functionality, the metabolite may be a hydroxylated or polyhydroxylated sulfonic acid with a shorter chain than AOS, although the precise chemical structure remains to be elucidated (Inoue et al., 1982).

B7. EFFECTS ON LABORATORY MAMMALS AND *IN VITRO* TEST SYSTEMS

Section summary

The oral LD_{50} for AOS sodium salt in mice was 3000 mg/kg. AOS are skin and eye irritants. Data from studies in experimental animals are limited, but no effects were observed in a long-term study in which oral doses of 250 mg/kg body weight per day were administered to rats. Fetotoxicity was observed in the progeny of rabbits administered a maternally toxic dose of 300 mg/kg body weight per day.

The available long-term studies are inadequate to evaluate the carcinogenic potential of AOS in experimental animals; however, in the limited studies available in which animals were administered AOS orally or on the skin, there was no evidence of carcinogenicity.

The limited data available also indicate that AOS are not genotoxic *in vivo* or *in vitro*.

B7.1 Single exposures

The LD_{50} values for AOS (sodium salt of sulfonated C_{15}-C_{18} *n*-olefin) in male ddy mice were 3000 mg/kg body weight by oral administration, 1660 mg/kg by subcutaneous injection, 170 mg/kg by intraperitoneal injection, and 90 mg/kg by intravenous injection. The toxic effects seen at high oral doses were reduced voluntary activity, diarrhoea, anaemia, dyspnoea, and respiratory collapse. Clonic convulsions followed by respiratory collapse were seen in animals given the material intravenously (Oba et al., 1968a).

B7.2 Short-term exposure

No data were available.

B7.3 Long-term exposure; carcinogenicity

B7.3.1 Mouse

The skin of Swiss-Webster mice was painted with 20% C_{14}-C_{18} AOS, 25% C_{14}-C_{18} AOS, 20% C_{14}-C_{16} AOS, 25% C_{14}-C_{16} AOS,

6.7 or 8.3% C_{16} 1,4-sultone, water, or acetone, or remained untreated. Animals were treated with 0.02 ml of test material on about 1 cm^2 of exposed skin three times per week for 92 weeks. Final necropsies were conducted when the survival of each group reached 30% (approx. 19 months). Histopathological examination showed no evidence of carcinogenicity with any test material (Haar, 1983).

B7.3.2 Rat

AOS (97.93% of a 60.4:39.6% (w/w) mixture of alkenyl sulfonate and hydroxyalkane sulfonate; chain-length distribution, 25% C_{14}, 45% C_{16}, 30% C_{18}) were fed to four groups of 50 male and 50 female CFY rats at a dietary level of 0, 1000, 2500, or 5000 ppm, corresponding to 49, 122, or 245 mg/kg body weight per day, for two years. No adverse clinical signs were seen, and survival rates were not affected by treatment. The rate of body weight gain was marginally lower during the second trimester of the study in both males and females receiving 5000 ppm, and food intake was marginally lower during the first year among females receiving 5000 ppm. During the remainder of the study, body weight gain and food consumption were similar to those of the control animals. Investigation of the eyes, blood, and urine of controls and of those receiving 5000 ppm several times during the experiment revealed no reaction to treatment; and no changes related to treatment were seen in gross appearance or organ weights of rats in any group killed after 104 weeks. Histological examination of a limited range of tissues did not provide evidence of toxicity or tumour induction that could be attributed to treatment (Hunter & Benson, 1976).

Groups of 40 male and 40 female Wistar rats were fed the following materials in the diet for 24-27 weeks: 1, 0.75, or 0.5% C_{14}-C_{18} AOS (corresponding to 500, 375, or 250 mg/kg body weight per day); 1, 0.75, or 0.5% C_{14}-C_{18} AOS (corresponding to 500, 375, or 250 mg/kg body weight per day); or 0.33, 0.25, or 0.16% C_{16}1,4-sultone (corresponding to 165, 125, or 80 mg/kg body weight per day). One control group consisted of 100 males and 100 females and another of 40 males and 40 females. No excess of tumours over that in controls was observed with any treatment (Haar, 1983).

In 70-week studies on Wistar rats, 0.5 ml of a 1.0, 10, or 30% aqueous solution of AOS or 0.5 ml of a 50% aqueous solution of a detergent based on AOS was applied dermally; 24 h after the application, each site was washed with warm water. No abnormal gross or histopathological findings were reported (Tomizawa, 1978).

These studies are summarized in Table 32.

B7.4 Skin and eye irritation; sensitization

AOS (C_{10}; purity, 99.21%) were applied as 0.5 g of a 20 or 30% solution once a day for 15 days to the backs of three male Wistar rats. The skin at the application site and the tissues of the tongue and oral mucosa of animals receiving the 30% solution were examined histologically 16 days after application. Body weight gain was reduced in the group given the 20% solution, and body weight was decreased in the group at 30%. Macroscopically, there were no abnormalities at the application site. Histologically, although atrophy of the stratum spinosum was noted, neither necrosis nor

Table 32. Carcinogenicity of alpha-olefin sulfonates (AOS) after long-term exposure

Species, strain, numbers per group	Test material (specification)	Route	Dosage	Results	Reference
Mouse, Swiss-Webster 40 M, 40 F	AOS, C_{14}-C_{18}	Dermal	0, 200, 250 mg/kg (water, acetone)	No gross or histopathological adverse effects on skin 3 times/week, 92 weeks	Haar (1983)
Mouse, Swiss-Webster 40 M, 40 F	AOS, C_{14}-C_{16}	Dermal	0, 200, 250 mg/kg (water, acetone)	No gross or histopathological adverse effects on skin 3 times/week, 92 weeks	Haar (1983)
Rat, CFY, 50 M, 50 F	AOS, C_{14}-C_{18} (a.i., 97-93%)	Oral (diet)	0, 0.1, 0.25, 0.5%,	No adverse effects 2 years	Hunter & Benson (1976)
Rat, X-MRC, 40 M, 40 F	AOS, C_{14}-C_{18}	Oral (diet)	0, 0.5, 0.75, 1.0%, 24-27 months	No excess of tumours in comparison with controls	Haar (1983)
Rat, X-MRC, 40 M, 40 F	AOS, C_{14}-C_{16}	Oral (diet)	0, 0.5, 0.75, 1.0%, 24-27 months	No excess of tumours in comparison with controls	Haar (1983)
Rat, Wistar, 10 M, 10 F	AOS, C_{16}-C_{19}	Dermal	0, 250, 2500, 7500 mg/kg bw, 3 times per week, 70 weeks	No gross or histopathological abnormalities	Tomizawa (1978)
Rat, Wistar, 10 M, 10 F	AOS-based detergent	Dermal	12.5 g/kg bw 3 times/week, 70 weeks	No gross or histopathological abnormalities	Tomizawa (1978)

M, male; F, female; a.i., active ingredient

inflammatory cell infiltration was present. No abnormalities of the tongue were observed, but severe atrophy was observed in the mucosa of the oral cavity. The local lesions caused by application of AOS were reported to be minimal in comparison with those induced by application of linear dodecylbenzenesulfate or lauryl sulfate (Sadai

& Mizuno, 1972).

Solutions of 0.05–4% AOS (sodium salt of sulfonated C_{15}–C_{18} *n*-alpha-olefin) were instilled at a dose of 0.1 ml into the eyes of one to three rabbits, and the eyes were examined after 24 h. No abnormal findings were observed with the 0.05% solution, but slight congestion was observed with 0.1% and marked reactions, including severe congestion and oedema, increased secretion, opacity of the cornea, and absence of the corneal reflex, were observed at $\geq$ 1% (Oba et al., 1968a).

Solutions of C_{14}–C_{19} olefin (84% C_{15}–C_{17}) and five other solutions consisting mainly of C_{10}, C_{12}, C_{14}, C_{16}, or C_{18} were instilled into the eyes of three rabbits at one of six concentrations ranging from 0.01 to 5%. The rabbits were examined over a period of 168 h. The materials elicited similar reactions. No abnormal reaction was seen with 0.05%; slight congestion was observed with 0.1% within 2 h after application of the solution; and marked congestion or oedema was observed with 0.5%, which disappeared by 24 h. In the groups treated with 1 or 5%, marked reactions, including severe congestion and oedema, increased secretion, turbidity of the cornea, and disappearance of the corneal reflex, continued for 24 h but had usually completely disappeared by 120 h (Iimori et al., 1972).

In 1973, the apparent sensitizing potential of AOS attracted attention (Haar, 1983). AOS can contain unsaturated gamma-sultones when manufactured under certain conditions, and these are strong sensitizers in guinea-pigs (Haar, 1983; Roberts & Williams, 1983; Roberts et al., 1990). When the levels of these sultones were reduced to low levels by altering the manufacturing techniques, AOS no longer caused sensitization (Haar, 1983; Oba et al., 1985; Roberts et al., 1990).

Skin sensitization was studied in guinea-pigs with pastes made of C_{14}–C_{16} AOS, a light-duty dishwashing detergent containing AOS, some consumer products containing AOS, and mixtures of these products with alkyl unsaturated sultone in sodium lauryl sulfate or hypochlorite bleach. The pastes, the dishwashing detergent, most of the consumer products, and the mixtures with hypochlorite bleach induced sensitization, the degree of response being related to the amount of unsaturated gamma-sultone present in the material tested (Bay & Danneman, 1985).

B7.5 Reproductive toxicity, embryotoxicity, and teratogenicity

AOS (C_{14}–C_{18}) were administered at a concentration of 0.2, 2, 300, or 600 mg/kg body weight per day to CD rats, CD-1 mice, and NZW rabbits orally once a day by gavage. Groups of 20 rats and mice were given AOS on days 6–15 of pregnancy, and groups of 13 rabbits were treated on days 6–18 of pregnancy. The doses of 0.2 and 2 mg/kg were estimated to be equivalent to 1–2 and 10–20 times the maximal amount of AOS to which humans are exposed. No adverse effects were seen in rat dams, even at the maximal dose. Mouse dams given 300 or 600 mg/kg showed piloerection, decreased movement, and inhibition of body weight gain; six dams at 600 mg/kg died. All rabbits given 600 mg/kg and one given 300 mg/kg died; anorexia and decreased body weight were seen initially in surviving dams given 300 mg/kg. Both mouse and rabbit dams given 0.2 or 2 mg/kg showed only initial inhibition of body weight gain. No adverse effects were seen on litter parameters of rats at any dose. In mice, total litter loss was found in five dams given 600 mg/kg and in six dams given 300 mg/kg; however, the average number of live fetuses in the other dams was no different from that in controls. The average body weights of the fetuses of dams given 300 or 600 mg/kg was significantly lower than that of controls. The incidence of major malformations was not significantly increased in rats, mice, or rabbits. There were no significant minor anomalies or skeletal variations (extra ribs) in rats at any dose. The offspring of mice at 600 mg/kg had a significant increase in delayed ossification. Those of rabbits at 300 mg/kg had a significant increase in skeletal anomalies and variations, although the incidence of skeletal variations was within the normal background range, and there was no delayed ossification. The effects of AOS on the fetuses, such as changes in litter parameters and delayed ossification, were considered to reflect the effects of AOS on the dams. There were no adverse effects on fetuses of mouse or rabbit dams given 0.2 or 2 mg/kg or on fetuses of rat dams given 0.2, 2, 300, or 600 mg/kg, where effects on the dams were either not observed or were minimal (Palmer et al., 1975b).

AOS and AOS-S (a synthetic detergent with AOS as the main ingredient) were applied to the shaven dorsal skin of mice at a dose of 0.5 ml/mouse per day of a 0.1% (the concentration of AOS usually found in detergents), 1%, or 5% aqueous solution of AOS or a 0.5% (equivalent to 0.1% AOS), 5%, or 25% aqueous solution of AOS-S on days 0–14 of pregnancy. Adverse effects on the dams and fetuses were found in a few cases. None of the dams died; the viability, body weight, and sex ratio of the fetuses did not differ from those of controls; and there were no malformations (Sawano, 1978).

B7.6 Mutagenicity and related end-points

AOS did not cause differential toxicity in *Bacillus subtilis* rec at a concentration of 20 µg/disc or reverse mutation in *Salmonella typhimurium* TA98 or TA100 at 10–100 µg/disc, in the presence or absence of metabolic activation (Oda et al., 1980).

One batch of AOS (C_{14}–C_{16}; 28.4% active ingredient) induced host-mediated mutagenicity at 283 mg/kg body weight in rats inoculated with *S. typhimurium* TA1530 but not in an assay with TA1534 or in plate incorporation assays with either strain (Arthur

D. Little Inc., 1993).

B7.7 Special studies

Rabbit erythrocytes were mixed with solutions containing various concentrations of AOS (sodium salt of sulfonated C_{15}–C_{16} *n*-alpha-olefin; average relative molecular mass, 338.5) at room temperature for 3 h. The 50% haemolytic concentration was 1.5 mg/litre (Oba et al., 1968a). The effects of AOS on methaemoglobin formation were studied in groups of three male mice given an oral or intraperitoneal dose of 0.3 or 3.0 g/kg body weight C_{15}–C_{18} AOS. The level of methaemoglobin in blood was measured 0.5, 1, 2, 3, and 24 h after administration of AOS. No significant increase was observed (Tamura & Ogura, 1969).

In an immunological study of AOS, a complex (HA) prepared by mixing AOS with human serum albumin (HSA) containing 30 mg of total protein was injected subcutaneously or intravenously into rabbits during a period of 2.5 months, and the anti-serum produced was subjected to the ordinary precipitation reaction. As a control, anti-AOS-serum, similarly prepared, was subjected to the same reaction. Minor positive reactions were seen in the HA-anti-HA and HSA-anti-HSA systems but not in the AOS-anti-HA or AOS-anti-AOS systems (Iimori & Ushiyama, 1971).

B8. EFFECTS ON HUMANS

Section summary

In patch tests, human skin can tolerate contact to solutions containing up to 1% AOS for 24 h with only mild irritation. AOS can cause delipidation of the skin surface, elution of natural moisturizing factor, denaturation of the outer epidermal layer proteins, and increased permeability and swelling of the outer layer. AOS did not induce skin sensitization in volunteers. There is no conclusive evidence that AOS induce eczema. No serious injuries or fatalities have been reported following accidental ingestion of detergent formulations that could contain AOS.

B8.1 Exposure of the general population

AOS surface-active agents are found in shampoos, dishwashing products, household cleaners, and laundry detergents. The composition of nonionic and ionic surfactants in these products varies between 10 and 30%. Surface-active agents can affect human skin and eyes.

B8.2 Clinical studies

B8.2.1 Skin irritation and sensitization

AOS are mildly to moderately irritating to human skin, depending on the concentration.

The relative intensity of skin roughness induced on the surface of the forearm was evaluated in volunteers by a circulation method consisting of contact with 1% solutions of C_{12}, C_{14}, C_{16}, and C_{18} AOS for 10 min. The skin response was characterized mainly on the basis of gross visible changes. C_{12} AOS induced more skin roughening than compounds with longer or shorter alkyl chains. The relative degree of skin roughening *in vivo* was correlated with the extent of protein denaturation measured *in vitro* (Imokawa et al., 1975a).

Primary skin irritation induced by a 1% aqueous solution (pH 6.8) of AOS containing 27% C_{15}, 25% C_{16}, 28% C_{17}, and 18% C_{18} (relative molecular mass, 338.5) was studied in a 24-h closed-patch test on the forearms of seven male volunteers. The intensity of skin irritation was scored by grading erythema, fissuring, and scales. The average score for AOS was 3.97 and that for a control (water) was 1.79. The same compound was evaluated at 0.3% for the relative intensity of skin lesions produced on the surface of the hands by an immersion test involving 30 repetitions of a 1-min dip and 1-min dry. The average score for AOS with regard to erythema, irritation, fissuring, scaling, and loss of suppleness was 5.75, while that for the water control was 2.5 (Oba et al., 1968a).

Skin irritation induced by a 1% aqueous solution of C_{14}, C_{16}, and C_{18} AOS was studied in a 24-h closed-patch test on the forearm and in a test in which the compound was dripped onto the interdigital surface for 40 min once daily for two consecutive days at a rate of 1.2–1.5 ml/min. Skin reactions were scored by grading erythema in the patch test and by grading scaling in the drip test. The score for AOS was 1 (slight erythema) in the patch test and 0.35 (minimal scaling) in the drip test (Sadai et al., 1979).

In sensitization tests on volunteers, AOS in a paste or in a detergent mixture containing up to 0.06% AOS and up to 0.002 ppm unsaturated g-sultone did not produce sensitization, although one subject had a strong dermal response, which was considered to be due to pre-existing sensitization. Two out of 264 subjects using a light-duty detergent containing AOS developed hand dermatitis and had positive reactions to AOS paste and/or unsaturated gamma-sultone in sodium lauryl sulfate in a patch test. Use of a hand dishwashing liquid containing AOS did not cause sensitization provided the level of unsaturated g-sultones was kept low (Bay & Danneman, 1985). Patch tests on 790 volunteers after four months' use of a dishwashing liquid showed no evidence of sensitization (Oba et al., 1985).

B8.2.2 Effects on the epidermis

The effects of AOS on the epidermal outer layer (stratum corneum) are similar to those of other surface-active agents (see section 8.2.2 of the monograph on LAS), including delipidation of the skin surface, elution of natural moisturizing factor, denaturation of stratum corneum protein, increased permeability, swelling of the stratum corneum, and inhibition of enzyme activities in the epidermis (Wood & Bettley, 1971; Imokawa et al., 1974; Okamoto, 1974; Imokawa et al., 1975a,b).

The effects of anionic surfactants on various types of proteins were studied using skin keratin as a filamentous protein, bovine serum albumin as a globular protein, acid phosphatase as an enzyme protein, and membrane lysosome as a membrane protein. The denaturing effects of surfactants were measured as liberation of sulfhydryl groups and enzyme inhibition. AOS were less potent than LAS or alkyl sulfates. A relationship was observed between denaturing potency, skin irritant action, and alkyl chain length (Imokawa & Katsumi, 1976; Imokawa & Mishima, 1976).

B8.2.3 Hand eczema

Skin reactions to a 0.04, 0.4, or 4.0% aqueous solution of AOS (25.0% C_{14}, 45.0% C_{16}, 30.0% C_{18})were evaluated in a 24-h closed-patch test on the lower back of 10 healthy volunteers and 11 patients with hand eczema (progressive keratosis palmaris). The incidence and intensity of skin reactions were significantly higher in the group with hand eczema than in a control group with normal skin (Okamoto & Takase, 1976a,b).

B8.2.4 Accidental or suicidal ingestion

No data were available that related specifically to AOS.

B9. EFFECTS ON OTHER ORGANISMS IN THE LABORATORY AND THE FIELD

Section summary

Limited data are available on the effects of AOS on environmental organisms. The 24-h LC_{50} values for daphnids were 19-26 mg/litre; the 48-h LC_{50} values ranged from 0.3 mg/litre for brown trout *(Salmo trutta)* to 6.8 mg/litre for golden orfe *(Idus idus melanotus)*, and the 96-h LC_{50} was 0.5-5.0 mg/litre for brown trout. One study suggested that AOS have little toxicity for birds.

B9.1 Microorganisms

No information was available.

B9.2 Aquatic organisms

B9.2.1 Aquatic plants

The EC_{50} values for $C_{16.4}$ AOS in the green alga *Selenastrum capricornutum* exposed for two to three days, based on growth, fell within the range 45-65 mg/litre (Yamane et al., 1984). The EC_{50} for C_{16}-C_{18} AOS on the growth of *S. capricornutum was* > 20 mg/litre (Konno & Wakabayashi (1987).

B9.2.2 Aquatic invertebrates

Daphnia magna and *Dapghnia pulex* less than 24 h old were exposed to C_{16}-C_{18} AOS under static conditions, in which the water was unchanged for the duration of the test, at a temperature of 20°C and a water hardness of 25 mg/litre $CaCO_3$. The 6-h LC_{50} values were > 64 and > 130 mg/litre, and the 24-h LC_{50} values were 19 and 26 mg/litre, for the two species respectively (Wakabayashi et al., 1988).

B9.2.3 Fish

The acute toxicity of AOS to fish is summarized in Table 33. The 48-h LC_{50} values ranged from 0.3 mg/litre for brown trout *(Salmo trutta)* to 6.8 mg/litre for golden orfe *(Idus idus melanotus);* the 96-h LC_{50} for brown trout was 0.5-5.0 mg/litre. Acute toxicity tended to increase with carbon chain length.

When eggs of rainbow trout *(Oncorhynchus mykiss)* and carp *(Cyprinus carpio)* were exposed to C_{16}-C_{18} AOS, the EC_{50} values, based on hatchability, were 4.9 for rainbow trout and 3.0 mg/litre for carp (Wakabayashi & Onizuka, 1986). In one-month old rainbow trout under semi-static conditions, the 14- and 28-day LC_{50} values for C_{16}-C_{18} AOS were 0.62 and 0.58 mg/litre. The

EC_{50} based on growth was 0.35 mg/litre (Wakabayashi & Mizorogi, 1989).

The time to lethality in goldfish *(Carassius auratus)* exposed to AOS was 2 h at a concentration of 5 mg/litre and 1 h at 10 mg/litre. Addition of 2100 mg/litre egg albumin increased the time to 100% lethality to 3 h and addition of 4200 mg/litre albumin increased the time to 6 h (Tomiyama, 1974).

B9.3 Terrestrial organisms

B9.3.1 Terrestrial plants

AOS were not toxic with respect to growth at the early life

stages of radish, Chinese cabbage, and rice when added in hydroponic culture at concentrations of 56, 56, and 32 mg/litre, respectively; concentrations of 100, 100, and 56 mg/litre were toxic (Takita, 1982).

B9.3.2 Terrestrial invertebrates

No information was available.

B9.3.3 Birds

No significant effect on egg quality was found after Leghorn chickens were fed a diet containing 200 mg/kg AOS for 45 days (Lopez-Zavala et al., 1975).

Table 33. Toxicity of alpha-olefin sulfonates (AOS) to fish

Species	Length, weight, or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	AOS chain length	End-point	Concn (mg/litre)	Reference
Masu trout (Oncorhynchus masou)	2 mo	Static[r]	8.5-9.6	30	NS	C_{16}-C_{18}	96-h LC_{50}	0.56	Wakabayashi et al. (1984)
Rainbow trout (Oncorhynchus mykiss)	40 d	Static[r]	8.8-10.9	25	NS		96-h LC_{50}	0.78	Wakabayashi et al. (1984)
	4 d	Static[r]	10	25	NS	C_{16}-C_{18}	96-h LC_{50}	0.61	Wakabayashi & Onizuka (1986)
	19 d	Static[r]	10	25	NS	C_{16}-C_{18}	96-h LC_{50}	0.98	
Brown trout (Salmo trutta)	2.8-5.8 cm	Flow	15	26-30	NS	C_{14}-C_{16}	48-h LC_{50}	2.5-5.0[b]	Reiff et al. (1979)
	2.8-5.8 cm	Flow	15	26-30	NS	C_{14}-C_{16}	96-h LC_{50}	2.5-5.0[b]	
	2.8-5.8 cm	Flow	15	26-30	NS	C_{16}-C_{18}	48-h LC_{50}	0.6[b]	
	2.8-5.8 cm	Flow	15	26-30	NS	C_{16}-C_{18}	96-h LC_{50}	0.5[b]	
	2-4 cm	Flow	15	250	NS	C_{14}-C_{16}	48-h LC_{50}	3.5[b]	
	2-4 cm	Flow	15	250	NS	C_{16}-C_{18}	96-h LC_{50}	3.1[b]	
	2-4 cm	Flow	15	250	NS	C_{14}-C_{16}	48-h LC_{50}	0.3-0.5[b]	
Goldfish (Carassius auratus)		Static	20		NS	C_{12}-C_{16}	6-h LC_{50}	11.2[c]	Gafa (1974)
		Static	20		NS	C_{14}-C_{18}	6-h LC_{50}	3.0[c]	

Table 33 (contd)

Species	Length, weight, or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	AOS chain length	End-point	Concn (mg/litre)	Reference
Golden orfe (Idus idus melanotus)	1.2-1.8 g	Static	20		NS	C_{14}-C_{16}	48-h LC_{50}	5.08	Mann (1976)
	1.2-1.8 g	Static	20		NS	C_{16}-C_{18}	48-h LC_{50}	1.44	
	5-7 cm	Flow	20	150	NS	C_{14}-C_{16}	48-h LC_{50}	5.7[b]	Reiff et al. (1979)
	5-7 cm	Flow	20	150	NS	C_{16}-C_{18}	48-h LC_{50}	1.9[b]	
		Flow	20	268	NS	C_{14}-C_{16}	48-h LC_{50}	3.7-6.8[b]	
		Flow	20	268	NS	C_{16}-C_{18}	48-h LC_{50}	1.0[b]	
		Flow	20	268	NS	C_{14}-C_{16}	96-h LC_{50}	3.4-4.9[b]	
		Flow	20	268	NS	C_{16}-C_{18}	96-h LC_{50}	0.9[b]	
Harlequin fish (Rasbora heteromorpha)		Flow	20	20	NS	C_{14}-C_{16}	48-h LC_{50}	4.8[b]	Reiff et al. (1979)
		Flow	20	20	NS	C_{16}-C_{18}	48-h LC_{50}	0.9[b]	
		Flow	20	20	NS	C_{14}-C_{16}	96-h LC_{50}	3.3[b]	
		Flow	20	20	NS	C_{16}-C_{18}	96-h LC_{50}	0.5[b]	
Medaka (Oryzias latipes)	175-332 mg	Static	21-22	25	6.7-7.1	C_{14}-C_{18}	6-h LC_{50}	6.2[b]	Kikuchi & Wakabayashi (1984)
	175-332 mg	Static	21-22	25	6.7-7.1	C_{14}-C_{18}	48-h LC_{50}	1.8[b]	
	175-332 mg	Static	21-22	25	6.7-7.1	C_{16}-C_{18}	6-h LC_{50}	2.7[b]	
	175-332 mg	Static	21-22	25	6.7-7.1	C_{16}-C_{18}	48-h LC_{50}	0.81[b]	
Carp (Cyprinus carpio)	3.5-5.5 cm	Static	21		7.5-7.8	Technical	24-h LC_{50}	3.2[c]	Lopez-Zavala et al. (1975)
	3.5-5.5 cm	Static	21		7.5-7.8	Technical	96-h LC_{50}	3.0[c]	
	2 d	Static[r]	20	25	NS	C_{16}-C_{18}	96-h LC_{50}	> 1.4	Wakabayashi & Onizuka (1986)
	15 d	Static[r]	20	25	NS	C_{16}-C_{18}	96-h LC_{50}	1.5	

Table 33 (contd)

Species	Length, weight, or age	Static or flow	Temp. (°C)	Hardness (mg/litre)[a]	pH	AOS chain length	End-point	Concn (mg/litre)	Reference
Carp (contd). (Cyprinus carpio)	50 d	Static[r] Static[r]	21	75	NS		96-h LC_{50}	1.0	Wakabayashi et al. (1984)
White tilapia (Tilapia melan opleura)	5-7 cm	Static	21		7.5-7.8	Technical	24-h LC_{50}	2.0[c]	Lopez-Zavala et al. (1975)
	5-7 cm	Static	21		7.5-7.8	Technical	96-h LC_{50}	2.0[c]	
Grey mullet (Mugil cephalus)		Static	20.6-22.0				96-h LC_{50}	0.70	Wakabayashi et al. (1984)

Static[r], static renewal: water changed at regular intervals; flow, flow-through conditions: concentration in water maintained continuously; static: water unchanged for duration of test

[a] mg/litre $CaCO_3$

[b] Measured concentration

[c] Nominal concentration

C. Alkyl sulfates

C1. SUMMARY

See Overall Summary, Evaluation, and Recommendations (pp. 7-21)

C2. IDENTITY, PHYSICAL AND CHEMICAL PROPERTIES, AND ANALYTICAL METHODS

C2.1 Identity

Chemical formula: $C_nH_{2n+1}O_4S\ Na$ (n = 10-8)

Chemical structure: $C_nH_{2n+1}OSO_3^-\ Na^+$ (n, integer)

Common names: Sodium alkylsulfate, sulfuric acid alkyl ester sodium salt, alkylsulfate sodium salt, alcohol sulfuric ester sodium salt, sodium dodecyl sulfate, sodium lauryl sulfate

Common trade names: Akyporox SAL SAS, Akyposal, Alphenate TFC 76, Alscoap LN, Aremsol, Berol, Cosmopon, Dehydag, Elfan, Emal, Empicol, Gardinol, Genapol CRT 40, Manro, Marlinat KT 50, Melanol LP 1, Monogen, Montopol CST, Montovol, Neopon LT, Nikkol, Nissan Persoft SK, Perlankrol ATL-40, Perlankrol, Polystep B, Rewopol, Sactipon, Sactol, Sandopan KD, Sermul, Stepanol WA 100, Sufatol, Sufetal, Sulfopon, Sunnol, Surfax, Swascol, Teepol HB 7, Tensopol Tesapon, Texapon, Ufarol AM 70, Zoharpon, Zorapol LS-30, (McCutcheon, 1993)

Abbreviations: AS, AS-Na, SDS

CAS Registry numbers: 151-21-3 (C_{12} AS), 1120-04-3 (C_{18} AS), 68130-43-8 (C_8-C_{18} AS)

Specification: AS are higher alcohol sulfuric ester salt types of anionic surfactants. Depending on which precursor alcohol is used as the raw material, the alkyl group is linear or branched, may contain a single homologue or a mixture of chain lengths, and is usually primary. The data presented are applicable mainly to linear alcohol sulfates and AS with predominantly single or similar type of branching.

C2.2 Physical and chemical properties

AS are white crystalline powders. Their physical properties differ widely depending on their alkyl groups, and they are usually produced and used as mixtures. The relationships between the critical micelle concentration, solubility, and alkyl chain length are shown in Table 34.

Table 34. Relationships between alkyl chain length, critical micelle concentration (CMC), and solubility

Alkyl chain length	CMC × 10^{-3} mol/litre[a,c]	Solubility/°C[b,c]
8	136	-
12	8.6	15
14	2.4	28
16	0.58	42
18	0.16	55

[a] From Evans (1956)

[b] Temperature at which 10 g of AS dissolve in 1 litre of water (Gotte, 1954)

[c] The solubility of surfactants in water, defined as the concentration of dissolved molecules in equilibrium with a crystalline surfactant phase, increases with rising temperature. For surfactants, there is a distinct, sharp bend (break-point) in the solubility-temperature curve. The steep increase in solubility above the sharp bend is caused by micelle formation. At above the critical micelle concentration, a micellar solution is formed. Under these conditions, higher levels than the aqueous solubility may be obtained.

AS are readily hydrolysed in hot acidic media. Compounds with an alkyl chain length of C_{10} (27°C), C_{12} (25°C), C_{14} (40°C), or C_{16} (40°C) have a surface tension of 40 dyne/cm at the temperatures shown in parentheses at concentrations greater than the critical micelle concentration, indicating a good ability to reduce surface tension (Dreger et al., 1944).

Cleansing capacity at 25°C increases with alkyl chain length up to C_{13} and then becomes constant up to C_{16}. In an actual detergent containing alkali builders and chelating agents, however, maximal

detergency was obtained with C_{14} compounds (Yamane et al., 1970).

C2.3 Analysis

C2.3.1 Isolation

Since AS are readily susceptible to hydrolysis in acidic media, special attention is required.

C2.3.2 Analytical methods

There is no officially recognized, specific procedure for the analysis of AS in environmental samples. The methods used for analysing linear alkylbenzene sulfonates (LAS) are commonly used for AS, except those involving high-performance liquid chromatography (HPLC), which is of limited use for detecting AS in environmental samples because AS do not effectively absorb ultra-violet radiation. An HPLC method for the analysis of AS after its conversion by derivatization into an ultra-violet-active species has been proposed (Utsunomiya et al., 1982). A modified analytical method has been developed that is based on measurement of methylene blue-active substances (MBAS) by HPLC. This method permits determination of AS at concentrations as low as 0.05 mg/litre (Takita & Oba, 1985). Trace enrichment followed by gas chromatography and flame ionization detection have been proposed for the sensitive determination of AS as their trimethylsilyl ethers in environmental samples (Fendinger et al., 1992a).

Non-specific methods used in the analysis of anionic surfactants in general, such as the methylene blue method, may be used for the analysis of AS (see also section 2.3 of the monograph on LAS).

C3. SOURCES OF HUMAN AND ENVIRONMENTAL EXPOSURE

Section summary

Few quantitative data are available on AS in the environment, but AS can be expected to mineralize rapidly in all environmental compartments and to be removed to a large extent during sewage treatment. Environmental concentrations in receiving surface waters, sediments, soils, estuaries, and the marine environment can be expected to be low.

C3.1 Natural occurrence

AS do not occur naturally.

C3.2 Anthropogenic sources

C3.2.1 Production levels and processes

AS are synthesized industrially. Worldwide consumption of AS in 1987 was about 117 000 tonnes in the United States, 56 000 tonnes in western Europe, and 46 000 tonnes in Japan (Richtler & Knaut, 1988). In western Germany in 1987, some 10 000 tonnes of AS and 87 000 tonnes of LAS were used (Schöberl et al., 1988). Worldwide consumption was estimated to be 289 000 tonnes in 1990 (Hewin International Inc., 1992; see Table 35).

Table 35. Estimated worldwide use of alkyl sulfates in 1990 (tonnes)

Region	Household products	Personal care products	Industrial and institutional use
North America	140 000	33 000	9 000
Western Europe	49 000	12 000	7 000
Japan	21 000	6 000	4 000
Rest of the world	-	4 000	4 000
Total	210 000	55 000	24 000

From Hewin International Inc. (1992)

AS were originally made by the sulfation of natural fatty alcohols. They are currently produced from both natural and synthetic fatty alcohols. Primary AS are usually manufactured by conventional sulfation of the parent alcohol with either sulfur trioxide or chlorosulfonic acid. The product of this reaction is then neutralized with an appropriate base (NaOH, Na_2CO_3, NH_4OH, or triethanolamines).

C3.2.2 Uses

Initially, AS were used as washing agents for wool or as active ingredients in heavy-duty laundry detergents. They are now used mainly in personal care products (shampoos, toothpastes, toiletries), household detergents (light-duty dishwashing detergents, heavy-duty laundry detergents), and industrial applications.

C4. ENVIRONMENTAL TRANSPORT, DISTRIBUTION, AND TRANSFORMATION

Section summary

AS can be expected to be transported into the environment by mechanisms similar to those that operate for LAS and alpha-olefin sulfonates (AOS). AS are readily biodegradable under aerobic

conditions, both in laboratory tests and under environmental conditions, and primary biodegradation is complete within two to five days. Less information is available on the effect of temperature on the biodegradation of AS than for LAS. The biodegradation kinetics of AS appear to be less affected by temperature than those of other surfactants. The whole-body bioconcentration factors are 2–73, depending on chain length. AS are taken up by fish mainly through the gills and are subsequently distributed to the liver and gall-bladder. After biotransformation, AS are excreted rapidly. They are not bioconcentrated or biomagnified in aquatic organisms.

C4.1 Transport and distribution between media

After use, AS are discharged into the environment in wastewater, like other detergent compounds, where they can undergo sewage treatment if such facilities are available. In countries where adequate wastewater treatment facilities are not available, AS released to the environment are removed by biodegradation and adsorption in the receiving surface water (see section 4.2 of the monograph on AOS).

Sorption equilibria were obtained rapidly (within 20 min) for pure homologues of AS (> 99%) with chain lengths of C_8, C_9, C_{10}, C_{11}, C_{12}, C_{13}, and C_{14}, suggesting that sorption is due to a hydrophobic bonding mechanism, as has been observed for other surfactants. Thus, sorption of AS to sediment is likely to be stronger for longer chain homologues than for shorter ones. The K_D values for C_{12} AS were 70 and 100 for two river sediments, whereas for C_{12} LAS on the same sediments they were 310 and 330 (Marchesi et al., 1991). Adsorption of AS therefore competes in kinetic terms with biodegradation as a mechanism for removal of AS from the environment, as is seen for surfactants in general.

C4.2 Biotransformation

C4.2.1 Biodegradation

C4.2.1.1 Biodegradation pathway; mechanism

Several species of bacteria have been found that can mineralize AS. AS with chains longer than six carbons are degraded by the initial action of a sulfatase enzyme, producing sulfate and the corresponding alcohol. The alcohol is readily oxidized by formation of an aldehyde, to produce carboxy acid, which can be further oxidized by ß-oxidation and in the citric acid cycle. Secondary ketones and hydroxy ketones of AS are produced as metabolites but have not been detected in simulated activated sludge. Biodegradation of short-chain homologues of AS may proceed by oxidation of the chain before hydrolysis of the ester bond by the sulfatase enzyme.

The metabolic pathway for biodegradation of C_{12} AS by *Pseudomonas* strains has been described (Hsu, 1965; Thomas & White, 1989). Initial liberation of the sulfate head produces dodecanol, which is further transformed into more polar metabolites, including dodecanal and dodecanoic acid. These products may be further metabolized by ß-oxidation, or they may be elongated to C_{14}, C_{16}, or C_{18} fatty acyl residues, which are then incorporated into lipid fractions such as phospholipids (Thomas & White, 1989).

C4.2.1.2 Biodegradation in the environment

The aerobic biodegradation of 20 mg/litre AS at 27°C was followed during a 10-day incubation period. Primary degradation, measured by the MBAS method, was complete within five days. The theoretical production of CO_2 reached 60–90% within 10 days (Itoh et al., 1979).

The biodegradation of AS at a concentration of 30 mg/litre was studied in a vessel containing activated sludge at a concentration of 100 mg/litre over a period of 12 days, by measuring chemical oxygen demand. All of the AS were lost within two days; the specific rate of biodegradation was calculated to be 20 mg/g per h (Pitter & Fuka, 1979).

The biodegradation of an initial concentration of 6 mg/litre C_{12} AS was studied by the die-away method, in which disappearance of the compound is followed over a given period. Less than 10% of the original amount remained in river water in the test vessel after 12 days' exposure, and complete degradation was reported within 21 days (Okpokwasili & Nwabuzor, 1988).

The capacity of epilithic (sampled from the surface of pebbles) and planktonic river bacterial populations to degrade C_{12} AS was studied under simulated environmental conditions. Samples were collected from four polluted sites and one clean site in a polluted river in South Wales, United Kingdom. In die-away tests, AS were degraded after an apparent lag at all four polluted sites, but degradation by the bacterial populations at the clean site was relatively slow. Quantification of the kinetic components that contributed to the die-away curves demonstrated that biodegradation of AS occurred at concentrations below its K_m by bacteria with exponential growth that are unaffected by addition of the test substrate. Degradation of AS in the clean sample followed a different pattern, but there was generally little or no growth on endogenous carbon. The authors concluded that the capacity of epilithic bacterial populations to degrade C_{12} AS is more stable than that of planktonic populations (Anderson et al., 1990).

Riverine bacteria that can grow in the presence of 0.5 mmol/litre C_{12} AS are widespread, and a greater incidence of

isolates resistant to C_{12} AS was recorded at a polluted site than in clean water. The ability of each culture to produce alkyl sulfatases, the enzymes that initiate degradation of AS, was also determined. Bacteria containing alkyl sulfatases were widespread, but a greater alkyl sulfatase yield was obtained from polluted site. The authors concluded that more strains at the polluted site had constitutive rather than inducible enzymes. An increased incidence of strains containing multiple alkyl sulfatases was also recorded at the polluted site (White et al., 1985).

In another study in South Wales, the distribution of planktonic bacteria capable of degrading 98.5% C_{12} was examined in water samples at sites along a river. The annual mean prevalence of such bacteria was 8.1–16.0% of the total number of isolates. The proportion of isolates that degrade AS in clean water was no different from that at polluted sites, and a lower density was recorded at the source owing to a reduction in overall numbers. A higher percentage of bacteria capable of degrading C_{12} AS was recorded in estuarine samples than in samples from the middle of the polluted river; however, when cell numbers were taken into account, the cell density was similar at all polluted sites on the river, including the estuary. The incidence of these isolates was not correlated with either biochemical oxygen demand or oxygen concentration, but the incidence tended to increase at the end of the summer. More than half of the isolates contained constitutive alkyl sulfatase enzymes, while they were induced or repressed in the remainder after exposure to AS. No variation in the proportions of type of enzyme regulation was seen between sampling sites or times (White et al., 1989).

The biodegradation of AS was also examined at three sites, above, at, and below a sewage works outfall on the South Wales river. Samples capable of degrading C_{12} AS after only one day's exposure were found at each site. No biodegradation of AS was reported at a pristine source site. The onset of biodegradation was more rapid following longer exposure of the river, suggesting the existence of an adaptive mechanism. A model of the die-away kinetics of degradation suggested that C_{12} AS were biodegraded by a bacterial population growing at the expense of endogenous carbon. The activity of the epilithic samples in degrading AS increased during the first four days of exposure at each site. The stabilized values (days 4–14) increased from the upstream site to the outfall, decreasing to intermediate values downstream. The sewage input had less effect on activities

in degrading AS than on bacterial cell densities. Little variation in growth characteristics was seen throughout colonization at the three sites. The authors concluded that the adaptation seen during exposure in the river was attributable to colonization of the epilithon by an existing population that degradedC_{12} AS and not to acquisition or adaptation of biodegrading capacity (Russell et al., 1991).

The half-life for primary degradation of 20 mg/litre C_{12} AS in seawater varied over a range of 0.26 to 0.34 days, and degradation was reported to follow first-order kinetics. Primary degradation was followed by an immediate increase in bacterial number and thymidine incorporation (Vives-Rego et al., 1987). C_{12} AS was found to be degraded rapidly in seawater, and 250 g/litre were found in sediment; at 25°C, 90% was degraded within five days. No lag phase was reported, and the degradation kinetics were reported to be first-order (Sales et al., 1987).

C_{15}–C_{16} AS were 98% removed at 15°C and 99% removed at 8°C (Gilbert & Pettigrew, 1984). Similarly, C_{12}–C_{15} and C_{12}–C_{14} AS were found (by the MBAS method) to be biodegraded during winter and spring in a trickling filter sewage treatment plant (Mann & Reid, 1971). These results suggest that temperature has no major effect on the removal of alkyl sulfates under environmental conditions.

Primary biodegradation of C_{12} AS was less affected by incubation temperature than that of other anionic surfactants in die-away tests with water from the Tama River, Japan. Primary biodegradation was complete within one day at temperatures of 21 and 27°C, within two days at 15°C, and within three days at 10°C (Kikuchi, 1985).

Over 99% of MBAS activity in activated sludge was lost in a 19-day OECD screening test and in the 28-day OECD confirmatory test. Mineralization of both C_{12}–C_{14} and C_{16}–C_{18} AS was complete, with 90–95% degradation for C_{12}–C_{14} AS and 77–88% for C_{16}–C_{18} AS in the two test systems (Steber & Wierich, 1987).

C4.2.1.3 Anaerobic degradation

Biodegradation of AS under anaerobic conditions has been reported in several studies, with 88% degradation of stearyl sulfate containing C_{14} AS in an anaerobic screening test (Birch et al., 1989) and 95% ultimate degradation of the same compound (Steber & Wierich, 1987).

C4.2.2 Abiotic degradation

No information was available.

C4.2.3 Bioaccumulation and biomagnification

Carp *(Cyprinus carpio)* were exposed to ^{35}S-C_{12} AS at a concentration of 0.85 mg/litre for up to 24 h. Within 1 h, AS was concentrated in the gills, hepatopancreas, and kidneys with concentration factors of 1.6, 1.4, and 1.5, respectively. After the initial uptake in the gills, the levels of AS fell, and other organs and tissues, such as the skin surface, muscle, brain, kidney, hepatopancreas, and gall-bladder showed gradual uptake over the exposure period. The concentration factors after 24 h ranged from 2.0 for the skin surface to 43 for gall-bladder. Blood and kidney also

showed uptake, but the levels after 24 h were less than those after 4 and 8 h, respectively. AS were lost rapidly from all tissues except the gall-bladder when the fish were kept in 'clean' water for 48 h (Kikuchi et al., 1978).

Carp maintained in water containing 0.5 mg/litre $^{35}S-C_{12}$ AS absorbed the compound within 1 h, and an equilibrium for the whole body and gall-bladder was reached within 24 h, with concentration factors of about 4 and 700, respectively. After 24 h, the levels of AS in hepatopancreas had decreased from the initial level. When the fish were transferred to 'clean' water, 50% of the AS was still present after 72 h (Wakabayashi et al., 1978).

When carp were exposed to $^{35}S-C_{12}$ AS at concentrations between 2.7 µg/litre and 40 mg/litre for up to 120 h, equilibrium was reached within 72 h, at concentration factors of 3.9–5.3, which were independent of the concentration of AS in solution (Wakabayashi et al., 1981).

In a study of the effect of chain length on the uptake of AS, carp were exposed to 0.5 mg/litre of $^{35}S-C_{12}$, $^{35}S-C_{14}$, or $^{35}S-C_{16}$ AS for 24 h. Absorption of AS reached a maximum within the exposure period. The whole-body concentration factors were 2.1, 11, and 73 for the three surfactants respectively, and thus increased with alkyl chain length. This tendency was also observed in gills and hepatopancreas, but the factors in the gall-bladder were almost the same for the three homologues. When fish were transferred to 'clean' water, the elimination rate decreased with increasing carbon chain length, and 50% of C_{16} AS was retained after 120 h (Wakabayashi et al., 1980).

The absorption, tissue distribution, metabolism, and route of excretion of 50 mg/litre C_{12} AS were studied in goldfish *(Carassius* auratus) exposed for 24 h. AS was absorbed mainly through the gills and was distributed rapidly throughout the body; it was absorbed to a lesser extent (20% of total) by cutaneous absorption and orally (8%). The highest concentration of AS was measured in the gall-bladder, mainly because of its small size. The greatest proportion of the absorbed AS was located in the body, gut, liver, and gall-bladder. The level of AS in the tissues fell by 38% over 24 h in unfed fish and by 68% in fed fish. The high concentration of AS in the liver and gall-bladder was thought to indicate metabolism of the compound in the liver. The metabolites of AS that were identified included successive products of ß-oxidation of the alkyl chain and butyric-4-sulfate (Tovell et al., 1975).

C4.3 Interaction with other physical, chemical, and biological factors

The presence of 1 mg/litre AS (chain length unspecified) had no significant effect on the uptake of mercury by phytoplankton (*Diogenes* sp.) or mussels (*Mytilus* sp.) (Laumond et al., 1973).

Exposure of bacteria to 20 mg/litre phenol and 0.5 mg/litre C_{12} AS resulted in a directly additive effect. Exposure to 2.5 mg/litre phenol and 0.5 mg/litre AS resulted in a synergistic effect. No interactive effects were reported between sodium cyanide and AS in the same test protocol (Dutka & Kwan, 1982).

C4.4 Ultimate fate following use

As no specific analytical method is available for AS, their concentrations in environmental samples have not been established. Like detergent compounds, AS are present in wastewater after use. A large proportion is removed during treatment of wastewater, mainly as a result of a combination of biodegradation and adsorption processes. As for other surfactants, these processes continue when AS are released into the environment.

C5. ENVIRONMENTAL LEVELS AND HUMAN EXPOSURE

Section summary

Data on the environmental concentrations of AS are limited. At sewage treatment plants where the influent concentrations of AS were < 0.01–0.7 mg/litre, the effluent contained predominantly C_{12} AS, at concentrations of < 0.005–0.1 mg/litre. Surface waters receiving treated wastewater contained AS at concentrations below the detection limit of 0.005 mg/litre.

Environmental levels

AS were measured at two sewage treatment plants in the United States where the influent concentrations were < 0.01–0.7 mg/litre, which were at least 2.4 times lower than those predicted on the basis of use of AS and per-capita wastewater in the United States. The predominant homologues of AS in untreated wastewater were C_{12}, C_{14}, and C_{15}. The effluent contained predominantly C_{12} AS, at concentrations of < 0.005–0.1 mg/litre, showing that removal exceeded 98% during rotating biological contact and activated sludge treatment. Surface waters receiving treated wastewater contained AS at concentrations below the detection limit of 0.005 mg/litre (Fendinger et al., 1992a,b).

C6. KINETICS

Section summary

AS are readily absorbed by the gastrointestinal tract after oral administration and are excreted principally in the urine, only minor

amounts being eliminated in the faeces. Penetration of AS through intact skin appears to be minimal. AS are extensively metabolized in various species to several metabolites. Butyric acid-4-sulfate has been identified as their major metabolite.

C6.1 Absorption, distribution, and excretion

In a study of the absorption of higher alcohol sulfates, ^{14}C-hexadecyl sulfate salts were administered orally to humans and dogs. After a single dose of 14.4 mg/kg bw of the salts to dogs, the maximal plasma concentration of hexadecyl sulfate (1.22–2.45 µg/ml) was reached within 30–60 min; 6 h later, the plasma concentration had decreased to about one-tenth of the peak value. Within 72 h, 50–79% of the administered dose had been excreted in the urine and 12–41% in the faeces. After a single dose of 360 mg to humans, the maximal plasma concentration was reached at 2 h, although there was marked variation between individuals (range, about 3.1–23 µmol/ml) (Merits, 1975).

Potassium dodecyl ^{35}S-sulfate was injected intravenously or intraperitoneally at 1 mg/ml to male and female rats. The proportions of the administered dose excreted in the urine and faeces and the amounts retained in the carcass after 24 h are shown in Table 36. Most of the radiolabel appeared in the urine of both male and female rats, although some was present as inorganic ^{35}S-sulfate. The intestinal flora do not play a significant role in the metabolism of potassium dodecyl ^{35}S-sulfate, since the distribution of radiolabel in the urine and faeces was similar in rats pretreated with antibiotics and in untreated rats. Whole-body autoradiograms of rats killed 5 min after administration of the compound by intraperitoneal injection showed significant amounts of radiolabel in the liver; the concentrations increased up to 30 min and then gradually declined, only trace amounts remaining after 4 h. The kidney was the only other organ in which any appreciable accumulation was reported (quantitative data not presented) (Denner et al., 1969).

In order to investigate the percutaneous absorption of AS, 0.5 ml of 25 mmol/litre sodium ^{14}C-dodecyl sulfate in water was applied to the dorsal skin (10 cm^2) of rats for 15 min. Heavy deposition of the surfactant on the skin surface and in the upper regions of the hair follicles was observed. The ^{14}C level in urine was calculated to be equivalent to a penetration of 0.26 µg/cm^2 per 24 h (Howes, 1975).

Table 36. Excretion of ^{14}C-alkyl sulfates by rats after injection of 1 mg/ml

Route of administration	Sex	Excretion (%)		
		Urine (total ^{35}S)	Faeces	
			Inorganic ^{35}S	Total ^{35}S
Intraperitoneal	Male	86.3	14.4	0.2
	Female	93.2	18.1	0.9
Intravenous	Male	95.6	23.5	-
	Female	97.4	11.4	-

From Denner et al. (1969)

In young swine administered sodium dodecyl ^{35}S-sulfate (3.3 mmol/animal) orally, the labelled compound was well absorbed from the intestine. Traces of radiolabelled sulfur were found only in bristles, bones, and bone marrow. The total amounts of ^{35}S retained in organs and tissues were 1.7% of the dose at 82 h, 0.6% at 200 h, and 0.18% at 10 weeks. About 90% of the sodium dodecyl sulfate was recovered in urine and about 10% in faeces at 140 h (Havermann & Menke, 1959).

Similar results were obtained in guinea-pigs in a study of the percutaneous absorption of 3 µmol sodium lauryl ^{35}S-sulfate in water through skin *in vivo*. Less than 0.4% of the dose was found to have penetrated the skin, on the basis of recovery of radiolabel in the urine, faeces, and expired air. The permeability constant was calculated to be 0.65 × 10^{-6} cm/min (Prottey & Ferguson, 1975).

In a study of the dermal absorption of some homologues of AS, ranging from octyl to octadecyl sulfate, by isolated human abdominal skin, no penetration of the dermis was detected (Blank & Gould, 1961).

The rates of excretion in urine and faeces after oral, intravenous, or intraperitoneal administration of ^{14}C- or ^{35}S-labelled C_{10}–C_{18} AS to rats, dogs, and humans are summarized in Table 37.

C6.2 Biotransformation

Potassium dodecyl ^{35}S-sulfate was extensively metabolized in rats to yield a single ester sulfate, identified as butyric acid 4-^{35}S-sulfate (III in scheme below), and inorganic ^{35}S-sulfate.

Table 37. Excretion of alkyl sulfates (AS) in the urine and faeces of rats, dogs, and humans

ASa	Species	Treatment	Length of treatment (h)	Excretion (%)		Reference
				Urine	Faeces	
^{35}S-AS(C_{10})-K	Rat	1 mg/rat ip	48	82.9	1.2	Burke et al. (1975)
				79.5	1.0	

^{35}S-AS(C_{11})-K	Rat	1 mg/200 g ip	48	98.2 90.6	2.5 7.3	Burke et al. (1976)
	Rat	1 mg/200 g po	48	75.1 88.7	14.3 5.7	
	Rat	1 mg/200 g iv	48	85.9 74.8	5.9 18.5	
^{35}S-AS(C_{12})-K	Rat	1 mg/rat ip	48	86.3 93.2	0.2 0.9	Denner et al. (1969)
	Rat	1 mg/rat po	48	98.7 106.9	0.7 0.5	
^{35}S-AS(C_{16})-EM	Rat	14.4 mg/kg po	96	94	5	Merits (1975)
^{14}C-AS(C_{16})-EM	Rat	14.4 mg/kg po	72	87	3	
^{35}S-AS(C_{16})-Na	Dog	2.9 mg/kg iv	72	83	3	
^{14}C-AS(C_{16})-TMA	Dog	4.4 mg/kg iv	48	50	41	

Table 37 (contd)

ASa	Species	Treatment	Length of treatment (h)	Excretion (%) Urine	Faeces	Reference
^{35}S-AS(C_{16})-EM	Dog	14.4 mg/kg po	72	52	37	
^{14}C-AS(C_{16})-EM	Dog	14.4 mg/kg po	72	65	26	
^{14}C-AS(C_{16})-EM	Human	250 mg po	72	80 20	7 73	
^{35}S-AS(C_{18})-K	Rat	1 mg/rat ip	48	77.1 73.9	1.1 2.6	Burke et al. (1975)
	Rat	1 mg/200 g po	48	76.7 68.8	4.1 6.1	
^{35}S-AS(C_{18})-Na	Rat	4 mg/rat po	48	95.3	2.2	Adachi et al. (1979)

[a] K, potassium salt; EM, erythromycin salt; TMA, trimethylammonium salt

These compounds were degraded by a process involving initial omega-oxidation followed by ß-oxidation of fatty acids with successive elimination of a C_2 fragment. The final product of degradation of potassium dodecyl ^{35}S-sulfate was potassium butyric acid 4-^{35}S-sulfate, which was excreted in urine. When this product was injected intraperitoneally into rats, it was mostly eliminated unchanged in the urine, but about 20% of the dose was present as an inorganic ^{35}S-sulfate. These findings suggest that the sulfate ester is hydrolysed *in vivo* (Denner et al., 1969).

Butyric acid 4-sulfate was hydrolysed nonenzymatically *in vitro* at pH 5.0 and above, and the 4-butyrolactone (IV) and inorganic SO_4^{2-} ion were liberated in approximately equimolar amounts (Ottery et al., 1970).

After administration of ^{14}C-hexadecyl sulfate to rats, dogs, and humans, the main metabolite was identified as the sulfate ester of 4-hydroxybutyric acid. A minor metabolic product, *tert*-^{14}C-butyrolactone, was also isolated from the urine of rats, dogs, and humans. The urine of dogs contained still another metabolite, which was isolated and identified as glycollic acid sulfate (V) (Merits, 1975).

$HOOC-CH_2-CH_2-CH_2OSO_3H$ $OC-CH_2-CH2CH_2$ $HOOC-CH_2OSO_3H$

Butyric acid 4-sulfate (III) 4-Butyrolactone (IV) Glycollic acid sulfate (V)

Qualitative analysis of ^{35}S in the urine of rats administered potassium decyl ^{35}-sulfate or potassium octadecyl ^{35}-sulfate intravenously showed that butyric acid 4-^{35}-sulfate was the major metabolite and inorganic ^{35}-sulfate a minor metabolite; no unchanged compound was detected (Burke et al., 1975).

Similar results were obtained when sodium octadecyl ^{35}-sulfate was administered orally to rats . It was suggested that alkylsulfates with even-numbered carbons, like C_{10}, C_{12}, C_{16}, and C_{18}, are degraded by a common pathway involving omega-oxidation followed by ß-oxidation, and finally excreted in urine as metabolized forms with C_4 or C_2 (Adachi et al., 1979).

The metabolism of surfactants with odd-numbered carbon chains, like C_{11} potassium undecyl ^{35}-sulfate, was also investigated in rats. Propionic acid 3-^{35}-sulfate was identified as the major metabolite in urine; pentanoic acid 5-^{35}-sulfate and inorganic ^{35}-sulfate were identified as minor metabolites (Burke et al., 1975, 1976).

C7. EFFECTS ON LABORATORY MAMMALS AND IN VITRO TEST SYSTEMS

Section summary

The oral LD_{50} values for AS in rats ranged from 1000 to

4120 mg/kg bw. AS irritate the skin and eye at concentrations of about 0.5% or more. Although the effects of short- and long-term exposure to AS in animals have been investigated, most of the studies are limited by inadequate histopathological examination or small group size. Toxic effects have been reported in rats administered AS in the diet or drinking-water at concentrations equivalent to $\geq$ 200 mg/kg per day.

Maternal toxicity and fetotoxic effects have been observed at a dose equivalent to 200 mg/kg per day.

The available long-term studies are inadequate to evaluate the carcinogenic potential of AS in experimental animals; however, in the limited studies available, in which animals were administered AS in the diet, there was no evidence of carcinogenicity.

On the basis of limited data, AS also do not appear to be genotoxic *in vivo* or *in vitro*.

7.1 Single exposures

The oral, intraperitoneal, intravenous, and dermal LD_{50} values for AS are summarized in Table 38. The acute oral toxicity of AS in rats and guinea-pigs may vary with the length of the alkyl chain, and compounds with shorter chains are less toxic. The low LD_{50} value for sodium lauryl sulfate after dermal application to rabbits may indicate rapid skin penetration.

There were no overt signs of poisoning, except diarrhoea in rats given sodium coconut alcohol sulfate orally (Brown & Muir, 1970); however, signs of central nervous stimulation, including tremors, tonic-clonic convulsions, and respiratory collapse, were observed in rabbits, guinea-pigs, and rats given lauryl sulfate dermally and in rabbits given the compound intravenously (Carson & Oser, 1964).

In animals that died after receiving large doses of AS, the main gross pathological findings were haemorrhage and congestion of the stomach wall and bloodstained urine. Histopathological examination of rats given the sodium sulfate derivative of 3,9-diethyltridecane-4-ol orally revealed congestion, cloudy swelling of convoluted tubules with marked toxic degeneration of the cells, and granular detritus in the kidneys of animals killed by the LD_{50}, whereas only congestion and cloudy swelling were seen in the kidneys of animals that survived the LD_{50}. At larger doses, similar severe kidney injury and necrosis of the intestinal villi of the entire mucosal surface of the small intestine were observed. Only minor injury was seen in the liver, and the other organs examined were normal (Smyth et al., 1941).

Table 38. Acute toxicity of alkyl sulfates (AS)

Species	Sex	Route	LD_{50}[a]	Test material	Reference
Mouse	NS	po	2900	C_8 sodium AS	Gloxhuber (1974)
			2200	C_{10} sodium AS	
			2700	C_{12} sodium AS	
			3000	C_{14} sodium AS	
			> 8000	C_{16} sodium AS	
			> 8000	C_{18} sodium AS	
Rat	M	po	4120	40% solution of sodium 2-ethylhexanol sulfate	Smyth et al. (1941)
	M	po	1250	25% solution of sodium 7-ethyl-2-methyl undecanol-4 sulfate	
	M	po	1425	25% solution of sodium 3,9-diethyl tridecanol-6 sulfate	
	M	po	2730	30% solution of sodium lauryl sulfate	
	F,M	po	1280 (C_{12-C15})	86% sodium laury sulfate	Walker et al. (1967)
	F,M	po	1000-2000	Sodium coconut alcohol sulfate (mainly C_{12})	Brown & Muir (1970)
	F,M	ip	210	Sodium lauryl sulfate	Epstein et al. (1939)
	F,M	Dermal	2000 (100% deaths)	30% slurry of sodium lauryl sulfate	Carson & Oser (1964)

Table 38 (contd)

Species	Sex	Route	LD_{50}[a]	Test material	Reference
Guinea-pig	F,M	po	1520	40% solution of sodium 2-ethylhexanol sulfate	Smyth et al., (1941)
	F,M	po	650	25% solution of sodium 7-ethyl-2-methyl undecanol-4 sulfate	
	F,M	po	425	25% solution of sodium 3,9-diethyl tridecanol-6 sulfate	
	F,M	Dermal	1200 (no deaths)	33% slurry of sodium lauryl sulfate	Carson & Oser (1964)
	F,M	Dermal	2000 (100% deaths)	33% slurry of sodium lauryl sulfate	

Rabbit	F,M	Dermal	580	33% slurry of sodium lauryl sulfate
	F,M	iv	121 (100% deaths)	33% slurry of sodium lauryl sulfate

M, male; F, female
[a] As active ingredient

C7.2 Short-term exposure

The results of short-term tests for toxicity with repeated doses are summarized in Table 39.

C7.2.1 Rat

C7.2.1.1 Administration in the diet

Groups of five male and five female Wistar rats were fed diets containing technical-grade sodium lauryl sulfate (purity, 98%) at a concentration of 0, 0.5, 1, or 2% (equivalent to 245, 490, or 980 mg/kg of diet per day) for two or four weeks. No abnormalities were seen in behaviour or food intake; but body weight gain was significantly suppressed in females at the highest dose, and haematological examination revealed a significant decrease in red blood cells at two weeks. Biochemical examination of the serum revealed a significant increase in the glucose level at two weeks in males given 2%, a significant increase in glutamate-oxalate transaminase at two weeks in females given 1 or 2%, significant increases in glutamate-pyruvate transaminase and alkaline phosphatase activities at four weeks in all females, and a significant decrease in cholinesterase activity at four weeks in females given 2%. Both the absolute and relative weights of the liver and thyroid were increased at two weeks in males and females given 2%, and those of the liver and left kidney were increased at four weeks in all females; the weights of the thymus were decreased in males given 2% at four weeks. Histopathological examination of rats with increased liver weight revealed slight swelling of liver cells and increased numbers of dividing liver cells. This finding was considered to be an adaptation to administration of the test material. Cylinders in the renal tubules, vacuolar degeneration of the epithelial cells of the renal tubules, periodic acid-Schiff stain-positive substances in the renal tubules, and atrophy of the renal glomeruli were observed mainly in rats given 1 or 2% (Oishi et al., 1974).

Groups of 25 albino rats (sex not specified) were given diets containing a sodium lauryl sulfate formulation (Iriumr) at a dose of 0, 30, or 60 mg/animal per day for eight weeks. The only abnormal sign in the experimental groups was soft stools. Histological examinations of the livers of four rats in each group revealed swelling of liver cells, compression of cellular cords, and prominent nuclei. These effects were particularly marked in rats given the high dose (Hatton et al., 1940).

Table 39. Results of short-term exposure of experimental animals to alkyl sulfates (AS)

Species, strain, numbers per group	Material	Route	Dosage	Results	Reference
Rat, Wistar, 10	AS, C_{12} (a.i. 98%)	Diet	0, 0.5, 1.0, 2.0%, 4 weeks	Changes in haematological parameters, serum enzyme activities, and liver; depressed body weight gain in females at highest dose; increased weights of liver, thyroid and kidney at highest dose; decreased thymus weight in males	Oishi et al. (1974)
Rat, 25	AS, C_{12} (Irium^{R})	Diet	30, 60 mg/rat per day, 5 weeks	Dose-related hepatic effects	Hatton et al. (1940)
Rat, Wistar, 5	AS, C_{12}	Diet	1.5%, 12 weeks	Changes in serum, renal, and hepatic enzyme activities; depressed body weight gain; increased liver weight	Ikawa et al. (1978)
Rat, Osborne-Mendel, 5 M	AS, C_{12}	Diet	9, 2, 4, 8%, 4 months	Diarrhoea, abdominal bloating; depressed body weight gain	Fitzhugh & Nelson (1948)
Rat, Carworth, 24	AS, C_{12}-C_{15} (a.i. 86%)	Diet	9, 0.04, 0.02, 0.1, 0.5%, 13 weeks	Increased liver weight in females at highest dose	Walker et al. (1967)
Rat, Wistar, 5, 10	AS	Drinking-water	0, 0.25, 0.5, 1.0, 2.0, 4.0%, 30 days	Renal changes; proteinuria; depressed body weight gain at 4% sodium 2-ethylhexanol sulfate	Smyth et al. (1941)
Rat, Wistar 15 M	AS (a.i.22.5%)	Dermal	5 mg/kg per day, 30 days	Dermal irritation; hepatic effects	Sakashita et al. (1974)

Table 39 (contd)

Species, strain, numbers per group	Material	Route	Dosage	Results	Reference
Rat, Wistar (NS) M	AS (a.i. 22.5%)	Dermal	5 mg/kg per day, 30 days	Hepatic degeneration	Sakashita (1979)
Rabbit 3 M, 3 F	AS, sodium lauryl sulfate	Dermal	6, 60, 150 mg/kg, 5 times/week, 3 months	Dermal irritation	Carson & Oser (1964)

a.i., active ingredient; M, male; F, female; NS, not specified
Groups of five male Wistar SPF rats were fed a diet containing

sodium dodecyl sulfate at a concentration of 1.5% (equivalent to 750 mg/kg of diet per day) for 2, 4, or 12 weeks, and were compared with a control group. Body weight gain was suppressed and relative liver weight significantly increased from two weeks. Biochemical analysis of serum revealed increased activities of alkaline phosphatase and glutamate-pyruvate transaminase and a decreased level of cholesterol. Enzymatic examinations of the liver showed decreased activity of glucose-6-phosphatase at 12 weeks, decreased activity of glucose-6-phosphate dehydrogenase and increased activity of lactate dehydrogenase at each observation time, and increased isocitrate dehydrogenase activity at 4 and 12 weeks. Examination of the renal cortex showed decreased activities of 5'-nucleotidase and Mg-ATPase at 12 weeks and increased isocitrate dehydrogenase activity at 4 and 12 weeks. Examination of the renal medulla showed decrease activities of Mg- and Na,K-ATPases and increased isocitrate dehydrogenase activity at 12 weeks (Ikawa et al., 1978).

Groups of five male Osborne-Mendel rats were given diets containing sodium lauryl sulfate at a concentration of 0, 2, 4, or 8% (equivalent to 1000, 2000, or 4000 mg/kg of diet per day) for four months. Significant inhibition of growth was observed with 4%; severe diarrhoea and marked abdominal bloating were noted at 8%, and all the rats died within two weeks. Autopsy revealed irritation of the gastrointestinal tract in rats fed 8% (Fitzhugh & Nelson, 1948).

Technical-grade sodium lauryl sulfate (86% w/w active ingredient; chain length distribution, C_{12}-C_{15}) was fed to four groups of 12 male and 12 female Carworth Farm 'E' rats at a dietary level of 0, 40, 200, 1000, or 5000 ppm (corresponding to 2, 10, 50, or 250 mg/kg bw per day) for 13 weeks. No abnormalities were observed in behaviour, body weight, food intake, haematological parameters, urinary pH or osmolality, serum urea or protein, or organ weights, except for a significant increase in the absolute weight of the liver in females fed 5000 ppm (Walker et al., 1967).

C7.2.1.2 Administration in the drinking-water

Groups of five or 10 male Wistar rats were given water containing sodium 2-ethylhexanol sulfate, sodium 7-ethyl-2-methyl undecanol-4 sulfate, or sodium 3,9- diethyl tridecanol-6 sulfate at a concentration of 0, 0.25, 0.5, 1, 2, or 4% for 30 days. Water intake was decreased at concentrations $\geq$ 2% of sodium 2-ethylhexanol sulfate and sodium 7-ethyl-2-methyl undecanol-4 sulfate and at $\geq$ 1% sodium 3,9-diethyl tridecanol-6 sulfate. Body weight gain was suppressed at 4% sodium 2-ethylhexanol sulfate. None of the rats died, and no haematological abnormalities were observed during the experiment. Proteinurea was seen at 2 and 4% sodium 2-ethylhexanol sulfate. The major histopatho-logical findings were renal changes, including light cloudy swelling and secretion in the renal tubules and congestion or dilation of Bowman's capsule. The no-effect doses were

0.44 g/kg bw per day of sodium 2-ethylhexanol sulfate, 0.1 g/kg bw per day of sodium 7-ethyl-2-methyl undecanol-4 sulfate, and 0.25 g/kg bw per day of sodium 3,9- diethyl tridecanol-6 sulfate (Smyth et al., 1941).

C7.2.1.3 Dermal application

A group of 15 male Wistar rats received 2 ml of a commercial preparation of AS (22.5% active ingredient) on their backs, and the livers of three rats were examined under the electron microscope three and 30 days later; a control group was available. Redness of the skin and wrinkles were observed in treated animals at 24 h; the redness subsequently increased, the dermis became lacerated, and bleeding occurred. These lesions reached a peak at 57 days but tended to regress about 10 days later. Five rats died within the first 19 days. Electron microscopy at three days revealed separation of the intercellular space, cells with a high electron density, elongation of mitochondria, swelling of the smooth-surfaced endoplasmic reticulum, and a decreased prevalence of fatty droplets. Electron microscopy at 30 days showed liver parenchymal cells filled with mitochondria, apparently abnormally divided and proliferated smooth-surfaced endoplasmic reticulum, abnormally rough-surfaced cells, a typical Golgi apparatus, myelin-like structures in bile canaliculi, and extracellular prolapse of mitochondria (Sakashita et al., 1974).

Electron microscopy of the liver was also performed after dermal application of a commercial preparation of AS (22.5% active ingredient) to male Wistar rats (number not specified) at a dose of 5 mg/kg active ingredient once a day for 30 days. Hepatic degeneration, seen as atrophy and a high density of liver cells, was observed; in cells, there was deformation of nuclei, mitochondria, and the Golgi apparatus, an increased number of lysosomes, and swelling of endoplasmic reticula (Sakashita, 1979).

As no information was given on the method of application (occluded or non-occluded), these results were not interpretable in terms of risk to human health.

C7.2.2 Rabbit

Sodium lauryl sulfate was applied dermally to three groups, consisting of two male and two female rabbits with intact skin and one male and one female rabbit with abraded skin, at a dose of 6, 60, or 150 mg/kg bw five times per week for three months. A control group consisted of one male and one female with intact skin and one male with abraded skin. Dose-related irritation of the skin was observed in all treated animals (Carson & Oser, 1964).

C7.3 Long-term exposure; carcinogenicity

C7.3.1 Mouse

In a study of the effects of AS on the carcinogenicity of benzo[a]pyrene (BaP), a 10% AS solution, a 0.3% BaP solution, and a 10% AS:0.3% BaP solution were applied to the backs of groups of 10 male and 20 female mice twice a week for one year. Skin tumours appeared in all mice treated with BaP or AS:BaP. The average ages at the appearance of skin tumours were 119 days in the group exposed to BaP and 102 days in that exposed to AS:BaP. It was concluded that AS accelerated the induction of tumours by BaP ($p < 0.1$). Untreated mice and vehicle (acetone) controls had no skin tumours; one female exposed to AS had a skin tumour, but this finding was not considered to be related to treatment (Yamamoto, 1977).

C7.3.2 Rat

C7.3.2.1 Administration in the diet

Three groups of 12 weanling male Osborne-Mendel rats were given food containing sodium lauryl sulfate at a concentration of 0.25, 0.5, or 1.0% for two years; there was a similar sized control group. No effects attributable to the test material were observed on growth, mortality, or the macroscopic or histopathological appearance of organs. No tumours were reported (Fitzhugh & Nelson, 1948). As there were few animals per group and no toxic effects at any dose, the observations are considered to be of limited value.

C7.3.2.2 Administration in the drinking-water

Groups of 4–11 white rats were given drinking-water containing sodium lauryl sulfate at a concentration of 0, 0.1, 0.25, 0.5, 1, 5, or 10% for 120 or 160 days. Dose-related increases in mortality occurred at doses $\geq$ 0.25%; at doses $\geq$ 5%, all rats died. Histological examination of rats exposed to doses $\geq$ 0.25% revealed marked inflammatory changes of the lumen of the oesophagus in those that died, but the changes were slight in surviving animals. No abnormalities were seen in the liver, kidney, or intestine. The intake of the materials was about 30 mg/animal per day in those given 0.1% and 150 mg/animal per day in those given 1.0% (Epstein et al., 1939).

Groups of 9 or 10 weanling male Wistar rats were given drinking-water containing technical-grade sodium lauryl sulfate at a concentration of 0, 0.05, or 0.25% for five months. Growth was not suppressed, even at the higher concentration, and the activities of serum enzymes, including glutamate-oxalate and glutamate-pyruvate transaminases, alkaline phosphatase and cholinesterase, were not affected. At 0.25%, the triglyceride level increased in the liver but decreased in serum, while hepatic and serum levels of cholesterol, phospholipids, and free fatty acids were unchanged. Increased weights of spleen, lung, and kidney were noted at 0.25%. Histopathologically diagnosed broncho-pneumonia, observed in all animals given 0.25% and two animals given 0.05%, was considered to be a characteristic effect of the test material (Fukazawa et al., 1978).

The results of long-term studies are shown in Table 40.

C7.4 Skin and eye irritation; sensitization

C7.4.1 Local irritation

C7.4.1.1 Skin

Groups of two to six white rats received a subcutaneous injection of 1 ml of one of 10 solutions of sodium AS, ranging from 0.125 to 10% and were observed for one week after the injection. No reactions occurred at 0.125%, but sloughing and subcutaneous lumps in the skin appeared in rats given doses $\geq$ 0.19%. In a study in which the diffusibility of trypan blue was used as an index of irritation, groups of five to nine white rats were given subcutaneous injections of 0.2 ml sodium AS at one of six concentrations ranging from 0.15 to 5%. Two hours after the injection, slight reactions were seen in animals given 0.15% and marked reactions in those given 2.5 or 5% (Epstein et al., 1939).

Groups of three albino rabbits received closed-patch applications of 5 ml of 1, 5, or 25% sodium lauryl sulfate solution on intact and abraded areas of shaven abdominal skin. Over a 14-day period, 10 applications were made to intact skin and three to abraded skin; additionally, small amounts of the material were applied daily to the intact ears of groups of three rabbits. Occluded application to the abdomen produced erythema and blistering, which was more severe on abraded skin. Application to the intact ear resulted in very slight erythema at the 1% concentration, very slight to slight erythema at 5%, and slight erythema with moderate to severe burns at 25% (Olson et al., 1962).

Sodium alcohol (coconut alcohol, mainly C_{12}) sulfate solutions of 0.1, 1.0, and 2.5% were applied in occluded tests in rabbits as 1 ml of each solution on the back three times on three days. Macroscopic and histological examination seven days after application revealed no abnormalities at 1.0% and moderate irritation at 2.5%. In open tests, 1 ml of each of the solutions was applied to the backs of rabbits and 0.5 ml to the backs of guinea-pigs five times a week for 4.5 weeks. No abnormal findings were seen in animals receiving 0.1 or 1.0% groups, but there was moderate irritation at 2.5% (Brown & Muir, 1970).

Table 40. Results of long-term exposure of experimental animals to alkyl sulfates (AS)

Species, strain, numbers per group	Material	Route	Dosage	Results	Reference

Mouse, ddy/SLC 10 M, 20 F	10% AS, 3% benzo[*a*]pyrene	Dermal	Twice per week, 1 year	Skin tumours	Yamamoto (1977)
Rat, Osborne-Mendel 10-12 M	1.0%AS, C_{12}	Diet	0, 0.25, 0.5, 1.0%, 2 years	No effects	Fitzhugh & Nelson (1948)
Rat, Wistar, 9-10	AS, C_{12}	Diet	0, 0.05, 0.25%, 5 months	Increased weights of spleen, lung, and liver at highest dose	Fukuzawa et al. (1978)
Rat, 4-11	AS, C_{12}	Diet	0, 0.1, 0.25, 0.5 1.0, 5.0%, 160 days	Oesophageal irritation	Epstein et al. (1939)

Groups of three male Wistar rats received applications of 0.5 g of a 20 or 30% solution of linear lauryl sulfate (C_{12}; purity, 98.91%) on the back once a day for 15 days. The skin at the application site and the tissues of the tongue and oral mucosa (to determine the effects of licking) of animals receiving the 30% solution were examined histologically 16 days after application. Body weight gain was inhibited in the group given the 20% solution; body weight was decreased in the group at 30%, and two rats had died by the end of the experiment. A dry, thick, yellowish-white or reddish-brown crust was observed after two to three days in animals given 20% and after one to two days in those given 30%. When the crust was abraded several days later, ulcers occurred at the abraded site, which remained unchanged for 16 days in animals at 20% group and were aggravated in those at 30%. Histological examination of the application site revealed severe necrosis extending from the epidermis to the upper layer of the dermis, dense inflammatory-cell infiltration into the upper layer of the dermis just below the necrotic area, diffuse inflammatory-cell infiltration throughout the dermis, swelling of collagenous fibres in the dermis, and sloughing. Histological examination of the tongue revealed necrosis extending from the surface to the middle epithelial layer of the mucosa, inflammatory-cell infiltration into the upper layer of the dermis, and sloughing. Histological examination of the mucosa of the oral cavity revealed thickening of the stratum corneum and germinative and slight degeneration (pale staining) of epithelial cells (Sadai & Mizuno, 1972).

The effects of sodium lauryl sulfate on oesophageal and gastric mucosa were studied in cats by irrigation and pledget techniques. In the irrigiation technique, the stomachs and oesophaguses of two cats were filled with 10 and 20% solutions of sodium lauryl sulfate, respectively, for 15 min, and then tissues were taken for histological examination. Pledgets soaked in 10 or 20% sodium lauryl sulfate solution were applied to the exposed oesophageal and gastric mucosa of two other cats for 10 min, and specimens were taken 90 min later. The 10% solution produced moderate injury to the oesophagus, consisting of intramucosal oedema and congestion and loss of superficial epithelial layers; in the stomach, there was hydropic degeneration, loss of surface mucosal cells, vascular congestion with submucosal oedema, and occasional focal ulceration. Treatment with the 20% solution resulted in more extensive damage, and particularly extensive submucosal oedema and disruption and erosion of the superficial mucosa of both the oesophagus and stomach (Berensen & Temple, 1976).

C7.4.1.2 Eye

Three drops of one of nine solutions of sodium lauryl sulfate ranging from 0.019 to 5.0% were instilled into the eyes of rabbits three times at 10-min intervals, and the rabbits were observed for 48 h. There were no abnormal findings at 0.038%, but slight chemosis and redness were seen at 0.075% and marked chemosis and redness at 5% (Epstein et al., 1939).

The minimal concentration of sodium lauryl sulfate that caused corneal necrosis (detected by fluorescein staining) after instillation into the eyes of rabbits was 0.1% (Smyth et al., 1941). In another study, two drops of a 1, 5, or 25% solution of sodium lauryl sulfate were instilled into both sides of the eyes of groups of three rabbits; 30 min later, one of the eyes was washed. Moderate corneal injury was observed in unwashed eyes of animals receiving the 5 or 25% solution; in washed eyes, either slight conjunctivitis or moderate corneal injury was observed at 25%, slight conjunctivitis at 5%, and only very slight conjunctivitis at 1% (Olson et al., 1962).

In an irritation test based on a method developed by the United States Food and Drug Administration, 0.1, 1, or 25% solutions of sodium coconut alcohol sulfate were instilled into the eyes of rabbits. No reaction was seen at 0.1%; mild conjunctivitis lasting for 48 h was seen at 1%, and severe conjunctivitis lasting for 72 h was observed at 25% group, but there was no permanent damage (Brown & Muir, 1970). Solutions of a synthetic alkyl sulfate and five AS consisting mainly of C_{10}, C_{12}, C_{14}, C_{16}, or C_{18}, were instilled at concentrations of 0.01–5% into the eyes of three rabbits, which were observed for 168 h. The materials caused similar reactions. No abnormalities were seen at 0.01%. Slight congestion and marked congestion or oedema were observed at 0.05 and 0.1% within 2 h, but these effects had disappeared 24 h later. In the groups given $\geq$ 0.5%, marked reactions were seen for 24 h, including severe congestion and oedema, increased lachrymal secretion, turbidity of the cornea, and disappearance of the corneal reflex, but these tended to regress and had disappeared completely by 120 h (Iimori et al., 1972).

C7.4.2 Skin sensitization

A 0.1% solution of a sodium lauryl sulfate derivative of coconut alcohol was applied to the skin or injected intradermally into groups of 10 guinea-pigs three times per week for three weeks. Ten days later the animals received challenge doses and were observed for 48 h. No reaction occurred in the group treated dermally, but a slight reaction was observed 24 h after the challenge in some of the guinea-pigs

treated intradermally (Brown & Muir, 1970).

C7.5 Reproductive toxicity, embryotoxicity, and teratogenicity

Daily doses of 0.2, 2, 300, or 600 mg/kg bw of AS were administered by gavage to CD rats, CD-1 mice, and NZW rabbits. Groups of 20 rats and mice were given AS on days 6–15 of pregnancy, and groups of 13 rabbits were treated on days 6–18 of pregnancy. The doses of 0.2 and 2 mg/kg bw per day were estimated to be equivalent to 1–2 and 10–20 times the maximal amount of AS to which humans are exposed. Three rats given 600 mg/kg bw died during the study, but the surviving rats and those given 300 mg/kg bw had only mild to moderate inhibition of body weight gain. Mice given 600 mg/kg bw showed severe effects, including anorexia and inhibition of body weight gain, and four animals died during the study; in those given 300 mg/kg bw, inhibition of body weight gain was mild to moderate. Rabbits given 600 mg/kg bw showed severe effects, including diarrhoea, anorexia, and reduced rate of body weight gain, and 11 died during the study; those given 300 mg/kg bw showed mild to moderate reduction of body weight gain. No toxic effects were seen in any of the animals given 0.2 or 2 mg/kg bw. No adverse effects were seen on litters of rats at any dose. Some mice and rabbits at each dose had total litter loss, but the other litter parameters did not differ from those of controls. No major malformations were seen at any dose in offspring of rats, mice, or rabbits, and the incidence of skeletal variations in offspring of rats given 600 mg/kg bw was significantly low. A high incidence of skeletal anomalies was seen in litters of mice given 600 mg/kg bw, and those of rabbits at 2.0 mg/kg bw had a significantly higher incidence of skeletal variations; however, the incidences of anomalies and variations were within the background range (Palmer et al., 1975a).

Groups of 21 ICR mice received applications of 15 mg/kg bw per day of a 0.4, 4, or 6% aqueous solution of AS (98% sodium dodecyl sulfate, 0.5% N_2SO_4, 0.1% NaCl, and 0.1% H_2O) to a 3 × 3-cm^2 area of shaven dorsal skin on days 6–13 of pregnancy. The 0.4% solution was equivalent to about 10–12 times the specified concentration used by humans, and the application area was equivalent to about one-seventh of the total surface area of the mouse. The body weight gain of dams exposed to the 4 or 6% solution was reduced; there were no deaths. The numbers of dams with surviving young were 19/21 in the control group, 20/20 at 0.4%, 17/20 at 4%, and 11/21 at 6%; the decrease in dams at 6% was significant. Fetal weights were significantly lower in dams at 4 and 6%, but there were no other differences from the control values. The incidence of cleft palate was fairly high in offspring of dams exposed to the 4 or 6% solution, and a tendency to delayed ossification was seen; however, none was significant (Takahashi et al., 1976).

A dose of 0.1 ml/day of a 2% aqueous solution of AS was applied to a 2 × 3-cm^2 area of shaven dorsal skin in groups of 20–26 ICR mice on days 1–17 of pregnancy. The same dose of a 20% solution was applied to a similar group up to the 10th day of pregnancy, and implantation was examined on the 11th day. In addition, 14 mice were injected subcutaneously with 2 mg/kg bw per day of AS on days 8–10 of pregnancy. The numbers of dams with implantations were 18/20 controls, 14/22 at 2%, 1/26 at 20%, and 13/14 at 2 mg/kg bw; the decrease at 20% was significant. There were no significant changes in litter parameters and no significant changes in the incidences of major malformations, minor anomalies, or skeletal variations. AS thus disturbed implantation and caused abortion at maternally toxic doses, but in surviving litters it had no effect on the size or numbers of fetuses, although low fetal weight and delayed ossification were observed. At doses that had no or only mild effects on the dams, no adverse effects were seen on the fetuses. The effects of AS on the fetus therefore appear to be secondary to the toxic effects on the dams (Nomura et al., 1980).

C7.6 Mutagenicity and related end-points

Sodium lauryl sulfate did not cause differential toxicity in *Bacillus subtilis* H17 (*rec*$^+$) or M45 (*rec*$^-$) at concentrations of 20–2000 µg/plate, and it did not induce reverse mutations in *Salmonella typhimurium* TA98 or TA100 at 1–500 µg/plate or in *Escherichia coli* WP2 *trp* at 10–1000 µg per plate (Inoue & Sunakawa, 1979).

Sodium lauryl sulfate, Dobanol 25 sulfate LCU, and Dobanol 25 sulfate HCB (aliphatic alcohol sulfates with chain lengths of C_{10}–C_{15}) were fed in the diet to groups of six male and six female Colworth/Wistar rats for 90 days at a concentration of 0.56 or 1.13%, the latter being the maximal tolerated dose. No effect was seen on chromosomes in bone-marrow cells (Hope, 1977).

After dodecyl sulfate was administered to male ddY mice intra-peritoneally at 50 mg/kg bw, the incidence of polychromatic erythrocytes with micronuclei in the bone marrow was similar in treated and control groups (Kishi et al., 1984).

C7.7 Special studies

Intravenous injection of 1 mg/min sodium decyl sulfate or 5.7 mg/min sodium dodecyl sulfate to cats increased pulmonary arterial pressure, caused a small increase in systemic vascular resistance, and reduced the ventilation volume per minute after about 5 min. Intravenous injection of 4.6 mg/min sodium octyl sulfate or 6.3 mg/min sodium tetradecyl sulfate had similar effects. The increase in pulmonary arterial pressure was considered to be due to a direct

effect on the smooth muscle of blood vessels and bronchi. The blood sugar level was unchanged (Schumacher et al., 1972).

The effects of sodium lauryl sulfate on histamine release from

mast cells were studied *in vitro* in peritoneal mast cells isolated from rats. Histamine was released at a concentration of 0.03 mmol/litre, and the critical micelle concentration in buffer at 22°C was 1.0 mmol/litre. Sodium lauryl sulfate and its mono- and tri-ethoxy derivatives had the most potent histamine releasing capacity of nine surfactants with a chain length of C_{12} (Prottey & Ferguson, 1975).

C8. EFFECTS ON HUMANS

Section summary

In patch tests, human skin can tolerate contact with solutions containing up to 1% AS for 24 h with only mild irritation. AS caused delipidation of the skin surface, elution of natural moisturizing factor, denaturation of the proteins of the outer epidermal layer, and increased permeability and swelling of the outer layer. They did not induce skin sensitization in volunteers, and there is no evidence that they induce eczema. No lasting injuries or fatalities have been reported following accidental ingestion of detergent formulations containing AS.

C8.1 Exposure of the general population

Surface-active agents are found in shampoos, dishwashing products, household cleaners, and laundry detergents, and AS are major components of these products. The composition of nonionic and ionic surfactants varies between 10 and 30%. Surface-active agents can affect human skin and eyes.

C8.2 Clinical studies

C8.2.1 Skin irritation and sensitization

AS can be mildly to moderately irritating to human skin. No data were available on sensitization.

The relative intensity of skin erythema produced on the lower back of volunteers was evaluated by applying concentrations of 0.2–5.4% of C_8, C_{10}, C_{12}, C_{14}, or C_{16} AS under a closed patch for 24 h or under a closed patch re-applied once daily for 10 days. C_{12} AS were more potent than AS with other alkyl chain lengths (Kligman & Wooding, 1967).

A circulation method was used to evaluate the relative intensity of skin roughness induced on the surface of the forearms of volunteers after application for 1 min of 1% aqueous solutions of AS with an alkyl chain length of C_8, C_{10}, C_{12}, or C_{14}. The potential to cause skin roughness increased with alkyl chain length, reaching maximal intensity at C_{12} (Imokawa et al., 1974, 1975a). In other studies, the relative degree of skin roughening was correlated with the extent of protein denaturation but not with irritating potential determined in a closed-patch test (Imokawa et al., 1975b).

Primary skin irritation induced by a 1% aqueous solution (pH 6.8) of dodecyl sulfate (relative molecular mass, 288.5) was studied in a 24-h closed-patch test on the forearms of seven male volunteers. The relative intensity of skin irritation was scored by grading erythema, fissuring, and scaling. The average score for AS was 4.86, whereas that for a water control was 1.79. Dodecyl sulfate was more irritating than either LAS or AOS (Oba et al., 1968a).

The intensity of skin irritation produced by a 1% aqueous solution of sodium AS was studied in a 24-h closed-patch test on the forearm and in a 40-min drip test on the interdigital surface in which the compound was dripped once daily for two consecutive days at a rate of 1.2–1.5 ml/min. Skin reactions were scored by grading erythema in the patch test and by grading scaling in the drip test. The average scores were 2.5 for primary skin irritation at 24 h in the patch test and 1 for scaling at two days in the drip test; in both tests, the control value was 0. AS was more irritating than LAS or AOS in the patch test, whereas the score of AS for skin scaling in the drip test was similar to that of LAS but higher than that of AOS (Sadai et al., 1979).

Moderate to intense erythema was produced on the forearms of 10 volunteers in a 24-h closed-patch test by a 10% aqueous solution of AS with an average chain length of C_{12}. The mean irritation scores were significantly higher at 26 h (2.85 out of 8 possible points) and at 28 h (2.88) than at 24 h (2.00), when the patches were removed. Irritation had decreased by 48 h, and a significant decrease in the intensity of inflammation was apparent at 96 h (Dahl & Trancik, 1977).

In a 48-h patch test on the upper arms of 100 pairs of twins (54 monozygotic, 46 dizygotic) with a solution of 0.5% C_{12} AS, no reaction was seen in 50% of the subjects, and slight reaction, ranging from noninflammatory changes to mild erythema, in the other 50%. The response was not related to the type of twin (Holst & Moller, 1975).

Application of aqueous 0.5, 1, or 2% solutions of AS with an average chain length of C_{12} to the backs of healthy male volunteers produced epidermal hyperplasia. Treatment with the 1% solution induced an approximately 30-fold increase in mitotic activity, which peaked 48 h after treatment. Application of either the 0.5 or the 2% solution induced similar but milder changes (Fisher & Maibach, 1975).

Skin permeability to C_8, C_{10}, C_{12}, C_{14}, C_{16}, and C_{18} AS prepared as 0.02, 0.5, and 1% solutions (0.58% C_8 and 0.74% C_{18}) was studied by a circulation method on the forearms of healthy

male and female volunteers. C_{12} AS attained maximum permeation, whereas the permeation of C_8 and C_{18} AS was of the same order as that of water. The authors pointed out the close relationship between permeation and irritation (Szakall & Schulz, 1960).

C8.2.2 Effects on the epidermis

The effects of AS on the stratum corneum include delipidation of the skin surface, elution of natural moisturizing factor, denaturation of protein of the stratum corneum, increased permeability, swelling of the stratum corneum, and inhibition of enzyme activities in the epidermis. These effects, and some others, constitute a potential hazard to the epidermis.

The water-holding capacity of thin sheets of callus isolated from the plantar surface of the human foot, with relative moisture contents of 76, 88, and 97%, was compared before and after immersion in water, AS, or soap solution. Water-holding capacity was measured as the weight of water taken up from each solution. The relative moisture content decreased after treatment with AS or soap solution (Blank & Shappirio, 1955).

Elution of natural moisturizing factor was compared for nine kinds of surfactants, including AS, in the arm immersion test, in patch tests, and by measuring eluted amino acids and protein, skin permeation, and freeing of sulfhydryl groups. AS induced a strong reaction in the immersion test and relatively strong reactions in the other tests. The author concluded that the immersion test was the best simulation of actual use (Polano, 1968).

A detergent consisting of long-chain AS was shown to denature stratum corneum protein and thus expose enclosed sulfhydryl groups (Anson, 1941). AS readily released sulfhydryl groups from stratum corneum obtained from abdominal skin taken at autopsy within 12 h of death, but there was no correlation between changes in epidermal permeability and the amounts of sulfhydryl released (Wood & Bettley, 1971). AS were the most effective surfactants with regard to denaturation of protein, measured as inhibition of invertase activity (Imokawa et al., 1974; Okamoto, 1974). AS were found to denature skin keratin (a filamentous protein), bovine serum albumin (a globular protein), acid phosphatase (an enzyme protein), and membrane lysozymes (membrane protein) (Imokawa & Katsumi, 1976). Sodium laurate was reported to produce swelling of the stratum corneum (Putterman et al., 1977).

AS with a hydrophobic chain length of C_{12} were maximally absorbed on human callus. Extraction of proteins from human callus was also a function of chain length: C_{12} and C_{14} AS were much more active than C_8, C_{10}, and C_{18} AS (Dominguez et al., 1977).

C8.2.3 Hand eczema

In a 24-h closed-patch test of 0.2–0.5% aqueous solutions of AS on the fingers of nine women with hand eczema, skin lesions were not exacerbated, although four women felt slight itching at the patch site (Sasagawa, 1963).

C8.2.4 Accidental or suicidal ingestion

Four members of a family accidentally ingested unknown quantities of a household detergent containing 24% lauryl sulfate, 60% sodium tripolyphosphate, and 16% anhydrous soap. Shortly after ingestion, all of the family members experienced abdominal pain and nausea. The 10-year-old daughter and 13-year-old son felt oropharyngeal pain, and the son was found at endoscopic examination to have a 2.5 × 2 cm oropharyngeal burn in the right posterior pharynx and first-degree burns of the oesophagus. The mother had erythema, friability, erythema and a few superficial erosions of the distal oesophagus, and gastritis evidenced by exudate and petechial lesions on the mucosa. The father had haematemesis on a few occasions. The mother, father, and son were examined about one month after the incident by an X ray examination after a barium meal; no strictures were found (Berenson & Temple, 1974).

C9. EFFECTS ON OTHER ORGANISMS IN THE LABORATORY AND THE FIELD

Section summary

AS have been studied in short- and long-term studies in the laboratory and in one study carried out under more realistic conditions. Their toxicity is dependent on alkyl chain length, but no data were available on the differential toxicity of linear and branched AS.

In aquatic organisms, the EC_{50} values for C_{12} AS in a community of marine microorganisms were 2.1–4.1 mg/litre. The NOEC values were 35–550 mg/litre (C_{16}/C_{18}) for *Pseudomonas putida and* 14–26 mg/litre (C_{12}–C_{16}/C_{18}) for green algae; and the EC_{50} values were > 20–65 mg/litre (C_{12}–C_{13}) for green algae and 18–43 mg/litre (C_{12}) for macrophytes.

In aquatic invertebrates, the L(E)C_{50} values were 4–140 mg/litre (C_{12}/C_{15}–C_{16}/C_{18}) for freshwater species and 1.7–56 mg/litre (all C_{12}) for marine species. The long-term NOECs were 16.5 mg/litre (C_{16}–C_{18}) for *Daphnia magna* and 0.29–0.73 mg/litre (chain length not specified) for marine species.

In fish, the LC_{50} values were 0.5–5.1 mg/litre (C_{12}–C_{16} or chain length not specified) for freshwater species and 6.4–16 mg/litre (all C_{12}) for marine species. In a 48-h study of *Oryzias latipes,*

chain length influenced LC_{50} values, the measured concentrations being 46 mg/litre for C_{12}, 2.5 mg/litre for C_{14}, and 0.61 mg/litre for C_{16}. This and other studies indicate that toxicity differs by a factor of five for two units of chain length.

In a flow-through study of the effect of C_{16}–C_{18} AS on a biocenosis, an NOEC of 0.55 mg/litre was observed. Many of the studies of toxicity in aquatic environments were carried out under static conditions. As AS are readily biodegraded, this design may result in underestimates of toxicity.

Few data were available on the effects of AS on terrestrial organisms. An NOEC of > 1000 mg/kg (C_{16}–C_{18}) was reported for earthworms and turnips.

C9.1 Microorganisms

During tests of biodegradation, marine bacteria used 20 mg/litre AS as a nutrient source. It was therefore concluded that its toxicity for the bacterial community studied is nil or very low (Vives-Rego et al., 1987). In a study of the effect of C_{12} AS on the metabolic activity of a marine microbial community, the EC_{50} values for toxic effects on thymidine incorporation and glucose metabolism were reported to be 4.1 and 2.1 mg/litre, respectively. AS also increased exoproteolytic activity (Vives-Rego et al., 1986).

The 30-min EC_{50} for C_{16}–C_{18} AS, based on oxygen consumption, was 35 mg/litre in *Pseudomonas putida* (Robra, 1976). The NOEC for cell reproduction in *Pseudomonas putida* exposed to C_{16}–C_{18} AS was 550 mg/litre (Bringmann & Kühn, 1977).

C9.2 Aquatic organisms

C9.2.1 Aquatic plants

C9.2.1.1 Freshwater algae

The phytoflagellate alga *Poterioochromonas malhamensis* was exposed to C_{12} AS at sublethal concentrations of 28.8, 57.6, 72, 86.4, 100.8, and 115.2 mg/litre (100, 200, 250, 300, 350, and 400 µmol/litre), being transferred every three to four days into fresh medium with a higher test concentration. The initial cell density in each medium was 0.1×10^6 cells/ml; the final cell density, after exposure to the highest concentration of AS, was 0.05×10^{6} cells/ml, which was similar to that reached after exposure of unacclimatized algal cultures to 200 µmol/litre AS. Exposure to AS at 57.6 mg/litre (240 µmol/litre) was reported to affect mitosis and cytokinesis, with the formation of cells containing up to 12 nuclei. Exposure of the alga to 50.4 mg/litre (175 µmol/litre) AS resulted in a 24% increase in telophases (binucleated cells). Cells with eight nuclei were also reported in this culture (Röderer, 1987).

The green alga *Selenastrum capricornutum* was exposed to analytical grade C_{12} AS at a concentration of 10, 20, 30, 40, 50, or 100 mg/litre in synthetic medium for three weeks. Growth was reduced by 30% at the lowest concentration (Nyberg, 1988).

The green alga *Chlamydomonas reinhardi* was exposed to 0.02, 0.2, or 2.0 mmol/litre of C_{10}, C_{12}, C_{14}, C_{16}, or C_{18} AS for 7–10 days. Photometric absorption (652 nm) by the exposed cultures was no different from that by controls for the first six days of exposure, although it was reduced slightly at 2 mmol/litre. The authors concluded that the AS were present at below the critical micelle concentration at all concentrations tested (Ernst et al., 1983).

The EC_{50} for growth of the green alga *Selenastrum capricornutum* exposed to C_{12} AS for two to three days was within the range 45–65 mg/litre (Yamane et al., 1984). An EC_{50} of 9 mg/litre C_{14} AS was found for growth of S. capricornutum (Konno & Wakabayashi, 1987).

C9.2.1.2 Macrophytes

The seven-day EC_{50} values for C_{12} AS in the duckweed Lemna minor under flow-through conditions were 43 mg/litre for frond count, 29 mg/litre for dry weight, and 18 mg/litre for root length.

The time-independent EC_{50} for growth rate/doubling time was 44 mg/litre (Bishop & Perry, 1981).

C9.2.2 Aquatic invertebrates

The acute toxicity of AS to aquatic invertebrates is summarized in Table 41. The 48-h LC_{50} values were 8–60 mg/litre for daphnids; the 96-h LC_{50} values ranged from 3.2 to 4.2 mg/litre for marine invertebrates.

The 48-h LC_{50} for lugworms *(Arenicola marina)* exposed to AS was calculated to be 15.2 mg/litre (95% confidence interval, 13.2–17.6). Tissues from lugworms exposed to AS at a concentration close to that of the LC_{50} were examined for changes in morphology by both light and electron microscopy: serious damage was found in the epidermic receptors and less serious damage in the caudal epidermis and gills. No morphological effects were reported on the thoracic epidermis or intestine. AS caused separation inside the caudal epithelial layer, resulting in holes in some caudal papillae. Deciliation of the epidermic receptors was also reported. The authors concluded that the physiological response of damaged epidermic receptors was reduced or blocked after exposure to AS. AS also induced fissures in the epithelial layer of the gills (Conti, 1987).

Caeriodaphnia dubia were exposed to C_{12} AS for three generations under static renewal conditions, with the following mean water parameters: temperature, 26.2°C; pH, 8.2; hardness, 94.4 mg/litre $CaCO_3$; and alkalinity, 82.2 mg/litre $CaCO_3$. The water was changed every second day. The LC_{50} for survival of three broods of *C. dubia* was calculated to be 41 ± 3.2 mg/litre. The mean EC_{50}, based on progeny produced, was calculated to be 36 ± 3.2 mg/litre. No statistically significant effects were reported after exposure to 83 mg/litre AS, although the size of later broods was reduced (Cowgill et al., 1990).

The effect of 0.25–10 mg/litre AS was studied on the growth and survival of eggs and larvae of oysters *(Crassostrea virginica)* and clams *(Mercenaria mercenaria)*. The minimal concentrations that caused a significant reduction in the number of fertilized eggs which developed into normal larvae two days after hatching were 0.73 mg/litre for clams and 0.29 mg/litre for oysters. The minimal concentration that caused a significant reduction in growth and survival between two and 12 or 14 days after hatching was 1.46 mg/litre for both species. The EC_{50} values, based on the development of fertilized clam and oyster eggs to normal straight-hinge larvae after 48 h, were calculated to be 0.47 mg/litre for clams and 0.37 mg/litre for oysters (Hidu, 1965).

After snails *(Lymnaea peregra)* were exposed to C_{12} AS at measured concentrations of 0.6–12 mg/litre for six days, a significant, dose-related reduction in the dry weight of shells was observed, but the organic content of shells was not significantly affected at any concentration (Tarazona & Nunez, 1987).

C9.2.3 Fish

The acute toxicity of AS to fish is also summarized in Table 41. The 48-h LC_{50} values were 0.5–51 mg/litre for medaka *(Oryzias latipes)*. A 96-h LC_{50} value of 1.7 mg/litre was reported for both rainbow trout *(Salmo gairdneri)* and sheepshead minnow *(Cyprinodon* variegatus). The acute toxicity of AS to fish tends to increase with increasing carbon-chain length.

Rainbow trout *(Oncorhynchus mykiss)* and goldfish *(Carrasius auratus)* were exposed to C_{12} AS at a concentration of 70 mg/litre at different levels of water hardness. Trout treated in hard water (300 mg/litre $CaCO_3$) died within 40–45 min; those treated in soft water (60 mg/litre $CaCO_3$) died after 3 h. Goldfish treated in hard water died within 90–110 min, whereas those treated in distilled water (no $CaCO_3$) were alive and apparently normal after 24 h (Tovell et al., 1974). When yearling rainbow trout were maintained in water containing C_{12} AS at a concentration of 100 mg/litre, the time to 50% lethality was calculated to be 4.9 h. The changes seen in the gills were typical of an acute inflammatory reaction: The gill epithelium was lifted away from the underlying tissue, and lymphocytes and granulocytes invaded the subepithelial spaces. Large numbers of epithelial cells died, but the epithelium was not punctured (Abel & Skidmore, 1975).

After exposure of the eggs of carp *(Cyprinus carpio)* to AS of various chain lengths from spawning to hatching, the LC_{50} values were calculated to be 18 mg/litre for C_{12} AS, 2.9 mg/litre for C_{14} AS, and > 1.6 mg/litre for C_{16} AS (Kikuchi et al., 1976).

The minimal avoidance concentration of AS, i.e. the concentration at which fish spend 65% of a 5-min period in clean water in order to avoid AS, was 7.1 µg/litre for medakas *(Oryzias latipes)* (*Hidaka et* al., 1984). The threshold concentrations for avoidance of AS by ayu *(Plecoglossus altivelis)* were 4.0 µg/litre of a formulation and 8.4 µg/litre of pure reagant AS (Tatsukawa & Hidaka, 1978). The environmental relevance of avoidance studies is questionable (see also section A9.3.3.4 of the monograph on LAS).

Larvae of the fathead minnow (Pimephales promelas) were exposed to C_{12} AS at a concentration of 1.2, 2.3, 4.6, 9.2, or 18.4 mg/litre for seven days under static renewal conditions. Survival and final dry weight were not significantly affected at concentrations up to and including 4.6 mg/litre; however, at 9.2 and 18.4 mg/litre, no fish

Table 41. Toxicity of alkyl sulfates (AS) to aquatic organisms

Species	Size or age	Static or flow	Temp. (°C)	Hardness or salinity	pH	AS chain length	End-point	Concn (mg/litre)	Reference
Eastern oyster (Crassostrea virginica)	Embryo	Static	20	25[a]		C_{12}	48-h LC_{50}	1.7[b]	Mayer (1987)
Mysid shrimp (Metamysidopsis swifti)	Juvenile	Static	25	30[a]		C_{12}	96-h LC_{50}	3.2[b]	
Mysid shrimp (Mysidopsis bahia)	Juvenile	Static	25	20[a]		C_{12}	96-h LC_{50}	4.2[b]	
	Adult	Static	22			C_{12}	96-h LC_{50}	6.62	Roberts et al. (1982)
Shrimp (Neomysis americana)	Adult	Static	22	20.0 ± 0.5[a]		C_{12}	96-h LC_{50}	7.24	
Copepod (Eurytemora affinis)	Adult	Static		10[a]		C_{12}	96-h LC_{50}	2.6	
(Acartia tonsa)	Adult	Static				C_{12}	96-h LC_{50}	0.55	
Scud						NS	72-h LC_{50}	9–46	Gilbert &

(Gammarus pulex)							Pettigrew (1984)
Water flea (Daphnia magna)	Static	20		C_{12}	24-h EC_{50}	17.4	Snell & Persoone (1989)
	Static	20		C_{12}	24-h EC_{50}	27.5	Persoone et al. (1989)
				C_{16}-C_{18}	24-h EC_{50}	27.5	Steber et al. (1988)
				C_{12}	24-h EC_{50}	10.5-24.3	Cowgill et al. (1990)

Table 41 (contd)

Species	Size or age	Static or flow	Temp. (°C)	Hardness or salinity	pH	AS chain length	End-point	Concn (mg/litre)	Reference
Water flea (Daphnia pulex)						C_{12}	24-h LC_{50}	15.0	Snell & Persoone (1989)
						C_{12}	24-h LC_{50}	9.5-20.5	Cowgill et al. (1990)
Mosquito (Aedes aegypti)	2nd/3rd stage	Static	25			C_{12}-C_{15}	24-h LC_{50}	4	van Emden et al. (1974)
Rainbow trout (Salmo gairdneri)		Flow	15	350-375[c]	8.3-8.5	NS	96-h LC_{50}	4.62	Fogels & Sprague (1977)
						NS	96-h LC_{50}	1.7	Gilbert & Pettigrew (1984)
Atlantic silverside (Menidia menidia)	59 mm	Static	22	10[a]		C12	96-h LC_{50}	6.4	Roberts et al. (1982)
Medaka (killifish) (Oryzias latipes)							48-h LC50	10	Tomiyama (1974)
	323 mg	Static[r]	23-24		5.6-5.8	C_{12}	24-h LC_{50}	70[b]	Kikuchi et al.
	323 mg	Static[r]	23-24		5.6-5.8	C_{12}	48-h LC_{50}	51[b]	(1976)
	323 mg	Static[r]	19-21		5.6-5.8	C_{14}	24-h LC_{50}	5.9[b]	
	323 mg	Static[r]	19-21		5.6-5.8	C_{16}	24-h LC_{50}	0.78[b]	
	323 mg	Static[r]	19-21		5.6-5.8	C_{12}	48-h LC_{50}	0.5[b]	
	approx. 262 mg	Static[r]	21-22		6.7-7.1	C_{12}	48-h LC_{50}	46[d]	Kikuchi &
	approx. 262 mg	Static[r]	21-22		6.7-7.1	C_{12}	48-h LC_{50}	2.5[d]	Wakabayashi
	approx. 262 mg	Static[r]	21-22		6.7-7.1	C_{12}	48-h LC_{50}	0.61[d]	(1984)

Table 41 (contd)

Species flow	Size or (°C)	Static or or salinity	Temp.	Hardness length	pH	AS chain (mg/litre)	End-point	Concn	Referenceage
Sheepshead minnow (Cyprinodon variegatus)	Juvenile	Static	25	20[a]		C_{12}	96-h LC_{50}	1.7[b]	Mayer (1987)
Fathead minnow (Pimephales promelas)	NS	Static	NS	80-400	7.4-8.2	NS	96-h LC_{50}	5-6	Henderson et al. (1959)
	< 30 d	Static	20			C_{15}	48-h LC_{50}	7.8	Cowgill et al.
	<30 d		17			C_{12}	24-h LC_{50}	7.7-9.7	(1990)
	<30 d		17			C_{12}	96-h LC_{50}	7.0-9.0	
	30±2 d		20			C_{12}	48-/96-h LC_{50}	38.0	
Carp (Cyprinus carpio)	4.4 mg	Static	22	25	7	C_{10}	12-h LC_{50}	180[b]	Kikuchi et al.
	4.4 mg	Static	22	25	7	C_{10}	48-h LC_{50}	13[b]	(1976)
	4.4 mg	Static	22	25	7	C_{12}	12-h LC_{50}	46[b]	
	4.4 mg	Static	22	25	7	C_{14}	48-h LC_{50}	5.0[b]	
	4.4 mg	Static	22	25	7	C_{16}	12-h LC_{50}	0.69[b]	
	4.4 mg	Static	22	25	7	C_{16}	48-h LC_{50}	0.69[b]	

Static, water unchanged for duration of test; NS, not specified; flow, flow-through conditions: AS concentration in water maintained continuously; static[r], static renewal: water changed at regular intervals

[a] Salinity (‰)

[b] Based on nominal concentrations

[c] Hardness expressed as mg/litre $CaCO_3$

[d] Based on measured concentrations

survived. When the test was repeated over an eight-day period, significantly reduced survival was seen at 4.6 mg/litre, but this result was variable, as some replicates did not show significant effects. The mean of the geometric means of the NOEC and LOEC values for the embryo-larval test was 3.8 mg/litre; the mean LC_{50} value was 5.5 mg/litre (Pickering, 1988).

An LC_{50} value of 38 mg/litre was reported for fathead minnows exposed to C_{12} AS for either 48 or 96 h. The authors suggested that the same value was obtained because the tests were not carried out aseptically and the C_{12} AS had degraded completely within 48 h (Cowgill et al., 1990).

C9.2.4 Tests in biocenoses

In a flow-through biocenosis test, 13 species of aquatic organisms were exposed to C_{16}-C_{18}AS. The species used represented several trophic levels: seven species of algae, four species of protozoa, and two species of rotifers. An NOEC of 0.55 mg/litre was reported for 'biocenotic toxicity'. The lowest concentration at which biocenotic toxicity was reported was 1.65 mg/litre (Guhl, 1987).

C9.3 Terrestrial organisms

No information was available.

APPENDIX I

APPENDIX I.

Reference values for intakes and body weights of laboratory animals, with conversion factors for deriving no-observed-adverse-effect levels (NOAELs) in milligrams per kilogram per day from doses administered as parts per million

Species	Body weight (kg)	Inhalation rate	Water consumption	Food consumption	Dose conversion[a]		
					Air (m^3/day)	Water (litres/day)	Food (g/day)
Mouse	0.03[b]	0.04[b]	0.006[b]	4[b]	1.33	0.20	0.13
Rat	0.35[b]	0.11[d]	0.05[b]	18[b]	0.31	0.14	0.05
Hamster	0.14[b]	0.13[b]	0.03[b]	12[b]	0.93	0.21	0.09
Guinea-pig	0.84[b]	0.40[b]	0.20[b]	34[b]	0.48	0.24	0.04
Rabbit	3.8[b]	2.0[b]	0.41[b]	186[b]	0.53	0.11	0.05
Rhesus monkey	8.0[b]	5.4[c]	0.53[b]	320[b]	0.68	0.07	0.04
Dog	12[b]	4.3[b]	0.61[b]	300[b]	0.36	0.05	0.03
Cat	1.5[d]	0.75[d]	0.15[e]	168[e]	0.50	0.10	0.11
Pig	80[e]	–	5.5[e]	2250[e]		0.07	0.03

From Health Canada (in press); most values have been rounded to two significant figures.
[a] Air: 1 mg/m^3 in air = *x* in mg/kg bw per day; water: 1 ppm (mg/litre) = *x* in mg/kg bw per day; food: 1 ppm in food = *x* in mg/kg bw per day
[b] From Calabrese & Kenyon (1991)
[c] Calculated from the minute volume of 220 ml/kg bw reported by Flecknell (1987)
[d] From Flecknell (1987); values are average of the ranges reported.
[e] From Canadian Council on Animal Care (1980–84); values are average of the ranges reported.

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ALKYLBENZENESULFATES A CHAINE DROITE ET COMPOSES VOISINS

1. RECAPITULATION, EVALUATION ET RECOMMANDATIONS GENERALES

1.1 Identité, propriété et méthodes d'analyse

Les alkylbenzènesulfonates à chaîne droite (appelé aussi alkylbenzènesulfonates linéaires ou ASL, les alpha-oléfine-sulfonates (AOS) et les alkylsulfates (AS)) sont des tensio-actifs anioniques dont les molécules sont caractérisées par la présence d'un groupement hydrophobe et d'un groupement hydrophile (polaire). Les produits du commerce sont des mélanges d'isomères et d'homologues de produits voisins, qui different par leurs propriétés physicochimiques et qui, sous leurs diverses formes, ont des applications variées.

L'analyse des ASL, des AOS et des AS peut se faire par des méthodes non spécifiques. On utilise généralement l'essai au bleu de méthylène, qui permet de mettre en évidence tout composé contenant un groupement anionique et un groupement hydrophobe. On peut donc être gêné par la présence d'autres substances lorsqu'on travaille sur des échantillons prélevés dans l'environnement; en outre, la sensibilité de la méthode n'est que de 0,02 mg/litre. On a mis au point d'autres méthodes non spécifiques qui peuvent se substituer à celles-ci mais on ne les utilise guère. En ce qui concerne les échantillons prélevés dans l'environnement, il n'existe de méthodes spécifiques que pour les ASL et les AS. En ce qui concerne les AOS, on dispose d'une méthode améliorée qui repose sur la réaction au bleu de méthylène et la chromatographie en phase liquide à haute performance (HPLC).

Les ASL sont des composés non volatils que l'on obtient par sulfonation des alkylbenzènes à chaîne droite. Les produits du commerce sont toujours constitués de mélanges d'homologues ayant des chaînes alkylées de différentes longueurs (C_{10}-C_{13} ou C_{14}) et d'isomères qui différent par la position du point d'attache de la chaine sur le noyau phényle (positions 2 à 5). Tous les homologues et isomères des ASL peuvent être dosés dans des échantillons environnementaux ou d'autres matrices au moyen de méthodes d'analyse spécifiques comme la HPLC, la chromatographie en phase gazeuse et la chromatographie en phase gazeuse couplée à la spectrométrie de masse.

Les AOS sont également des dérivés non volatils produit par sulfonation des alpha-oléfines. Ils consistent dans le mélange de deux types de composés, les alcène-sulfonates de sodium et les hydroxyalcane-sulfonates de sodium, avec une chaine alkylée en C_{14}-C_{18}.

Egalement non volatils, les AS s'obtiennent en traitant par l'acide sulfurique, les alcools d'origine oléochimique ou pétrochimique. Ce sont des mélanges d'homologues avec une chaîne alkylée en C_{10}-C_{18}. On met actuellement au point des méthodes d'analyse spécifiques pour la surveillance de l'environnement.

1.2 Sources d'exposition humaine et environnementale

On utilise les ASL, les AOS et les AS comme principes actifs de divers produits d'entretien ou d'hygiène personnelle, ou encore, pour certaines applications spéciales. Après usage, ces détergents sont rejetés dans l'environnement avec les eaux usées.

Il peut y avoir exposition professionnelle à ces composés. Quant à l'exposition de la population humaine en général et des êtres vivants dans leur milieu naturel, elle dépend du type d'application de ces substances (ou d'autres tensio-actifs), des pratiques locales en matière de traitement des effluents et des caractéristiques du milieu récepteur.

En 1990, la consommation mondiale de ces produits d'établissait à 2 millions de tonnes pour les ASL, 86 000 tonnes pour le AOS et 289 000 tonnes pour les AS.

1.3 Concentrations dans l'environnement

1.3.1 Alkylbenzènesulfonates à chaîne droite

On peut doser les ASL à l'aide de méthodes spécifiques et sensibles dans pratiquement tous les compartiments du milieu où ils sont susceptibles de se trouver. Leur concentration diminue progressivement selon la séquence suivante: eaux usées > effluents traités > eaux de surface > mer.

Dans les zones où l'on utilise principalement des ASL comme tensio-actifs, leur concentration est généralement de 1-10 mg/litre dans les eaux usées, de 0,05-0,1 mg/litre dans les effluents traités par voie biologique, de 0,05-0,6 mg/litre dans les effluents traités sur lit filtrant, de 0,005-0,05 mg/litre dans les eaux de surface situées au-dessous de déversoirs d'égouts (avec des concentrations qui tombent rapidement à 0,01 mg/litre en aval du déversoir), de < 1-10 mg/kg dans les sédiments de cours d'eau ($\leq$ 100 mg/kg dans les sédiments très pollués à proximité des zones de décharge), de 1-10 g/kg dans les boues d'égouts, de < 1 5 mg/kg dans les sols amendés à l'aide de boues d'égouts (initialement 5-10 mg/kg; on a trouvé des concentrations $\leq$ 50 mg/kg après d'importants épandages de boues, d'ailleurs non représentatifs). La concentration des ASL dans les eaux estuarielles varie de 0,001 à 0,01 mg/litre, mais elle peut être beaucoup plus élevée là où il y a déversement direct d'eaux usées. En mer, à distance du rivage, les concentrations vont de < 0,001 à

0,002 mg/litre.

Il est à noter que la concentration de ASL varie considérablement dans l'environnement. Ces variations sont dues à la diversité des méthodes d'analyse, des points de prélèvement (qui vont de zones très polluées où sont déversés des effluents insuffisamment traités à des secteurs où l'effluent a subi un traitement intensif), des périodes de prélèvement (ce qui selon le cas peut signifier une différence du simple au double) et enfin, des volumes de ASL consommés.

La surveillance de l'environnement montre que les ASL ne s'accumulent pas au cours du temps dans les différents compartiments du milieu. La concentration dans le sol, loin d'augmenter, diminue au contraire par suite de la minéralisation. Comme les ASL ne se décomposent pas en anaérobiose stricte (pour donner naissance à du méthane), on ne peut pas en conclure qu'ils subissent une minéralisation dans les sédiments anaérobies. Au taux actuel d'utilisation, les ASL parviennent dans les différents compartiments de l'environnement à un rythme sensiblement égal à celui de leur assimilation, ce qui crée les conditions d'un état stationnaire.

1.3.2 Les alpha-oléfine-sulfonates et alkyle-sulfates

Les données dont on dispose sur la concentration des AOS dans l'environnement sont limitées en raison de la difficulté à analyser les échantillons prélevés dans le milieu. En général, on peut déceler la présence des tensio-actifs anioniques au moyen de méthodes colorimétriques non spécifiques (comme celles qui sont basées sur la réaction au bleu de méthylène), mais la présence d'autres substances est gênante et ces méthodes ne permettent pas de procéder à un dosage spécifique des alpha-oléfine-sulfonates. Une méthode spécifique de dosage des AS dans l'environnement est en cours de mise au point.

Les études effectuées en laboratoire indiquent que les AOS et les AS sont rapidement minéralisés dans tous les compartiments de l'environnement et presque totalement éliminés des effluents au cours du traitement de ces derniers. Leur concentration dans les eaux de surface, les sédiments, le sol, les eaux estuarielles et le milieu marin est probablement faible. C'est précisément ce que l'on a constaté pour la concentration des AOS dans l'eau des rivières.

1.4 Transport, distribution et transformation dans l'environnement

Aux températures inférieures à 5-10°C, la cinétique de biodégradation des ASL, des AOS et des AS est ralentie en raison de la réduction de l'activité microbienne.

1.4.1 Alkylbenzène-sulfonates à chaîne droite

Les voies de pénétration des ASL dans l'environnement varient selon les pays, mais la porte d'entrée principale est constituée par la décharge des stations d'épuration des eaux usées. Lorsque ces stations sont inexistantes ou fonctionnent mal, il peut y avoir décharge directe dans les rivières, les lacs et la mer. L'épandage de boues d'égout sur les terrains agricoles peut également constituer une voie de pénétration de ASL dans l'environnement.

A mesure qu'ils pénètrent dans l'environnement, les ASL en sont éliminés par divers mécanismes qui vont de l'adsorption à la biodégradation ultime. Les ASL sont adsorbés sur les surfaces colloïdales et les particules en suspension, et l'on a mesuré des coefficients d'adsorption de 40-5200 litres/kg selon le milieu et la structure des ASL en cause. Ils subissent une biodécomposition dans les eaux de surface (demi-vie 1-2 jours), dans les sédiments aérobies (1-3 jours) ainsi que dans les écosystèmes marins et estuariels (5-10 jours).

Lors du traitement primaire des effluents, environ 25% des ASL (de 10-40%) s'adsorbent sur les boues résiduelles et sont rejetés avec elles. Ils ne sont pas éliminés au cours de la digestion anaérobie des boues mais au cours du traitement aérobie, leur demi-vie étant alors de 10 jours. Après épandage des boues sur le sol, les ASL sont générale-ment décomposés à hauteur de 90% en l'espace de trois mois, la demi-vie étant de l'ordre de 5-30 jours.

Le facteur de concentration des ASL dans le corps entier varie de 100 à 300 pour l'ensemble des ^{14}C-ASL et ^{14}C-métabolites. Ils sont captés par les poissons essentiellement à travers les branchies et se répartissent ensuite dans le foie et la vésicule après biotransformation. Les ASL sont rapidement excrétés et rien n'indique par conséquent qu'ils subissent une bioamplification.

1.4.2 alpha-Oléfine-sulfonates

Les données relatives au transport, à la distribution et à la transformation des AOS dans l'environnement sont encore moins nombreuses que dans le cas des ASL. On peut toutefois penser que les AOS sont transportées dans l'environnement à peu près comme les ASL, les AS et les autres détergents tensio-actifs et que leur destinée y est analogue à celles des ASL et des AS. En aérobiose, elles subissent une biodécomposition rapide et cette biodécomposition primaire est achevée en 2 à 10 jours, en fonction de la température. On ne dispose que de données limitées sur la bioaccumulation des AOS; en tout état de cause elles ne s'accumulent pas chez les poissons. On ne dispose d'aucune donnée sur leur décomposition en milieu abiotique.

1.4.3 Alkylsulfates

Les AS sont transportés dans l'environnement par des mécanismes analogues à ceux qui sont à l'oeuvre dans le cas des ASL et des AOS. Ils sont facilement biodégradable en aérobiose ou en anaérobiose, que ce soit au laboratoire ou dans l'environnement; la biodécomposition primaire est achevée en l'espace de 2 à 5 jours. Les facteurs de

bioconcentration pour le corps entier varient de 2 à 73 ainsi qu'avec la longueur de la chaîne des différents homologues. Chez les poissons, les AS sont captés, distribués, biotransformés et excrétés de la même manière que les ASL et ne se concentrent pas dans les autres organismes aquatiques.

1.5 Cinétique

Les ASL, les AOS et le AS sont facilement résorbés dans les voies digestives, après quoi ils se répartissent dans l'ensemble de l'organisme où ils sont largement métabolisés. Les ASL subissent une omega- et une ß-oxydation. Les composés initiaux et leurs métabolites sont principalement excrétés par la voie rénale, encore qu'une certaine proportion de la dose absorbée puisse l'être également pas la voie fécale, après métabolisation et passage dans les voies biliaires. Les ASL, les AOS et les AS ne sont absorbés qu'en quantités minimes par voie percutanée lorsque la peau est intacte, mais un contact prolongé peut altérer l'intégrité de la barrière épidermique, ce qui permet une résorption plus importante; à fortes concentrations, il peut y avoir réduction du temps de pénétration.

1.6 Effets sur les animaux de laboratoire et sur les systèmes d'épreuve *in vitro*

On a relevé, pour la DL_{50} des sels de sodium des ASL, des valeurs allant de 404 à 1470 mg/kg de poids corporel chez le rat et de 1259 à 2300 mg/kg de poids corporel chez la souris, ce qui incite à penser que les rats sont plus sensibles que les souris à l'action toxique des ASL. Chez la souris, on a obtenu une DL_{50} de 3000 mg/kg de poids corporel pour un sel de sodium d'AOS. Chez le rat, les valeurs de la DL_{50} par voie orale allaient de 1000 à 4120 mg/kg de poids corporel pour les AS. Les ASL, les AOS et les AS sont irritants pour la peau et les yeux.

Lors d'études subchroniques au cours desquelles on a administré à des rats des ASL dans leur nourriture ou leur eau de boisson à des concentrations quotidiennes correspondant à plus de 120 mg/kg de poids corporel, on a observé des effets minimes, qui consistaient notamment en modifications des paramètres biochimiques et altérations histopathologiques au niveau du foie. Bien que lors d'une étude, on ait observé des modifications ultrastructurales dans les hépatocytes à des doses plus faibles, ces modifications se sont révélées réversibles. D'ailleurs, les autres études n'ont pas révélé de tels

effets aux mêmes doses, mais il n'est pas exclu que lors de l'étude initiale, les organes aient fait l'objet d'un examen plus minutieux. Des effets ont également été observés sur la fonction de reproduction chez des animaux auxquels on avait administré des doses quotidiennes > 300 mg/kg; il s'agissait d'une réduction du taux de grossesse et d'une certaine mortalité dans les portées. Après application cutanée de longue durée à des rats de solutions de ASL à plus de 5% et application, également cutanée, du même type de solution à des cobayes à raison de 60 mg/kg de poids corporel pendant 30 jours, on a observé des modifications biochimiques et histopathologiques. Des applications cutanées répétées de solutions de teneur $\geq$ 0,3% de ASL ont produit des effets toxiques sur les foetus ainsi que sur la reproduction, mais les doses étaient également toxiques pour les femelles gestantes.

On n'a guère de données résultant d'études sur des animaux de laboratoire qui permettraient d'évaluer les effets potentiels des AOS chez l'homme. Aucun effet n'a été observé sur des rats ayant reçu, pendant une longue durée, des doses quotidiennes de 250 mg/kg de poids corporel en administration orale; toutefois une dose quotidienne de 300 mg/kg de poids corporel, toxique pour les femelles gestantes, a entraîné des effets foetotoxiques chez des lapins. L'application topique d'AOS sur la peau et les yeux de divers animaux de laboratoire a produit des effets localisés.

Les effets d'une exposition à long et à court terme aux AS ont été étudiés à plusieurs occasions sur l'animal mais la plupart des études en question pêchent par les insuffisances des examens histopathologiques ou la trop petite taille des groupes; en outre, les doses les plus élevées utilisées dans les études à long terme n'ont pas produit le moindre effet toxique, de sorte qu'il n'a pas été possible d'établir la valeur de la dose sans effets nocifs observables. Cependant, lorsqu'on a administré à des rats des concentrations quotidiennes de ces substances correspondant à 200 mg/kg de poids corporel ou davantage, par incorporation à leur nourriture ou à leur eau de boisson, on a systématiquement observé un certain nombre d'effets. En outre, l'application topique sur la peau ou les yeux d'AS à des concentrations égales ou supérieures à environ 0,5%, a donné lieu à une irritation localisée. Par ailleurs à fortes concentrations, on observe des effets toxiques sur les femelles gestantes ainsi que sur les foetus.

La plupart des études à long terme ne se prêtent pas à l'évaluation du pouvoir cancérogène des ASL, des AOS et des AS chez l'animal de laboratoire en raison de facteurs tel que le nombre trop faible d'animaux, un nombre de doses limité, la non détermination de la dose tolérée maximale, et, en outre, un examen histopathologique limité dans la majorité des cas. Dans les travaux où les effets anatomo-pathologiques ont été convenablement étudiés, on n'a pas déterminé la dose tolérée maximale et les doses employées n'ont pas produit d'effets toxiques. Toutefois et compte tenu de ces réserves,

on peut retenir que les études au cours desquelles on a administré à des animaux des ASL, des AOS et des AS par voie orale, n'ont pas révélé de signes de cancérogénicité; quant aux études à long terme consistant en applications topiques d'AOS par badigeonnage cutané, elles n'ont pas non plus révélé la présence d'effets imputables à ces substances.

Sur la base de ces données limitées, il ne semble pas que ces composés soient génotoxiques *in vivo* ou *in vitro.*

1.7 Effets sur l'homme

L'application d'un timbre cutané imprégné de solution contenant jusqu'à 1% de ASL, d'AOS ou d'AS pendant 24 heures montre que la peau humaine supporte le contact avec cette substance au prix d'une légère irritation. Ces tensio-actifs provoquent une délipidation de l'épiderme, une élution du facteur d'humidification naturelle, ainsi qu'une dénaturation des protéines de la couche épidermique externe, dont ils augmentent la perméabilité et dont ils provoquent le gonflement. Ni les ASL, ni les AOS, ni les AS n'ont provoqué de sensibilisation cutanée chez les volontaires et rien n'indique de façon concluante qu'ils puissent provoquer un eczéma. On n'a pas signalé de lésions graves ou mortelles consécutives à l'ingestion accidentelle de ces tensio-actifs.

1.8 Effets sur l'environnement

1.8.1 Alkylbenzène-sulfonates à chaîne droite

1.8.1.1 Milieu aquatique

Les ASL ont été très largement étudiés tant au laboratoire (études à court et à long terme) que dans des conditions plus proches de la réalité (études sur le micro- et le mésocosme et études en situation réelle). En général, la diminution de la longueur de la chaîne alkylée ou une plus grande intériorisation du groupement phényle s'accompagnent d'une diminution de la toxicité. Les observations effectuées sur des poissons et sur des daphnies montrent que lorsque la longueur de la chaîne diminue d'une unité (par exemple lorsqu'elle passe de C_{12} à C_{11}), la toxicité est approximativement divisée par deux.

Les résultats des tests en laboratoire sont les suivants:

-- *Microorganismes:* Les résultats sont très variables en raison de l'utilisation de systèmes d'épreuve très divers (par exemple inhibition des boues activées, cultures mixtes et espèces individuelles). Les valeurs de la CE_{50} vont de 0,5 mg/litre (une seul espèce) à > 1000 mg/litre. Dans le cas des microorganismes, il n'existe pas de relation linéaire entre la longueur de la chaîne et la toxicité.

-- *Plantes aquatiques:* Les résultats dépendent largement de l'espèce. En ce qui concerne les plantes d'eau douce, les valeurs de la CE_{50} se situent entre 10 et 235 mg/litre (C_{10}-C_{14}), dans le cas des algues vertes; entre 5 et 56 mg/litre ($C_{11,1}$-C_{13}), dans le cas des algues bleu-vert; entre 1,4 et 50 mg/litre ($C_{11,6}$-C_{13}) pour les diatomées et entre 2,7 et 4,9 mg/litre ($C_{11,8}$) pour les macrophytes. Il semble que les algues marines soient même encore plus sensibles. Dans le cas des algues, il n'y a probablement pas non plus de relation linéaire entre la longueur de la chaine et la toxicité.

-- *Invertébrés:* Les valeurs de la CE_{50} et de la CL_{50} (exposition aiguë) pour au moins 22 espèces d'eau douce se situent entre les limites suivantes: 4,6-200 mg/litre (longueur de chaine non précisée; C_{13}) dans le cas des mollusques; 0,12-27 mg/litre (longueur de chaine non précisée; $C_{11,2}$-C_{18}) dans le cas des crustacés; 1,7-16 mg/litre (longueur de chaine non précisée; $C_{11,8}$) dans le cas des vers et enfin 1,4-270 mg/litre (C_{10}-C_{15}) dans le cas des insectes. Dans le cas d'une exposition chronique, les valeurs de la CE_{50} et de la CL_{50} sont de 2,2 mg/litre ($C_{11,8}$) pour les insectes et de 1,1-2,3 mg/litre ($C_{11,8}$-C_{13}) pour les crustacés. La concentration sans effets chroniques observables (basée sur la mortalité ou des effets sur la fonction de reproduction) est de 0,2 à 10 mg/litre (longueur de chaîne non précisée; $C_{11,8}$) pour les crustacés. Il semble que les invertébrés marins soient plus sensibles, avec des valeurs de la CL_{50} allant de 1 à plus de 100 mg/litre (dans presque tous les cas, C_{12}) pour 13 espèces et avec une concentration sans effets observables de 0,025 à 0,4 mg/litre (longueur de chaine non précisée dans l'ensemble des tests) dans le cas des sept espèces étudiées

-- *Poissons:* Pour 21 espèces d'eau douce, les valeurs de la CL_{50} aiguë se situent entre 0,1 et 125 mg/litre (C_8-C_{15}); les valeurs de la CE_{50} et/ou de la CL_{50} pour une exposition chronique sont, pour deux espèces, respectivement égales à 2,4 et à 11 mg/litre (longueur de chaîne non spécifiée; $C_{11,7}$); quant à la concentration sans effets observables, elle va de 0,11-8,4 à 1,8 mg/litre (longueur de chaine non précisée; $C_{11,2}$-C_{13}) pour deux espèces. Dans ce cas encore, les poissons de mer se révèlent plus sensibles, avec des valeurs de la CL_{50} aiguë allant de 0,05 à 7 mg/litre (longueur de chaîne non spécifiée; $C_{11,7}$) pour six espèces et des valeurs de la CL_{50} chronique allant de 0,01 à 1 mg/litre (longueur de chaîne non précisée) pour deux espèces. Dans la plupart des publications, la longueur de la chaine n'est pas précisée. Pour des espèces marines, on a également fait état d'une concentration sans effets observables < 0,02 mg/litre (C_{12}).

Les produits communément utilisés dans le commerce ont en moyenne, une chaîne latérale en C_{12}. Des composés ayant diverses longueurs de chaîne ont été étudiés sur *Daphnia magna* et sur des poissons, mais dans le cas des autres organismes d'eau douce, c'est en général des

composés dont la longueur de chaine moyenne est de $C_{11,8}$ qui ont été utilisés. Les valeurs caractéristiques de la CE_{50} et de la CL_{50} aiguë

pour les ASL en C_{12} sont 3-6 mg/litre chez *Daphnia magna* et 2-15 mg/litre chez les poissons d'eau douce; celles de la concentration sans effets observables pour une exposition chronique sont de 1,2 à 3,2 mg/litre pour *Daphnia magna* et de 0,48-0,9 mg/litre pour les poissons d'eau douce. Chez les poissons de mer, les valeurs caractéristiques de la CL_{50} aiguë pour des ASL en C_{12} sont de < 1-6,7 mg/litre.

Les organismes halophiles et en particulier les invertébrés, se révèlent être plus sensibles aux ASL que les organismes d'eau douce. Chez les invertébrés, l'action séquestrante des ASL sur le calcium peut affecter la biodisponibilité de cet ion pour la morphogénèse. Les ASL exercent un effet général sur le transport ionique. Les produits de biodécomposition et les sous-produits des ASL sont 10 à 100 fois plus toxiques que les composés de départ.

Les résultats obtenus dans des conditions plus proches de la réalité sont les suivants: on a étudié les ASL au moyen de toute sorte de tests en eau douce et à plusieurs niveaux trophiques, notamment dans des enceintes lacustres (organismes inférieurs), dans des écosystèmes modèles (sédiments et réseaux hydrographiques), des cours d'eau en aval et en amont des déversoirs de stations d'épuration des eaux usées et enfin, des cours d'eau expérimentaux. Dans presque tous les cas on a utilisé des ASL en C_{12}. Les algues se sont révélées être plus sensibles en été qu'en hiver, les valeurs de la CL_{50} à 3 heures étant de 0,2 à 8,1 mg/litre après la photosynthèse, alors que dans les écosystèmes modèles, on n'observait aucun effet sur l'abondance relative des populations d'algues à la concentration de 0,35 mg/litre. Selon ces études, la valeur de la concentration sans effets observables se situe de 0,24 à 5 mg/litre selon l'organisme et le paramètre étudié. Ces résultats sont en assez bon accord avec ceux des épreuves en laboratoire.

1.8.1.2 Milieu terrestre

On dispose de données sur les végétaux et les lombrics. Pour sept espèces de plantes étudiées dans des solutions nutritives, on a obtenu des valeurs de la concentration sans effets observables qui se situent dans les limites < 10-20 mg/litre; pour trois espèces étudiées sur sol d'après leur croissance, on a obtenu 100 mg/kg (C_{10}-C_{13}). Pour les lombrics, la CL_{50} à 14 jours était > 1000 mg/kg.

1.8.1.3 Oiseaux

Une étude sur des poulets qui recevaient une nourriture contenant de ces substances, a permis de fixer à > 200 mg/kg la dose sans effets observables (d'après la qualité des oeufs).

1.8.2 alpha-Oléfine-sulfonates

On dispose de données limitées concernant les effets des AOS sur les organismes aquatiques et terrestres.

1.8.2.1 Milieu aquatique

On ne dispose que des résultats des épreuves en laboratoire:

-- *Algues:* Valeur de la CE_{50} : > 20-65 mg/litre (C_{16}-C_{18}) pour les algues vertes

-- *Invertébrés:* Valeur de la CL_{50} : 19 et 26 mg/litre (C_{16}-C_{18}) pour la daphnie

-- *Poissons:* Pour neuf espèces de poissons on a obtenu des valeurs de la CL_{50} aiguë de 0,3-6,8 mg/litre (C_{12}-C_{18}). Sur la base d'études à court terme effectuées sur la truite de mer *(Salmo trutta)*, l'ide rouge *(Idus melanotus)* et le rasbora (Rasbora heteromorpha), on peut conclure que la toxicité des composés en C_{14}-C_{16} est environ cinq fois plus faible que celle des composés en C_{16}-C_{18}, avec des valeurs de la CL_{50} (à toutes les concentrations mesurées) de 0,5-3,1 (C_{16}-C_{18}) et de 2,5-5,0 mg/litre (C_{14}-C_{16}). Deux études à long terme effectuées sur la truite arc-en-ciel ont montré que le paramètre le plus sensible était la croissance, et qu'il permettait d'obtenir une CE_{50} de 0,35 mg/litre. Pour ce qui est des poissons de mer, on a obtenu pour le mulet gris ou muge *(Mugal cephalus)*, une valeur de la CL_{50} à 96 heures de 0,70 mg/litre.

1.8.2.2 Milieu terrestre

Une étude portant sur des végétaux en solution nutritive a montré que la concentration sans effets observables se situait dans les limites 32-56 mg/litre. Dans une autre étude, portant cette fois sur des poulets qui recevaient les AOS dans leur nourriture, on a obtenu une valeur > 200 mg/kg pour la concentration sans effets observables (d'après la qualité des oeufs).

1.8.3 Alkyl-sulfates

1.8.3.1 Organismes aquatiques

Les AS ont fait l'objet d'études à court et à long terme et d'une étude dans des conditions plus proches de la réalité. On constate encore que leur toxicité dépend de la longueur de la chaîne latérale alkylée; par contre on ne dispose d'aucune donnée qui indiquerait l'existence d'une différence de toxicité entre les AS à chaine droite et les AS à chaîne ramifiée.

Les résultats des épreuves de laboratoire sont les suivants:

-- *Microorganismes:* Les valeurs de la CE_{50} dans une communauté marine étaient de 2,1-4,1 mg/litre (C_{12}). Pour *Pseudomonas putida,* les concentrations sans effets observables étaient de 35-550 mg/litre (C_{16}-C_{18}).

-- *Végétaux aquatiques:* Les valeurs de la CE_{50} s'établissaient comme suit: > 20-65 mg/litre (C_{12}-C_{13}) pour les algues vertes et 18-43 mg/litre (C_{12}) pour les macrophytes. Les concentrations sans effets observables s'établissaient à 14-26 mg/litre (C_{12}-C_{16}/C_{18}) chez les algues vertes.

-- *Invertébrés:* Les valeurs de la CE_{50} et de la CL_{50} se situaient entre 4 et 140 mg/litre (C_{12}/C_{15}-C_{16}/C_{18}) pour les espèces d'eau douce et entre 1,7 et 56 mg/litre (tous les composés en C_{12}) chez les espèces marines. La concentration sans effets observables pour *Daphnia magna* était de 16,5 mg/litre (C_{16}/C_{18}) en exposition chronique, les valeurs se situant entre 0,29 et 0,73 mg/litre (longueur de chaine non précisée) pour les espèces marines.

-- *Poissons:* Les valeurs de la CL_{50} se situaient entre 0,5 et 5,1 mg/litre (longueur de chaine non précisée ou C_{12}-C_{16}) pour des espèces d'eau douce et entre 6,4 et 16 mg/litre (tous les composés en C_{12}) pour les espèces marines. On n'a pas eu connaissance d'études à long terme.

Il est à noter que nombre de ces travaux ont été effectués dans des conditions statiques. Comme les AS sont facilement biodégradables, il est possible qu'on en ait sous estimé la toxicité. Lors d'une étude de 48 heures sur *Oryzias latipes,* on a obtenu pour la CL_{50} des valeurs respectivement égales à 46, 2,5 et 0,61 mg/litre (mesures de concentrations) pour des composés en C_{12}, C_{14} et C_{16}. Cette étude et d'autres, montrent que la toxicité s'accroît d'un facteur 5 lorsque la longueur de la chaîne augmente de deux unités. Une étude dynamique sur une biocénose, avec des composés en C_{16}-C_{18} a permis d'obtenir une concentration sans effets observables de 0,55 mg/litre.

1.8.3.2 Organismes terrestres

On a fait état, pour les lombrics et les navets, de concentrations sans effets observables de valeur > 1000 mg/kg (C_{16}-C_{18}).

1.9 Evaluation des risques pour la santé humaine

Les ASL sont les tensio-actifs les plus largement utilisés pour la fabrication de détergents et de produits de nettoyage; les AOS et les AS entrent également dans la composition des détergents et des

produits destinés à l'hygiène personelle. La principale voie d'exposition humaine est donc le contact cutané. Cependant de petites quantités de ASL, d'AOS et d'AS peuvent être ingérées avec l'eau de boisson ou sous forme de résidus subsistant sur les ustentsiles de cuisine et dans les aliments. Bien que les données sur ce point soient limitées, on peut estimer à environ 5 mg/personne la quantité de ASL ingérée quotidiennement de cette manière. Quant à l'exposition professionnelle à ces trois catégories de produits, elle peut intervenir lors de la préparation des différentes substances qui en contiennent, mais on ne dispose d'aucune donnée sur les effets qu'une exposition chronique à ces composés pourrait avoir sur l'homme.

Les ASL, les AOS et les AS peuvent irriter la peau par suite d'un contact répété ou prolongé aux concentrations qui sont celles des produits non dilués. Chez le cobaye, les AOS peuvent provoquer une sensibilisation cutanée lorsque la concentration en sultone gamma-insaturée dépasse environ 10 ppm.

Les études à long terme sur animaux de laboratoire dont on connaît les résultats sont insuffisantes pour permettre d'évaluer le pouvoir cancérogène des ASL, des AOS et des AS, et ce, pour différentes raisons: conception même de ces études, trop petit nombre d'animaux utilisés et doses administrées trop faibles, enfin examens histopathologiques trop succints. Compte tenu de ces réserves, les résultats fournis par les études au cours desquelles les animaux ont reçu des ASL, des AOS ou des AS par voie orale, ne comportent aucun signe de cancérogénicité; par ailleurs l'application d'AOS aux animaux par badigeonnage cutané, a également donné des résultats négatifs. Ces composés ne se révèlent pas non plus génotoxiques *in vivo* ou *in vitro,* encore que peu d'études aient été publiées sur ce point.

Des études sub-chroniques au cours desquelles des rats avaient reçu des ASL dans leur nourriture ou leur eau de boisson à des concentrations quotidiennes correspondant environ à 120 mg/kg de poids corporel, ont révélé la présence d'effets minimes, notamment des altérations biochimiques et des modifications histopathologiques au niveau du foie; toutefois d'autres études au cours desquelles des animaux avaient été exposés plus longtemps à des doses plus élevées n'ont pas mis d'effets en évidence. L'application cutanée de ASL a provoqué une intoxication générale ainsi que des effets localisés.

La dose journalière moyenne de ASL absorbée par la population générale, telle qu'on peut l'évaluer sur la base d'estimations de l'exposition de cette population par l'intermédiaire de l'eau de boisson, des ustensiles de cuisine et des aliments, est probablement beaucoup plus faible (de l'ordre de trois ordres de grandeur) que les concentrations qui se révèlent produire des effets insignifiants sur les animaux de laboratoire.

Les effets des AOS observés sur l'homme à l'occasion des quelques études dont on a connaissance, rapellent ceux qui ont été mis en évidence chez des animaux de laboratoire exposés aux ASL. Comme on ne dispose pas de données suffisantes pour évaluer la dose journalière

moyenne d'AOS absorbée par la population générale ni sur les concentrations susceptibles de produire des effets chez l'homme et l'animal, il n'est pas possible de savoir avec certitude si l'exposition aux AOS présentes dans l'environnement représente un risque pour la santé humaine. Les concentrations d'AOS présentes dans les milieux auxquels l'homme pourrait être exposé, sont de toute manière plus faibles que celles des ASL, du fait de la moindre utilisation des AOS.

Des effets ont été observés systématiquement à l'occasion de quelques études à portée limitée effectuées sur des rats à qui l'on avait fait ingérer quotidiennement des AOS soit avec leur nourriture, soit dans leur eau de boisson à des concentrations supérieures ou égales à 200 mg/kg de poids corporel. Des applications topiques répétées ou prolongées produisent également des effets localisés sur la peau et les yeux. On ne dispose pas non plus de données suffisantes pour évaluer la dose journalière moyenne d'AS absorbée par la population générale. Toutefois, étant donné que les tensio-actifs à base d'AS ne sont pas utilisés aussi abondamment que ceux qui contiennent des ASL, il est probable que la dose d'AS absorbée est au moins mille fois plus faible que celle qui produit des effets sur l'animal.

1.10 Evaluation des effets sur l'environnement

Les ASL, les AS et les AOS sont utilisés en grandes quantités et rejetés dans l'environnement avec les eaux usées. Pour évaluer le risque qui leur est attaché, il faut comparer les concentrations auxquelles l'exposition peut se produire avec celles qui ne provoquent aucun effet indésirable, cette comparaison pouvant être faite pour un certain nombre de milieux présents dans l'environnement. En ce qui concerne les tensio-actifs anioniques en général, les plus importants de ces milieux sont constitués par les stations de traitement des eaux usées, les eaux de surface, les sols amendés au moyen de sédiments et de boues d'égout, ainsi que les eaux estuarielles et marines. Les composés subissent une biodécomposition (depuis les premiers stades jusqu'à leur dégradation ultime) ainsi qu'une adsorption, qui réduisent leur concentration dans l'environnement ainsi que leur biodisponibilité. Le racourcissement de la chaîne latérale alkylée et la disparition de la structure du composé initial conduisent à des composés qui sont moins toxiques que les molécules de départ. Il importe d'en tenir compte lorsqu'on compare les résultats des épreuves en laboratoire aux effets qui pourraient se produire dans l'environnement. En outre, lorsqu'on évalue le risque associé à l'exposition, dans l'environnement, à ces trois types de tensio-

actifs anioniques, il faut que les comparaisons entre les différentes épreuves de toxicité portent sur des composés dont la chaîne latérale à la même longueur.

Les effets des ASL sur les organismes aquatiques ont été très largement étudiés. Lors des épreuves de laboratoire effectuées en eau douce, ce sont les poissons qui se sont révélés les plus sensibles; ainsi la concentration sans effets observables pour un cyprin d'Amérique du Nord, *Pimephales promelas,* est d'environ 0,5 mg/litre (C_{12}); tous ces résultats ont été confirmés lors d'épreuves effectuées dans des conditions plus proches de la réalité. Pour ce qui est du phytoplancton, des épreuves de toxicité aiguë sur trois heures ont donné, pour la CE_{50}, des valeurs de 0,2-0,1 mg/litre (C_{12}-C_{13}), alors qu'on n'a constaté aucun effet sur l'abondance relative du plancton dans d'autres tests effectués à la concentration de 0,24 mg/litre ($C_{11,8}$). Il semble que les espèces marines soient légèrement plus sensibles que la plupart des autres groupes taxonomiques.

Ces trois types de composés anioniques se retrouvent dans l'environnement à des concentrations qui varient dans de larges limites. De ce fait, il n'est pas possible de procéder à une évaluation du risque écologique qui soit d'une portée générale. Toute évaluation du risque doit s'appuyer sur une connaissance suffisante de l'exposition et des concentrations agissantes dans l'écosystème étudié.

Pour ce qui est de l'évaluation du risque imputable à la présence d'AS et d'AOS dans l'environnement, il faudra encore réunir des données précises sur l'exposition à ces composés. C'est pourquoi on utilise des modèles pour étudier l'exposition à ces produits dans les différents milieux qui en sont les récepteurs. En ce qui concerne les organismes aquatiques, les données toxicologiques sur les AS et les AOS sont relativement rares, notamment dans les cas d'exposition chronique à des concentrations constantes. Celles dont on dispose montrent que cette toxicité est analogue à celle des autres tensio-actifs anioniques.

Les organismes aquatiques halophiles se révèlent plus sensibles que les organismes dulçaquicoles à ces composés; toutefois leur concentration est plus faible dans l'eau de mer, sauf au débouché des émissaires d'eaux usées. La destinée et les effets de ces composés, qui sont présents dans les effluents déversés en mer, n'ont pas été étudiés en détail.

Pour évaluer la sûreté écologique de tensio-actifs tels que les ASL, les AOS et les AS, il faut comparer les concentrations effectives dans l'environnement à celles qui ne produisent aucun effet. Les besoins en matière de recherche sont déterminés non seulement par les propriétés intrensèques de tel ou tel produit chimique mais aussi par les modalités ou les tendances de sa consommation. Tous ces facteurs

peuvent varier fortement d'une région à l'autre, aussi l'appréciation et l'évaluation des risques doivent-elles être effectuées région par région.

1.11 Recommandations pour la protection de la santé humaine et de l'environnement

1. Comme il peut y avoir exposition à des poussières sur les lieux de travail (au cours de la fabrication et de la préparation des différentes formules), il faut veiller à ce que les précautions habituelles d'hygiène et sécurité du travail soient respectées afin d'assurer la protection des travailleurs.

2. La composition des préparations destinées à la consommation des ménages et à l'usage industriel doit être étudiée pour éviter tout danger, en particulier lorsqu'il s'agit de produits destinés au nettoyage ou au lavage du linge à la main.

3. L'exposition à ces produits dans l'environnement et les effets qu'ils peuvent avoir doivent faire l'objet d'une surveillance appropriée afin que l'on puisse reconnaître à temps la présence de tout concentration excessive dans tel ou tel milieu.

1.12 Recommandations pour les recherches futures

Santé humaine

1. Etant donné que le contact cutané est la principale voie d'exposition humaine aux ASL, aux AOS et aux AS et que l'on ne dispose pas d'études à long terme suffisantes sur la toxicité cutanée ou la cancérogénicité de ces produits chez les animaux de laboratoire, il est recommandé de procéder à des études à long terme convenablement conçues au cours desquelles il sera procédé à l'application de ces composés sur la peau des animaux.

2. En raison de l'absence de données définitives sur la génotoxicité des AOS et des AS, il conviendrait de procéder à des études supplémentaires *in vivo* et *in vitro*.

3. En raison de l'insuffisance des études existantes concernant les effets toxiques de ces produits sur la reproduction et le développement, il conviendrait d'effectuer, sur des animaux de laboratoire, des études qui permettent d'obtenir des résultats définitifs sur la valeur des concentrations agissant ou au contraire, sans effets des ASL, des AOS et des AS.

4. Etant donné que l'on ne connaît pas de façon suffisamment précise l'exposition aux ASL, aux AOS et aux AS, il faudrait surveiller l'exposition de la population générale à ces produits, en particulier lorsque ces tensio-actifs sont utilisés pour le nettoyage et le lavage du linge à la main.

5. Etant donné que les ASL, les AOS et les AS peuvent favoriser le transport d'autres produits chimiques dans les différents milieux qui composent l'environnement et en faire varier la biodisponibilité et la toxicité dans les eaux de surface, les sédiments, les cours d'eau et les sols auxquels l'être humain pourrait se trouver exposé, il conviendrait d'étudier les interactions de ces produits avec d'autres substances présentes dans l'environnement et les conséquences qui en découlent pour la santé humaine.

Sûreté écologique

6. Des études supplémentaires devraient être effectuées afin d'élucider les mécanismes de l'adsorption et de la désorption des AOS et des AS. Elles devraient également porter sur le partage des ASL, des AOS et des AS entre les particules colloïdales en solution ou en suspension dans l'eau. Il faudrait effectuer une modélisation mathématique des coefficients de sorption et valider les modèles obtenus en fonction des paramètres physicochimiques.

7. En cas d'exposition à des sols amendés à l'aide de boues d'égout ou à des sédiments de rivière, il faudrait étudier la biodécomposition des AOS et des AS dans ces milieux. L'étude des sédiments (dans les zones d'aérobiose et d'anaérobiose) devrait s'effectuer en aval des points où sont rejetées des eaux traitées ou non traitées ou des émissaires d'évacuation.

8. Il faudrait surveiller au niveau régional et national les concentrations en ASL, AOS et AS dans l'environnement afin d'obtenir des données sur l'exposition. Il faudrait également mettre au point des méthodes d'analyse permettant de déceler la présence de faibles teneurs en AOS et en AS dans les compartiments appropriés de l'environnement.

9. Il faudrait établir des bases de données nationales sur la concentration des ASL, AOS et AS dans les eaux usées et les cours d'eau ainsi que sur les différents types de stations d'épuration, leur implantation et leur efficacité, afin de mieux étudier l'impact des décharges dans l'environnement.

10. Il faudrait effectuer des études à long terme sur la toxicité des AOS et des AS pour les poissons (espèces d'eau douce et espèces marines) et des invertébrés aquatiques, afin d'en établir la sensibilité relative.

ALKILSULFONATOS LINEALES Y SUSTANCIAS RELACIONADOS

1. RESUMEN GENERAL, EVALUACION Y RECOMENDACIONES

1.1 Identidad y métodos analíticos

Los alkilsulfonatos lineales (ASL), los alpha-olefinsulfonatos (AOS) y los alkilsulfatos (AS) son sustancias tensioactivas aniónicas con moléculas que se caracterizan por tener un grupo hidrófobo y uno hidrófilo (polar). Las mezclas comerciales están formadas por isómeros y homólogos de compuestos relacionados entre sícon distintas

propiedades fisicoquímicas, obteniéndose formulaciones con diversas aplicaciones.

Los ASL, los AOS y los AS se pueden analizar por métodos no específicos. El ensayo que se suele utilizar es el de las sustancias que reaccionan con el azul de metileno, es decir, todas las que contienen un grupo aniónico e hidrófobo. Por consiguiente, si se utiliza para muestras del medio ambiente se producen interferencias analíticas; por otra parte, la sensibilidad de este método es de unos 0,02 mg/litro. Aunque se han buscado alternativas no específicas a este método, su uso no es habitual. En el análisis del medio ambiente sólo hay métodos específicos para los ASL y los AS. Para el análisis de los AOS se dispone de un método mejorado basado en la reactividad del azul de metileno y la cromatografía líquida de alto rendimiento (HPLC).

Los ASL son sustancias no volátiles que se forman por la sulfonación del alkilbenceno lineal. Los productos comerciales son siempre mezclas de homólogos con la cadena alkilo de distintas longitudes (C_{10}-C_{13} o C_{14}) e isómeros que difieren en las posiciones del anillo de fenilo (2-5 fenil). En las muestras del medio ambiente y en otras matrices se pueden determinar todos los homólogos e isómeros de los ASL por medio de métodos analíticos específicos como la HPLC, la cromatografía de gases y la cromatografía de gases-espectrometría de masas.

Los AOS son sustancias no volátiles producidas por la sulfonación de las alpha-olefinas. Son mezclas de dos compuestos, el alkensulfonato de sodio y el sulfonato de hidroxialkano, con longitudes de la cadena alkilo de C_{14}-C_{18}.

Los AS son compuestos no volátiles producidos por la sulfatación de alcoholes oleoquímicos o petroquímicos. Son mezclas de homólogos con longitudes de la cadena alkilo de C_{10}-C_{18}. Se están perfeccionando métodos analíticos específicos para la vigilancia del medio ambiente.

1.2 Fuentes de exposición humana y ambiental

Los ASL, los AOS y los AS se utilizan como ingredientes activos en productos de uso doméstico y de aseo personal y en aplicaciones especializadas. Una vez utilizadas, dichas sustancias detergentes pasan al medio ambiente en las aguas residuales.

Se dan casos de exposición en el trabajo a estas sustancias. La exposición de la población humana general y de los organismos del medio ambiente depende de la aplicación de los ASL, los AOS y los AS (y de otras sustancias tensioactivas), de las prácticas de tratamiento de las aguas residuales y de las características del medio ambiente al que llegan.

En 1990, el consumo mundial fue de unos dos millones de toneladas de ASL, 86 000 toneladas de AOS y 289 000 toneladas de AS.

1.3 Concentraciones en el medio ambiente

1.3.1 Alkilsulfonatos lineales

Las concentraciones de ASL se han determinado cuantitativamente por medio de un método analítico sensible específico en casi todos los compartimentos del medio ambiente en los que pueden estar presentes. Las concentraciones disminuyen progresivamente en el siguiente orden: aguas residuales > efluente tratado > aguas superficiales > mar.

En las zonas donde los ASL son las sustancias tensioactivas predominantes utilizadas, las concentraciones suelen ser de 1-10 mg/litro en las aguas residuales, 0,05-0,1 mg/litro en los efluentes sometidos a un tratamiento biológico, 0,05-0,6 mg/litro en los efluentes tratados con un filtro de goteo, 0,005-0,05 mg/litro en las aguas superficiales por debajo de los desagües de aguas residuales (con concentraciones que disminuyen con rapidez a 0,01 mg/litro corriente abajo del desagüe), < 1-10 mg/kg en los sedimentos fluviales ($\leq$ 100 mg/kg en los sedimentos muy contaminados cerca de las zonas de vertido), 1-10 g/kg en los fangos de alcantarillado y < 1-5 mg/kg en los suelos tratados con fangos (al principio 5-10 mg/kg; se ha registrado una concentración de $\leq$ 50 mg/kg después de aplicaciones anormalmente elevadas de fangos). Las concentraciones de ASL en las aguas de estuario son de 0,001-0,01 mg/litro, aunque hay niveles más elevados en los lugares donde se vierten directamente aguas residuales. Las concentraciones en el agua marina cercana a la costa son < 0,001-0,002 mg/litro.

Hay que señalar que las concentraciones de ASL en el medio ambiente varían mucho. Esto se debe a diferencias en los métodos analíticos, las características de los lugares de muestreo (que van desde zonas muy contaminadas con un tratamiento inadecuado de las aguas residuales hasta zonas donde dichas aguas se someten a un

tratamiento a fondo), la estación (los valores pueden ser en una el doble que en otra) y el consumo de ASL.

La vigilancia del medio ambiente pone de manifiesto que no se ha producido acumulación de ASL en sus compartimentos a lo largo del tiempo. Las concentraciones en el suelo no aumentan con el tiempo, sino que disminuyen debido a la mineralización. Los ASL no se degradan en condiciones estrictamente anaerobias (para formar metano), por lo que no se puede concluir que estén mineralizados en sedimentos anaerobios. Con la utilización presente, el ritmo de asimilación de ASL en todos los compartimentos del medio ambiente que los reciben es igual al ritmo de entrada, por lo que la situación es estable.

1.3.2 alpha-Olefinsulfonatos y alkilsulfatos

Los datos disponibles sobre las concentraciones de AOS en el medio ambiente son limitados debido a la dificultad para analizarlos en las muestras de dicho medio. Hay métodos colorimétricos no específicos (como el basado en el azul de metileno) que permiten detectar sustancias tensioactivas aniónicas en general, pero se ven afectados por interferencias analíticas y no son idóneos para determinar concentraciones determinadas de AOS. Se está preparando un método específico para medir los AS en muestras del medio ambiente.

En estudios de laboratorio se ha observado que los AOS y los AS se mineralizan con rapidez en todos los compartimentos del medio ambiente y prácticamente se eliminan del todo de las aguas residuales durante el tratamiento. Las concentraciones en el agua superficial, los sedimentos, el suelo, el agua de estuario y el medio marino son probablemente bajas. Se ha comprobado que la concentración de AOS en el agua fluvial es pequeña.

1.4 Transporte, distribución y transformación en el medio ambiente

A temperaturas por debajo de 5-10°C, la cinética de la biodegradación de los ASL, los AOS y los AS se reduce debido a la disminución de la actividad microbiana.

1.4.1 Alkilsulfonatos lineales

Las vías de entrada de los ASL en el medio ambiente varían de un país a otro, pero la principal es el vertido de las depuradoras de aguas residuales. Cuando no hay depuradoras o son inadecuadas, las aguas residuales se pueden verter directamente en los ríos, los lagos o el mar. Otra vía de entrada de ASL en el medio ambiente es la dispersión de fangos de alcantarillado en las tierras cultivadas.

Durante su recorrido hasta llegar al medio ambiente, los ASL se eliminan mediante una combinación de adsorción y biodegradación primaria y final. Los ASL se adsorben sobre superficies coloidales y partículas en suspensión, con unos coeficientes medidos de adsorción de 40-5200 litros/kg, en función de los medios y de la estructura de los ASL. Se biodegradan en el agua superficial (semivida de 1-2 días), los sedimentos aerobios (1-3 días) y los sistemas marinos y de estuarios (5-10 días).

Durante el tratamiento primario de las aguas residuales se adsorbe alrededor del 25% (intervalo, 10-40%) de los ASL en los fangos residuales y se elimina con ellos. No se eliminan durante la digestión anaerobia de los fangos, sino durante su tratamiento aerobio, con una semivida de unos 10 días. Tras la aplicación de fangos al suelo, en general se degrada el 90% de los ASL en tres meses, con una semivida de 5-30 días.

Los factores de concentración en el organismo completo para los ASL oscilan entre 100 y 300 para la suma de los ASL-^{14}C y los metabolitos de ^{14}C. Los peces los absorben sobre todo por las branquias, distribuyéndose después al hígado y la vesículas biliar tras la biotransformación. Los ASL se excretan con rapidez, por lo que no hay pruebas de que se produzca bioampliación.

1.4.2 alpha-Olefinsulfonatos

Los datos disponibles sobre el transporte, distribución y transformación en el medio ambiente para los AOS son más escasos que para los ASL. Cabe suponer que los AOS llegan al medio ambiente de manera análoga a la establecida para los ASL, los AS y otras sustancias tensioactivas detergentes, y su destino en él es semejante al de los ASL y los AS. En condiciones aerobias se biodegradan fácilmente y la biodegradación primaria se completa en 2-10 días, en función de la temperatura. Son limitados los datos disponibles sobre la bioacumulación de los AOS; en peces no se observó ninguna. No hay datos relativos a la degradación abiótica.

1.4.3 Alkilsulfatos

Los AS llegan al medio ambiente por mecanismos análogos a los de los ASL y los AOS.Son fácilmente biodegradables en condiciones aerobias y anaerobias en el laboratorio y en el medio ambiente; la biodegradación primaria se termina en 2-5 días. El factor de bioconcentración en el organismo entero oscila entre 2 y 73 y varía con la longitud de la cadena de los homólogos de los AS. Los peces absorben, distribuyen, biotransforman y excretan los AS de la misma manera que los ASL y no se produce bioconcentración en los organismos acuáticos.

1.5 Cinética

Los ASL, los AOS y los AS se absorben fácilmente en el aparato digestivo y se distribuyen ampliamente por todo el organismo, con una metabolización extensa. En los ASL se produce omega- y ß-oxidación. Las sustancias originales y los metabolitos se excretan sobre todo a través de los riñones, aunque una parte de la cantidad absorbida se puede excretar en forma de metabolitos en las heces por excreción biliar. Parece que por la piel intacta solamente se absorben cantidades mínimas de ASL, AOS y AS, aunque el contacto prolongado puede poner en peligro la integridad de la barrera cutánea, permitiendo así una mayor absorción; las concentraciones elevadas pueden reducir el tiempo necesario para la penetración.

1.6 Efectos en los animales de laboratorio y en los sistemas de prueba *in vitro*

Los valores de la DL_{50} por vía oral para las sales sódicas de los ASL fueron de 404-1470 mg/kg de peso corporal en ratas y de 1259-2300 mg/kg en ratones, lo cual parece indicar que las ratas son

más sensibles que los ratones a la toxicidad de los ASL. En ratones se midió para una sal sódica de AOS una DL_{50} por vía oral de 3000 mg/kg de peso corporal. Los valores de la DL_{50} de AS por vía oral en ratas fueron de 1000-4120 mg/kg de peso corporal. Los ASL, AOS y AS irritan la piel y los ojos.

Se han descrito efectos mínimos, entre ellos alteraciones bioquímicas y cambios histopatológicos en el hígado, en estudios de toxicidad subcrónica en los que se administraron ASL a ratas con los alimentos o el agua de beber en concentraciones equivalentes a dosis superiores a 120 mg/kg de peso corporal al día. Aunque en un estudio se observaron cambios estructurales de las células hepáticas a dosis menores, al parecer eran reversibles. En otros estudios no se detectaron efectos con dosis análogas, pero tal vez el examen de los órganos fuera más detenido en el primer estudio. Se han notificado efectos en la reproducción, por ejemplo menor tasa de gestación y pérdida de crías, en animales que recibieron dosis > 300 mg/kg al día. Se observaron cambios histopatológicos y bioquímicos tras la aplicación cutánea de larga duración a ratas de soluciones > 5% de ASL y después de la aplicación durante 30 días de 60 mg/kg de peso vivo en la piel de cobayas. La aplicación cutánea repetida de soluciones $\geq$ 0,3% de ASL indujo efectos fetotóxicos y en la reproducción, pero también se observó toxicidad materna.

Son escasos los datos disponibles de estudios en animales experimentales que permitan evaluar los posibles efectos de los AOS en el ser humano. No se observó ningún efecto en ratas que recibieron por vía oral dosis de 250 mg/kg de peso corporal al día en aplicación crónica, pero se apreció fetotoxicidad en conejas a las que se administró una dosis tóxica para la madre de 300 mg/kg de peso corporal al día. La aplicación de AOS a la piel y los ojos de animales experimentales indujo efectos locales.

Aunque se han investigado en varios estudios los efectos de la exposición de corta y larga duración de animales a los AS, en la mayoría de los casos el examen histopatológico fue inadecuado o el tamaño de los grupos pequeño; por otra parte, las dosis más altas utilizadas en los estudios de larga duración no produjeron ningún efecto tóxico, de manera que no se pudo establecer un NOAEL. Sin embargo, se han descrito habitualmente efectos en ratas que recibían AS en los alimentos o el agua de beber a concentraciones equivalentes a 200 mg/kg de peso corporal al día o más. Se han observado efectos locales en la piel y los ojos tras la aplicación tópica de concentraciones aproximadas del 0,5% de AS o más. A concentraciones más elevadas se han registrado efectos de toxicidad materna y fetotóxicos.

La mayoría de los estudios de larga duración son inadecuados para evaluar el potencial carcinogénico de los ASL, los AOS y los AS en animales experimentales, debido a factores como el pequeño número de animales, el número limitado de dosis, la ausencia de una dosis tolerada máxima y la limitación del examen histopatológico en la mayoría de los estudios. En los casos en que se describieron de manera apropiada los hallazgos patológicos no se utilizaron dosis toleradas máximas y las dosis no produjeron efectos tóxicos. Teniendo presentes estas limitaciones, sin embargo, en los estudios en los que se administraron por vía oral ASL, AOS y AS no se obtuvo ninguna prueba de carcinogenicidad; en estudios de larga duración de aplicación de AOS en la piel con un pincel no se observó ningún efecto.

Según los limitados datos disponibles, no parece que estas sustancias tengan efectos genotóxicos *in vivo* o *in vitro*.

1.7 Efectos en el ser humano

Los resultados obtenidos en pruebas de parche demuestran que la piel humana puede tolerar el contacto con soluciones de ASL, AOS o AS de hasta un 1% durante 24 horas con la única reacción de una irritación leve. Estas sustancias tensioactivas provocaron la pérdida de lípidos de la superficie de la piel, la elución del factor hidratante natural y la desnaturalización de las proteínas de la capa epidérmica externa y aumentaron la permeabilidad y la hinchazón de esta capa. Los ASL, los AOS y los AS no indujeron sensibilización cutánea en voluntarios y no se ha encontrado ninguna prueba definitiva de que induzcan la formación de eczemas. No se han comunicado lesiones graves ni muertes tras la ingestión accidental de estas sustancias tensioactivas por personas.

1.8 Efectos en el medio ambiente

1.8.1 Alkilsulfonatos lineales

1.8.1.1 Medio acuático

Los ASL han sido objeto de amplios estudios tanto en el laboratorio (estudios de corta y larga duración) como en condiciones más naturales (microcosmos y mesocosmos y estudios sobre el terreno). En general, la disminución de la cadena alkilo o la posición más interna del grupo fenilo van acompañadas de una menor toxicidad. Las observaciones en peces y en *Daphnia* indican que al disminuir la longitud de la cadena en una unidad (por ejemplo de C_{12} a C_{11}) la toxicidad se reduce prácticamente a la mitad.

Los resultados de las pruebas de laboratorio han sido los siguientes:

-- *Microorganismos:* Los resultados son muy variables debido al uso de diversos sistemas de prueba (Por ejemplo, inhibición de fango activado; cultivos mixtos y especies individuales). Los valores de la CE_{50} oscilan entre 0,5 mg/litro (especie única) y > 1000 mg/litro. Para los microorganismos no hay relación lineal entre la longitud de la cadena y la toxicidad.

-- *Plantas acuáticas:* Los resultados dependen mucho de las especies. Para los organismos de agua dulce, los valores de la CE_{50} son de 10-235 mg/litro (C_{10}-C_{14}) en las algas verdes, de 5-56 mg/litro ($C_{11,1}$-C_{13}) en las algas cianofíceas, de 1,4-50 mg/litro ($C_{11,6}$-C_{13}) en las diatomeas y de 2,7-4,9 mg/litro ($C_{11,8}$) en las macrofitas; al parecer las algas marinas son aún más sensibles. En las algas es probable que no haya relación lineal entre la longitud de la cadena y la toxicidad.

-- *Invertebrados:* Los valores de la $CL(E)_{50}$ aguda por lo menos en 22 especies de agua dulce son de 4,6-200 mg/litro (longitud de la cadena sin especificar; C_{13}) para los moluscos; 0,12-27 mg/litro (sin especificar; $C_{11,2}$-C_{18}) para los crustáceos; 1,7-16 mg/litro (sin especificar; $C_{11,8}$) para los gusanos; y 1,4-270 mg/litro (C_{10}-C_{15}) para los insectos. Los valores de la $CL(E)_{50}$ crónica son de 2,2 mg/litro ($C_{11,8}$) para los insectos y 1,1-2,3 mg/litro ($C_{11,8}$-C_{13}) para los crustáceos. La concentración crónica sin efectos observados (NOEC; basada en la letalidad o los efectos en la reproducción) es de 0,2-10 mg/litro (sin especificar; $C_{11,8}$) para los crustáceos. Parece que los invertebrados marinos son más sensibles, con valores de la CL_{50} de 1 a > 100 mg/litro (casi siempre C_{12}) para 13 especies y NOEC de 0,025-0,4 mg/litro (sin especificar en todas las pruebas) para siete especies ensayadas.

-- *Peces:* Los valores de la CL_{50} aguda son de 0,1-125 mg/litro (C_8-C_{15}) para 21 especies de agua dulce; los valores de la $CL(E)_{50}$ crónica son de 2,4 y 11 mg/litro (sin especificar; $C_{11,7}$) para dos especies; y las NOEC de 0,11-8,4 y 1,8 mg/litro (sin especificar; $C_{11,2}$-C_{13}) para dos especies. También en este caso los peces marinos parecen ser más sensibles, con valores de la CL_{50} aguda de 0,05-7 mg/litro (sin especificar; $C_{11,7}$) para seis especies y de la CL_{50} crónica de 0,01-1 mg/litro (sin especificar) para dos especies. En la mayoría de los informes no se indicaba la longitud de la cadena. Para especies marinas se señaló una NOEC de < 0,02 mg/litro (C_{12}).

La longitud media de la cadena de los productos utilizados habitualmente en el comercio es C_{12}. Se han probado compuestos de numerosas longitudes de cadena en *Daphnia magna* y en peces, pero la longitud utilizada en otros organismos de agua dulce ha solido ser la de $C_{11,8}$. Los valores típicos de la $CL(E)_{50}$ para el ASL C_{12} son de 3-6 mg/litro en *Daphnia magna* y de 2-15 mg/litro en peces de agua dulce, y las NOEC crónicas típicas son de 1,2-3,2 mg/litro para *Daphnia* y de 0,48-0,9 mg/litro para los peces de agua dulce. Los valores típicos de la CL_{50} de los ASL con cadenas de esta longitud son en los peces marinos < 1-6,7 mg/litro.

Los organismos de agua salada, en particular los invertebrados, parecen ser más sensibles que los de agua dulce a los ASL. En los invertebrados, la acción inhibidora de los ASL sobre el calcio puede afectar a la disponibilidad de este ión para la morfogénesis. Los ASL tienen un efecto general sobre el transporte iónico. Los productos de la biodegradación y los subproductos de los ASL son 10-100 veces menos tóxicos que las sustancias de las que proceden.

Los resultados obtenidos en condiciones más reales son los siguientes: Se han utilizado ASL en todas las pruebas de agua dulce a varios niveles tróficos, como recintos cerrados en lagos (organismos inferiores), modelos de ecosistemas (sistemas de sedimentos y agua), ríos por debajo y por encima del desagüe de depuradoras de aguas residuales y corrientes experimentales. En casi todos los casos se emplearon ASL C_{12}. Al parecer las algas son más sensibles en verano que en invierno, puesto que los valores de la CE_{50} en tres horas fueron de 0,2-8,1 mg/litro después de la fotosíntesis, mientras que en los modelos de ecosistemas no se observó ningún efecto en la abundancia relativa de las comunidades de algas con 0,35 mg/litro. Los niveles sin efecto en estos estudios fueron de 0,24-5 mg/litro, en función del organismo y del parámetro ensayado. Estos resultados prácticamente coinciden con los de las pruebas de laboratorio.

1.8.1.2 Medio terrestre

Se dispone de información acerca de las plantas y las lombrices de tierra. Las NOEC para siete especies de plantas en pruebas realizadas con soluciones de nutrientes son < 10-20 mg/litro; la correspondiente a tres especies en suelo, mediante pruebas basadas en el crecimiento fue de 100 mg/litro (C_{10}-C_{13}). La CL_{50} en 14 días fue para las lombrices de tierra > 1000 mg/kg.

1.8.1.3 Aves

En un estudio con pollos tratados en la alimentación se obtuvo una NOEC (basada en la calidad de los huevos) > 200 mg/kg.

1.8.2 alpha-Olefinsulfonatos

Los datos acerca de los efectos de los AOS en los organismos acuáticos y terrestres son limitados.

1.8.2.1 Medio acuático

Solamente se dispone de datos de pruebas de laboratorio:

-- *Algas:* Los valores de la CE_{50} que se han descrito para las algas verdes son > 20-65 mg/litro (C_{16}-C_{18}).

-- *Invertebrados:* Para *Daphnia* se han notificado valores de la

CL_{50} de 19 y 26 mg/litro (C_{16}-C_{18}).

-- *Peces:* Los valores de la CL_{50} son de 0,3-6,8 mg/litro (C_{12}-C_{18}) para nueve especies de peces. De los estudios de corta duración realizados en la trucha común *(Salmo trutta), Idus melanotus* y *Rasbora heteromorpha,* cabe concluir que la toxicidad de los compuestos C_{14}-C_{16} es unas cinco veces inferior a la de los C_{16}-C_{18}, con valores de la CL_{50} (todas las concentraciones medidas) de 0,5-3,1 (C_{16}-C_{18}) y 2,5-5,0 mg/litro (C_{14}-C_{16}). En dos estudios de larga duración en la trucha arcoiris se comprobó que el crecimiento era el parámetro más sensible, con una CE_{50} de 0,35 mg/litro. En un pez marino, el pardete *(Mugal cephalus)*, el valor de la CL_{50} en 96 horas fue de 0,70 mg/litro.

1.8.2.2 Medio terrestre

En un estudio de plantas con soluciones de nutrientes, la NOEC fue de 32-56 mg/litro. En un estudio con pollos tratados en la alimentación, se notificó una NOEC (basada en la calidad de los huevos) > 200 mg/kg.

1.8.3 Alkilsulfatos

1.8.3.1 Organismos acuáticos

Se han realizado estudios de los AS de corta y larga duración y uno en condiciones más reales. Su toxicidad también depende de la longitud de la cadena alkilo; no se disponía de información sobre diferencias de toxicidad entre los AS lineales y ramificados.

Los resultados de las pruebas de laboratorio son los siguientes:

-- *Microorganismos:* Los valores de la CE_{50} en un conjunto de microorganismos marinos fueron de 2,1-4,1 mg/litro (C_{12}). Las NOEC en *Pseudomonas putida* fueron de 35-550 mg/litro (C_{16}-C_{18}).

-- *Plantas acuáticas:* Los valores de la CE_{50} fueron > 20-65 mg/litro (C_{12}-C_{13}) en algas verdes y de 18-43 mg/litro (C_{12}) en macrofitas. Las NOEC fueron de 14-26 mg/litro (C_{12}-C_{16}/C_{18}) en algas verdes.

-- *Invertebrados:* Los valores de la $CL(E)_{50}$ fueron de 4-140 mg/litro (C_{12}/C_{15}-C_{16}/C_{18}) en especies de agua dulce y de 1,7-56 mg/litro (todos C_{12}) en especies marinas. La NOEC crónica en *Daphnia magna* fue de 16,5 mg/litro (C_{16}/C_{18}) y en especies marinas de 0,29-0,73 mg/litro (longitud de la cadena sin especificar).

-- *Peces:* Los valores de la CL_{50} fueron de 0,5-5,1 mg/litro (longitud de la cadena sin especificar o C_{12}-C_{16}) en especies de agua dulce y de 6,4-16 mg/litro (todos C_{12}) en especies marinas. No había estudios de larga duración.

Hay que señalar que muchos de estos estudios se llevaron a cabo en condiciones estáticas. Los AS son fácilmente biodegradables, por lo que se puede haber infravalorado su toxicidad. En un estudio de 48 horas con Oryzias latipes, los valores de la CL_{50} fueron de 46, 2,5 y 0,61 mg/litro (concentraciones medidas) para los compuestos C_{12}, C_{14} y C_{16} respectivamente. Este y otros estudios indican que la toxicidad difiere en un factor de cinco por cada dos unidades de longitud de la cadena. En un estudio de biocenosis de paso de corriente con compuestos de C_{16}-C_{18} se observó una NOEC de 0,55 mg/litro.

1.8.3.2 Organismos terrestres

Se han notificado valores de la NOEC > 1000 mg/kg (C_{16}-C_{18}) en lombrices de tierra y en nabos.

1.9 Evaluación del riesgo para la salud humana

Los ASL son los agentes tensioactivos más utilizados en detergentes y productos de limpieza. También se utilizan AOS y AS en detergentes y en productos de aseo personal. Por consiguiente, la principal vía de exposición humana es el contacto cutáneo. Pueden ingerirse pequeñas cantidades de ASL, AOS y AS con el agua potable y debido a la presencia de residuos en utensilios y alimentos. Aunque la información de que se dispone es limitada, la ingesta diaria de ASL por esos medios se puede estimar en unos 5 mg/persona. Puede producirse exposición en el trabajo a los ASL, AOS y AS durante la formulación de diversos productos, pero no hay datos acerca de los efectos de una exposición crónica a estas sustancias en el ser humano.

Los ASL, AOS y AS pueden irritar la piel después de un contacto cutáneo repetido o prolongado con concentraciones análogas a las presentes en los productos sin diluir. En los cobayas los AOS pueden inducir sensibilización cutánea cuando el nivel de sulfona g insaturada es superior a unas 10 ppm.

Los estudios disponibles de larga duración en animales experimentales son insuficientes para evaluar el potencial carcinogénico de los ASL, AOS y AS, debido a factores como el diseño del estudio, el uso de un número pequeño de animales, el ensayo de dosis insuficientes y lo limitado del examen histopatológico. En los escasos estudios en los que se administró ASL, AOS o AS a animales por vía oral no se observaron signos de carcinogenicidad; también fueron negativos los resultados de los estudios de larga duración en los que se administraron AOS mediante aplicación cutánea. Estas sustancias no parecen ser genotóxicas *in vivo* o *in vitro,* aunque se tienen noticias de pocos estudios.

Se han descrito efectos mínimos, entre ellos alteraciones bioquímicas y cambios histopatológicos hepáticos, en estudios subcrónicos en los que se administraron ASL a ratas en la alimentación o el agua de beber a concentraciones equivalentes a una dosis aproximada de 120 mg/kg de peso corporal al día, aunque no se observó ningún efecto en estudios en los que los animales estuvieron expuestos a dosis más elevadas durante períodos más largos. La aplicación cutánea de ASL ocasionó tanto toxicidad sistémica como efectos locales.

La ingesta diaria media de ASL de la población general, con arreglo a estimaciones limitadas de la exposición por medio del agua potable, utensilios y alimentos probablemente sea muy inferior (unas tres veces menor) a los niveles con los que se ha observado que inducen efectos leves en los animales experimentales.

Los efectos de los AOS observados en el ser humano en los escasos estudios disponibles son parecidos a los descritos en los animales expuestos a los ASL. Debido a que son insuficientes los datos para estimar la ingesta diaria media de AOS de la población general y los relativos a los niveles que inducen efectos en el ser humano y en los animales, no es posible evaluar con suficiente confianza si la exposición a los AOS en el medio ambiente representa un riesgo para la salud humana. Sin embargo, los niveles de AOS en medios a los que puede estar expuesto el ser humano probablemente sean inferiores a los de ASL, puesto que se utilizan menos.

Se han descrito repetidamente efectos en un pequeño número de estudios limitados en ratas que recibieron AS en la alimentación o en el agua de beber en concentraciones equivalentes a dosis de 200 mg/kg de peso corporal al día o más. Se han observado efectos locales en la piel y en los ojos tras una aplicación tópica repetida o prolongada. Los datos disponibles son insuficientes para estimar la ingesta diaria media de AS de la población general. Sin embargo, dado que no se utilizan tanto agentes tensioactivos con AS como los que contienen ASL, la ingesta de AS será probablemente como mínimo tres veces inferior a las dosis que se ha demostrado que inducen efectos en los animales.

1.10 Evaluación de los efectos en el medio ambiente

Los ASL, los AOS y los AS se utilizan en grandes cantidades y se liberan en el medio ambiente por medio de las aguas residuales. Para evaluar el riesgo es preciso comparar las concentraciones de exposición con las que no producen efectos adversos, y esto se puede hacer para varios compartimentos del medio ambiente. Para los agentes tensioactivos aniónicos en general, los compartimentos más importantes son las depuradoras de aguas residuales, las aguas superficiales, los suelos tratados con sedimentos y fangos y los medios estuarinos y marinos. Se produce tanto biodegradación (primaria y final) como adsorción, por lo que disminuyen las concentraciones y la biodisponibilidad en el medio ambiente. Con la reducción de la longitud de la cadena y la pérdida de la estructura original se forman sustancias menos tóxicas que la primera. Es importante tener en cuenta estos aspectos a la hora de interpretar los resultados de laboratorio con los posibles efectos en el medio ambiente. Por otra parte, al evaluar el riesgo asociado con la exposición del medio ambiente a estos tres compuestos aniónicos se debe establecer una comparación con los resultados de las pruebas de toxicidad de sustancias cuya cadena tenga la misma longitud.

Se han realizado abundantes pruebas de los efectos de los ASL en los organismos acuáticos. En las pruebas de laboratorio con agua dulce parece que los peces eran las especies más sensibles; la NOEC para Pimephales promelas fue de unos 0,5 mg/litro (C_{12}), y estos resultados se confirmaron en pruebas realizadas en condiciones más reales. en el fitoplancton se han observado diferencias: en ensayos

de toxicidad agua de tres horas los valores de la CE_{50} fueron de 0,2-0,1 mg/litro (C_{12}-C_{13}), mientras que no se detectaron efectos en la abundancia relativa en otras pruebas con 0,24 mg/litro ($C_{11,8}$). Parece que las especies marinas eran ligeramente más sensibles que la mayoría de los otros grupos taxonómicos.

En el medio ambiente hay una amplia gama de concentraciones de las tres sustancias aniónicas, como se ha puesto de manifiesto en las numerosas mediciones de los ASL. Debido a esta amplia gama, no se puede hacer una evaluación del riesgo de estas sustancias para el medio ambiente de aplicación general. Para evaluar el riesgo se deben conocer de manera apropiada las concentraciones de exposición y las que tienen efectos en el ecosistema que interesa.

Se necesitan datos precisos sobre la exposición a los AS y los AOS si se quiere hacer una evaluación del riesgo para el medio ambiente. Por consiguiente se están utilizando modelos a fin de evaluar las concentraciones de exposición en los compartimentos del medio ambiente que los reciben. Los datos sobre la toxicidad de los AS y los AOS para los organismos acuáticos, especialmente después de una exposición crónica a concentraciones estables, son relativamente escasos. Los datos disponibles indican que la toxicidad de estos productos es análoga a la de otras sustancias tensioactivas aniónicas.

Los organismos de agua salada parecen ser más sensibles que los de agua dulce a estos compuestos; sin embargo, su concentración es menor en el agua del mar, excepto cerca de los desagües de alcantarillados. No se han investigado con detalle su destino y sus efectos en las aguas residuales vertidas en el mar.

Si se desea evaluar la inocuidad para el medio ambiente de agentes tensioactivos como los ASL, los AOS y los AS hay que comparar las concentraciones reales en el medio ambiente con las que no tienen

ningún efecto. Las necesidades de investigación se determinan no sólo por las propiedades intrínsecas de un producto químico, sino también por sus características o la tendencia del consumo. Estos varían considerablemente entre las distintas zonas geográficas, por lo que la evaluación debe ser de ámbito regional.

1.11 Recomendaciones para la protección de la salud humana y el medio ambiente

1. Puesto que en el lugar de trabajo se puede producir exposición al polvo (durante la elaboración y formulación), deben utilizarse prácticas normalizadas de higiene del trabajo a fin de asegurar la protección de la salud de los trabajadores.

2. La composición de las formulaciones para uso privado e industrial se debe diseñar de manera que se evite el riesgo, especialmente en las formulaciones utilizadas para la limpieza o el lavado a mano.

3. La exposición y los efectos en el medio ambiente se deben vigilar de manera apropiada con objeto de tener una indicación pronta de cualquier acumulación excesiva en los compartimentos pertinentes del medio ambiente.

1.12 Recomendaciones de nuevas investigaciones

Salud humana

1. Debido a que la piel es la principal vía de exposición humana a los ASL, los AOS y los AS y a que no se dispone de estudios adecuados de larga duración acerca de la toxicidad cutánea o la carcinogenicidad en animales experimentales, se recomienda la realización de estudios de larga duración debidamente diseñados de aplicación cutánea de estas sustancias.

2. Ante la falta de datos definitivos sobre la genotoxicidad de los AOS y los AS, deben llevarse a cabo nuevos estudios *in vivo* e *in vitro*.

3. A la vista de la insuficiencia de los estudios disponibles sobre la toxicidad en la reproducción y el desarrollo, se han de realizar estudios definitivos en animales de laboratorio a fin de obtener datos relativos a los efectos de los ASL, los AOS y los AS y los niveles con efectos y sin ellos.

4. Puesto que la exposición a los ASL, los AOS y los AS no está debidamente definida, se debe vigilar la exposición de la población general, en particular cuando estas sustancias tensioactivas se utilizan en la limpieza y el lavado a mano.

5. Debido a que los ASL, los AOS y los AS pueden potenciar el transporte de otras sustancias químicas y regular su biodisponibilidad y toxicidad en las aguas superficiales, los sedimentos fluviales y los suelos a los que puede estar expuesto el ser humano, deben investigarse las interacciones con otras sustancias químicas del medio ambiente y las consecuencias para las personas.

Inocuidad para el medio ambiente

6. Deben realizarse nuevos estudios sobre los mecanismos de adsorción y desorción de los AOS y los AS. También se debe estudiar el reparto de los ASL, los AOS y los AS entre las partículas coloidales disueltas y suspendidas en el agua. Hay que elaborar modelos matemáticos de los coeficientes de sorción y validarlos con arreglo a parámetros fisicoquímicos.

7. Se han de realizar estudios de la biodegradación de los AOS y los AS en suelos tratados con fangos y en sedimentos fluviales (zonas aerobias y anaerobias) corriente abajo de los vertidos de aguas residuales tratadas y sin tratar.

8. Se deben vigilar en los ámbitos regional y nacional las concentraciones de ASL, AOS y AS en el medio ambiente, a fin de obtener información acerca de la exposición. Se han de preparar métodos analíticos para la detección de niveles bajos de AOS y AS en los compartimentos pertinentes del medio ambiente.

9. Hay que organizar bases de datos nacionales sobre las concentraciones de ASL, AOS y AS en las aguas residuales y en los ríos y sobre los tipos, la eficacia y el lugar de las depuradoras de aguas residuales, con objeto de facilitar la evaluación de los efectos de los vertidos de estas sustancias tensioactivas en el medio ambiente.

10. Deben realizarse estudios de la toxicidad de los AOS y los AS en los peces (de agua dulce y marinos) y los invertebrados acuáticos para establecer la sensibilidad relativa de estas especies.

See Also:
Toxicological Abbreviations

12. JUSTIFICATION STATEMENT

Justification Statement:

Sodium dodecylbenzene sulfonate (SDBS), when used as an active ingredient within the formulation of the Ecolab product Antimicrobial Fruit and Vegetable Treatment (AFVT), is a very effective option to help control pathogens (*Escherichia coli O157:H7*, *Listeria monocytogenes* and *Salmonella enterica*) in the wash water or on the surface of processed fruits and vegetables. AFVT also helps control spoilage and decay causing organisms present in the wash water for raw agricultural commodities (RACs).

From a food safety perspective, AFVT was specifically developed for the food retail environments such as restaurants, cafeterias, food service operations, commissaries and kitchens; AFVT provides these organic users with a reliable tool to aid in the combat against microorganisms that cause foodborne illness outbreaks. AFVT has been thoroughly tested against *Escherichia coli O157:H7*, *Listeria monocytogenes* and *Salmonella enterica*, which are major contributors to the foodborne outbreaks we experience in the United States. Healthcare costs continue to rise, people continue to get sick, become hospitalized and may even die as a result of some of these foodborne illnesses. AFVT can help control the spread of these outbreaks, help protect the organic brand and maintain the integrity of the National Organic Program.

AFVT has been reviewed and cleared for safe use by the Food and Drug Administration (FDA) and also registered with the Environmental Protection Agency (EPA) for use as an antimicrobial produce wash.

AFVTs unique dispensing system also provides users with a controlled dispensing system that not only protects the user from unnecessary exposure, but also ensures the correct amount of chemical is delivered to the wash sink for maximum effectiveness and consistent results.

There are other options available to the organic community that are considered “natural” (citric, lactic), but those substances alone do not provide the same level of protection at similar use concentrations as AFVT. There are also synthetic options currently allowed for use in treating organic fruits and vegetables (acidified sodium chlorite and peracetic acid), however, these products are marketed to, and primarily used in industrial/commercial food processing establishments and not in restaurants, kitchens, etc. AFVT will now help the food retail customers in their fight against food borne illnesses.

In closing, Ecolab requests that SDBS, the active ingredient in the product AFVT, be added to the list of 7 CFR 205.605(b) and allowed as an active synthetic ingredient for use in organic handling operations, based on its contribution and associated benefits within the AFVT formulation.

13. CONFIDENTIAL BUSINESS INFORMATION

Confidential Business Information:

Page 15 – Formulary information for Antimicrobial Fruit & Vegetable Treatment (AFVT) has been omitted from within the product's EPA Confidential Statement of Formula (CSF). Ecolab considers this to be Confidential Business Information (CBI). The upper right hand corner of Page 15 has been marked with the phrase "CBI DELETED."

Page 17 – Formulary information for Antimicrobial Fruit & Vegetable Treatment (AFVT) has been omitted from within the product's EPA Confidential Statement of Formula (CSF). Ecolab considers this to be Confidential Business Information (CBI). The upper right hand corner of Page 17 has been marked with the phrase "CBI DELETED."

Page 19 – Formulary information for Antimicrobial Fruit & Vegetable Treatment (AFVT) has been omitted from within the product's EPA Confidential Statement of Formula (CSF). Ecolab considers this to be Confidential Business Information (CBI). The upper right hand corner of Page 19 has been marked with the phrase "CBI DELETED."

Page 21 – Formulary information for Antimicrobial Fruit & Vegetable Treatment (AFVT) has been omitted from within the product's EPA Confidential Statement of Formula (CSF). Ecolab considers this to be Confidential Business Information (CBI). The upper right hand corner of Page 21 has been marked with the phrase "CBI DELETED."

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