

## SIDS INITIAL ASSESSMENT REPORT

For

**20<sup>th</sup> SIAM**

Paris, France, 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<sub>10-16</sub> Monoalkylbenzene sulfonic acid, sodium salt
  - 68411-30-3 C<sub>10-13</sub> Alkylbenzene sulfonic acid, sodium salt
  - 69669-44-9 C<sub>10-14</sub> Alkyl deriv benzene sulfonic acid, sodium salt
  - 85117-50-6 C<sub>10-14</sub> Monoalkylbenzene sulfonic acid, sodium salt
  - 90194-45-9 C<sub>10-13</sub> Alkyl deriv benzene sulfonic acid, sodium salt
  - 127184-52-5 4-C<sub>10-13</sub>-sec Alkyl deriv benzene sulfonic acid, sodium salt
3. **Sponsor Country:** United States
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
  - 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](http://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 SIDS Program?

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. Comments on environmental portion required extensive review of aquatic toxicity data and the entire environmental section has been revised based on the comments provided on the document for SIAM 17. The revised document has been reviewed by U.S. EPA. 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:

August 15, 2003; revised document submitted January 21, 2005.

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## SIDS Initial Assessment Report

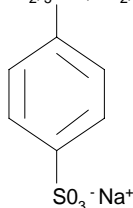
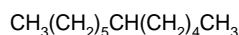
### 1 IDENTITY

#### 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
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	90194-45-9	C <sub>10-13</sub> Alkyl deriv benzene sulfonic acid, sodium salt
	127184-52-5	4-C <sub>10-13</sub> -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 predominantly linear, ranging from 87% to 98%. The structure of C<sub>12</sub>-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<sub>11,3</sub>) to 356 (C<sub>12,6</sub>)

The approximate weight percentage of the alkyl chain varies somewhat regionally as shown below.

Region	<C <sub>10</sub>	C <sub>10</sub>	C <sub>11</sub>	C <sub>12</sub>	C <sub>13</sub>	C <sub>14</sub>	>C <sub>14</sub>	Range of Averages	Weighted Average*
<b>Canada</b> 68081-81-2	≤1	<16	19-39	20-50	5-27	<3	<1	11.8	11.8
<b>Europe</b> 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
<b>Japan</b> 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
<b>United States</b> 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, having average alkyl chain lengths ranging from C<sub>11,3</sub> to C<sub>12,6</sub>, with the predominant materials having average alkyl chain lengths ranging from C<sub>11,6</sub> to C<sub>12,6</sub>. The material is 87-98% 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. 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 U.S., Europe, and Japan incorporated to increase LAS yields also reduce the amount of DATS present.

### 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	198.5°C	Experimental (C <sub>12.0</sub> )	Dossier 2.1a (2)
Boiling point	Decomposition onset at 444°C	Experimental (C <sub>12.0</sub> )	Dossier 2.2a (2)
Relative density	1.06 g/cm <sup>3</sup>	Experimental (C <sub>11.6</sub> )	Dossier 2.3a (4)
Bulk density	450-550 kg/m <sup>3</sup>	Experimental (C <sub>11.6</sub> , C <sub>12.0</sub> )	Dossier 2.3b,c (4)
Vapor pressure	3-5 x 10 <sup>-13</sup> Pa at 25°C	Calculated as C <sub>12</sub>	Dossier 2.4a,d (4,2)
Partition coefficient n-octanol/water (log value)	3.32	Calculated as C <sub>11.6</sub>	Dossier 2.5a (2)
Critical micelle concentration	0.1 g/L	Experimental (C <sub>12</sub> )	Dossier 2.6Aa (2)
Water solubility	250 g/L	Experimental (C <sub>11.6</sub> )	Dossier 2.6Ab (2)
pH	10.0 ± 1	1% solution (C <sub>12.0</sub> )	Dossier 2.6Ba (4)
Henry's law constant	6.35 x 10 <sup>-3</sup> Pa m <sup>3</sup> /mole	Calculated as C <sub>12</sub>	Dossier 2.13A (2)

Pure LAS is a solid at ambient temperatures. The melting point for LAS has been experimentally determined. EPI Suite calculations (dossier 2.1b-e) 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 K<sub>ow</sub> 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 K<sub>ow</sub>. The most reliable calculated value for C<sub>11.6</sub> LAS (log K<sub>ow</sub> = 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

Commercial LAS consists of more than 20 individual homologues and isomers, representing different alkyl chain lengths and aromatic ring positions along the linear alkyl chain; however, the ratio of the various components is relatively constant across the various detergent and cleaning applications. Because of the close consistency of the mixtures, their commercial uses, physico-chemical properties, fate and health and environmental effects, LAS is supported as a category rather than as individual CAS numbers in this assessment.

## 2 GENERAL INFORMATION ON EXPOSURE

### 2.1 Production Volumes and Use Pattern

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, 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**

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%	-	-



**Table 3. Percentage of LAS in Different Types of Institutional and Industrial 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%

\*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, 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. 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. E-FAST modeling of U.S. manufacturing facility effluent discharges (see Annex, 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.<sup>1</sup>

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 or in leachate from landfills. Based on its temperature of decomposition, LAS is unlikely to enter the environment from incineration of sludge.

E-FAST modeling of down-the-drain disposal in the U.S. (see Annex, Format C, Modeling Evaluation #2) resulted in estimated median and 7Q10 (low flow) stream concentrations of 0.099 and 1.3 µg/L, respectively.<sup>1</sup>

<sup>1</sup> U.S. EPA did not evaluate the EFAST modelling results and therefore, can make no conclusions regarding these values.

### 2.2.2 Photodegradation

LAS does not undergo rapid photodegradation under environmental conditions. This has been demonstrated by studies that indicate the presence of photoactivating materials (and typically high intensity light spectrum) are required to produce a measurable rate of photodegradation of LAS in aqueous systems (Matsuura and Smith 1970; Hidaka et al 1985; Hermann et al. 1997). Because LAS is rapidly biodegraded in surface waters (see below) and has low vapor pressure ( $3-5 \times 10^{-13}$  Pa), photodegradation in surface waters likely plays only a minor role, if any, as a removal mechanism.

### 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 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  $^{14}\text{C}$  LAS, 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 a longer chain ( $\text{C}_{13}$ ) 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  $\text{C}_{10}$  to  $\text{C}_{14}$  LAS homologues and two different soil types. In the most recent laboratory study, Elsgaard et al. (2001b) showed more than 73% primary biodegradation of LAS 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).

### 2.2.5 Transport between Environmental Compartments

Games (1982) reported that  $K_d$  values for LAS increased with increasing alkyl chain length of LAS homologues.  $K_d$  values (L/kg) for activated sludge ranged from 220 ( $\text{C}_{10}$  LAS), 1000 ( $\text{C}_{11}$  LAS), 3070 ( $\text{C}_{12}$  LAS) to 9330 ( $\text{C}_{13}$  LAS).  $K_d$  values for river sediment ranged from 41 ( $\text{C}_{10}$  LAS), 100 ( $\text{C}_{11}$  LAS), 330 ( $\text{C}_{12}$  LAS), 990 ( $\text{C}_{13}$  LAS) to 2950 ( $\text{C}_{14}$  LAS). Traina et al. (1996) also reported that  $\log K_{oc}$  values (L/kg) for LAS and dissolved humic substances increased with increasing alkyl chain length: 4.02 ( $\text{C}_{10}$  LAS), 4.83 ( $\text{C}_{12}$  LAS) and 5.49 ( $\text{C}_{14}$  LAS). Based on the  $\text{C}_{11}$  and  $\text{C}_{12}$  LAS-activated sludge data, Feijtel et al. (1999) estimated the  $K_d$  value for commercially representative  $\text{C}_{11.6}$  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  $K_d$  value (L/kg) for  $\text{C}_{12}$  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) results in a  $K_d$  value for  $\text{C}_{11.6}$  LAS and activated sludge of 2500 L/kg.

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) 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.

Based on these two modelling studies, LAS transport between environmental compartments is primarily determined by inputs to the various compartments, biodegradation rates in water (see below) and soil, and water-sediment transfer.

### 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). 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). SPCs also biodegrade as demonstrated by the rapid and complete biodegradation of LAS (to  $\text{CO}_2$ ,  $\text{SO}_4^{2-}$ , and water) under aerobic conditions documented below. [See change here...Done.]

An extensive database of studies is available demonstrating rapid and complete biodegradation of LAS in freshwater under aerobic conditions (dossier section 3.5). The two studies summarized in Table 4 demonstrate that LAS passes standard tests for ready biodegradability, including the 10-day biodegradation window. 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 as 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	DOC Removal	C <sub>11.6</sub>	93%	28	Schoeberl 1993
DOC Die-Away, Directive 79/83/EEC, Appendix V, C.4-A	DOC Removal	C <sub>11.6</sub>	94%	28	Schoeberl 1993

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) 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/L). They 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.

### 2.2.7 Bioaccumulation

The bioaccumulation potential of LAS has been investigated. Early studies, e.g., Kimerle et al. 1981, used <sup>14</sup>C-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-C<sub>10</sub> LAS) to almost 1000 L/kg (2-phenyl-C<sub>13</sub> 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 = C<sub>11.6</sub>) and a representative environmental sample (filtered Mississippi river water, average alkyl chain length = C<sub>10.8</sub>). The respective BCFs were 87 and 22 L/kg, indicating that the bioconcentration potential of LAS is low and 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<sub>11.5</sub> (range C<sub>10.7-11.9</sub>). 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 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. [Are there any quantitative values for the levels in marine waters? Values added above.]

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<sub>3</sub>) in which the LAS levels in the digested sludge (30,200 mg/kg) likely represent 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).

### **2.3 Human Exposure – To be revised based on comments at SIAM 17 (November 2003)**

## **3 HUMAN HEALTH HAZARDS – TO BE REVISED BASED ON COMMENTS AT SIAM 17 (NOVEMBER 2003)**

## 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. Kimerle and Swisher (1977) demonstrated 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**

Individual LAS Homologues	48-hour LC <sub>50</sub> (mg/L)	
	<i>D. magna</i> (Dossier, section 4.2Af)	Fathead minnow (Dossier, section 4.1r)
C <sub>10</sub>	12.3	43.0
C <sub>11</sub>	5.7	16.0
C <sub>12</sub>	3.5	4.7
C <sub>13</sub>	2.0	0.4
C <sub>14</sub>	0.7	0.4

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<sub>50</sub> 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<sub>11</sub>, C<sub>11.6</sub>, and C<sub>13</sub> were tested in accordance with the OECD 201 protocol under GLP conditions (Verge and Moreno 1996a, dossier section 4.3d,e). The resultant EC<sub>50</sub> 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<sub>50</sub> values to be 270, 111, 48, 30, and 18 mg/L for the pure C<sub>10</sub>, C<sub>11</sub>, C<sub>12</sub>, C<sub>13</sub>, and C<sub>14</sub>, 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<sub>ow</sub> and supported by considerable experimental data. Although it is extremely difficult to accurately measure log K<sub>ow</sub>s for surfactants because of their strong preference for the oil-water interface, log K<sub>ow</sub>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<sub>ow</sub> 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<sub>11.6</sub> 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<sub>10</sub> to C<sub>14</sub>. Van de Plassche et al. commented that the range of LC<sub>50</sub> 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<sub>50</sub> values for fish was only provided for one species (*Pimephales promelas*, 0.40-100 mg/L) as an example of the wide ranges found but these values. 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 is due primarily to the wide range of materials tested and differences in test designs.

**Table 9. Geometric Mean Fish Toxicity Results**

Species	Geometric Mean LC <sub>50</sub> (mg/L)	Number of Records
<i>Lepomis macrochirus</i> (bluegill sunfish, dossier section 4.1c)	3.0	88
<i>Pimephales promelas</i> (fathead minnow, dossier section 4.1d)	3.2	35
<i>Leusiscus idus melanotus</i> (golden orfe, dossier section 4.1e)	2.9	11
<i>Carassius auratus</i> (goldfish, dossier section 4.1f)	9.5	46
<i>Oncorhynchus mykiss</i> (rainbow trout, dossier section 4.1f)	3.0	10
<i>Oryzias latipes</i> (medaka, dossier section 4.1f)	13	5
<i>Poecilia reticulata</i> (guppy, dossier section 4.1f)	3.8	9

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<sub>11.6</sub>-C<sub>11.8</sub>) and valid test methods. LC<sub>50</sub> 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)**

Taxon	LC <sub>50</sub> /EC <sub>50</sub> /IC <sub>50</sub> (mg/L)	Reference
Fish ( <i>Lepomis macrochirus</i> ), LC <sub>50</sub> (dossier, section 4.1a) [96 hr. exposure]	1.67	Lewis and Perry 1981
<i>Daphnia magna</i> , EC <sub>50</sub> (dossier, section 4.2Aa) [48 hr. exposure]	1.62	Hooftman and van Drongelen Sevenhuijsen 1990
Algae ( <i>Selenastrum capricornutum</i> ), IC <sub>50</sub> (dossier, section 4.3a) [96 hr. exposure]	29.0	Lewis 1986; Lewis and Hamm 1986

### 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<sub>10</sub> to C<sub>14</sub>. Similar to the results with fish, the range of invertebrate EC<sub>50</sub> 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<sub>50</sub> 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*. The geometric mean EC<sub>50</sub> based on 139 records was determined to be 4.7 mg/L (dossier, section 4.2Ac).

The HERA search (HERA 2004) also found 20 daphnid studies on commercial LAS, of which 11 studies were on currently relevant LAS (C<sub>11.6</sub>-C<sub>11.8</sub>) and followed standardized test methods (Annex 2). EC<sub>50</sub> 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 (C<sub>11.6</sub>-C<sub>11.8</sub>) and followed standardized test methods (Annex 2). The range of ErC<sub>50</sub> 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<sub>50</sub> 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 (dossier 4.1q)**

Taxon	Geometric Mean LC <sub>50</sub> (mg/L)	Alkyl Chain Length	Number of Records
All spp.*	4.36	C <sub>11.7-12.0</sub>	36
Fish	1.58	C <sub>11.7-12.0</sub>	6

\* Data from fish, crustacea, algae and other species.

### Chronic Toxicity Test Results

#### *Freshwater Species*

The chronic toxicity to freshwater aquatic organisms of commercial LAS with C<sub>10-13</sub> alkyl chains and average carbon lengths close to C<sub>11.6</sub> has been reviewed by van de Plassche et al. (1999) and the geometric mean NOEC values, normalized to C<sub>11.6</sub> LAS, from this review are provided in Table 12. 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 the study representing the value closest to the geometric mean determined by van de Plassche et al. for five species for which multiple studies were available. Robust summaries were also prepared on nine species for which only a single study was available. The NOEC values from these studies, including additional chronic data identified, are shown in Table 12. Available NOEC values ranged from 0.25 to 3.4 mg/L. The endpoints affected included behavior, growth, mobility, mortality, and reproduction, depending on the species tested.

Table 12. Chronic Aquatic Toxicity for Freshwater Species

Species	Endpoint (Exposure Period)	Available NOEC [LOEC] (mg/L) Closest to van de Plassche et al. (1999) Geometric Mean	LAS Alkyl Chain Length	Available NOEC Normalized to C <sub>11.6</sub> LAS <sup>1</sup>	Van de Plassche et al. (1999) Geometric Mean NOEC (mg/L), Normalized to C <sub>11.6</sub> LAS, (range <sup>2</sup> ), [Number Studies]
<b>Fish</b>					
<i>Brachydanio rerio</i> , dossier 4.5.1a	Mortality, behavior (14 d)	2.0	11.8	2.4	2.3 [1]
<i>Lepomis macrochirus</i> , dossier 4.5.1m	Growth (28 d)	1.0	11.6	1.0	-- <sup>3</sup>
<i>Oncorhynchus mykiss</i> <sup>4</sup>					0.34 (0.19-0.89) [7]
<i>Pimephales promelas</i> , dossier 4.5.1b	Fry survival (30 d)	1	12.3	1.87	0.87 (0.3-2) [14]
<i>Poecilia reticulata</i> , dossier 4.5.1c	Mobility (28 d)	3.2	N/A <sup>5</sup>	3.2	3.2 [1]
<i>Tilapia mossambica</i> , dossier 4.5.1e	Reproduction (90 d)	0.25	N/A <sup>5</sup>	0.25	0.25 [1]
<b>Aquatic Invertebrates</b>					
<i>Brachionus calyciflorus</i> , dossier 4.5.2i	Survival (2 d)	1.4	12.1	2.19	-- <sup>3</sup>
<i>Ceriodaphnia</i> sp., dossier 4.5.2b	Reproduction (7 d)	2.68	11.8	3.2	3.2 [1]
<i>Chironomus riparius</i> , dossier 4.5.2o	Survival & Emergence (24 d)	2.4	11.8	2.87	2.8 [1]
<i>Daphnia magna</i> , dossier 4.5.2c	Reproduction (21 d)	1.18	11.8	1.41	1.4 (0.3-10) [12]
<i>Paratanytarsus parthenogenica</i> , dossier 4.5.2h	Survival & Population Size (28 d)	3.4	N/A <sup>5</sup>	3.4	3.4 [1]
<b>Algae</b>					
<i>Chlamydomonas reinhardtii</i> <sup>4</sup>					12 [1]
<i>Chlorella kessleri</i> , dossier 4.3r	Growth (15 d)	3.1	11.8	3.71	3.5 [1]
<i>Microcystus aeruginosa</i> , dossier 4.3s	Growth (4 d)	0.3 <sup>6</sup>	11.6	0.3	0.80 (0.3-10.7 <sup>7</sup> ) [4]
<i>Plectonema boryanum</i> <sup>3</sup>					15 [1]
<i>Scenedesmus subspicatus</i> , dossier 4.3f	Growth (3 d)	2.4	11.6	2.4	7.7 (0.8-105 <sup>7</sup> ) [4]
<i>Selenastrum capricornutum</i> , dossier 4.3a	Growth (4 d)	0.5	11.8	0.58	3.8 (1-39 <sup>7</sup> ) [9]

<sup>1</sup> The normalization procedure is described in Annex 3.

<sup>2</sup> Feijtel & van de Plassche, 1995

<sup>3</sup> Not reviewed by van de Plassche et al. (1999).

<sup>4</sup> No valid study identified.

<sup>5</sup> Not available.

<sup>6</sup> EC<sub>50</sub> value divided by 3; as documented in Annex 3, the average EC<sub>50</sub>/NOEC ratio for LAS is 3.

<sup>7</sup> Range includes EC<sub>50</sub> values divided by 3.

Table 12 also provides the available NOEC values normalized to C<sub>11.6</sub> LAS by the QSAR procedures used by van de Plassche et al. (1999) and described in detail in Annex 3. These normalized NOEC values range from 0.25 to 3.71 mg/L for the 14 species for which we were able to document reliable values. The similarity of these values, as shown in Table 12, 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<sub>5</sub>. The HC<sub>5</sub> value calculated by van de Plassche et al., from the NOEC data shown in Table 12, 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<sub>5</sub> value of 0.36 mg/L (Annex 3). Applying these same methods to the available NOEC data, normalized to C<sub>11.6</sub> LAS (Table 12), gave an HC<sub>5</sub> value of 0.43 mg/L (Annex 3). Because these values are based on NOEC data from 14 or more species of fish, algae and several groups of invertebrates, these values are all considered to be valid estimates of the HC<sub>5</sub> for LAS. Based on goodness of fit, the best HC<sub>5</sub> values are 0.43 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). Results are shown in Table 13.

**Table 13. Chronic Aquatic Toxicity Data for Marine Species (dossier 4.5.2s)**

Genus (and species)	Geometric mean NOEC (mg/L)
<b>Fish</b>	
<i>Limanda (yokohamae)*</i>	0.05
<b>Aquatic Invertebrates</b>	
<i>Arbacia</i>	0.45
<i>Arcatia</i>	0.30
<i>Asterias</i>	0.35
<i>Botrylloides</i>	1.94
<i>Botryllus</i>	0.75
<i>Chaetopterus</i>	0.45
<i>Crassostrea (virginica)*</i>	0.025
<i>Crassostrea</i>	0.04
<i>Molgula</i>	0.90
<i>Mysidopsis (bahia)*</i>	0.12
<i>Mysidopsis</i>	0.20
<i>Mytilus (edulis)*</i>	0.025
<i>Mytilus</i>	0.04
<i>Spisula</i>	0.80
<b>Algae</b>	
<i>Dunaliella</i>	0.11
<i>Laminaria</i>	5.00

\*Normalized to C<sub>11.6</sub> 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 C<sub>11</sub>, C<sub>11.6</sub> and C<sub>13</sub>) 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 EC<sub>50</sub> values of 760, 550 and 650 mg/L for the C<sub>11</sub>, C<sub>11.6</sub>, and C<sub>13</sub> commercial materials, respectively, and 1042-1200, 740-782, 500-723, 700-795, and 900-1045 mg/L for the C<sub>10</sub>, C<sub>11</sub>, C<sub>12</sub>, C<sub>13</sub>, and C<sub>14</sub> 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 EC<sub>50</sub> values of 107-152 mg/L for a commercial LAS sample (dossier 4.4c). Studies with the bacterium *Pseudomonas putida* reported EC<sub>50</sub> 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 EC<sub>0</sub>/EC<sub>10</sub>/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).

### 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 sediment spiked with commercial LAS with an average alkyl chain length C<sub>11.8</sub> (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 LAS sorbed to sediment by repeated additions for 80 days (Bressan et al. 1989). All animals survived and were actively filter-feeding at sediment concentrations beginning at 750 mg/kg and 200 mg/kg at the end of the test. Similarly, a tubificid, *Branchiura sowerbyi*, was exposed for 220 days to sediment spiked with 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. According to Marin et al. (1994), no effects were observed in the marine mussel, *M. galloprovincialis*, at 132 mg/kg (initial concentration). The LAS concentration decreased by 90% by the end of the exposure but the kinetics were not reported so the results can not be used directly to determine a NOEC value. Most recently, GLP studies have been conducted with *Lumbriculus variegatus* (an oligochaete worm) and *Caenorhabditis elegans* (a nematode worm) to finalize the effects assessment of sediment associated LAS (Comber et al. 2004). After 28 days of exposure to sediment spiked with radiolabeled LAS, the resultant survival, reproduction and growth NOEC for *L. variegatus* 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 sediments spiked with non-radiolabeled LAS based on effects on egg production.

**Table 14. Results of Sediment Exposures**

Species	Test Duration (days)	NOEC (mg/kg)	Reference (Reliability)
<b>Freshwater</b>			
<i>Chironomus riparius</i>	24	319	Pittinger et al. 1989, dossier 4.5.2° (2)
<i>Anodonta cygnea</i>	80	200	Bressan et al. 1989, dossier 4.5.2p (2)
<i>Branchiura sowerbyi</i>	220	-*	Casellato et al. 1992, dossier 4.5.2q (4)
<i>Lumbriculus variegatus</i>	28	81	Comber et al. 2004, dossier 4.5.2r (2)
<i>Caenorhabditis elegans</i>	3	100	Comber et al. 2004, dossier 4.5.2s (2)
<b>Marine</b>			
<i>Mytilus galloprovincialis</i>	7	-*	Marin et al. 1994, dossier 4.5.2u (2)

\* The range of exposure concentrations was too low to derive a useful toxicity value.

### 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 (greater than or equal to 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. An integrated model stream ecosystem (Experimental Stream Facility, ESF) that did not have these design limitations was used to test a C<sub>12</sub>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 (0.37 mg/L if normalized to C<sub>11.6</sub> 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 12), and the resultant HC<sub>5</sub> values (0.36-0.43 mg/L for C<sub>11.6</sub> LAS).

**Table 15. Results of Model Ecosystem Studies**

Type of Ecosystem	Avg. Alkyl Chain Length	Exposure Duration	Most Sensitive Endpoint (Species)	NOEC (mg/L)	Reference (Reliability)
Experimental Stream	C <sub>12</sub>	56 days	Increased drift, reduced benthic abundance (Invertebrates)	0.27	Belanger et al. 2002, dossier 4.7 (1)
Artificial Stream	C <sub>11.52</sub>	28 days	Population density (invertebrates)	≥0.12	Tattersfield et al. 1995, 1996, dossier 4.7b (4)
Experimental Stream	C <sub>11.9</sub>	45 days	No effects observed (Periphyton, detritus, invertebrates, snails, amphipods and fish)	>0.36	Fairchild et al. 1993, dossier 4.7 (2)
Outdoor Ponds	C <sub>12</sub>	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 <sub>11.9</sub>	28 days	Microbial function	0.5	Larson and Maki 1982, dossier 4.7 (2)
Aquaria with sediment and activated sludge effluent	C <sub>11.9</sub>	28 days	Growth (Bluegill sunfish)	1.0	Maki 1981, dossier 4.7i (2)
In Situ River	C <sub>11.9</sub>	21 days	Photosynthesis inhibition (phytoplankton)	9.8	Lewis et al. 1993, dossier 4.7j (2)
Bottles filled with lake water	C <sub>11.8</sub> C <sub>13.3</sub>	3 hours/ month for 6 months	Photosynthesis inhibition (phytoplankton)	3.4* 1.9*	Lewis and Hamm 1986, dossier 4.7 (2)

\* EC<sub>50</sub> 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). Additional information is available from other investigations of LAS toxicity on terrestrial invertebrates (Holmstrup and Krogh 2001; Mieure et al. 1990). These data are summarized in Table 16. In these studies, 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 18 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. Hence, these values are likely to be overly conservative and the use of the values for hazard assessment may not be appropriate.

**Table 16. Results of LAS Exposures on Soil Invertebrates (in mg/kg dry weight)**

Species	Endpoint	NOEC	LOEC	L/EC <sub>10</sub>	L/EC <sub>50</sub>	Reference (Reliability)
<i>Aporrectodea caliginosa</i>	Adult Survival	278	793	329	535	Holmstrup and Krogh 2001, dossier 4.6.1b (2)
	Juvenile Survival	>397	>397	>397	>397	
	Juvenile Growth	278	397	105	354	
<i>Aporrectodea longa</i>	Adult Survival	278	793	329	535	Holmstrup and Krogh 2001, dossier 4.6.1b (2)
	Juvenile Survival	397	793	296	517	
	Juvenile Growth	79	278	84	349	
<i>Enchytraeus albidus</i>	Adult survival	<750	750	511	1400	Gejlsbjerg et al., 2001; dossier 4.6.1f (2)
	Reproduction	750	1500	447	1143	
<i>Enchytraeus albidus</i>	Adult Survival	198	397	194	430	Holmstrup and Krogh 2001, dossier 4.6.1b (1)
	Reproduction	20	40	6	41	
<i>Eisenia foetida</i>	Reproduction			383	558	Jensen et al. 2001, dossier 4.6.1a (4)
<i>Eisenia foetida</i>	Body Weight	250	500		>1000	Mieure et al. 1990, dossier 4.6.1c (2)
<i>Folsomia candida</i>	Adult survival	1000	2500	750	1338	Gejlsbjerg et al., 2001; dossier 4.6.1f (2)
	Reproduction	500	1000	480	1143	
<i>Folsomia candida</i>	Reproduction			18	91	Jensen et al. 2001, dossier 4.6.1a (4)
<i>Folsomia fimetaria</i>	Adult Survival	>793	>793	>793	>793	Holmstrup and Krogh 2001, dossier 4.6.1b (1)
	Reproduction	278	278	85	424	
<i>Folsomia fimetaria</i>	Adult survival	>1000	>1000	>1000	>1000	Holmstrup and Krogh, 1996, dossier 4.6.1e (2)
	Juvenile survival	500	700	196	570	
	Reproductive output	500	1000	147	737	
	Juvenile growth	<200	200	163	896	
	Molting frequency	<300	300	185	923	
<i>Folsomia fimetaria</i>	Reproduction			96	442	Jensen et al. 2001, dossier 4.6.1a (4)
<i>Hypoaspis aculeifer</i>	Adult Survival	>793	>793	>793	>793	Holmstrup and Krogh 2001, dossier 4.6.1b (2)
	Reproduction	278	793	82	236	
<i>Hypogastrura assimilis</i>	Reproduction	79	278	99	421	Holmstrup and Krogh 2001, dossier 4.6.1b (1)
<i>Isotoma viridis</i>	Growth			41		Jensen et al. 2001, dossier 4.6.1a (4)
<i>Lumbricus terrestris</i>	Body Weight/ Burrowing	667	1333		>1333	Mieure et al. 1990, dossier 4.6.1d (2)
<i>Platynothrus peltifer</i>	Reproduction	320			467	Jensen et al. 2001, dossier 4.6.1a (4)



**Terrestrial Toxicity – Plants** (dossier section 4.6.2)

Several studies have been conducted in which terrestrial plants have been exposed to LAS-spiked soils. These studies are summarized in Table 17. In these studies, LAS was added as aqueous solutions and not associated with sludge, which would be the normal route of exposure for agricultural soil.

**Table 17. Results of LAS Exposure on Terrestrial Plants (in mg/kg dry weight)**

Species	Endpoint	EC <sub>10</sub>	EC <sub>50</sub>	NOEC	Reference (Reliability)
<i>Amaranthus retroflexus</i>	Growth		142		Jensen et al. 2001, dossier 4.6.2a (4)
<i>Avena sativa</i>	Growth	50	300		Jensen et al. 2001, dossier 4.6.2a (4)
<i>Avena sativa</i>	Emergence of Seedlings			50	European Commission 2000, dossier 4.6.2f (4)
<i>Brassica rapa</i>	Growth		134		Jensen et al. 2001, dossier 4.6.2a (4)
<i>Brassica rapa</i>	Growth	90	200		Jensen et al. 2001, dossier 4.6.2a (4)
<i>Brassica rapa</i>	Emergence of Seedlings			50	European Commission 2000, dossier 4.6.2d (4)
<i>Chenopodium album</i>	Growth		164		Jensen et al. 2001, dossier 4.6.2a (4)
<i>Galinsoga parviflora</i>	Growth		90		Jensen et al. 2001, dossier 4.6.2a (4)
<i>Helianthus annuus</i>	Growth		289		Jensen et al. 2001, dossier 4.6.2a (4)
<i>Lycopersicum esculentum</i>	Emergence of Seedlings			50	European Commission 2000, dossier 4.6.2e (4)
<i>Malvia pusila</i>	Growth		204		Jensen et al. 2001, dossier 4.6.2a (4)
<i>Nigella arvensis</i>	Growth		132		Jensen et al. 2001, dossier 4.6.2a (4)
<i>Phaseolus aureus</i>	Growth		316		Jensen et al. 2001, dossier 4.6.2a (4)
<i>Sinapis alba</i>	Growth	200	300		Jensen et al. 2001, dossier 4.6.2a (4)
<i>Sorghum bicolor</i>	Growth		137		Jensen et al. 2001, dossier 4.6.2a (4)
<i>Solanum nigrum</i>	Growth		169		Jensen et al. 2001, dossier 4.6.2a (4)
Grass, Beans, Radishes	Biomass			-*	Figge and Schoberl 1989, dossier 4.6.2b (2)
Potatoes	Biomass			-*	Figge and Schoberl 1989, dossier 4.6.2b (2)
Radish, Tomato, Oats	Growth		>77.1	25.7	European Commission 2000, dossier 4.6.2c (4)

\* The exposure concentration tested was too low to derive a useful toxicity value.

**Terrestrial Toxicity – Avian**

One non-guideline study is available in which the effects of LAS 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.

### **Terrestrial Toxicity – Field Studies**

Jensen and Krogh (1999) 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 microarthropods and earthworms after sludge application resulting in LAS soil concentrations of 15 mg/kg dry weight. Brandt et al. (2003) found that 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), 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 vapour pressure ( $3\text{-}5 \times 10^{-13}$  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<sub>11.6</sub> LAS. Based on two Fugacity III modelling studies, LAS transport between environmental compartments is primarily determined by inputs to the various compartments, biodegradation rates in water and soil, and water-sediment transfer. 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 biodegradation of LAS under aerobic conditions, 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. LAS is effectively removed in biological wastewater treatment (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<sub>2</sub>, SO<sub>4</sub><sup>2-</sup>, and water. LAS does not generally degrade under anaerobic conditions. The bioconcentration factor decreases with decreasing average alkyl chain lengths (from almost 1000 for 2-phenyl-C<sub>13</sub> LAS to 2 for 6-phenyl-C<sub>10</sub> LAS). The BCF for currently produced C<sub>11.6</sub> LAS is 87 L/kg, with rapid clearance. The BCF decreases with decreasing average alkyl chain lengths and was 22 L/kg for filtered Mississippi River water (average alkyl chain length of surface water fingerprint = C<sub>10.8</sub>).

Ecotoxicity data are extensively available for LAS, with several comprehensive reviews having been completed. The lowest valid acute LC<sub>50</sub>/EC<sub>50</sub>/ErC<sub>50</sub> values based on a review of the aquatic toxicity data on commercially representative LAS (C<sub>11.6</sub>-C<sub>11.8</sub>) 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 LC<sub>50</sub> values >1000 mg/L for fish and *D. magna*. Chronic aquatic toxicity data have been evaluated for five freshwater species in which multiple studies were reported and nine freshwater species for which single studies were reported. Available NOEC values range from 0.25 to 3.4 mg/L for freshwater species. Geometric mean NOEC values for marine species ranged from 0.025 to 5.0 mg/L. Based on the mesocosm studies, a NOEC of 0.27 mg/L (0.37 mg/L if normalized to C<sub>11,6</sub> 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, and the resultant HC<sub>5</sub> values (0.36-0.43 mg/L for C<sub>11,6</sub> LAS).

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.

NOEC values for sediment exposures were greater than or equal to 81 mg/kg dry matter.

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.

Field studies indicate no adverse effects of LAS in sludge-amended soil from LAS levels of 15 mg/kg dry matter in the soil or 31,300 mg/kg dry matter in sludge.

Maximal LAS sludge levels reported in monitoring studies were also generally less than 20,000 mg/kg dry matter. Average LAS concentrations in sludge from US sewage treatment plants ranged from 150 mg/kg dry matter for aerobic digesters to 10,500 mg/kg dry matter for anaerobic digesters, with similar LAS sludge levels reported in European monitoring studies. In sludge-amended agricultural soils, LAS concentrations are generally less than 15 mg/kg dry weight immediately after sludge spreading, less than 2 mg/kg in fields spread two to three months previously and less than 1 mg/kg in fields spread the previous year.

## 5 RECOMMENDATIONS

The chemicals in the LAS category are currently of low priority for further work.

### **Agreed at SIAM 17:**

**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.

### **To be discussed at SIAM 20:**

**Environmental:** The chemicals in the LAS category possess properties indicating a hazard for aquatic species. However, they are of low priority for further work due to ready and/or rapid biodegradation and limited potential for bioaccumulation. Countries may desire to investigate any exposure scenarios that were not presented by the Sponsor country.

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## 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 alkyl benzene 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  $\leq 28$  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  $\mu\text{g/L}$  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  $\mu\text{g/L}$  for river water samples collected under low dilution (worst case) conditions below treatment plant mixing zones and range from non-detect ( $< 0.1 \mu\text{g/L}$ ) to 28  $\mu\text{g/L}$  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  $3.5 \times 10^{-5}$  to  $9.3 \times 10^{-7}$  mg/kg/day. Similarly, the results of the dermal exposure modeling for various activities range from  $5.6 \times 10^{-2}$  to  $4.7 \times 10^{-5}$  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**

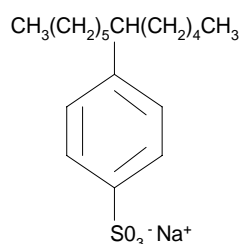
<b>(1) Date of Submission</b>	2003-11-06	
<b>(2) Identity of Organization</b>	Industry Coalition for the SIDS Assessment of LAS John E. Heinze, Ph.D., Manager 529 14 <sup>th</sup> Street, NW, Suite 807 Washington, DC 20045, USA 202-737-0171 (tel) 202-737-8406 (fax) <a href="mailto:jheinze@johnadams.com">jheinze@johnadams.com</a>	
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**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<sub>10-16</sub> Monoalkylbenzene sulfonic acid, sodium salt  
 68411-30-3 C<sub>10-13</sub> Alkylbenzene sulfonic acid, sodium salt  
 69669-44-9 C<sub>10-14</sub> Alkylbenzene sulfonic acid, sodium salt  
 85117-50-6 C<sub>10-14</sub> Monoalkylbenzene sulfonic acid, sodium salt  
 90194-45-9 C<sub>10-13</sub> Alkyl derivatives benzene sulfonic acid, sodium salt  
 127184-52-5 4-C<sub>10-13</sub>-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<sub>12</sub>-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

The report covers exposure from manufacturing and consumer/commercial/industrial use for all LAS volumes produced and used in the United States.

### IV. Summary

#### (1) 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 alkyl benzene 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  $\leq 28$  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  $\mu\text{g/L}$ . Results of extensive environmental monitoring evaluations in the United States indicate that measured surface water concentrations were generally below 50  $\mu\text{g/L}$  for river water samples collected under low dilution (worst case) conditions below treatment plant mixing zones and range from non-detect ( $<0.1 \mu\text{g/L}$ ) to 28  $\mu\text{g/L}$  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 SIAR). Modeled estimates of environmental exposure leading to indirect human exposure from drinking water and fish consumption range from 3.5E-5 to 9.3E-7 mg/kg/day. Similarly, the results of the dermal exposure modeling for various activities range from 5.6E-2 to 4.7E-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%).

#### (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)**
<b>Surface Water Monitoring</b>		
Mississippi River	2.21	270*
50 U.S. Rivers	43 to 46	270*
<b>Manufacturing Effluent Modeling</b>		
Aquatic	50th percentile facility	
Mean stream conc.	4.8	270*
7Q10 Stream conc.	13	270*
Drinking Water Consumption		
50 <sup>th</sup> percentile facility	9.3E-7	85**
Fish Consumption		
50 <sup>th</sup> percentile facility	3.5E-5	85**
<b>Consumer Use Modeling</b>		
Aquatic		
Median flow	9.9E-2	270*
7Q10 flow	1.3	270*
Drinking Water Consumption		
7Q10 flow	1.9E-6	85**
Fish Consumption		
7Q10 flow	7.2E-7	85**
<b>Consumer Use – Dermal Modeling</b>		
<i>Diluted and undiluted laundry and dishwashing products and hard surface cleaning products</i>		
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**
<i>Laundry product residual on clothing</i>		
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**
<i>Face and Hand Soap product residual after washing</i>		
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
<p><b>(1) Process Description</b></p> <p>LAS is produced from the sulfonation of linear alkyl benzene (LAB) to make an intermediate, LAB sulfonic acid. The acid is produced primarily by oleum or air/SO<sub>3</sub> 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).</p>
<p><b>(2) General Description of Potential Releases and Exposures</b></p> <p>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<sub>2</sub>/SO<sub>3</sub> 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.</p> <p>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.</p>
<p><b>(3) Discussion of Factors that Mitigate or Exacerbate Releases and Exposures</b></p> <p>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.</p> <p>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.</p> <p>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.</p>
<p><b>(4) Remarks</b></p> <p>Product formulation, the blending of LAS with other ingredients, is not expected to result in workplace exposures that exceed those for LAS manufacturing facilities.</p>

## 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:

<u>Product Type</u>	<u>Concentration in Products in US/Canada</u> (range)
---------------------	--

Laundry detergents (dry)	5-25 %
Dishwashing detergents (liquids)	5-10 %
General cleaners	1-5 %
Disinfectant cleaners (liquids)	5-10 %

<u>Product Type</u>	<u>Concentration in Products in Europe</u> (range)
---------------------	---

Laundry detergents (dry)	5-10 %
Laundry detergents (liquids)	10-25 %
Pre-washes	10-25 %
Dishwashing detergents (liquids)	25-50 %

<u>Product Type</u>	<u>Concentration in Products in Japan</u> (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  $\leq 28$  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:** Quantitative estimation of occupational exposures from commercial products containing LAS is beyond the scope of this document.

### Consumer Use

#### (13) Function/ Product Use Description

LAS has wide-spread and dispersive use as a surfactant in the following consumer products.

<u>Product Type</u>	<u>Concentration in Products in US/Canada</u> (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 %

<u>Product Type</u>	<u>Concentration in Products in Europe</u> (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 %

<u>Product Type</u>	<u>Concentration in Products in Japan</u> (range)
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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 ( $3 \times 10^{-13}$  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  $\leq 28$  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.

Inhalation exposures are not modeled for LAS, as they do not contribute significantly to total exposure.

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 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, 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  $\text{mg}/\text{m}^3$ . HERA (2002) reported an air concentration of 0.35  $\text{mg}/\text{m}^3$  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  $4.0 \times 10^{-5}$   $\text{mg}/\text{kg}/\text{day}$  from this pathway, which is several orders of magnitude below the  $5.0 \times 10^{-3}$  to  $1.0 \times 10^{-3}$  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  $\text{mg}/\text{kg}$  (mean =  $0.23 \pm 0.19$   $\text{mg}/\text{kg}$ ) while NOEC values for sediment exposure are  $\geq 81$   $\text{mg}/\text{kg}$ .

**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<sub>11.1</sub> (range C<sub>10.2-12.0</sub>).

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<sub>11.5</sub> (range C<sub>10.7-11.9</sub>).

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<sub>12</sub> 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<sub>11.8-11.9</sub>

**(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](http://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 50<sup>th</sup> percentile represents a facility on a mid-size stream with average flow.

**Aquatic exposure -**

50<sup>th</sup> 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 -**

50<sup>th</sup> percentile facility -

Average Daily Dose (ADD) =

9.3E-07 mg/kg/day (chronic non-cancer)

**Fish consumption exposure –**

50<sup>th</sup> 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 50<sup>th</sup> 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 50<sup>th</sup> 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](http://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 50<sup>th</sup> 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<sup>2</sup>)
- PC: product concentration (g/cm<sup>3</sup>)
- 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.

## 1. Exposure during the activity/use of diluted and undiluted laundry and dishwashing products, and diluted and undiluted hard surface cleaning products

$$\frac{[FQ \times CA \times PC \times FT \times CF \times TF \times DA]}{BW} \times PF$$

	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 <sup>h</sup>	1 <sup>h</sup>	1 <sup>h</sup>	3 <sup>h</sup>	0.14 <sup>h</sup>	1 <sup>h</sup>	1 <sup>h</sup>
Contact Area (CA) (cm <sup>2</sup> )	360 <sup>b</sup>	360 <sup>b</sup>	1680 <sup>f</sup>	1680 <sup>f</sup>	1680 <sup>f</sup>	1680 <sup>f</sup>	180 <sup>j</sup>
Product Concentration (PC) (g/cm <sup>3</sup> )	0.6 <sup>a</sup>	1 <sup>a</sup>	0.01 <sup>a</sup>	0.0015 <sup>a</sup>	0.9 <sup>g</sup>	0.01 <sup>a</sup>	1 <sup>a</sup>
Film Thickness (FT) (cm)	0.0024 <sup>c</sup>	0.0024 <sup>c</sup>	0.0024 <sup>c</sup>	0.0024 <sup>c</sup>	0.0024 <sup>c</sup>	0.0024 <sup>c</sup>	0.0024 <sup>c</sup>
Conversion Factor (CF) (1000 mg/g)	1000	1000	1000	1000	1000	1000	1000
Time Scaling Factor (TF) (unitless)	0.007 <sup>d</sup>	0.007 <sup>d</sup>	0.007 <sup>d</sup>	0.03 <sup>d</sup>	.00035 <sup>d</sup>	0.014 <sup>h</sup>	0.014 <sup>h</sup>
Dermal Absorption (DA) (%)	100% <sup>i</sup>	100% <sup>i</sup>	100% <sup>i</sup>	100% <sup>i</sup>	100% <sup>i</sup>	100% <sup>i</sup>	100% <sup>i</sup>
Female body weight (BW) (kg)	60 <sup>e</sup>	60 <sup>e</sup>	60 <sup>e</sup>	60 <sup>e</sup>	60 <sup>e</sup>	60 <sup>e</sup>	60 <sup>e</sup>
LAS concentration in product formulation (PF) <sup>g</sup> (%)	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)



## 2. Exposure to laundry and fabric conditioning product residual on clothing

$$\frac{[A \times PR \times PT \times DA \times CF] \times PF}{BW}$$

	Liquid Laundry Detergent	Dry Laundry Detergent	Tablet Laundry Detergent	Fabric conditioner (dryer-sheet)
Amount Per Use (A) (g/day or g/wash)	121 <sup>a</sup>	121 <sup>a</sup>	135 <sup>a</sup>	3 <sup>a</sup>
Percent Retained on Clothing (PR) (%)	1% <sup>a</sup>	1% <sup>a</sup>	1% <sup>a</sup>	10% <sup>a</sup>
Percent Transferred from Clothing to Skin (PT) (%)	1% <sup>a</sup>	1% <sup>a</sup>	1% <sup>a</sup>	1% <sup>a</sup>
Dermal Absorption (DA) (%)	100% <sup>b</sup>	100% <sup>b</sup>	100% <sup>b</sup>	100% <sup>b</sup>
Conversion Factor (CF) (1000 mg/g)	1000	1000	1000	1000
Female body weight (BW) (kg)	60 <sup>c</sup>	60 <sup>c</sup>	60 <sup>c</sup>	60 <sup>c</sup>
LAS concentration in product formulation (PF) <sup>g</sup> (%)	1-25% <sup>d</sup>	5-25% <sup>d</sup>	5-25% <sup>d</sup>	0.1 – 0.5% <sup>d</sup>

References:

- a: SDA Habit and Practice Survey
- b: Default assumption
- c: EU Technical Guidance Document, 1996
- d: LAS Coalition Survey, Min-Max values

## 3. Exposure to face and hand soap residual after use

$$\frac{[FQ \times A \times PR \times DA \times CF] \times PF}{BW}$$

	Bar Soap Hand	Bar Soap Face
Frequency of Use (FQ) (use/day)	6 <sup>a</sup>	1 <sup>a</sup>
Amount Per Use (A) (g/use)	0.36 <sup>a</sup>	0.27 <sup>a</sup>
Percent Retained on Skin (PR) (%)	1% <sup>c</sup>	1% <sup>c</sup>
Dermal Absorption (DA) (%)	100% <sup>b</sup>	100% <sup>b</sup>
Conversion Factor (CF) (1000 mg/g)	1000	1000
Female body weight (BW) (kg)	60 <sup>c</sup>	60 <sup>c</sup>
LAS concentration in product formulation (PF) <sup>g</sup> (%)	1-5% <sup>d</sup>	1-5% <sup>d</sup>

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****1. Exposure during the activity/use of diluted and undiluted laundry and dishwashing products and diluted and undiluted hard surface cleaning products**

	<b>Potential Dermal Exposure (mg/kg/day)<sup>a</sup></b>
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

<sup>a</sup> range based on minimum and maximum product concentration values

**2. Exposure to laundry and fabric conditioning product residual on clothing**

	<b>Potential Dermal Exposure (mg/kg/day)<sup>a</sup></b>
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

<sup>a</sup> range based on minimum and maximum product concentration values

**3. Exposure to face and hand soap residual after use**

	<b>Potential Dermal Exposure (mg/kg/day)<sup>a</sup></b>
Bar Soap – Hand	3.6E-3 to 1.8E-2
Bar Soap - Face	5.0E-4 to 2.3E-3

<sup>a</sup> 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%).

**Annex 1 References**

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Valtorta, L., Radici, P., Calcinai, D., and Cavalli, L. 2000. Recent developments of LAB/LAS. Riv. It. Sostanze Grasse. LXXVII:73-76.

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**7 ANNEX 2 & ANNEX 3 (LANDSCAPE ORIENTATION)**

**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 CaCO <sub>3</sub> /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, 0.13, 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)



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	Static/flow through	# replicates	Indiv./rep	Nominal conc (mg/L)	Test T range (°C)	Hard. (mg CaCO <sub>3</sub> /L)	Measured conc.	Control mortality	Remarks/deviation from protocol
				GLP								
11. Holman and Macek, 1980	4.1		US EPA 1975 EPA-660/3-75-009	No					40	MBAS		C <sub>11.7</sub> ; 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	
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 (°C)	Hard. (mg NaHCO3/L)	Measured conc.	Control 96h count	Remarks/deviation from protocol
23. 43235, P&G 1991	35.5	96 Hr	<i>Selenastrum capricornutum</i>	Bionomics	OECD 201	Yes	Duplicate tests and quadriuplicate controls	10 <sup>4</sup> cells/ml	Control, 1.0, 3.1, 10, 32, 99, 180, 320, 560	21-22	150	measured	3.610 <sup>6</sup> cells/ml	White precipitate highest concentrations
24. Lewis, 1986; Lewis and Hamm, 1986	29	96 Hr	<i>Selenastrum capricornutum</i>		ASTM, 1984	No				21.2-25.6	137			Low value; dossier 4.3(a)
25. Verge and Moreno, 1996	163	72 Hr	<i>Scenedesmus subspicatus</i>		OECD, 1984	No	Triplicate test concentrations and six control replicates	10 <sup>4</sup>		21-22		Nominal		Dossier 4.3(d)
26. Scholz, 1992	127.9	72 Hr	<i>Scenedesmus subspicatus</i>		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	<i>Scenedesmus subspicatus</i>		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)

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**List of Published References**

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11. Holman, W. and Macek, K., 1980; An aquatic safety assessment of Linear Alkylbenzene Sulfonate (LAS): Chronic effects on Fathead minnows. Transactions of the American Fisheries Society 109, 122-131.

16. Taylor, M.J.; Effect of Diet on the Sensitivity of *Daphnia magna* to Linear Alkylbenzene Sulfonate, Aquatic Toxicology and Hazard Assessment: Seventh Symposium, ASTM STP 854, R.D. Cardwell, R. Purdy, and R.C. Bahner, Eds, American Society for Testing and Materials, Philadelphia, 1985, pp 53-72.

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18. Lewis, M.A. and Suprenant, D., 1983; Comparative Acute Toxicities of Surfactants to Aquatic Invertebrates. Ecotoxicology and Environmental Safety, 7, 313-322 (1983).

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.

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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**

<b>Paper</b>	<b>Reason</b>
<b>Fish – <i>Lepomis macrochirus</i></b>	
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
<b>Fish – <i>Pimephales promelas</i></b>	
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

<b>Algae</b>	
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

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**Annex 3 – Derivation of the HC<sub>5</sub> Value****Linear Alkylbenzene Sulfonate (LAS)**  
Industry Coalition for the SIDS Assessment of LAS  
September 15, 2004**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<sub>5</sub>, is the lower 5<sup>th</sup> 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<sub>5</sub> 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).

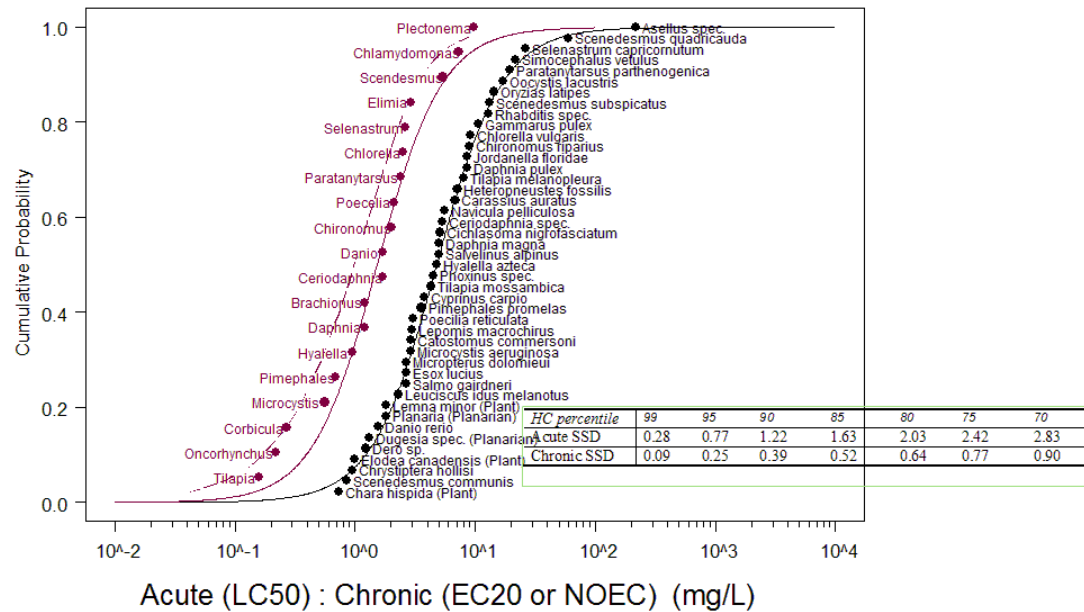
Consequently, the available chronic data and the van de Plassche et al data were plotted using log-logistic distributions. The fitted NOEC distribution is shown by the solid line in the distribution function. Lower 95% confidence limits on the fitted NOEC distribution function (dashed lines) were calculated 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<sub>5</sub> (HC<sub>5, 50% confidence interval</sub>) value.

The available chronic toxicity data and the data of van de Plassche et al. (1999) are presented in Table 12 of this SIAR. For *Microcystis aeruginosa*, dossier 4.3s, the NOEC was calculated by dividing the EC<sub>50</sub> value by 3. As documented below (data from BKH 1993), the average EC<sub>50</sub>/NOEC ratio for LAS is 3, and thus this calculation of the NOEC value from the EC<sub>50</sub> is supported by a large database of information.



Actual C12 - LAS A:C ratios (water column) ~ 3



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23 February 2004

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All NOEC values were normalized to C<sub>11.6</sub> 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.

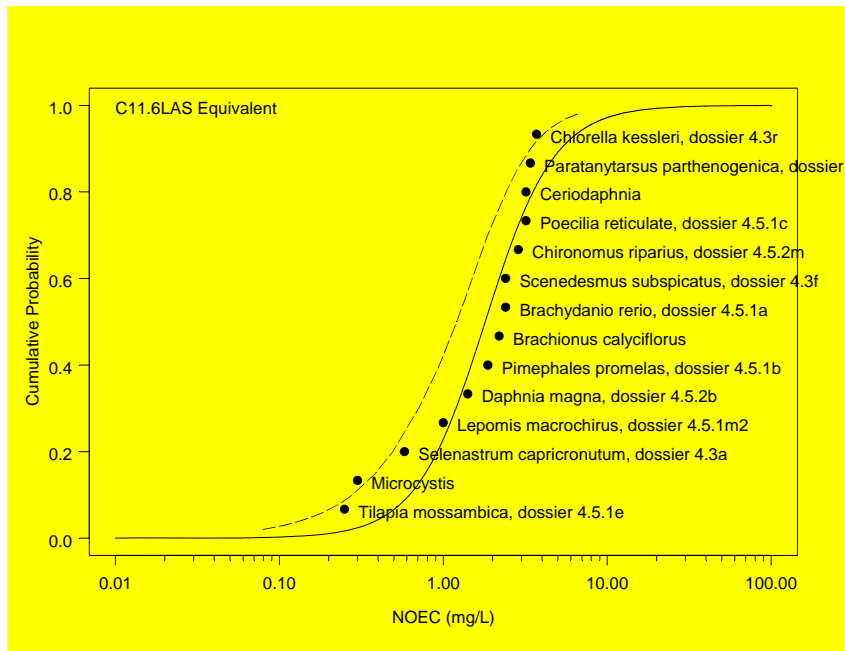
## Results

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 12 of this SIAR. Using the log-logistic distribution of the normalized NOEC data, the  $HC_5$  value calculated is 0.43 mg/L. The data used ("Available Chronic Values"), the cumulative probability distribution of the data and the  $HC_5$  calculation are shown below.

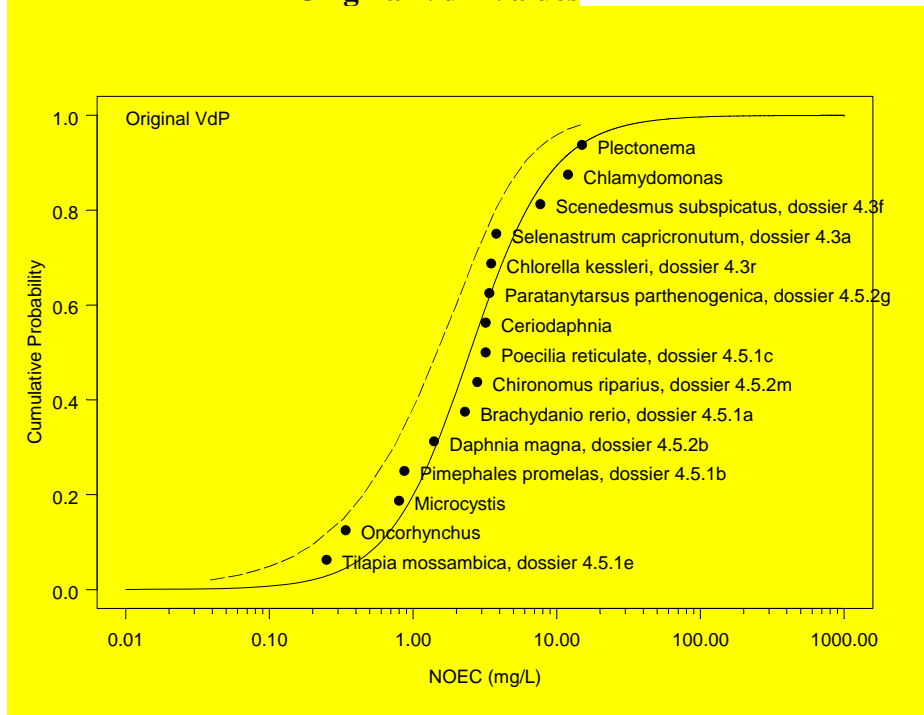
Original VdP Values (Table 12)	NOEC (mg/L)	Available Chronic Values	NOEC (mg/L)
<b>Fish</b>		<b>Fish</b>	
Brachydanio rerio (Not reviewed by van de Plassche et al.)	2.3	Brachydanio rerio, dossier 4.5.1a	2.4
Oncorhynchus mykiss (geometric mean)	0.34	Lepomis macrochirus, dossier 4.5.1m (No valid study identified)	1
Pimephales promelas (geometric mean)	0.87	Pimephales promelas, dossier 4.5.1b	1.87*
Poecilia reticulata	3.2	Poecilia reticulata, dossier 4.5.1c	3.21
Tilapia mossambica	0.25	Tilapia mossambica, dossier 4.5.1e	0.25
<b>Aquatic Invertebrates</b>		<b>Aquatic Invertebrates</b>	
(Not reviewed by van de Plassche et al.)		Brachionus calyciflorus, dossier 4.5.2h	2.19
Ceriodaphnia sp.	3.2	Ceriodaphnia sp., dossier	3.2
Chironomus riparius	2.8	Chironomus riparius, dossier 4.5.2n	2.87
Daphnia magna (geometric mean)	1.4	Daphnia magna, dossier 4.5.2b	1.41*
Paratanytarsus parthenogenica	3.4	Paratanytarsus parthenogenica, dossier 4.5.2g	3.4
<b>Algae</b>		<b>Algae</b>	
Chlamydomonas reinhardi	12	(No valid study identified)	
Chlorella kessleri	3.5	Chlorella kessleri, dossier 4.3r	3.71
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, dossier 4.3f	2.4*
Selenastrum capricornutum (geometric mean)	3.8	Selenastrum capricornutum, dossier 4.3a	0.58*

\*Available study closest to VdP geometric mean

**Available Chronic Data Distribution**



**Original VdP Values**



**Log-Logistic Calculation**

Compound Group	Statistical Parameters			
	Intercept (u) (mean)	Scale (sigma) Variability	K-S Test p-value	HC5
Available Chronic Values	0.589	0.4841	0.6675	0.433129819
Original VdP Values	0.911	0.6531	0.8655	0.363486427

**Discussion**

The HC<sub>5</sub> 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 its 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 12 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 and algae. LAS’s nonspecific mode of action does not suggest that other taxonomic groups such as higher aquatic plants would differ substantially in their sensitivity.
- 5) Minimum sample size – The database consists of NOEC values on at least 13 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 12). For the available data set, the study closest to the geometric mean value of van de Plassche et al. 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<sub>5</sub> value with 50% confidence limits.
- 9) Estimation of NOEC – The HC<sub>5</sub> 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<sub>5</sub> values and the mesocosm data, as discussed in the SIAR, section 4.1 Aquatic Effects.
- 10) Deviations from recommendations – The only deviation is that the data set does not include higher plants. LAS’s nonspecific mode of action suggests that higher aquatic plants would not differ substantially in their sensitivity compared to the other groups tested (fish, crustaceans, insects, a rotifer and algae). The available data on terrestrial plants is discussed in section 4.2 of the SIAR.

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