Institute for Health and Consumer Protection

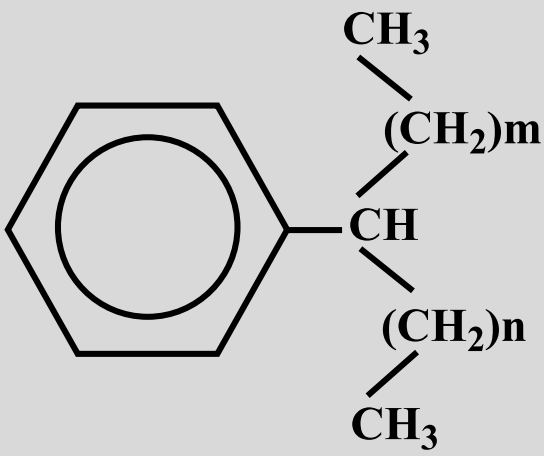
European Chemicals Bureau

Existing Substances

European Union Risk Assessment Report

CAS No.: 67774-74-7 | EINECS No.: 267-051-0

benzene, C_{10-13} alkyl derivs.



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European Union Risk Assessment Report

BENZENE C_{10-13} ALKYL DERIVS.

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RISK ASSESSMENT

Cataloguing data can be found at the end of this publication

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RISK ASSESSMENT

Final report, 30 June 1997

Italy

Rapporteur for the risk evaluation of Benzene C_{10-13} alkyl derivs is the Ministry of Public Health, in co-operation with the Italian National Health Institute (Istituto Superiore di Sanità – ISS). Responsible for the risk evaluation and subsequently for the contents of this report is the rapporteur.

The scientific work on this report has been prepared by the Italian National Health Institute (Istituto Superiore di Sanità – ISS), by order of the rapporteur.

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Date of Last Literature Search :	**1995**
Review of report by MS Technical Experts finalised:	**September, 1997**
Final report:	**June, 1997**

Foreword

We are pleased to present this Risk Assessment Report which is the result of in-depth work carried out by experts in one Member State, working in co-operation with their counterparts in the other Member States, the Commission Services, Industry and public interest groups.

The Risk Assessment was carried out in accordance with Council Regulation (EEC) 793/93[1] on the evaluation and control of the risks of "existing" substances. "Existing" substances are chemical substances in use within the European Community before September 1981 and listed in the European Inventory of Existing Commercial Chemical Substances. Regulation 793/93 provides a systematic framework for the evaluation of the risks to human health and the environment of these substances if they are produced or imported into the Community in volumes above 10 tonnes per year.

There are four overall stages in the Regulation for reducing the risks: data collection, priority setting, risk assessment and risk reduction. Data provided by Industry are used by Member States and the Commission services to determine the priority of the substances which need to be assessed. For each substance on a priority list, a Member State volunteers to act as "Rapporteur", undertaking the in-depth Risk Assessment and recommending a strategy to limit the risks of exposure to the substance, if necessary.

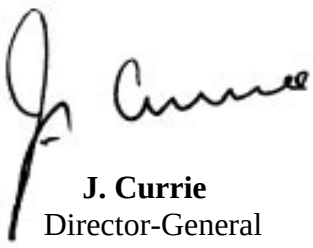
The methods for carrying out an in-depth Risk Assessment at Community level are laid down in Commission Regulation (EC) 1488/94[2], which is supported by a technical guidance document[3]. Normally, the "Rapporteur" and individual companies producing, importing and/or using the chemicals work closely together to develop a draft Risk Assessment Report, which is then presented at a Meeting of Member State technical experts for endorsement. The Risk Assessment Report is then peer-reviewed by the Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE) which gives its opinion to the European Commission on the quality of the risk assessment.

If a Risk Assessment Report concludes that measures to reduce the risks of exposure to the substances are needed, beyond any measures which may already be in place, the next step in the process is for the "Rapporteur" to develop a proposal for a strategy to limit those risks.

The Risk Assessment Report is also presented to the Organisation for Economic Co-operation and Development as a contribution to the Chapter 19, Agenda 21 goals for evaluating chemicals, agreed at the United Nations Conference on Environment and Development, held in Rio de Janeiro in 1992.

This Risk Assessment improves our knowledge about the risks to human health and the environment from exposure to chemicals. We hope you will agree that the results of this in-depth study and intensive co-operation will make a worthwhile contribution to the Community objective of reducing the risks from exposure to chemicals overall.

H.J. Allgeier
Director-General
Joint Research Centre



J. Currie
Director-General
Environment, Nuclear Safety and Civil Protection

[1] O.J. No L 084, 05/04/199 p. 0001 - 0075
[2] O.J. No. L 161, 29/06/1994 p. 0003 – 0011
[3] Technical Guidance Document, Part I-V, ISBN 92-827-801[1234]

0 OVERALL RESULTS OF THE RISK ASSESSMENT

CAS-No. 67774-74-7
EINECS-No. 267-051-0
IUPAC name Benzene C_{10-13} alkyl derivs.

Overall result of the risk assessment:

( ) i) There is need for further information and/or testing
(X) ii) There is at present no need for further information and/or testing of for risk reduction measures beyond those which are being applied already
( ) iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account

Conclusion ii) is reached because:

	PEC/PNEC	
	Local	**Regional**
- The PEC in the effluents of sewage treatment plants does not exceed the PNEC (micro-organisms)	$4.5 \cdot 10^{-4}$	-
- The PEC in surface waters does not exceed the $PNEC_{aquatic\ organism}$		
Using calculated data	0.68	0.093
Using monitoring data	0.53	-
- The PEC in sediments does not exceed the $PNEC_{sediment\ organisms}$		
Using calculated data	0.75	0.19
Using monitoring data	0.014	-
- The PEC in soil does not exceed the $PNEC_{terrestrial\ organisms}$		
Using calculated data	0.26	0.0022
Using monitoring data	0.09	-
- No concern for workers. The margins of safety range from 46 (dermal exposure) to more than 100 (inhalation exposure)		
- For consumers the margins of safety are very high, more than 8000		
- For men exposed indirectly via the environment the margins of safety do not indicate concern (MOS > 10^5)		

CONTENTS

1 GENERAL SUBSTANCE INFORMATION

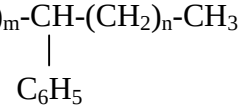
Introduction

Very similar substances have been previously considered in the OECD HPV programme and an OECD/SIDS risk assessment document has been finalised in USA. The document refers to various mixtures of linear alkylbenzenes (LAB) containing dodecylbenzene (123-01-3) and undecylbenzene (6742-54-7). US manufacturers produce various mixtures of long-alkyl chain LAB with the alkyl group in the range of C_{10} - C_{16} carbon atoms. The CAS registry numbers used by US manufacturers of these materials are: 68648-87-3, 129813-58-7, 68442-69-3, 129813-59-8, 129813-60-1, 68648-86-2. An exposure profile on LAB (Ref. 43) has been also produced for the US EPA by an independent consultant under an EPA contract (May, 1995).
These documents have been taken into account and all information considered pertinent was incorporated in the present risk assessment report of the European LAB, which consists of mixtures of linear alkylbenzenes having an alkyl chain group restricted to the range of C_{10}-C_{13} carbon atoms, and which are produced by the European manufacturers under the CAS registry number of 67774-74-7.

Identification of the substance

CAS-No.:	67774-74-7
EINECS-No.:	267-051-0
IUPAC name:	Benzene, C_{10-13} alkyl derivs.
Synonyms:	Linear Alkylbenzene, LAB
Empirical formula:	$C_6H_5C_n H_{2n+1}$ n = 10 - 13

Structural formula:



CH_3-$(CH_2)_m$-CH-$(CH_2)_n$-CH_3 (with C_6H_5 on the CH)

m + n = 7 - 10

Molecular weight: 239-243

Average alkyl carbon number: C = 11.6

Physical status: Liquid

LAB is a mixture of C_{10}-C_{13} alkyl chain homologues with all position isomers of the aromatic ring along the linear alkyl chain, except the terminal ones.

Purity/impurities, additives

Purity :	86 - 99% Purity is defined as the degree of the product linearity, namely the percent content of alkylates with C_{10}-C_{13} linear side alkyl chains. Depending on the production processes the commercial LAB contains two types of non linear alkylates as co-products.
Tetralins :	0.5 - 8%
Isoalkylbenzenes :	1 - 6%

They are an integral part of LAB commercial product contributing to the special performances of the sulphonated derivative (LAS) (Ref. 1).
The most common LAB on the market (ca. 75%) has a low tetralin content (< 0.5%).

Physico-chemical properties

Melting point:	< - 70°C	(DIN, Ref. 2)
Boiling range:	278 - 314°C at 1013 hPa	(ASTM, Ref. 3)
Density:	0.856 - 0.866 g/cm^3	(ASTM, Ref. 3)
Vapour pressure:		
at 25°C:	0.013 hPa	(ASTM, Ref. 4)
at 300°C:	3.99 hPa	(Calculated, Ref. 5)
Partition coefficient (log Pow):	7.5 - 9.12 at 25°C	(Calculated, Ref. 6)
Water solubility:	0.041 mg/l	(GLP, Ref. 5)
Flash point:	140°C	(ASTM, Ref. 4)
Flammable limits in air:	0.45 - 10.7 vol%	(DIN, Ref. 8)
Explosive properties:	none	(EEC,GLP, Ref. 7)

Classification

Classification according to Annex I

The substance is not included in Annex I.

Proposal of the competent authority

Human health effects

No classification is proposed for human health effects.

Environmental effects

The Classification and Labelling Working Group for the Environment (Dir. 92/32EEC amending for the seventh time Dir. 67/548/EEC) agreed to classify this substance N; R50, and this will be published in the 26th ATP of the Directive.

2 GENERAL INFORMATION ON EXPOSURE

2.1 MANUFACTURING

The commercial products are produced by three different technologies (Annex 1):

1. A mixture of n-paraffins and chloroparaffins, resulting from a partial chlorination of n-paraffins in a multistage or pipe reactor with chlorine gas, is fed with benzene in excess into a reactor where a $AlCl_3$- catalysed reaction is performed. The catalyst, suspended or dissolved in the crude alkylate, is then separated, while the benzene and unconverted n-paraffins are recovered by distillation and recycled to the previous reaction stage (Fig. 1).
2. n-Olefins are directly fed into the alkylation stage with benzene in excess in presence of $AlCl_3$ catalyst. The raw alkylate is then separated from the spent catalyst and subsequently washed with demi-water. In the separation section benzene is extracted and recycled, while some n-paraffins are separated (Fig. 1).
3. n-Paraffins are partially converted to internal n-olefins by catalytic dehydrogenation. The resulting mixture of n-paraffins and n-olefins is selectively hydrogenated to reduce diolefins and fed into an alkylation reactor together with benzene in excess and hydrofluoric acid as a catalyst in the Friedel - Craft reaction.
   In the next sections of the plant HF, benzene and unconverted n-paraffins are recovered and recycled to the preceding reaction stage (Fig. 2).

For all three processes, in the final stage of distillation, the LAB is separated from the heavy alkylate.

2.2 PROCESSING AND USE

LAB is almost entirely (> 99%) utilised as intermediate in the production of Linear Alkylbenzene Sulfonates (LAS). Some LAB also finds minor use as solvent and binder in speciality applications, e.g. cable oil, ink industry, paint and varnishes, insulating and electricity.
Some of these uses have been documented. Sweden, for example, for a series of different products has registered that LAB has been used for 43 - 66 ton in 1993 and for 48 ton in 1995. Denmark claimed that LAB as such (solvent?) has been used in cleaning products in quantities which have substantially decreased from 65 t/y in the mid-eighties to 12 t/y in 1995 and to 9 t/y until April 1996. These figures demonstrate that LAB in uses different from that of its transformation to LAS, is trivial, well below to 1% of the LAB production capacity and that it can be neglected in the risk assessment.
LAS is manufactured by LAB sulphonation and neutralisation of the corresponding sulphonic acid (Annex 2). LAB with a stream of SO_3 (Fig. 1) or oleum (Fig.2) are fed in equicurrent to the top of a multi-pipe reactor provided with a cooling jacket for the circulation of thermostated water. The sulphonic acid is discharged from the bottom of the reactor and is ready for the transport and/or the neutralisation.
Only a very small amount of LAB (typically 0.5%) remains in LAS as unsulphonated matter (Ref. 9, 38).
Manufacturers use LAS in laundry detergents (granular and liquid), in some all-purpose cleaners, in some liquid dishwashing detergents, and in industrial and institutional cleaners.

3 ENVIRONMENT

3.1 ENVIRONMENTAL EXPOSURE

3.1.0 General discussion

Manufacturing and processing/use

LAB production (1995)
Western Europe: 450 ktonnes/y
There are 5 production sites of LAB in Europe at present time (1995), 3 in Italy (Augusta - Sicily, Porto Torres - Sardinia and Mantova) for a total capacity of ca. 230 kt/y, 1 in Spain (S. Roque - Cd) for a capacity of ca. 180 kt/y and 1 in Germany (Ibbenbüren) for a capacity of ca. 40 kt/y. (see **Table 3.1**)
Part of this European LAB production is consumed in Europe and an other part is exported outside Europe.

Table 3.1 Production sites of LAB in Europe.

Country	Production (1995) (kt/y)
Italy (3 sites)	230
Spain	180
Germany	40

LAB consumption (1995)
Western Europe: 280 ktonnes/y (of which about 20% are imported extra-EEC).
This figure compares with a world-wide consumption of about 1800 kt/y.

LAB export
About 230 kt/y of the European LAB production are exported world-wide.
LAB is manufactured and processed in closed systems (see Annex 1, 2), where no emissions take place because, in addition to the LAB low vapour pressure, all plant units are protected by pressure security valves linked to the factory blow down, in turn connected with a flare. Releases can be due mainly to tank breathing and spills at work place. These were evaluated to be less than 1 ton/y by an exposure profile prepared for USA LAB production (Ref.43). Because European LAB production is of the same order of magnitude and obtained with identical processes as those of USA, we expect equivalent amount of releases. Any wastes or spills generated are collected and incinerated.
All factory effluents are loaded to treatment plants, so that we assume a negligible entry in the aquatic system from LAB manufacturing and processing.

Possible discharge via downstream products
A small amount of LAB (typically 0.5%) is estimated to remain in LAS used as surfactant in detergent formulations (Ref. 9, 38).

LAS consumption (1995)
Western Europe: 400 kt/y.
LAB is converted to LAS in all European countries mainly by big detergent manufacturers.

In the powdered detergent manufacture the low vapour pressure of LAB at 300°C suggests minimal environmental entry to the air from the spray drying treatment at this temperature. Use of improved tower scrubbers assures that this potential release is small.
The main release of LAB is in domestic sewage as unsulphonated matter of LAS in detergents. We can estimate, assuming a LAS consumption in Europe of 400 kt/y, a release in the sewage for LAB of max. 2. kt/y, which are removed by biological sewage treatments plants (STPs) with an efficiency of 95-98%, with a range of 69-98% as reported in literature studies for various types of STP (including trickling filters).

Behaviour in the environment

a) Degradation

Aerobic biodegradation
LAB biodegrades readily. A biodegradation test, recently conducted using a manometric respirometric method, shows a biodegradation of 64.1% after 28 days incubation (GLP, OECD 301 F, Ref. 40).
An OECD 301 B test indicates a biodegradation of 67% (measured by CO_2 evolution), after 28 days. An adapted inoculum was used. An emulsifier to disperse the poorly soluble LAB (Ref. 10) was added.
Another degradation test (Shake Flask Carbon Evolution Procedure) shows a biodegradation of 56-61% after 35 days, but the degradation is limited, probably because the test was conducted at LAB concentration far exceeding the solubility concentration (Ref. 5).
For this reason studies in more natural systems (Standard River Die-away Test) were carried out using lower LAB concentrations (100-500 ppb) and GC analytical determination. The results show a primary biodegradation of > 90% and a half-life of 4-15 days (GLP, Ref. 5).
Sewage treatment plants remove most of LAB released in sewage. Average percent removals from > 69% to > 98% for trickling filter and activated sludge plants respectively are reported (Ref. 5).
In sludge amended soils the LAB measured half-life is 15.3 days with a primary degradation of 98% after 103 days, measured by a final GC-MS detection analysis (Ref. 11).

Anaerobic biodegradation
A test conducted following the ECETOC Technical Report n° 28 shows a biodegradation of > 70% (Ref. 12).

Photodegradation
Photochemical transformation studies of acetonitrile solutions of LAB in direct sunlight indicate no significant direct photolysis or chemical transformation (EPA, GLP, Ref. 5).

b) Distribution

Volatilisation
Measurement of Henry's Log Constant was made using procedures similar to those of Mackay. The result shows a value of 95 $Pa \cdot m^3/mol$ which means a moderate volatilisation from the water medium (GLP, Ref. 5).

Adsorption/desorption
Organic carbon/water partition coefficient (K_{oc}) has been measured to be $2.2 \cdot 10^4$. This value was calculated by the solid/water partition coefficients measured in four types of soil with

different organic carbon content (from 0.4 to 2%) by addition of ^{14}C-labelled C_{12} alkylbenzene. The alkyl length (C_{12}) of the radiolabelled standard represents the average alkyl chain length ($C_{11.6}$) of the commercial LAB. The K_{oc} values of the different LAB homologues have been measured. The soils were analysed by combustion and liquid scintillation counting (ASTM, GLP, Ref. 5).
The solid/water partition coefficient (soil, sediment, suspended matter) K_p can be calculated as follows:

$$K_p = f_{oc} \cdot K_{oc}$$

where:
f_{oc} = weight fraction of organic carbon in the solid matter of different compartments. Recommended values by EU Technical Guidance Document (TGD) are 0.02 for soil, 0.05 for sediment and 0.1 for suspended matter.
$K_{p\ soil}$ = 440.0
$K_{p\ sediment}$ = 1100.0
$K_{p\ suspended\ matter}$ = 2200.0

LAB can be defined as a high adsorptive substance.
The dimensionless form of Kp or the total compartment-water partitioning coefficients can be derived from the definition of the soil (see TGD) and are:

$K_{soil\text{-}water}$ = 660 (m^3/m^3)
$K_{susp.\text{-}water}$ = 551 (m^3/m^3)
$K_{sed.\text{-}water}$ = 551 (m^3/m^3)

c) Accumulation
The log P_{ow} = 7.5 - 9.12 would predict a high potential bioaccumulation in fish but the measured BCF of 35 in a test on *Lepomis macrochirus* means a low bioconcentration (ASTM, GLP, Ref. 13).
This BCF test was conducted using as test material a radiolabelled C12 alkylbenzene. 150 fishes (of averaged weight 6 g) were placed in two 100 litres aquaria (acetone control and ^{14}C test material at nominal concentration of 0.1 mg/l) containing 70 litres of test solution. Actual concentration (0.092 mg/l) was checked by ^{14}C scintillation counting.
The uptake phase was conducted until steady state was reached, namely (when the whole fish from three 24 hour sampling intervals did not contain significantly different concentrations of ^{14}C test material using analysis of variance. The depuration phase was conducted until ^{14}C concentration in fish were 10% of the steady state concentration reached in the uptake phase.
Water from aquaria was sampled at 2, 12, 24, 48, 72 and 96 hours in the uptake phase and every 24 hours in the 96 hour depuration phase.
Whole fish were sampled at 2, 4, 12, 24, 48, 72 and 96 hours during depuration and at 96 hours time. Fish were collected and dissected into gall bladder, viscera and remaining fish portions.
Apparent ^{14}C LAB steady state concentration was reached in whole fish tissue after 48 hours. The BCF, calculated by BIOFAC (computer program for characterising the rates of uptake and clearance of chemicals) method, was determined to be 35. Based on the mean exposure concentration of 0.092 mg/l and the steady state whole fish residue concentration of 2.3 µg/g, the plateau BCF was 25. Both values are essentially identical and are significantly less than the BCF predicted on the basis of log P_{ow}.

This is still a conservative value, because the type of measurement (radiolabelled ^{14}C) includes not only the parent molecule but any possible metabolites.
Analysis of various tissues taken at 96 hours showed ^{14}C LAB concentration of 115 µg/g in the gall bladder, 7.1 µg/g in the viscera and 1.3 µg/g in the remaining fish.

Table 3.2 LAB bioconcentration kinetics according to BIOFAC.

BCF	Uptake phase		Depuration phase	
K1/K2	K1 (d^{-1})	90% steady state (d)	K2 (d^{-1})	50% steady state (d)
35	12	6.7	0.34	2.0

The reason why the measured BCF is lower than the predicted one can be explained by the high metabolisation rate of the substance by the fish. Although there is no direct proof in this study of LAB metabolism, several clues suggest presence of metabolism. First, the rates of uptake and depuration are different from the rates of chemicals, which persist in biological tissue. Persistent chemicals have slow, continued uptake and extremely retarded depuration with half-lives extending to 100 days. In contrast, the uptake time of 90% of steady state for LAB was less than a week and the time to clear 50% of the steady state whole fish concentration was two days. Furthermore there are similarities in the uptake and depuration kinetics data for LAB and its sulphonated derivative LAS, which is known to be metabolised. The relative distribution of [^{14}C] from LAB and LAS in the tissues and organs is the same, with the gall bladder being the site of highest concentration.
This situation should indicate that the chemical is metabolised in the liver and eliminated via biliary excretion and in the urine.
This interpretation is also supported by the findings from studies conducted on radiolabelled LAB to determine its distribution, metabolism and excretion in warm - blooded animals (rats), where some metabolites were separated by TLC analysis and identified (Ref. 18, 19, 20).
There are no experimental data on LAB bioaccumulation in other compartments; however one can calculate the BCFs using the programme EUSES.
The value for bioaccumulation in earthworms is derived from the octanol/water partition coefficient (K_{ow}), according to Connell and Markwell.
The EUSES calculates the following BCFs:

Table 3.3 Euses calculations.

Medium	BCF
Earthworms	326
Meat	0.08
Milk	0.025

3.1.1 Aquatic compartment (including sediment) and

3.1.2 Terrestrial compartment

Using the tables of the Technical Guidance Document of European Commission (TGD) and assigning to LAB production and processing the same “main category” lc, one can estimates the releases in waste water are 0.3% for the production and 0.7% for the processing, and the releases in soil equal to 0.01%.

This would mean the following total LAB releases:

in waste water	production :	1350 tons	(450 kt · 0.3%)
	processing :	1960tons	(280 kt · 0.7%)
in soil	production :	45 tons	(450 kt · 0.01%)
	processing :	28 tons	(280 kt · 0.01%)

These amounts of LAB releases are high in comparison with experimental ones, which are reported to be negligible, and which are related to a life cycle inventory (LCI) study on surfactants (Ref. 39) and refer to the actual emissions into the environment. In fact, if one considers the entire life cycle of the LAS production, namely from crude oil and through paraffins and olefins to LAB and LAS production, the total waterborne emissions of hydrocarbons (paraffins, olefins and LAB) related to processes amount to 0.0025 kg for 1000 kg of LAS (Ref. 39). For a total production of ca. 400 ktons of LAS in Europe 1.0 t/y as maximum release of hydrocarbons in water are estimated. Most of this total process related waterborne emissions of hydrocarbons comes from the production of refinery products, namely from the distillation, desalting and hydrotreating step. The waterborne emissions of hydrocarbons in the LAB production and sulphonation steps are estimated to be no more than 10% of this total hydrocarbon figure, namely 100 kg/y, as shown by the LCI study on surfactants, and their intermediates carried out by Franklin Ass. (Franklin Ass. reports on intermediates and surfactants, 1993-1994).

One should consider, at any rate, that this amount is not only LAB but corresponds to a total hydrocarbon release. These emissions are very trivial and can be neglected in comparison with those due to LAB content in LAS.

In fact the main release of LAB is in domestic sewage because of its presence (typically 0.5%) as unsulphonated matter in LAS. One estimates, assuming a LAS consumption in Europe of 400 kt/y, a release in sewage for LAB of 2.0 kt/y.

A different approach, which gives a more realistic waterborne release estimate of the only LAB from the European LAB/LAS production, is as follows. The only process unit, for which there is contact between LAB and water, is the aluminium trichloride ($AlCl_3$) alkylation process (see Fig. 1 of Annex 1) which is involved in about 33% of the total European LAB production (150 kt vs. 450 kt).

The contact between LAB and water occurs during the washing of the raw alkylate and the treatment of the quenched catalytic system. The total amount of water involved in this LAB production phase, which is then discharged for being STP treated, is at most 2100 l H_2O for 1 ton of LAB production. Assuming that LAB reaches its saturation concentration (0.04 mg/l) in these waters, one can make the following estimates of waterborne LAB release:

$$2100 \cdot 0.04 = 84 \text{ mg LAB for 1 tonne of LAB production}$$

For 150 kg/y of LAB production from $AlCl_3$ process one has a total LAB release of 12.6 kg/y, namely 0.04 kg/day.

This is the maximum amount of LAB waterborne emissions for the LAB/LAS European production, estimated to be released into a STP process. This amount is relative to a 150 kt/y LAB production, quite closed to a local scenario, which suggests to consider half of the total European production (B Tables of TGD). This experimentally LAB release estimate (0.04 kg/d) is well below that calculated for a local scenario (0.15 kg/d), relative to the use of LAS containing detergents, as shown below.

Calculations according to TGD

The most relevant LAB emission into the environment is in sewage due to the use of detergents containing LAS, in which LAB is present as a residue (typically 0.5%).
It is possible to calculate the LAB emissions from the LAS consumption, assuming on a conservative base that all LAB contained in LAS is released into the sewage and reaches the treatment plants without any biodegradation in sewers.

Table 3.4 LAS consumption and LAB release.

LAS consumption (kt/y)	LAB release (kt/y)
Europe	Europe
400	2.0

Total releases of LAB in kg/d to waste waters are estimated as follows:

Table 3.5 Total release of LAB to waste waters.

Scale	Release	Comment
Local	0.15	calculated for a 10,000 eq. population on the basis of the European LAS consumption, 400 Kt/y, and a population of 370 millions in Europe.
Regional	296	for 20 millions of equivalent population.
Continental	5480	calculated on the basis of European consumption of LAS.

Local model

a) Calculation of the STP influent concentration
Following TGD equations one can calculate the concentration in untreated waste water:

$$C\ local_{inf.} = \frac{E\ local_{water} \cdot 10^6}{Effluent_{STP}} = 0.075\ mg/l$$

where:
- $E\ local_{water} = 0.15$ kg/d, local emission rate
- $Effluent_{STP} = 2.0 \cdot 10^6$ l/d, effluent discharge rate of STP based on an average waste water flow of 200 l per capita per day for a population of 10000 inhabitants.

b) Calculation of the STP effluent concentration
The equation is as follows:

$$C\ local_{eff.} = C\ local_{inf.} \cdot F\ STP_{water} = 0.0045\ mg/l$$

where:
- $F\ STP_{water} = 0.06$, fraction of emission directed to water by STP, calculated according to Appendix II of TGD.

c) Calculation of the emission to air from the STP
The indirect emission to air is zero being zero the fraction of the emission to air from STP calculated according to Appendix II of TGD.

d) Calculation of the STP sludge concentration

The equation is as follows:

$$C_{sludge} = \frac{F\,STP_{sludge} \cdot E\,local_{water} \cdot 10^6}{\text{Sludge rate}} = 93 \text{ mg/kg}$$

where:

- $F\,STP_{sludge}$ = 0.88, fraction of emission directed to sludge by STP, calculated according to Appendix II of TGD.
- Sludge rate = 1420 kg/d^{-1}, rate of sludge production

The Sludge rate can be estimated from the outflows either of primary and secondary sludge as follows:

$$\text{Sludge rate} = 2/3 \cdot Suspconc._{inf.} \cdot Effluent_{STP} + Surplus_{sludge} \cdot Capacity_{STP}$$

where:

- $Suspconc_{inf.}$ = 0.45 kg/m^3, conc. of susp. matter in STP influent
- $Effluent_{STP}$ = 2000 m^3/d, effluent discharge rate of STP
- $Surplus_{sludge}$ = 0.011 kg/d/eq, surplus sludge per inhabitant equivalent
- $Capacity_{STP}$ = 10000 equivalent population

e) Calculation of the STP concentration for evaluation of inhibition to micro-organism

Assuming homogeneous mixing in aeration tank, the dissolved concentration of the substance is equal to the effluent concentration (0.0045 mg/l).

f) Calculation of PEC_{local} for the aquatic compartment

The local concentration is calculated as follows:

$$PEC\,local_{water} = \frac{C\,local_{eff.}}{(1 + Kp_{susp} \cdot SUSP_{water} \cdot 10^{-6}) \cdot \text{DILUTION}} + PEC_{regional\ water} = 0.0005 \text{ mg/l}$$

where:

- $C\,local_{eff.}$ = 0.0045 mg/l, concentration of chemical in STP effluent
- Kp_{susp} = 2200 l/kg,solid-water partitioning coefficient of suspended matter
- $SUSP_{water}$ = 15 mg/l, concentration of suspended matter in the river
- DILUTION = 10 dilution factor

g) Calculation of PEC_{local} for sediment

The concentration in bulk sediment can be derived from the corresponding water body concentration , assuming a thermodynamically partition equilibrium:

$$PEC\,local_{sed} = \frac{K_{susp.\text{-}water}}{RHO_{susp.}} \cdot PEC\,local_{water} \cdot 1000 = 0.24 \text{ mg/kg}$$

where:

- $PEC\,local_{water}$ = 0.0005 mg/l
- $K_{susp.sed}$ = 551 (m^3/m^3), suspended matter-water partitioning coefficient
- $RHO_{susp.}$ = 1150 kg/m^3, bulk density of suspended matter

h) Calculation of PEC_{local} for the aquatic and sediment compartment without considering STP treatment

Assuming that no water treatment exists one can calculate the PECs for the aquatic and sediment compartments in these conditions.
These data, of course, are only indicative and will not be used in the exposure assessment (TGD pg. 287). In this case the fraction of the emission to waste water, directed to effluent ($F\ STP_{water}$) should be set to 1, namely $C\ local_{eff.} = C\ local_{inf.} = 0.075$ mg/l.
For the calculation referring to the expression in the above f) paragraph:

$PEC\ local_{water} = 0.0074$ mg/l + $PEC_{regional\ water} = 0.0075$ mg/l

Assuming this figure as $PEC\ local_{water}$, an equivalent calculation according to the expression of g) paragraph gives:
$PEC\ local_{sed.} = 3.59$ mg/kg

i) Calculation of PEC_{local} for the soil compartment

For sludge application to agricultural soil an application rate of 5000 kg/ha/y dry weight is assumed while for grassland a rate of 1000 kg/ha/y should be used.
The PEC in agricultural soil is used for two purposes:

- Characterisation of risk to terrestrial ecosystem
- Calculation of indirect exposure to humans via crops and cattle products.

Therefore, for exposure of endpoints, the concentration in soil needs to be averaged over a certain time period. Different averaging times should be considered:

- A period of 30 days after application of sludge for the ecosystem
- A period of 180 days to determine biomagnification effects and indirect exposure to man.

The local concentration in soil is defined as the averaged concentration over a certain time period t.
The starting concentration a t = 0 in soil due to one sludge application in the year can be calculated as follows:

$$C_{0\ soil} = \frac{C_{sludge} \cdot APPL_{sludge}}{DEPTH_{soil} \cdot RHO} = 0.14\ mg/kg$$

where:

- C_{sludge} = 93 mg/kg, conc. in the sludge
- $APPL_{sludge}$ = 0.5 kg/m^2, dry sludge application rate
- $DEPTH_{soil}$ = 0.2 m, mixing depth of soil
- RHO = 1700 kg/m^3, bulk density of wet soil

The average exposure LAB concentration over a certain period of time can be calculated considering the first order biodegradation rate of the chemical in the top soil.
Summation of all concentrations over a certain day period and dividing by the corresponding days gives the average daily concentration. This is achieved by integrating the equation given in the TGD, which simplifies to the following expression if we neglect the contribution of aerial deposition:

$$C_{avg.\ soil} = \frac{C_{0\ soil}}{k \cdot t} (1 - e^{-kt}) \text{ expressed in mg/kg}$$

where:
- k (d^{-1}), first order rate constant in top soil
- t (d), averaging time

LAB monitoring studies in sludge amended soil (REF. 11) indicate a biodegradation rate in sludge amended soils corresponding to a half-life of 15 days, namely $k = \ln 2/t_{0.5} = 0.046\ d^{-1}$. Consequently we can calculate the $C_{avg.}$, namely the PEC local in agricultural soil as follows:

Table 3.6 PEC local in agriculture soil.

Averaging time (d)	PEC $local_{soil}$
30	0.076
180	0.017

In the case of grassland the averaging time suggested by TGD is 180 days and the sludge application rate and the mixing depth of soil are 0.1 m and 0.1 kg/m^2 respectively. Taking into account these different figures we can calculate:

$C_{0\ grassland} = 0.055$ mg/kg

and assuming the same biodegradation rate of LAB used for the agricultural soil ($t_{0.5} = 15$ d) one obtains for an averaging time of 180 days a value of:

PEC $local_{grassland} = 0.0066$ mg/kg

l) Calculation of concentration in groundwater

The concentration in groundwater is calculated for indirect exposure of humans through drinking water.

The concentration in pore water of agricultural soil is taken as an indication of potential groundwater level. This is a worst-case assumption, neglecting transformation and dilution in deeper soil layers.

$$\text{PEC local}_{grw} = \text{PEC local}_{porew.} = \frac{\text{PEC local}_{agr.\ soil} \cdot RHO_{soil}}{k_{soil\text{-}water} \cdot 1000} = 4.4 \cdot 10^{-5}\ \text{mg/l}$$

where:
- PEC $local_{agr.\ soil} = 0.017$ mg/kg
- $RHO_{soil} = 1700\ kg/m^3$, bulk density of wet soil
- $k_{soil\text{-}water} = 660\ m^3/m^3$, soil-water partitioning coefficient

In brief, the LAB overall results of the local model are as shown in **Table 3.7**.

Table 3.7 LAB overall results of the local model.

$C_{inf.}$	0.075 mg/l
$C_{eff.}$	0.0045 mg/l
C_{sludge}	93 mg/kg
$PEC_{micro\text{-}organism}$	0.0045 mg/l
PEC_{water}	0.0005 mg/l
$PEC_{sediment}$	0.24 mg/kg
PEC_{soil} (av. time: 30 d)	0.076 mg/kg
PEC_{soil} (av. time: 180 d)	0.017 mg/kg
$PEC_{grw.}$	$4.4 \cdot 10^{-5}$ mg/l

Regional model

The predicted LAB concentration (PEC) in the environmental compartments at regional level can be estimated by the EUSES programme. It is necessary to introduce some data directly into the programme, using a non-standard procedure, namely:

- the LAB emission figure (2000 t/y) as a production volume, considering that the entire volume is used as a substance with "Industry category" = 5 personal/domestic and "use category" = 9 cleaning/washing agents;
- the figures related to the local emission to wastewater, avoiding that the programme calculates these emissions at production step.
- of the total LAB regional emissions (296 kg/d), the figure (204 kg/d) to waste waters (70%) and the figure (89 kg/d) to surface waters (30%).

The programme calculates the regional emissions to various compartments assuming that 70% of wastewater is treated in a biological STP and the remaining 30% released into surface waters.

EUSES calculations for regional PECs in different compartments are as follows:

Table 3.8 Euses calculations for regional PECs.

Compartments	**PECs**
Surface water	$7 \cdot 10^{-5}$ mg/l
Sediment	0.06 mg/kg
Agricultural soil	$6.5 \cdot 10^{-4}$ mg/kg
Natural soil	$7 \cdot 10^{-7}$ mg/kg
Groundwater	$1.6 \cdot 10^{-6}$ mg/l

The flow sheets of the EUSES computerised summary results are in http://ecb.ei.jrc.it

Monitoring data

Aquatic compartment

In literature it is possible to find reliable data regarding USA (Ref. 5). The highest concentrations of LAB would be expected in the receiving waters of sewage treatment plant effluents.

Monitoring of total LAB (dissolved + adsorbed in suspended solids) was conducted in 10 typical sewage treatment plants (STP) selected on conservative basis because their effluents receive low dilutions in receiving waters (worst case). LAB in these downstream waters ranged from non-detectable (< 0.0001 mg/l) to a value of 0.001 mg/l. This last value is related to a trickling filter STP that is known to be less efficient than an activated sludge (AS) STP. In fact considering only the (AS) STPs the worst monitoring LAB data resulted to be 0.0004 mg/l, which is in good agreement with the calculated local one.

Sediment compartment

The highest concentration of LAB found in sediments in USA (Ref. 5) is 0.66 mg/kg (on dry basis). This value is related to the above mentioned monitoring and refers to a site just below a trickling filter STP.

More than twenty measurements of LAB are reported in a Japanese study of 1987 (Ref. 44). The values range from 0.01 to 15.8 mg/kg. Only two sediment samples show high LAB concentration (12.1 and 15.8 mg/kg). All the others show an average value below 2.5 mg/kg. One should consider, however, that the LAB used in Japan at that time (1987) had a definitely higher molecular weight (high content of C_{14} alkyl homologue) than that used nowadays in Europe. This means a high adsorptive capacity of this LAB. In addition all sediment measurements were related to rivers receiving almost only untreated domestic waste.

The most reliable data of LAB in sediments, consistent with the present situation in Europe, are those recently (1994) published by the UK Department of the Environment and obtained by several UK river sediments (Ref. 14). The LAB data range from 0.001 mg/kg (upstream of the discharge point) to 0.01 - 0.02 mg/kg (downstream of the sewage plant).

All these values are referred to dry sediment. To compare them with PECs calculated the above data should be multiplied by 0.2 (volume fraction of solids in sediment). In other words the highest value of the most reliable UK measurements become:

$$0.02 \cdot 0.2 = 0.004 \text{ mg/kg of wet sediment}$$

This value is significantly lower than the calculated one.

Soil compartment

The measured data for activated sludge ranges from 58 to 78 mg/kg (Ref. 11); however the most representative value should be near to 10 mg/kg, which is an average of several measurements done recently by the UK Dept. of Environment (Ref. 14).

Monitoring data of sludge amended soils in UK indicate a range of 0.005 - 0.044 mg/kg of LAB. The measurements were done about six months after the sludge application (Ref. 11).

Again these values are referred to dry soil. To make reference to wet soil the values should be multiplied by 0.6 (volume fraction of solids in soil), namely:

$$(0.005 - 0.044) \cdot 0.6 = 0.003\text{-}0.026 \text{ mg/kg of wet soil}$$

These data are consistent with the calculated ones for the local sites (0.017 mg/kg).

3.1.3 Atmosphere

Due to the very low vapour pressure of LAB and the fact that it is manufactured and processed in closed processes, no atmospheric emissions are expected.

Using the tables included in the Technical Guidance one can estimate releases in air from

production and processing are zero. EUSES calculates for both scenarios a very negligible PEC_{local} (100m from STP) = $3.2 \cdot 10^{-6}$ mg/m^3.

3.1.4 Non compartment specific effects relevant to the food chain

Exposure levels are calculated, assuming a scenario whereby 50% of the food is sourced from the local environment and 50% from the regional environment.

Exposure concentration for fish eating-predators
The value is calculated to be 0.09 mg/kg, based on fish BCF (measured) and averaged concentrations in surface water, namely:

$$PEC_{oral\text{-}fish} = PEC_{water} \cdot BCF_{fish} = 0.01 \text{ mg/kg}$$

where :
- $PEC_{water} = 1/2 (PEC_{local} + PEC_{regional}) = 0.00029$ mg/l
- $BCF_{fish} = 35$

Exposure concentration for earthworm eating-predators
The value is calculated to be 2.87 mg/kg, based on earthworm BCF (calculated) and averaged concentrations in agricultural soil (av. timing: 180 d), namely:

$$PEC_{oral\text{-}worm} = PEC_{soil} \cdot BCF_{worm} = 2.87 \text{ mg/kg}$$

where :
- $PEC_{soil} = 1/2 (PEC_{local} + PEC_{regional}) = 0.0088$ mg/kg
- $BCF_{worm} = 326$

3.2 EFFECTS ASSESSMENT: Hazard identification and dose (concentration) - response (effect) assessment

3.2.1 Aquatic compartment

LAB has a very low solubility in water (0.041 mg/l), therefore one must take into account this property in conducting bioassays.

Experimental data of acute toxicity on organisms of different trophic levels.

Decomposers (micro-organisms)
Two tests conducted on *Pseudomonas putida* show an EC_{10} at concentrations exceeding the saturation level (8.8 and 10 mg/l) after 6 and 18 hours (DIN 38412, Ref. 15).

Primary consumers
Daphnia magna

Tests conducted at nominal concentrations in static systems for three LABs with average molecular weights of 236, 244 and 262 show LC_{50} 48h = 0.009-0.08 mg/l (EPA, GLP, Ref. 5).

These tests were carried out using as a carrier solvent either acetone (1 ml/l) or dimethylformamide (0.25 ml/l).
Other tests on a commercial product (mol. w. 240) show no effects at the concentration of 3.8 mg/l and 1000 mg/l, the last with an emulsifier (DIN, Ref. 41).
Other tests, conducted at the saturated concentration of pure homologues obtained via commercial LAB fractionation, show no adverse effects after 48 h (OECD Guideline 202, part 1, Ref. 16).
A recent test (March 1997), commissioned to RBM of Ivrea and carried out according to EC.C2 method and in compliance with GLP on the typical European LAB at measured saturated concentrations and without use of a carrier solvent, indicate no adverse effects after 48 h (Ref. 47).
The tests carried out with the help of a carrier are the only ones, which show an apparent high acute toxicity of LAB. It is worth mentioning, however, that these tests, because of the use of a carrier, cannot be considered environmentally related and are not in line with the OECD suggestions which indicate that tests should be near to real world as far as possible. Therefore, the several other tests, carried out at the saturated concentration not only of the LAB mixture but also of pure homologues and showing no adverse effects, should be considered more reliable. The fact that the tests carried out with carrier show a toxicity result below the solubility limit of LAB, not evident in the other tests, would indicate that the toxicity mechanism for LAB in presence of a carrier is different.

Other crustacea

Mysidopsis bahia (after 96 h), *Gammarus fasciatus* (96 h), *Paratanytarsus* (48 h) are not affected at nominal concentration (1000 mg/l) up to and exceeding the water solubility with a solvent carrier (EPA, GLP, Ref. 5).
In addition no adverse effects were also found in measured saturated solutions of n-decyl-, n-undecyl- and n-dodecyl-benzene using *Chaetogammarus marinus* after 96 h (Ref. 46).

Sediment dwelling organisms

Chironomus tentans larvae are not affected after 96 h at nominal concentration (1000 mg/l) up to and exceeding the water solubility with a solvent carrier (EPA, GLP, Ref. 5).

Secondary consumers
Fish

Tests, conducted on Salmo gairdneri, Pimephales promelas and Lepomis macrochirus, show no adverse effects after 96 h at nominal concentration (1000 mg/l) up to and exceeding the water solubility with a solvent carrier (EPA, GLP, Ref. 5).
A test on *Leuciscus idus melanotus* shows no adverse effects after 48 h at nominal concentration (1000 mg/l) up to and exceeding the water solubility using an emulsifier (DIN 38412, GLP, Ref. 17).

Primary producers
Algae

Selenastrum capricornutum is not affected after 96 h at nominal concentration (1000 mg/l) up to and exceeding the water solubility with a solvent carrier (EPA, GLP, Ref. 5).

Experimental data of prolonged toxicity on organisms of different trophic levels.

Primary consumers
Daphnia magna

One-generation chronic tests (21 days) in clean water and at measured concentrations were conducted in flow-through conditions using acetone as a solvent for two LABs with mol. w. of 236 and 262 (EPA, GLP, Ref. 5).
Survival and reproduction are recorded and assessed three times; growth established at day 21. Concentration was monitored via a GC procedure.
The lowest no effect level measured for LAB is 0.0075 mg/l.
The use of a carrier as acetone (1 ml/l) could affect the long-term toxicity of LAB and throws some doubt whether to accept or not this very low effect value. This value, incidentally, is below the LAB solubility. The recent results of acute tests on *Daphnia magna* carried out on the European LAB cut at measured concentrations confirm that the use of solvent affects the toxicity negatively (Ref. 47). The same arguments, given above for the acute toxicity results on *Daphnia magna* obtained using a carrier, hold here as well.

Sediment dwelling organisms (Chironomus tentans larvae)

A midge chronic study (14 days) was conducted with ^{14}C-labelled LAB under flow-through conditions with a solvent and a small amount of river sediment as substrate. No effects were noted to the organisms exposed to concentrations of up to 0.125 mg/l (GLP, Ref. 5).

To calculate the corresponding risk characterisation it is better to refer to the aquatic toxicity derived following the equilibrium partitioning (see 3.3.1).

Conclusion
Surface water

One prolonged toxicity test on Daphnia is available. A 4-day alga test, covering LAB exposure over several alga generations, which can be considered as a prolonged test, is also reported.
According to the TGD, if there are only two long-term tests on different trophic levels but the chronic data are available for the most sensitive species, an assessment factor of 10 can be applied to the lowest NOEC. This is particularly important if the substance does not have a potential to bioaccumulate.
In the case of LAB *Daphnia* is recognised to be the most sensitive species on acute basis and because the BCF is low (35, see 3.1.0) it is highly probable that *Daphnia* is also the most sensitive species in chronic tests.
PNEC thus is equal to 0.00075 mg/l.

Sediment

To calculate the PNEC it is better to refer to the aquatic toxicity following the equilibrium partitioning:

$$PNEC_{sediment} = \frac{K_{sed\text{-}water}}{RHO_{sed}} \cdot PNEC_{aquatic\ organisms} \cdot 1000 = 0.32\ mg/kg$$

where :

- $K_{sed\text{-}water} = 551\ m^3/m^3$
- $RHO_{sed} = 1300\ kg/m^3$
- $PNEC_{aquatic\ organisms} = 0.00075\ mg/l$

3.2.2 Terrestrial compartment

Because no toxicity data on terrestrial organisms are available, it is possible to extrapolate the toxicity data from the aquatic organisms using the equilibrium partitioning method:

$$PNEC_{terrestrial\ organisms} = \frac{K_{soil\text{-}water}}{RHO_{soil}} \cdot PNEC_{aquatic\ organisms} \cdot 1000 = 0.29\ mg/kg$$

where

- K_{soil} = 660 m^3/m^3
- RHO_{soil} = 1700 kg/m^3
- $PNECa_{quatic\ organisms}$ = 0.00075 mg/l

3.2.3 Atmosphere

No data on atmospheric contamination of organisms are available.
The data of inhalation tests on mammals (4.2.2. and 4.2.6.) are the only ones available for air compartment.

3.2.4 Non compartment specific effects relevant to the food chain

Organisms to be protected in both aquatic and terrestrial ecosystem are predating organisms at the end of the food chain:
$PNEC_{oral}$ for predators can be calculated from the oral toxicity data of mammals as follows:

$$PNEC_{oral} = \frac{NOAEL_{mammals,\ oral,\ chr} \cdot 10\ (*)}{10\ (**)} = 50\ mg/kg_{\ food}$$

Where:

- $NOAEL_{mammals,\ oral,\ chr}$ = 50 $mg/kg_{\ bw}$/day
- 10 (*) is a conversion factor from $mg/kg_{\ bw}$/day to $mg/kg_{\ food}$
- 10 (**) is the assessment factor applied for chronic tests

3.3 RISK CHARACTERISATION

3.3.1 Aquatic compartment

Micro-organisms
The calculated xenobiotic concentration in the aeration tank of STP (0.0045 mg/l) is compared with the PNEC for micro-organisms. In this case we have a NOEC > 10 mg/l. Even if we assume PNEC = 10 mg/l the result is a negligible hazard quotient for the STP micro-organisms.

$$PEC/PNEC = 0.0045/10 = 4.5 \cdot 10^{-4}$$

Aquatic phase

The following hazard quotients for local and regional models, based on calculated data, are obtained:

$$PEC/PNEC_{local} = 0.0005 / 0.00075 = 0.68$$

$$PEC/PNEC_{regional} = 7 \cdot 10^{-5} / 0.00075 = 0.093$$

If we use the worst monitoring data, 0.001 mg/l, (see 3.1.1) one obtains a $PEC/PNEC_{local}$ = 1.3. This is, however, the worst case, because the monitoring data refer to a trickling filter STP effluent which receives no or low dilution in the receiving river. If we refer to the worst LAB monitoring of the activated sludge (AS) STP effluent, namely 0.0004 mg/l, the $PEC/PNEC_{local}$ becomes equal to 0.53, which reflects more closely the actual environmental situation and is consistent with the calculated one.

$$PEC/PNEClocal = 0.0004 / 0.00075 = 0.53$$

Sediment phase

PEC/PNEC for sediment can be calculated as follows, based on the equilibrium partitioning:

$$PEC/PNEC_{sediment} = \frac{PEC_{sediment} \cdot RHO_{sed.}}{PNEC_{aquatic\ organisms} \cdot K_{sed.-water} \cdot 1000}$$

where the following values have been used:

- $K_{sed.-water}$ = 551 m^3/m^3
- $PEC_{sediment}$ = 0.24 and 0.06 mg/kg (local and regional)
- PNEC = 0.00075 mg/l
- $RHO_{sed.}$ = 1300 kg/m^3

The hazard quotients for sediment deriving from the calculated exposures are as follows:

Table 3.9 Hazard quotients for sediment.

Model	$PEC/PNEC_{sediment}$
Local	0.75
Regional	0.19

A PEC/PNEC of 0.014 is calculated using the environmental concentration (0.0044 mg/kg) coming from European monitoring (Ref. 14), which is the worst case available value measured in UK

If on the contrary we use the Japanese average monitoring data (0.5 mg/kg) the PEC/PNEC becomes 1.6 and using the worst monitoring data (3.16 mg/kg) is 10. Therefore, it is evident that in Japan exists a potential risk as far as sediments are concerned. However, this is the situation monitored in 1987 with a LAB different from that used in Europe now and in cases where no water treatment of domestic waters occurred. It is advisable that the present situation is checked (**conclusion ii**).

3.3.2 Terrestrial compartment

The PNEC for terrestrial organisms is calculated as follows:

$$PEC_{soil}/PNEC_{soil} = \frac{PEC_{soil} \cdot RHO_{soil}}{PNEC_{aquatic\ organisms} \cdot K_{soil\text{-}water} \cdot 1000}$$

where the following values have been used:
- $K_{soil\text{-}water}$ = 660 m^3/m^3
- PEC_{soil} = 0.076 (av. time : 30 d) and $6.5 \cdot 10^{-4}$ mg/kg (local and regional)
- RHO_{soil} = 1700 kg/m^3

The estimated quotients for local and regional models are as follows:

Table 3.10 Quotients for local and regional models.

Model	$PEC/PNEC_{soil}$
Local	0.26
Regional	0.0022

If we use the worst monitoring value of sludge amended soil (0.026 mg/kg) (Ref. 11) the local PEC/PNEC value is below 1, namely 0.09 (**conclusion ii**).

3.3.3 Atmosphere

No data of atmospheric contamination on organisms are available. Due to the very low vapour pressure of LAB and the fact that it is manufactured and processed in closed systems, atmospheric emissions are not expected.
EUSES calculates a negligible local PEC at 100 m from STP.

3.3.4 Non compartment specific effects relevant to the food chain

To assess the potential hazard of bioaccumulation through the food chain, the hazard for worm eating birds or mammals and for fish eating predators is examined.
The hazard quotients are as follows:
- $PEC_{fish}/PNEC_{predator\ in\ food}$ = 0.0002
- $PEC_{worm}/PNEC_{predator\ in\ food}$ = 0.057

where :
- PEC_{fish} and PEC_{worm} are 0.01 and 2.87 mg/kg, the averaged concentrations at local and regional scale (see 3.1.4)
- $PNEC_{predator\ in\ food}$ = 50 mg/kg (see 3.2.4).

There is at present no need for further information and/or testing or for risk reduction measures beyond those, which are being applied already (**conclusion ii**).

4 HUMAN HEALTH

4.1 HUMAN HEALTH (Toxicity)

4.1.1 Exposure assessment

4.1.1.0 General discussion

As already said in 3.1.0, in 5 production sites located in 3 different European countries, LAB is manufactured and processed in closed systems, where no direct handling by the individual operators takes places and where the low vapour pressure and the location of the units (open air for the production plants and large, spacious buildings for the process plants, with large openings) minimise the potential risk of inhalation. The production plants are also protected by pressure security valves linked to the factory blow down, in turn connected with a flare. The rigorous procedures to control the exposure to benzene (alkylation of benzene is a step in the production of LAB), guarantee negligible levels of lower vapour pressure hydrocarbons such as LAB.
Technicians working at plant unit, operators in charge to transfer LAB via pumping through closed pipelines (from production to process units, through storage tanks, tank-cars and/or delivery ships), in taking samples for analysis and in maintenance activities, are required to wear safety goggles and gloves to avoid any eye or skin contact in case of accidental leakage.
One possible exposure is for consumers, during the use of detergents containing approximately 0.05% of unsulphonated LAB, assuming 10% of LAS in detergents.

4.1.1.1 Occupational exposure

Because no monitoring data are available, EASE model was used to estimate the possible exposure in workplace, both for production and transformation, assuming that no personal protective equipment (PPE) is used, including respiratory protective equipment (RPE).
Whether you assign the category of use “closed system” (with the possibility to be breached) or “non-dispersive use” to the processes, assuming that the control level is “full containment”, the output of the model is the same. A process “non-dispersive use” with full containment is actually considered a “closed system”.

Inhalation exposure
The range calculated for vapour concentration is 0-0.1 ppm (0-0.998 mg/m^3).

Dermal exposure
Assuming that the processes are “closed system” or “non-dispersive use”, a very low exposure is predicted in both cases, because no direct handling takes place.
Personnel exposed to a hypothetical dermal contact could be via sampling and tank filling activity. These operations are conducted wearing PPE and last a very short period of time over the working day. In some production plants the sampling is totally automated.
In the case of plant maintenance, other personnel are involved for some hours (an average of 15 hours as a total for at least 3 workers at production plant) to cover the maintenance during the annual, or less frequent, plant shut down. Also in this operation personnel are required to wear PPE.
Considering that direct handling occurs, with incidental contact level, a range of exposure of 0-0.1 mg/cm^2/day is predicted. Assuming that the body parts involved are hands (840 cm^2 of skin), a maximum exposure of 84 mg/day (1.2 mg/kg/day assuming a body weight of 70 kg).

4.1.1.2 Consumer exposure

The LAB traces, present in detergents, which can come into the contact with the consumer are mainly in hand-dishwashing and hand-washing liquids.
On the basis of different assumptions, detergent manufacturers have calculated for the total dermal exposure a maximum value of $5.9 \cdot 10^{-3}$ mg/kg/day and an oral exposure of $1.9 \cdot 10^{-4}$ mg/kg/day (see Annex 3).
The exposure of $5.9 \cdot 10^{-3}$ mg/kg/day is the sum of the exposure due to hand washing of dishes and laundry; $1.9 \cdot 10^{-4}$ mg/kg/day is the exposure due to deposits on dishes. The latter scenario is very conservative, assuming that the uptake of the film containing residual LAB is total, without considering events such as rinsing, wiping etc.
The models used for calculating these exposures are those described in the TGD for the dermal route and in ECETOC Technical Report No. 58 for the oral route.

4.1.1.3 Indirect exposure via environment

The indirect exposure is assessed by estimating the total daily intake of a substance by consumption of food, water and inhalation of air, based on the predicted environmental concentrations in all compartments.

Table 4.1 Find here below the EUSES calculations for PECs local and regional:

PECs (mg/kg)		
	Model	
	Local	Regional
Fish	0.0193	$2.5 \cdot 10^{-3}$
Stem of plant	$2.0 \cdot 10^{-4}$	$9.5 \cdot 10^{-5}$
Root of plant	$4.0 \cdot 10^{-3}$	$1.3 \cdot 10^{-3}$
Grass	$2.0 \cdot 10^{-4}$	$9.6 \cdot 10^{-5}$
Milk	$2.6 \cdot 10^{-5}$	$7.4 \cdot 10^{-6}$
Meat	$8.2 \cdot 10^{-5}$	$2.3 \cdot 10^{-5}$
Drinking water	$2.8 \cdot 10^{-4}$	$3.6 \cdot 10^{-5}$

Table 4.2 The total daily intakes are calculated by EUSES as follows:

Daily uptake (mg/kg body weight)		
	Model	
	Local	Regional
Air	$2.4 \cdot 10^{-6}$	$1.0 \cdot 10^{-6}$
Drinking water	$7.9 \cdot 10^{-6}$	$1.0 \cdot 10^{-6}$
Fish	$3.2 \cdot 10^{-5}$	$4.1 \cdot 10^{-6}$
Stem of plant	$3.2 \cdot 10^{-6}$	$1.6 \cdot 10^{-6}$
Root of plant	$2.5 \cdot 10^{-4}$	$7.3 \cdot 10^{-6}$
Meat	$3.5 \cdot 10^{-7}$	$1.0 \cdot 10^{-7}$
Milk	$2.07 \cdot 10^{-7}$	$6.0 \cdot 10^{-8}$
Total human dose	$2.5 \cdot 10^{-4}$	$1.5 \cdot 10^{-5}$

4.1.2 Effects assessment: Hazard identification and Dose (concentration) - response (effect) assessment

4.1.2.1 Toxico-kinetics, metabolism and distribution

A study has been conducted to determine the distribution, metabolism and excretion of 2-(^{14}C)-phenyl dodecane in male and female rats after intravenous, oral and dermal administration (96 hr). Metabolism was studied by thin-layer chromatography analysis, distribution by whole-body autoradiography and excretion by liquid scintillation counting.

Intravenous route

The distribution, elimination and metabolism of radiolabelled material have been investigated following a single intravenous administration of 2-(^{14}C)-phenyl dodecane to 5 male and 5 female rats at a nominal concentration of 1 mg/kg body weight (Ref. 18).

Irrespective of sex, radioactivity was widely distributed into tissues, extensively metabolised and rapidly excreted.

Over a period of 96 h, approximately 80 and 86% of the administered radioactivity was recovered in the excreta of male and female rats respectively. Of the total radioactivity recovered, ca.73% (males) and 88% (females) was eliminated in urine, the majority within the first 24 h, i.e. ca. 67 and 84% respectively. Faecal excretion was low with only ca. 9% and 5% of the administered radioactivity being eliminated by 96 h in male and female animals respectively.

Metabolism of 2-(^{14}C)-phenyl dodecane was rapid, with up to 9 radiolabelled components resolved by TLC. Two components (visualised on the TLC autoradiogram but not resolved by the linear analyser) accounted for ca. 50% of the urinary radioactivity. Glucuronide or sulphate conjugates were not detected but non-specific breakdown of one component was observed when urine was incubated at 37°C.

Five regions of interest were detected when faecal extracts were profiled. The extracts were highly concentrated (to increase quantities of radioactivity for TLC) with resulting high levels of endogenous material present. However, results suggest that as much as 68% of the recovered radioactivity was present as parent compound.

Whole-body autoradiography showed that radioactivity was widely distributed between tissues at early sampling times but was mainly associated with the organs of metabolism and excretion. No sex differences were apparent. Radioactivity was not detected in blood after 4 h (male) and 8 h (female). Of note there was a volatile fraction of radiolabelled material associated with the liver (particularly at 0.5 h post-dose). It is highly likely that this is unchanged parent compound.

Much of the radioactivity was eliminated by 24 h, but a feature of its disposition was its persistence in organs of high lipid content (skeletal and brown fat) and those tissues having oily and/or secretive properties (Harderian, preputial, clitoral, lachrymal and salivary glands) for up to 96 h. Also of interest was the presence of radioactivity in the stenos gland (a gland of high metabolic activity present in the epithelial lining of the nasal cavity).

Oral route

The absorption, distribution, metabolism and elimination of radiolabelled material have been investigated following a single oral administration of 2-(^{14}C)-phenyl dodecane to 5 male and 5 female rats at a nominal dose level of 10 mg/kg body weight (Ref.19).

Irrespective of sex, radioactivity was well absorbed, widely distributed between tissues, extensively metabolised and then rapidly excreted.

Urinary elimination indicated that >50% of the administered dose was absorbed following oral administration. At 4 to 8 h post-dose, blood radioactivity concentrations were at peak. At this time radiolabelled material with chromatographic characteristics similar to the parent test substance was detected in urine.

High levels of radioactivity were also apparent in the bile ducts at early sampling times, thus it is highly likely that more than 50% of the administered dose was absorbed.

Over a period of 96 h, approximately 75 and 89% of the administered radioactivity was recovered in the excreta of male and female animals respectively. Of the total radioactivity recovered, ca 49% (males) and 56% (females) was eliminated in urine, the majority within the first 24 h, i.e. 44 and 49% respectively.

Faecal elimination in males and females accounted for only ca 19% and 26% of the recovered dose.
Metabolism of 2-(^{14}C)-phenyl dodecane was relatively rapid and extensive with up to 9 radiolabelled components resolved by thin layer chromatography (TLC). Two components (visualised on the TLC autoradiograms but not resolved by the linear analyser) accounted for ca. 50% of the urinary radioactivity. Neither glucoronide nor sulphate conjugates were detected in urine. Of the administered radioactivity, 5 to 7% was chromatographically eluted with the parent material at 8 h post-dose. Mass spectroscopy tentatively identified the most polar of the metabolites as either 4-phenyl pentanoic acid or 4-phenyl pentylthioamide but no convincing structure could be assigned to the other metabolites.
Up to five regions of interest were resolved when faecal extracts were profiled. The largest region accounted for 58 to 67% of the radioactivity applied to the TLC plates and co-chromatographed with parent compound.
Whole-body autoradiography showed that radioactivity was widely distributed between tissues but was mainly associated with the organs of metabolism and excretion. No sex differences were apparent. Moderate levels of radioactivity were detected in the blood up to and including 8 h post-dose in animals of each sex. Of note there was a relatively volatile fraction of radiolabelled material associated with the contents of the stomach and upper intestinal tract at 4 and 8 hours. It is assumed that this was unchanged 2-(^{14}C)-phenyl dodecane.
Much of the radioactivity was eliminated by 48 h, but a feature of its disposition was its persistence in organs of high lipid content (skeletal and brown fat) and those tissues, having oily and/or secretive properties (Harderian, preputial, clitoral, lachrymal and salivary glands) for up to 96 h. The radioactivity present in the skeletal and brown fat (at 48 h and 96 h post dose) had chromatographic characteristics similar to unchanged test material. Also of interest was the presence of radioactivity in the stenos gland (a gland of high metabolic activity present in the epithelial lining of the nasal cavity).
At no time after dosing was radioactivity detected in the central nervous system (other than in the pituitary and blood sinuses of the brain).

Dermal route

The dermal absorption, distribution, metabolism and elimination of radiolabelled material have been investigated following a single percutaneous administration of 2-(^{14}C)-phenyl dodecane to 5 male and 5 female rats at a nominal dose volume of 200 µL of a 1% (w/v) solution, equivalent to approximately 2 mg/animal (Ref. 20).
Irrespective of sex, radioactivity was poorly but continuously absorbed through the skin throughout the 96 h duration of the study. However, that radioactivity which did penetrate was well distributed between tissues (at low levels), extensively metabolised and eliminated.
Over a period of 96 h, approximately 10% (males) and 8% (females) of the dermally applied radioactivity was recovered in excreta. Most of the radioactivity (ca. 72% and 77%, in males and females respectively) was eliminated in urine at a fairly constant rate throughout the experimental period. Faecal elimination of radioactivity was lower and accounted for only 19% and 11% of the total dose absorbed in males and females respectively.
In the male animal killed at 96 h post-dose, approximately 78% of the administered radioactivity was rinsed from the skin whereas ca. 15% remained on the treatment dose site. Equivalent values from the female animal were ca. 74% and ca. 14%.
Metabolism of 2-(^{14}C)-phenyl dodecane was virtually complete with up to 9 radiolabelled components resolved by thin-layer chromatography (TLC). Two radioactive components running very close together (visualised on the TLC autoradiograms but not resolved by the linear analyser) accounted for ca. 40 to 50% of the applied radioactivity. Neither glucuronide

or aryl sulphate conjugates were detected. Only very low concentrations of radioactivity (0.35 to 3.24%) co-chromatographed with parent material.
Concentrations of radioactivity in faecal extracts were so low as to preclude metabolite profiling although the proportions of radioactivity in the organic solvents imply that the extractable radioactivity had a lipid solubility greater than the aqueous one.
Although only a small proportion of the administered dose was absorbed through the skin, radioactivity was widely distributed throughout the body. Levels of radioactivity in the organs of metabolism and excretion increased up to 24 h post-dose and then remained relatively constant throughout the experimental period. Of note there were the moderate levels of radioactivity in the bile ducts throughout all kill times.
Radioactivity was also distributed into a number of organs having a high lipid content (skeletal and brown fat) and those tissues having oily and/or secretive properties (Harderian, preputial, clitoral, lachrymal and salivary glands). As in the case of organs of metabolism and excretion, peak levels of radioactivity were observed in these tissues between 24 and 96 h post-dose.
At no time after dosing was radioactivity observed in the central nervous system (other than in the pituitary).

4.1.2.2 Acute toxicity

Oral
The LD_{50} value after a single oral administration by gavage in rats indicates LD_{50} > 5000 mg/kg. No deaths were observed. Pilo-erection was observed shortly after dosing in all treated rats (OECD, GLP, Ref. 21).

Dermal
After a single dermal administration in rats: LD_{50} > 2000 mg/kg. No deaths were observed. No signs of systemic toxicity were observed. Terminal autopsy findings were normal. (OECD, GLP, Ref. 22).

Inhalation
LC_{50} value in rats was > 1.82 mg/l (administered as an aerosol containing > 90% particles with diameter less than 10 microns) in one test (no deaths were observed) (GLP, Ref. 23) and 71 mg/l in another test (administered as an aerosol) (Ref. 24).
LAB is not classifiable as either toxic or harmful under current EU legislation.

4.1.2.3 Irritation

Skin
Animal data

The available information on rabbits gives an irritating property ranging from negligible to slight.
One test conducted on six rabbits after an application of 4 h of the undiluted substance shows the following values: a maximum average score of 0.5 for erythema at 24 and 48 h (0 at 72 h) and a score of 0 for oedema (EEC, Ref. 25).
Another test in the same conditions shows an averaged score of 1.1 (24, 48, 72 h) for erythema and 0 for oedema (OECD, Ref. 26).

Human data

A study (repeated insult patch test) was conducted on 205 volunteers to evaluate the potential hazard of dermal contact of LAB (irritation and sensitisation) after repeated application (ref. 31).

Approximately 0.2 ml of the test material, as 100% and 50% in corn oil, was placed on the webril pad of a Parke - Davis Readi - Bandage. The patch was then applied to a designated site. The adhesive was pressed all around to assure firm contact of the test material with the skin and to form a seal to retard the loss of moisture. During the first week 4 applications of 24 h of the undiluted LAB were followed by observations.
In the second and third week 50% LAB in corn oil was applied to the same volunteers changing the application sites (8 applications of 24 h).
During the fourth (challenge) week a series of 4 applications on virgin sites of 50% LAB in corn oil were done to observe if any reaction of sensitisation occurred.
In this study, a numerical grade from 0 to 4 for irritation was used according to these criteria:

0 - No visible irritation, or no difference from surrounding, untreated skin
1 - Erythema confined to the contact site which exceeds that of the untreated skin.
2 - Erythema confined to the contact site which definitely exceeds that of untreated skin, papules may or may not be present
3 - Erythema, with some degree of induration, and papules may or may not be present
4 - Erythema, induration, with one or more complications such as: extension beyond margins of contact area, vesiculation, ulceration.

After 24 h of continuous application of 100% LAB with the occluded patch the following grades of irritation were observed:
Grade 1 in 51/205 individuals, grade 2 in 6/205, grade 3 in 5/205.

After 1 week of repeated applications (4 applications) of 100% LAB in the same pre-treated sites, 87/205 individuals showed signs of irritation (70/205 of grade 1, 11/205 of grade 2, 6/205 of grade 3).
After 2 weeks of 24 h applications (4 per week) of 50% LAB in corn oil, on the same pre-treated sites, only 3/205 individuals showed signs of irritation (2/205 of grade 1 and 1/205 of grade 3).
Despite the repeated applications, the skin showed its ability to return to the normal condition.
Observations of minimal irritation after 24 h of continuous contact of the substance with an occluded patch and in addition after repeated doses are not indicative of a significant irritative capability, especially when the continuity of that irritation is interrupted by the return of the skin to its normal conditions.

Based on the above data and on the animal data (rabbit test), LAB is not classifiable as a skin irritant under EU legislation.

Eye
The available studies report conjunctive congestion as the only effect of instillation of an undiluted sample of LAB into the eyes of six rabbits. The scores range from 0.44 (OECD, Ref. 28) to 1 (EEC, Ref. 29), which indicates negligible irritant properties.
LAB is not classifiable as an eye irritant under current EU legislation.

4.1.2.4 Corrosivity

See 4.1.2.3. It is not corrosive.

4.1.2.5 Sensitisation

Animal data
A Magnusson and Kligman Maximisation Test on guinea pigs showed no sign of sensitisation (20 animals for treated group, 20 animals for control group). LAB at 20% concentration was used for the induction period and LAB at 5 and 10% concentration for the challenge exposure (OECD, Ref. 30).

Human data
(See 4.1.2.3)
With reference to the study before reported (Ref. 31) the induction period was followed by a challenge period (a series of 4 applications for 1 week). No individuals showed a skin sensitisation reaction either with undiluted or diluted sample.
LAB is not classifiable as a skin sensitiser under EU legislation.

4.1.2.6 Repeated dose toxicity

Inhalation
Four groups of 15 male and 15 female Sprague-Dawley rats per group were each exposed to mean exposure levels of 0, 102, 298, or 580 mg LAB per cubic meter of air in 10 m^3 inhalation chambers, six hours per day over an approximate 14-week period (70 exposure days).
Hypoactivity, irritation of the eyes and/or nose, and respiratory difficulties, above all in the high exposure and some mid-exposure animals, were observed during the exposure periods. Discharges or secretions from or about the nose, mouth, and eyes, hypoactivity, inflammation around the mouth, redness around the ears, and integumentary conditions were observed during non-exposure periods.
Decreases of mean body weight in mid- and high exposure animals during the study were also observed. The urine pH in high exposure males decreased. Hematology es were all within the normal biological limits for the rat.
Decreased glucose and protein levels coincided with reduced body weights observed in the mid-exposure females and high exposure animals. The increased alkaline phosphatase, SGOT, LDH, and SGPT levels in high exposure females could not be explained in the absence of related gross and microscopic pathology changes.
An increased liver weight was, however, observed in these animals. Increased relative organ weights were considered coincidental to the decreased mean body weights in the mid- and high exposure animals. A sub-acute multifocal inflammation of the alveoli in high exposure animals was observed.
The “no-adverse-effect” exposure level for rats receiving 70 six-hour exposures over an approximate three-month period was 102 mg/m^3 (GLP, EPA/TSCA, Ref. 32).

Oral
Rats were fed with a diet containing LAB at various concentrations up to 20000 ppm (2%) during 4 weeks.
Reduction in body weight and food consumption were observed at all exposure levels. No gross pathological changes were noted.
Histopathology was not carried out. The lowest dose tested in this study (GLP, EPA/TSCA, Ref. 33) is 2500 ppm, corresponding to 125 mg/kg bw.

4.1.2.7 Mutagenicity

4.1.2.7.1 *In vitro* studies

Bacterial studies

There are two tests conducted on Salmonella thyphimirium TA 1535, 100, 1537 and 98 strains with and without metabolic activation (S9 hepatic fraction):

1. LAB concentrations in DMSO: 0, 100, 1000, 4000, 8000 and 10000 µg/plate (EEC B14, Ref. 34);

2. LAB concentrations in DMSO: 0.3, 12, 60, 300, 1000, 3000 µg/plate. The highest concentration produced evidence of either toxicity or insolubility (GLP, EPA/TSCA, Ref. 35).

3.

The results of both tests were negative.

Mammalian cells studies

V79/HGPRT gene mutation assay

LAB concentrations in DMSO from 0 to 1 mM were tested in the absence or presence of S9 activation.

There were no statistically significant increases in mutation frequencies compared to the negative control (EEC B14, Ref. 34)

CHO/HGPRT gene mutation assay

LAB concentrations in ethanol from 100 to 2000 µg/ml were tested in a CHO cell line in the absence or presence of metabolic activation (S9 hepatic fraction). Cytotoxicity was significant at and above 1250 µg/ml with and without metabolic activation.

There were no statistically significant increases in mutation frequencies for the substance compared to the negative control (GLP, EPA/TSCA, Ref. 35).

Mitotic recombination in Saccharomyces cerevisiae

LAB concentration tested was 0, 1, 4, 6, 8, 10 mg/ml DMSO in presence or absence of metabolic activation (S9 hepatic fraction). Results showed that LAB did not induce any genetic effect in the D7 strain (EEC B14, Ref. 34).

4.1.2.7.2 *In vivo* studies

Rat bone marrow chromosome assay

LAB was given via gavage undiluted or dissolved in corn oil. The solutions were given once to three groups of 18-24 male and female rats at dosages of 1200, 4000 and 12,700 mg/kg bw. A significant mean body weight loss was found in the groups treated with the highest dose. No statistically significant increases in chromosomal aberration or gaps were observed in the treated groups at any of the sampling times.

Both mean chromosome numbers and mean mitotic indices were similar in test and vehicle control groups (GLP, EPA/TSCA, Ref. 35).

4.1.2.8 Carcinogenicity

A study was reported by Iversen (Ref. 36) where groups of 32 hairless hr/hr Oslo mice were exposed for 18 months to skin painting with a mixture of linear alkylbenzenes predominantly C_9 and C_{10} at different concentrations.

The experiments were carried out with negative and positive control groups according to the following two protocols:

1. An initial single application of a carcinogen DMBA, (7.12-dimethylbenz (alpha) anthracene), in two different doses (25.6 and 51.2 µg in 100 µl acetone), followed by long-term painting of 20% and 40% of LAB in acetone solution (100 µl) twice a week.
2. A complete carcinogenesis protocol: long-term applications of 20%, 40% and 80% of LAB alone in acetone solution (100 µl) twice a week.

The conclusions were that this LAB produced skin tumours and lymphomas in animals pre-treated with the carcinogen but not in animals receiving no pre-treatment. However the concentrations of LAB used by Iversen produced severe irritation and even ulceration with abnormal multiplication of cells when applied to skin.
Many investigations have shown that prolonged hyperplasia can promote skin tumours in mice (Ref. 42).
The dose levels used by the investigation (20,40 and 80%) exceeded the maximum tolerated dose (MTD) by factors of 4, 8 and 16, based on a previously reported study (Ref. 27) where MTD was determined to be 5% LAB applied twice weekly.
It is widely accepted that cell mutation is involved in chemical carcinogenesis in mouse skin. *In vitro* studies conducted on C_{10}-C_{14} LABs show an overwhelming lack of genotoxic effects which can lead to DNA mutations. The lack of such activity suggests that, if any effects like those observed in Iversen's study were to be observed with these materials, it would not be the result of any direct mutation of DNA. It is also being recognised that certain chemicals, which do no exhibit genotoxic activity, can produce tumours in the presence of severe irritation. A candidate for the primary mutagenic event for such chemicals could be oxidative DNA damage. Such damage could be produced by increased metabolic activity due to enhanced proliferative activity or the result of oxidative enzymes released by inflammatory cells (Ref. 45). Both of these conditions may exist in the presence of severe skin irritation.
Regarding the lymphomas Iversen added all the groups treated together and compared them with a historical control. The validity of this approach is questionable.
In addition different types of lymphoma recorded were combined. The histological types observed were recorded only as B cell lymphomas and lymphomas NOS (not otherwise specified) without further description.
LAB is clearly not classifiable as a carcinogen according to the complete carcinogenesis study.

Maximum tolerated dose (MTD)

10 groups of 10 mice (5 male and 5 female) were dosed for 8 weeks by skin painting the clipped back with various LAB concentration and application frequencies.
LAB was administered (dose volume of 0.05 ml per animal) at concentration of 1, 2, 5, 10, 15, 20% (v/v in acetone) twice per week and at 100% twice per week, once per week, once every 2 weeks and once every 4 weeks. Further groups of 5 male and 5 female mice were dosed with acetone twice per week as control.
It was intended to use the results for the selection of a maximum tolerable dose (MTD) suitable for a long-term dermal exposure study in mice. The effects observed were hyperplastic and inflammatory lesions.
The LOAEL was defined as 5% twice weekly or 100% weekly for the 8-week period. The NOAEL was defined as 2% concentration twice per week or 100% once every two weeks (GLP, Ref. 27).

4.1.2.9 Toxicity to reproduction

Reproductive (fertility) and developmental toxicity (teratogenicity)
A two-generation reproduction study and a developmental study were conducted on rats using single daily doses provided by gastric intubation using corn oil as vehicle (GLP, Ref. 37).

Reproductive toxicity
In the reproductive toxicity study to groups of 30 rats/sex/group were given doses of 0, 5, 50 and 500 mg/kg/d. F_0 animals received a 10-weeks premating treatment period and were then mated to produce a single litter; F_1 adults were selected from the F_1 litters. F_1 animals were dosed for 11 weeks before mating to produce a single litter (Ref. 37).

At 500 mg/kg/d decreases in weight gains during premating and early lactation were found in F_0 females and during premating and gestation, respectively for males and females, in both generations. Decreases were also found in litter size, pup viability at birth survival, through day 4 of postnatal life, and weights on day 14 and 21.
At 50 mg/kg/d only a reduction in F_1 of pup weight gain at day 7 was observed but this effect had returned to normal at day 14 and 21. This temporary reduction in pup weight only occurred in one generation, i.e. F_1, and was thus not consistent across generations.
Adult and weaned pups received a gross post-mortem examination. Histopathology studies were conducted on reproductive tissues, tissues with gross lesions, and the pituitary gland taken from each adult in the control and high dose groups.
No adverse effects of treatment were evident from the gross post-mortem and histopathological evaluations.
The significant findings only at 500 mg/kg/d (for F_0 and F_1 adults and F_1 and F_2 litters) and the non consistent effects of treatment at lower dose, show that the NOAEL for reproductive toxicity is 50 mg/kg/d for both parental and neonatal animals.

Developmental toxicity
In this study to groups of 24 mated females were given doses of 0, 125, 500 and 2000 mg/kg/day from day 6 to 15 of gestation.
Dams were terminated at gestation day 20 and foetuses were examined for external soft tissues and skeletal defects (Ref. 37).

The only effect noted at 125 mg/kg/d was a slight decrease in maternal weight gain, which was not significant. The decreases in maternal weight gain were significant at 500 and 2000 mg/kg/d; however, compensatory increases in weight gain occurred during the post-treatment period.
Ossification variations and delayed ossification increased significantly at 2000 mg/kg/day (79.7% of foetuses with variations and delayed ossification and 57.3% in the control group) and were above control level at 500 mg/kg/d.
There were no significant differences between control and treated groups in the number of foetuses with malformations.
The substance should not be considered as a developmental toxicant since an increased incidence of ossification variations and delayed ossification only at dose levels causing maternal toxicity cannot be considered as specific effects on prenatal development.

4.1.3 Risk characterisation

4.1.3.0 General aspects

LAB produces only slight acute irritation to the skin and eye of rabbits. Repeated doses produced inflammatory lesions of the skin of rats.
LAB is not classified as an irritant under current EU legislation.
LAB does not produce sensitisation either in experimental animals or in human volunteers. LAB is not classified as a skin sensitiser under EU legislation.
There is no evidence for an accumulation in the body by intravenous, oral and dermal route in rats. The skin contact results in only a small degree of percutaneous absorption (10% of the dose).
LAB is assumed to be rapidly and extensively eliminated principally in urine, showing only a negligible affinity to the tissues with a high lipid content or secretive actions. Moreover metabolism of the absorbed quantity is rapid and complete.
No deaths were observed in acute oral and dermal toxicity limit tests on rats (at 5000 and 2000 mg/kg respectively) and a very low inhalation toxicity was found (LC_{50} = 71 mg/l). LAB is not classified either toxic or harmful under current EU legislation.
Rodents exposed via inhalation to LAB for 14 weeks exhibit general eye and nose irritation, with depression of body and organ weights and elevation of hepatic enzymes in females only for the highest concentration tested. The NOAEL is = 0.1 mg/l.
Depressed weight gains in parental animals and in litter are observed in a two generation reproduction study on rats at highest dose (500 mg/kg/d).
Decreases were also found in litter size, pup viability at birth, survival and weights, however no significant effects on fertility occurred. The significant findings only at 500 mg/kg/d (for F_0 and F_1 adults and F_1 and F_2 litters) and the non-consistent effects of treatment at the lower dose, show that the NOAEL for reproductive toxicity is 50 mg/kg/d for both parental and neonatal animals.
Ossification variation and delayed ossification are found in a developmental study, however no malformations were noted.
The substance should not be considered as a developmental toxicant since an increased incidence of ossification variations and delayed ossification only at dose levels including maternal toxicity cannot be considered as specific effects on prenatal development. LAB does not have any unusual or selective reproductive or developmental toxicity.
LAB is both non-mutagenic and non-clastogenic, because it does not exhibit activity in test systems *in vitro* and *in vivo*.
One author reports that LAB shows no skin tumourogenic or carcinogenic effects in itself and does not promote tumours induced by pre-treatment with a carcinogenic substance. However it is claimed that LAB seems to enhance the malignant lymphomas and skin tumours induced by the carcinogenic substance.
The results of this study can be misinterpreted because of high LAB concentration, resulting in hyperplastic and inflammatory lesions that is a sign that the maximum tolerable dose (MTD) has been exceeded, according to the EPA Dermal Carcinogenesis Criteria. Several authors suggest that irritation and mild-long standing inflammation may enhance the carcinogenicity of small doses of a carcinogen.
In addition the investigation combined different histological type of lymphomas.
LAB is clearly not classifiable as a carcinogen according to the complete carcinogenesis study.

4.1.3.1 Workers

Inhalation
The low vapour pressure of LAB and the closed system processes limit exposure by inhalation.
The maximum of exposure predicted of 0.1 ppm (0.988 mg/m^3) (see 4.1.1.1) can be compared with the NOAEL for inhalation of 102 mg/m^3 (see 4.1.2.6).
The margin of safety for inhalation is thus higher than 100.
(**conclusion ii**)

Dermal
The maximum dermal exposure, assuming that direct handling occurs, is predicted to be 1.2 mg/kg/d (see 4.1.1.1).
The margin of safety can be calculated using the oral NOAEL (50 mg/kg/d) (see 4.1.2.9) derived from reproductive toxicity, assuming that the bioavailability for humans and the animal model and for the two exposure routes are similar.
In addition the results from toxico-kinetic studies indicate that LAB is slowly absorbed through the skin, metabolised and eliminated quite completely in urine, without any accumulation.
The margin of safety, in case of direct handling with incidental contact level, is calculated to be 41.6.
In addition the use of proper handling procedures should avoid any possibility of exposure for workers (**conclusion ii**).

4.1.3.2 Consumers

The margin of safety for chronic dermal toxicity can be calculated using the oral NOAEL (50 mg/kg/d) derived from reproductive toxicity (see 4.1.2.9).
Taking into account the consumer's exposure (see 4.1.1.2.) it is possible to calculate MOSs (Margins of Safety) for dermal and oral toxicity, which in the worst case are as follows:

Margin of Safety for dermal exposure $= 50 / 5.9 \cdot 10^{-3} = 8475$
Margin of Safety for oral exposure $= 50 / 1.9 \cdot 10^{-4} = 263158$

These values represent a very high margin of safety (**conclusion ii**).

4.1.3.3 Man exposed indirectly via the environment

Using again a NOAEL of 50 mg/kg/day and uptake data as reported in 4.1.1.3, namely a total human dose of $2.5 \cdot 10^{-4}$ mg/kg and $1.5 \cdot 10^{-5}$ mg/kg for local and regional models respectively, we can calculate the MOS for indirect exposure as follows:

Table 4.3 Mos for indirect exposure.

Model	MOS
Local	$2.0 \cdot 10^5$
Regional	$3.3 \cdot 10^6$

These values represent a very high margin of safety (**conclusion ii**).

4.2 HUMAN HEALTH (Physico-chemical properties)

4.2.1 Exposure assessment

Regarding the physico-chemical properties for which LAB should represent a hazard for man, the only possible exposure occurs in the work place at plant units, in the storage places and during the transport.

4.2.2 Effect assessment

4.2.2.1 Explosivity

A test conducted on LAB showed no explosive properties (GLP, EEC A.14, Ref. 7) (**conclusion ii**).

4.2.2.2 Flammability

LAB is not a flammable substance because its flash point is 140°C (closed cup) (ASTM, Ref. 4) (**conclusion ii**).

4.2.2.3 Oxidising properties

No oxidising properties are expected for LAB, due to its hydrocarbon nature (**conclusion ii**).

5 RESULTS

Environment

(X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied

Consumers

(X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied

Workers

(X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied

Indirect exposure via the environment

(X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied

Human health (physico-chemical properties)

(X) ii) There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied

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GLOSSARY

Standard term / Abbreviation	Explanation / Remarks and Alternative Abbreviation(s)
Ann.	Annex
AF	assessment factor
BCF	bioconcentration factor
bw	body weight / Bw, b.w.
°C	degrees Celsius (centigrade)
CAS	Chemical Abstract System
CEC	Commission of the European Communities
CEN	European Committee for Normalisation
CEPE	European Committee for Paints and Inks
d	day(s)
d.wt.	dry weight / dw
DG	Directorate General
DT_{50}	period required for 50 percent dissipation (define method of estimation)
DT_{50lab}	period required for 50 percent dissipation under laboratory conditions (define method of estimation)
DT_{90}	period required for 90 percent dissipation (define method of estimation)
$DT_{90field}$	period required for 90 percent dissipation under field conditions (define method of estimation)
EC	European Communities
EC	European Commission
EC_{50}	median effective concentration
EEC	European Economic Community
EINECS	European Inventory of Existing Commercial chemical Substances
EU	European Union
EUSES	European Union System for the Evaluation of Substances
f_{oc}	organic carbon factor (compartment depending)
g	gram(s)
gw	gram weight
GLP	good laboratory practice
h	hour(s)
ha	Hectares / h
HPLC	high pressure liquid chromatography
IARC	International Agency for Research on Cancer
IC_{50}	median immobilisation concentration or median inhibitory concentration 1 / explained by a footnote if necessary
ISO	International Standards Organisation
IUPAC	International Union for Pure Applied Chemistry
kg	kilogram(s)
kPa	kilo Pascals
K_{oc}	organic carbon adsorption coefficient
K_{ow}	octanol-water partition coefficient
Kp	solid-water partitioning coefficient of suspended matter
l	litre(s) / L
log	logarithm to the basis 10

$L(E)C_{50}$	lethal concentration, median
m	meter
µg	microgram(s)
mg	milligram(s)
MOS	margins of safety
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
NOEL	no observed effect level
OECD	Organisation for Economic Co-operation and Development
OJ	Official Journal
pH	potential hydrogen -logarithm (to the base 10) of the hydrogen ion concentration $\{H^+\}$
pKa	-logarithm (to the base 10) of the acid dissociation constant
pKb	-logarithm (to the base 10) of the base dissociation constant
Pa	Pascal unit(s)
PEC	predicted environmental concentration
PNEC(s)	predicted no effect concentration(s)
$PNEC_{water}$	predicted no effect concentration in water
(Q)SAR	quantitative structure activity relation
STP	sewage treatment plant
TGD	Technical Guidance Document[1]
UV	ultraviolet region of spectrum
UVCB	Unknown or Variable composition, Complex reaction products or Biological material
v/v	volume per volume ratio
w/w	weight per weight ratio

[1] Commission of the European Communities, 1996. Technical Guidance Documents in Support of the Commission Directive 93/67/EEC on risk assessment for new substances and the Commission Regulation (EC) No 1488/94 on risk assessment for existing substances. Commission of the European Communities, Brussels, Belgium. ISBN 92-827-801[1234]

Annex 1 Flow diagrams for the production of LAB by $AlCl_3$ and HF processes

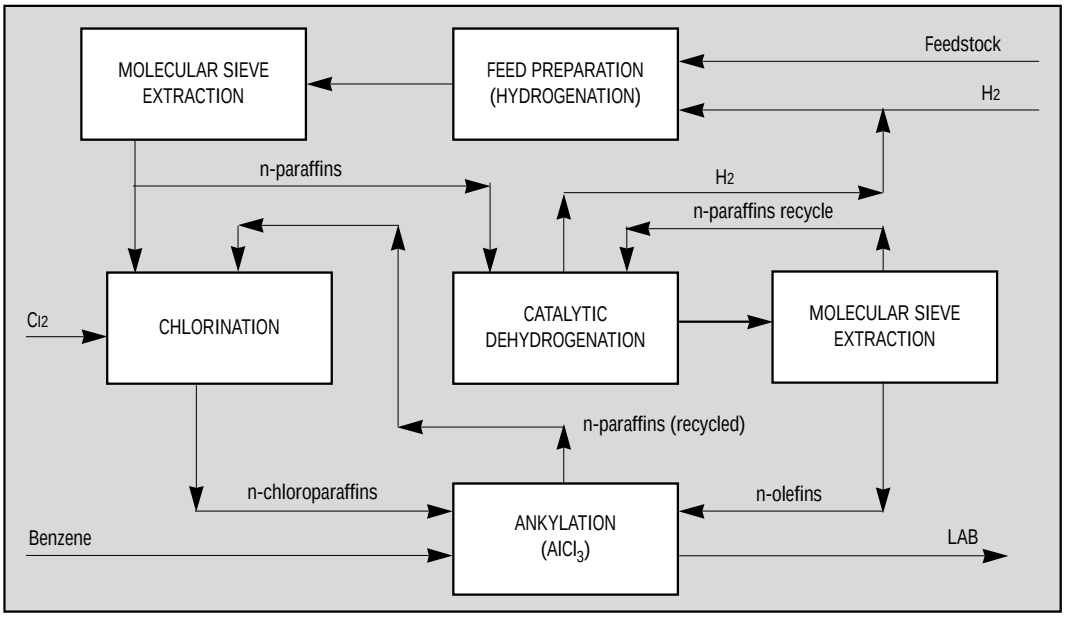

Figure 1.1 Flow diagram for the production of LAB by the $AlCl_3$ process.

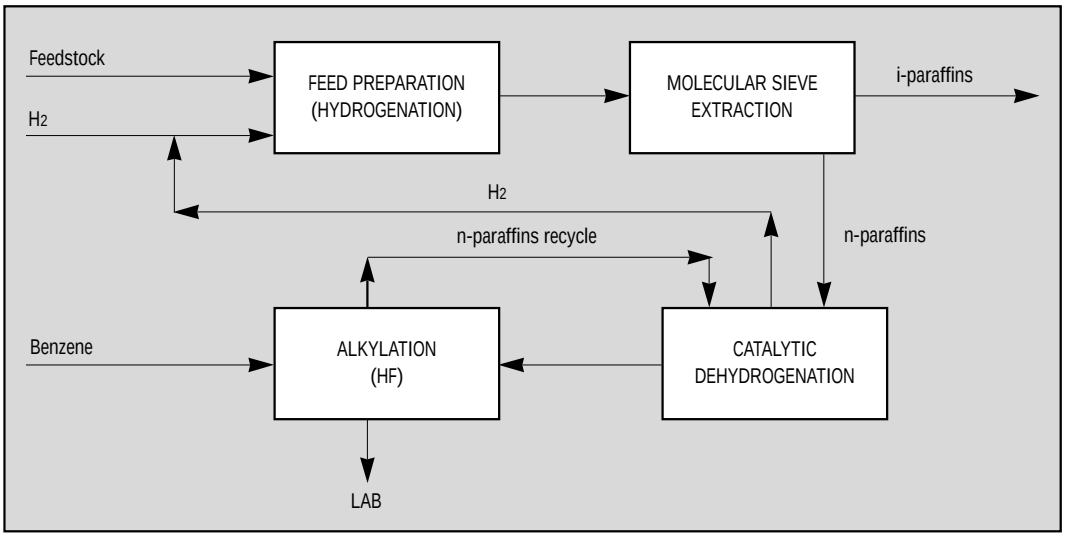

Figure 1.2 Flow diagram for the production of LAB by the HF process.

Annex 2 Sulphonation plant diagram

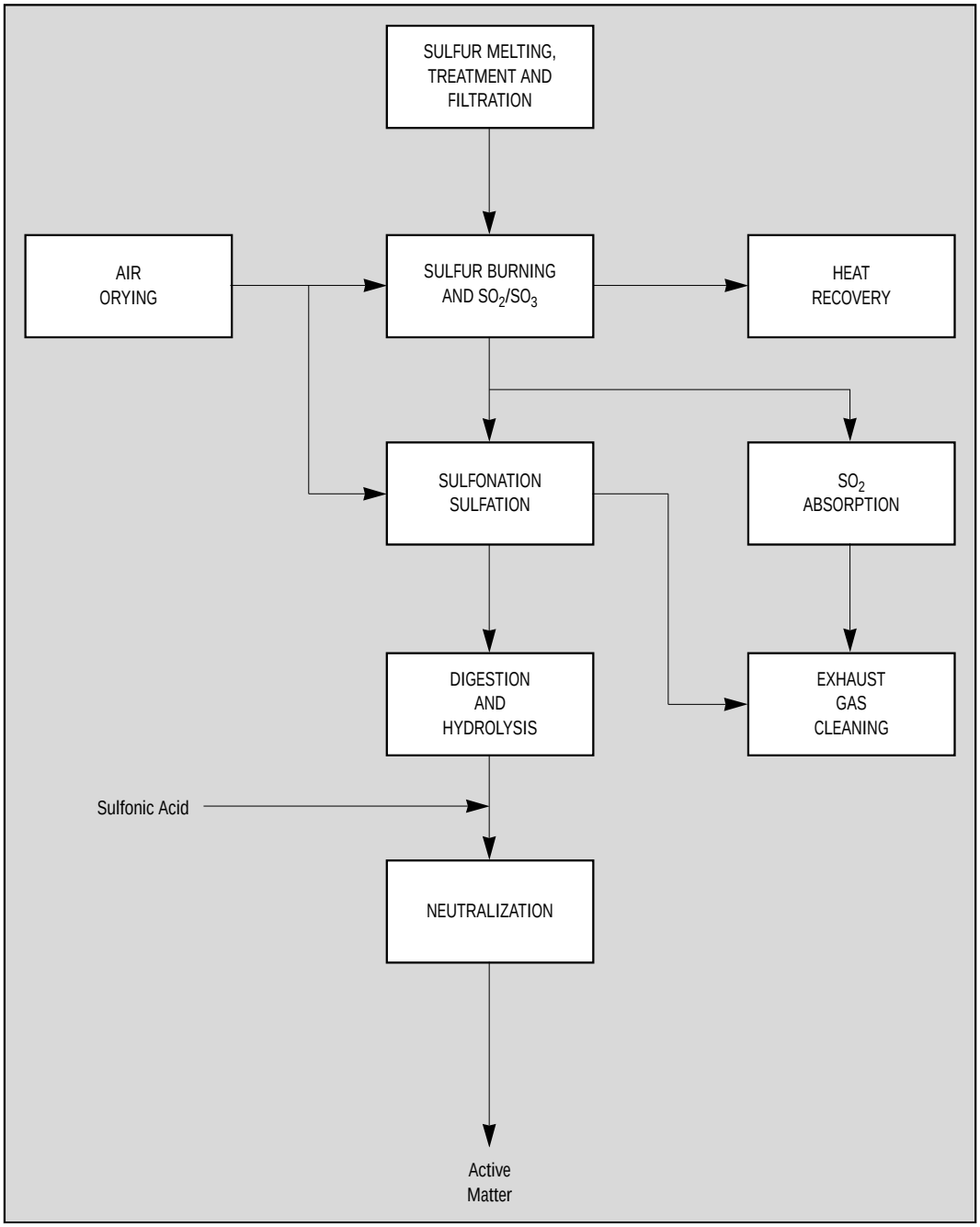

Figure 2.1 Sulphonation-sulphation plant with sulphur burning.

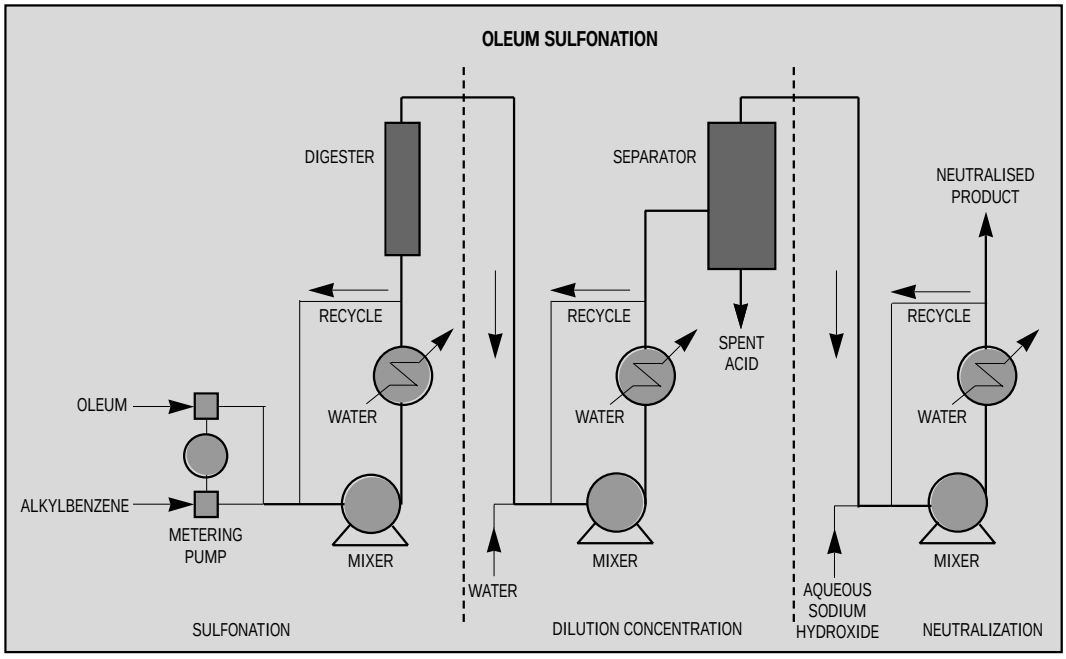

Figure 2.2 20% oleum sulphonation, a four-stage process.

Annex 3 From detergents manufacturers

BENZENE, C_{10-13} ALKYL DERIVATIVES

CAS# 67774-74-7

CONSUMER EXPOSURE TO LAB

Linear Alkyl Benzene (LAB), is used in the manufacture of the surfactant material, linear alkylbenzene sulphonate (LAS) following a reaction with sulphuric acid. The LAS is used in certain household detergent products such as hand dishwashing products and some laundry detergents. Only residual amounts (typical range estimated to be 0.1 – 1%) of LAB remain in the LAS and hence in the consumer product.

Considering a variety of scenarios and product uses, it is reasonable to consider that the tasks with the greatest chance of exposure of the consumer to LAB are ***hand dishwashing*** (dermal exposure) and ***use of dishes and other cooking utensils after dishwashing*** (oral exposure). Dermal exposure is also possible during ***handwashing of clothing*** with some light-duty laundry detergents. Consumer exposure via inhalation is not considered relevant due to the very low vapour pressure of LAB and the fact that only trace levels of LAB are present in consumer products.

Using available data on typical product usage from industry and the models suggested in the EU *Technical Guidance Document*, the following estimates of the potential consumer exposure to LAB for a "worst case" scenario were obtained:

1. **Total Dermal Exposure = 5,9 · 10^{-3} mg LAB/kg BW · day**
2. **Total Oral Exposure = 1.9 · 10^{-4} mg LAB/kg BW · day**

These estimates are very conservative since they assume 100% uptake of the "film" of product containing residual levels of LAB which may contact the skin or oral cavity. Typical events such as rinsing, wiping etc. are also not considered in the estimation of these "worst case" consumer exposure values.

The details are provided in the following sections and additional data and model parameters are explained in the Appendix.

CONSUMER EXPOSURE TO LAB - (see Appendix I)

1. Dermal Exposure Assessment during Hand Dishwashing:

An estimation of dermal exposure for the consumer is made using the EU *Technical Guidance Document* (Existing Chemicals Risk Assessment). The models described in the document are used with default values for some parameters and the additional models described *in USES Version 1.0* are also used.

Explanations for this scenario are provided in Appendix I.

LAB can be considered as a substance in a non-volatile medium (dishwashing liquid) which is diluted for normal use.

Assuming a "worst case" scenario using upper levels of ranges, the concentration (mg/cm^3) of LAB in the end volume of the dishwashing solution is:

$$\mathbf{C_{der} = q \cdot w_f \cdot V_e^{-1}}$$

$$= \frac{\mathbf{15\ g \cdot 0.0015}}{\mathbf{5000\ cm^3}}$$

$$\mathbf{C_{der} = 4.5 \cdot 10^{-3}\ mg\ LAB/cm^3}$$

Uptake via the skin is not calculated for such a scenario in the *Technical Guidance Document* since the proportion of the entire quantity of the substance in contact with the consumer's skin (hands and forearms) during this task is unknown.
The *USES Version 1.0* proposes an equation to calculate dermal uptake based on the assumption that a continuous film of the dishwashing solution with a constant substance concentration is deposited on the skin.
The *USES* model does not consider removal of the "film" through rinsing and/or wiping the skin dry after completion of the task. In addition, using the "worst case" assumption, the model assumes that the bioavailability of LAB for dermal uptake is 1 (i.e. 100% of the deposited film is absorbed!). No account is taken of the actual skin permeability of LAB or of the task duration. The calculation is thus very conservative.

$$U_{derm} = \frac{C_{der} \cdot THICKNESS_{derm} \cdot AREA_{derm} \cdot BIO_{derm} \cdot N_{events}}{BW}$$

$$= \frac{4.5 \cdot 10^{-3}\ mg \cdot 0.01\ cm \cdot 1980\ cm^2 \cdot 1 \cdot 2}{cm^3 \cdot 70\ kg}$$

$$\mathbf{U_{derm} = 2.5 \cdot 10^{-3}\ mg\ LAB/kg\ BW \cdot day}$$

CONSUMER EXPOSURE TO LAB – (see Appendix II)

1. Dermal Exposure Assessment during Handwashing of Laundry:

An estimation of dermal exposure for the consumer is made using the *EU Technical Guidance Document* (Existing Chemicals Risk Assessment). The models described in the document are used with default values for some parameters and the additional models described in *USES Version 1.0* are also used.
Explanations for this scenario are provided in Appendix II.
LAB can be considered as a substance in a non-volatile medium (light-duty laundry product) which is diluted for normal use.
Assuming a "worst case" scenario using upper levels of ranges (i.e. up to 25% LAS in the laundry product and a concentration of 1.2 g LAS/l of wash-water), then the concentration of LAB (mg/cm^3) in the diluted product for handwash laundry is:

$$\mathbf{C_{der} = 1.2 \cdot 10^{-2}\ mg\ LAB/cm^3}$$

Uptake via the skin is not calculated for such a scenario in the *Technical Guidance Document* since the proportion of the entire quantity of the substance in contact with the consumer's skin (hands and forearms) during this task is unknown.

The *USES Version 1.0* proposes an equation to calculate dermal uptake based on the assumption that a continuous film of the handwashing solution with a constant substance concentration is deposited on the skin of the consumer.
The *USES* model does not consider removal of the "film" though rinsing and/or wiping the skin dry after completion of the task. The calculation below also assumes that the task (hand laundering) is performed daily (n = 1) which is conservative. In addition, using the "worst case" assumption, the model assumes that the bioavailability of LAB for dermal uptake is 1 (i.e. 100% of the deposited film is absorbed!). No account is taken of the actual skin permeability of LAB or of the task duration. The calculation is thus very conservative.

$$U_{derm} = \frac{C_{der} \cdot THICKNESS_{derm} \cdot AREA_{derm} \cdot BIO_{derm} \cdot N_{events}}{BW}$$

$$= \frac{1.2 \cdot 10^{-2}\ mg \cdot 0.01\ cm \cdot 1980\ cm^2 \cdot 1 \cdot 1}{cm^3 \cdot 70\ kg}$$

$$\mathbf{U^{derm} = 3.4 \cdot 10^{-3}\ mg\ LAB/kg\ BW \cdot day}$$

<u>CONSUMER EXPOSURE TO LAB</u> – (see Appendix III)

2. <u>Oral Exposure Assessment due to Deposits on Dishes, Cooking Utensils etc. after Dishwashing:</u>

The EU *Technical Guidance Document* package does not describe a suitable model for estimating the potential oral intake due to residual deposits of a substance on dishes, cooking utensils etc. after hand dishwashing with a product containing the substance of interest. USES Version 1.0 only describes scenarios for a substance migrating from an article into food or drink or for a substance unintentionally swallowed. The ECETOC *Technical Report #58* describes a simple model for estimating potential oral intake via exposure to deposits on dishes etc. and this model is used here.
Explanations for this scenario are provided in Appendix III.
The ECETOC model does not consider rinsing of dishes with clean water; evaporation of substances from wet dishes or wiping dishes dry with a towel. All of these typical events would significantly reduce the amount of residue actually remaining on the dish surface after washing. Further, the model assumes that all the residue remaining on the dish is ingested during re-use of the dish and that the substance is then completely bioavailable once ingested by the consumer. Thus, the calculation is very conservative.

$$I_{oral} = A \cdot FA_{oral} \cdot S_{dish} \cdot BW^{-1}$$

$$A = \frac{4.5 \cdot 10^{-3}\ mg\ LAB \cdot 0.25\ cm^3}{cm^3 \cdot 450\ cm^2}$$

$$= 2.5 \cdot 10^{-6}\ mg\ LAB \cdot cm^{-2}$$

$$I_{oral} = \frac{2.5 \cdot 10^{-6}\ mg \cdot 1 \cdot (12 \cdot 450\ cm^2)}{cm^2 \cdot 70\ kg}$$

$$\mathbf{I_{oral} = 1.9 \cdot 10^{-4}\ mg\ LAB/kg\ BW \cdot day}$$

Appendix I - (see EU TGD and USES 1.0)

Additional data:

- Typical level of residual LAB in LAS = 0.1 – 1%
- Typical level of LAS in a dishwashing product = 5 – 15%
- Product use concentration for dishwasher = 0.3% (15 g product in 5 l of water)
- Surface area of exposed skin (hands and forearms) = 1980 cm^2
- Assume the number of events or jobs per day = 2

Model Parameters:

Average concentration of substance (LAB) in the product [$mg \cdot cm^{-3}$]	C_{der}
Amount of product used [g]	q
Weight fraction of substance (LAB) in product [-]	wf
Final volume of diluted product [cm3]	Ve
Uptake via the skin per period [$mg \cdot kg\ BW^{-1}\ period^{-1}$]	U_{derm}
Thickness of the film layer on skin [default = 0.01 cm]	$THICKNESS_{derm}$
Surface area of skin exposed [cm^2]	$AREA_{derm}$
Bioavailability for dermal exposure (default = 1)	BIO_{derm}
Number of events per period (usually, events $\cdot$ day^{-1})	N_{events}
Average human bodyweight [default = 70 kg]	BW

Appendix II - (see EU TGD and USES 1.0)

Additional data:

- Typical level of residual LAB in LAS = 0.1 – 1%
- Typical level of LAS in a handwash laundry product = 5 – 25%
- Typical level of LAS in wash solution = 1.2 g/l
  = 0.012 g/l of LAB assuming maximum leve of 1% LAB in LAS
- Surface area of exposed skin (hands and forearms) = 1980 cm^2
- Number of events of jobs per day = 1

Model Parameters:

Average concentration of substance (LAB) in the product [$mg \cdot cm^{-3}$]	C_{der}
Amount of product used [g]	q
Weight fraction of substance (LAB) in product [-]	wf
Final volume of diluted product [cm^3]	V_e
Uptake via the skin per period [$mg \cdot kg\ BW^{-1} \cdot period^{-1}$]	U_{derm}
Thicknes of the film layer on skin [default = 0.01 cm]	$THICKNESS_{derm}$
Surface area of skin exposed [cm^2]	$AREA_{derm}$
Bioavailability for dermal exposure (default = 1)	BIO_{derm}
Nmber of events per period (usually, events $\cdot$ day^{-1})	N_{events}
Average human bodyweight [default = 70 kg]	BW

Appendix III - (see ECETOC Technical Report #58))

Additional data:

- Typical level of residual LAB in LAS = 0.1 – 1%
- Typical level of LAS in a dishwashing product = 5 – 15%
- Product use concentration for dishwasher = 0.3% (15 g product in 5 l of water)
- Similar to C_{der} in dermal calculation, concentration of LAB = $4.5 \cdot 10^{-3}$ mg/cm^3
- Assume that a volume of dishwasher solution remains on the plate face = 0.25 cm^3
- Assume that the area of one side of a plate = 450 cm^2
- Assume that the total amount of dishes, cooking utensils used/day = 12 plates

Model Parameters:

Amount of substance ingested [mg $\cdot$ kg BW^{-1} $\cdot$ period^{-1}]	I_{oral}
Amount of substance deposited per unit are a [mg $\cdot$ cm^{-2}]	A
Fraction of deposited substance ingested (default = 1)	FA_{oral}
Area of dishes in contact with substance [cm^2]	S_{dish}
Average human bodyweight [default = 70 kg]	BW

European Commission

EUR 19011 – European Union Risk Assessment Report benzene C_{10-13} alkyl derivs, Volume 3

Editors: B.G. Hansen, S.J. Munn, G. Schoening, M. Luotamo, A. van Haelst, C.J.A. Heidorn, G. Pellegrini, R. Allanou, H. Loonen

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The report provides the comprehensive risk assessment of the substance Benzene C_{10-13} alkyl derivates. It has been prepared by Italy in the frame of Council Regulation (EEC) No. 793/93 on the evaluation and control of the risks of existing substances, following the principles for the assessment of risks to man and the environment, laid down in Commission Regulation (EC) No. 1488/94.

The evaluation considers the emissions and the resulting exposure to the environment and the human population in all life cycle steps. Following the exposure assessment, the environmental risk characterisation for each protection target in the aquatic, terrestrial and soil compartment has been determined. For human health the scenarios for occupational exposure, consumer exposure and humans exposed indirectly via the environment have been examined and the possible risks have been identified.

The risk assessment for Benzene C_{10-13} alkyl derivates concludes that there is no concern for the environment and/or for human health. There is at present no need for further information and/or testing or for risk reduction measures beyond those which are being applied already.

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European Union Risk Assessment Report

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