Human & Environmental Risk Assessment
on ingredients of
European household cleaning products

Fatty Acid Salts (Soap)

Environmental Risk Assessment

Draft

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1. Contents

2. Executive Summary

Fatty acid salts (soap) are widely used in household cleaning products, cosmetics, lubricants (and other miscellaneous industrial applications) and coatings. Uses in household cleaning products, the scope of this HERA assessment, include fabric washing products, fabric conditioners, laundry additives, and surface and toilet cleaners. These uses cover chain lengths of C10-22 predominantly with counterions of sodium and potassium.

According to data received from a survey conducted among detergent formulator companies, an overall annual tonnage of 71306 tonnes of fatty acid salts for use in HERA applications was estimated. This was compiled using data from 4 out of the 6 main formulator companies. This value is estimated to cover greater than 80% of the tonnage used within the HERA use categories. Calculations of PEC in the risk assessment have been based on 71306 tonnes per annum. A scaling factor of 1/0.8 = 1.25 is used as a final calculation of risk characterisation ratios to convert these values into estimates for total use in HERA applications.

There are a number of acute data for fatty acids and fatty acid salts to aquatic organisms although there is a predominance of data for fatty acid. There are few toxicity values for terrestrial organisms. Data availability / quality covering all the taxonomic groups for specific fatty acid salt chain lengths is poor. The chronic data set is very limited.

For chain lengths >C12, solubility decreases to a degree where an adverse effect would not be expected in the environment due to reduced biovailability. Data for longer chain lengths have been generated using solvents which makes interpretation more difficult.

The data set for environmental fate includes standard biodegradation studies (looking at aerobic and anaerobic degradation), some degradation in surface water studies and field monitoring data.

Removal from wastewater was determined using measured monitoring data. The PNEC values for C10 and C12 were determined from measured toxicity data. For chain lengths >C12 all observed toxicity values were above the limit of solubility and were not used in PNEC derivation. In determining the PNECs for these chain lengths, assumptions were made based on the toxicity values for shorter more soluble chain lengths. The PNEC values for the longer chain lengths are likely to be conservative since the concentration of the soluble fraction will be lower than that at which toxicity would be observed. PNEC and PEC calculations are further complicated by the predominance of calcium and magnesium ions in waste water leading to rapid formation and predominance of relatively insoluble Ca and Mg salts that will not be bioavailable.

By means of higher tier exposure and effects data, it could be shown that the use of fatty acid salts in HERA applications (household detergents and cleaning products) poses no concern in any environmental compartment. The risk characterisation ratios are considered conservative. This is largely due to the conservative nature of the derived PNEC values for chain lengths >C12 as described above.

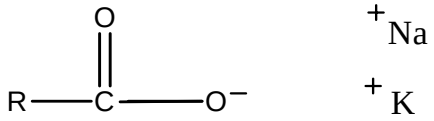
3. Substance Characterisation

Fatty acid salts are a widely used class of anionic surfactants. The applications which are covered by the scope of HERA include use in fabric washing products, fabric conditioners, laundry additives, and surface and toilet cleaners. In addition, there are a number of uses which are not covered by HERA. These include cosmetics, soap bars, lubricants (and other miscellaneous industrial applications) and use in coatings.

3.1. CAS No and Grouping information

The category for this assessment is defined as the salts of monocarboxylic acids bearing a straight, even numbered fatty acid chain, ranging in number of carbon atoms from 10 to 22. The C16 to C22 members of the group may be saturated or unsaturated (unsatd) with a carbon-carbon double bond.

The fatty acids salts grouping consists of a sequence of single molecule products differing in length of the carbon chainlength and commercial mixtures that are composed of fatty acids salts with a range of carbon chain lengths. The chemical structure of the category is:



where R contains from 9 to 21 carbon atoms and the higher fatty acid chain lengths may be saturated or unsaturated, with potassium or sodium salts included.

3.2. Chemical structure and composition

Table 1 covers the CAS numbers provided by 4 out 6 formulator companies. Although clearly important from a regulatory perspective, the environmental assessment is not based on CAS Nos., but on the product composition and specifically carbon chain length distribution - which is key to the environmental profile of this family. Whilst fatty acids are used in the initial starting list of materials, the final formulation of products covered through this assessment can be expected to contain only fatty acid salts. Thus, the salts of fatty acids only are considered here. Data for fatty acids have been used only for (comparative) read across purposes in the absence of data for the salts.

Table 1 – Chemicals, CAS Numbers, Synonyms, and Structural Composition

CAS No.	Compound	Synonyms	Chain length
Fatty Acid Salts			
629-25-4	Dodecanoic acid, sodium salt	Sodium laurate	12
143-18-0	9-Octadecanoic acid, potassium salt	Oleic acid, potassium salt; Potassium oleate	18
143-19-1	9-Octadecanoic acid, sodium salt	Oleic acid, sodium salt; Sodium oleate	18
822-16-2	Octadecanoic acid, sodium salt	Stearic acid, sodium salt; Sodium stearate	18
2272-11-9	9-Octadecanoic acid (Z)-, compd with 2-aminoethanol (1:1)	Monoethanolamine oleate	20
85408-69-1	Fatty acids, C8-C18 and C16-18 unsatd. Sodium salts	-	16-18
Fatty Acids			
143-07-7	Dodecanoic acid	Lauric acid	12
90990-09-3	Fatty acids, C10-14	-	10-14
67701-01-3	Fatty acids, C12-18	-	12-18
67701-03-5	Fatty acids, C16-18	-	16-18
67701-06-8	Fatty acids, C14-18 and C16-18 unsatd	-	14-18
85711-54-2	Fatty acids, rape oil	-	18-22
68424-37-3	Fatty acids C14-C22	-	14-22

Due to the limited availability of measured physico-chemical data for the fatty acid salts, these data have been generated mostly using predicted values from the EPIWIN program (see Appendix I). The EPI suite of tools was developed by the EPA Office of Pollution Protection Toxics and Syracuse Research Corporation. As part of this suite the program (WSKOWWIN) estimates the water solubility (WSol) of an organic compound using the compounds log octanol-water partition coefficient (Kow).

The available data demonstrate that the melting point increases with increasing chain length. Unsaturation results in decreased melting points in comparison to the saturated analogue. The salts of the fatty acids generally have higher melting points compared to their corresponding fatty acid.

The relevance of the boiling point endpoint for the salts of the fatty acids is questionable, as these chemicals are expected to decompose prior to reaching boiling temperatures. For saturated linear fatty acids, the boiling point increases with increasing carbon chain length.

The vapour pressure of the salts of single or mixed fatty acids are expected to be low. Due to lack of measured data for the fatty acid salts predicted values based on estimated log Kow have been generated by EPIWIN. Available measured data for members of the fatty acids themselves indicate that these chemicals have very low vapour pressures (Appendix Ic). Predictions generated by EPIWIN for the fatty acids indicate that the program overestimates vapour pressure.

For fatty acids the partition co-efficient increases with increasing chain length.

Available data for the salts of the fatty acids indicate that the salts, not unexpectedly, have much greater water solubility than the free acids, which demonstrate that water solubility

decreases with increasing chain length.
Physical-Chemical data are provided in Appendix I.

3.3 Manufacturing Route and Production/Volume Statistics

According to data received from AISE the estimated annual tonnage of fatty acids salts produced for use in household cleaning products in Europe is 71306 tons. This has been compiled from 4 out of the 6 main formulator companies.
Soaps are produced by the saponification of fat with alkali. The production process was invented by Leblanc in 1791, when he found a process for producing soda (Na_2CO_3) and thus NaOH became commercially available for the saponification of fatty acids (Moreno *et al.* 1993; Bruschweiler *et al.* 1988). The saponification of fats is given in figure 1.
Where R = C9 – C21 aliphatic chains

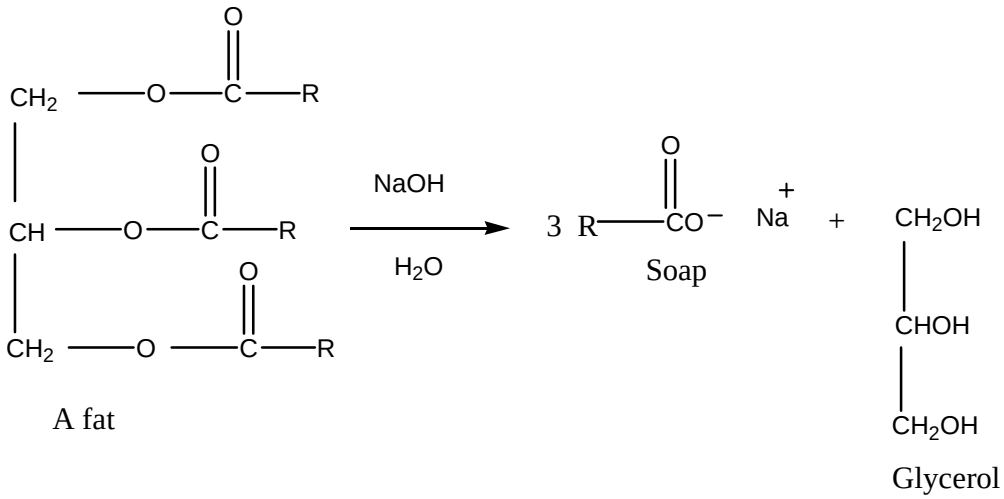


Figure 1: Saponification of fats (from BKH, 1994)

The crude soap curds contain glycerol and excess alkali but purification can be effected by boiling with a large amount of water, followed by precipitation of the pure sodium carboxylate salts on addition of sodium chloride (McMurry, 1984 *cited in* BKH, 1994).

3.4. Use applications summary

Tonnage used in HERA applications (HERA Tonnage)
To determine the total fatty acid salt tonnage used in products falling within the scope of HERA (i.e., household detergents and cleaning products), a survey was conducted among detergent formulator companies (data from members of AISE). The data received from the 4 of the 6 major fatty acid salt formulators provided an overall estimated annual tonnage of 71306 tonnes for HERA applications. This value is estimated to cover greater than 80% of the tonnage used within the HERA use categories. Calculations of PEC in the risk assessment have been based on 71306 tonnes per annum. A scaling factor of 1/0.8 = 1.25 is used as a final calculation of risk characterisation ratios to convert these values into estimates for total

use in HERA applications.

In addition, the data provided an estimated distribution between carbon chain lengths. This chain length distribution is not derived for 100% of the total tonnage but for one which is greater than 80% of the total. The distribution is shown in Table 2.

Table 2. Tonnage of fatty acid salts within the scope of HERA, determined via AISE survey

	Estimated Carbon Distribution of Fatty acid salts (% weight)	Tonnage of fatty acid salts (tonnes/annum (tpa))*
C10	1.1	784
C12	37	26526
C14	12	8414
C16	17	12336
C18	32	22675
>C18 **	0.8	570
Total		71306

* These values are calculated from % chain distribution and tonnage of 71306 tonnes per annum.

** This equates to predominantly C22

Total use of fatty acid salts (to include both HERA and non HERA uses) is estimated to be 701,000 tonnes/year (BKH review, 1994)

4. Environmental Assessment

Industry has sponsored several publications summarising environmental data on soaps (BKH, 1994). In addition, the majority of data have been collated from other databases e.g. IUCLID, ECOTOX and through literature searches (see also search strategy, Appendix II)

4.1. Environmental Exposure Assessment

The calculation for the following risk assessment is based on the estimated fatty acid salt tonnage of 71,306 tonnes/year in HERA applications. The chain length distribution was obtained from the AISE survey of formulators. This tonnage scenario is further referred to as 'HERA tonnage'.

Table 3. HERA Tonnage of Fatty acid salts

	Tonnage of Fatty acid salts (tonnes/year)
C10	784
C12	26526
C14	8414
C16	12336
C18	22675
>C18 (C22)	570
Total	71306

This was compiled using data from 4 out of the 6 main formulator companies. This value is estimated to cover greater than 80% of the tonnage used within the HERA use categories. Calculations of PEC and consequent risk characterisation ratios in the risk assessment have been based on 71306 tonnes per annum. A scaling factor of 1/0.8 = 1.25 is used as a final calculation to convert these values into estimates for total use in HERA applications.

It is recognised that the majority of the total European fatty acid salt tonnage is ultimately released in the same way as the HERA volume, down-the-drain to the environment. As such, although not within the scope of HERA, a more conservative assessment using the total European usage estimate (i.e. 701,000tonnes/year) (BKH review, 1994) and same chain length distribution as for HERA tonnage is also presented in an addendum (Section 4.4).

Data Reliability

Data reliability values have been assigned according to the HERA Methodology document. This advocates the use of the scoring system derived by Klimisch *et. al*. (1997).

Exposure Pathway and Detergent Scenario

The “HERA detergent scenario” was used for the environmental exposure calculations. The entire tonnage was assumed to follow the domestic down-the-drain pathway to the environment. For the calculation of the EUSES regional tonnage, 7% of the EU tonnage was assigned to the region (replacing the default 10%), and the local emissions were not increased by a factor 4, but by a factor 1.5. Further explanation on and justification for these values can be found in chapter 2.6 of the HERA methodology document.

4.1.1. Environmental Fate

A review of degradation data is based on the BKH Report for NVZ (1994) covering CAS numbers for the fatty acids and fatty acid salts on IUCLID, ECOTOX. In addition, reviews by Swisher (1987) and Verschueren (1973) and other literature sources were consulted.

Biodegradation Properties

The fate of fatty acid salts in aqueous systems is complicated by the fact that there are a numbers of water soluble and water insoluble groups and combinations of these. In practice whilst the use of Na salts are by far the most common use of soap in finished products, the predominance of calcium and magnesium ions in waste water leads to rapid formation and predominance of relatively insoluble Ca and Mg salts (Swisher, 1987; Prats *et al*, 1996).

Overall conclusions were drawn from the reviews and literature and were summarised in Swisher (1987) as follows:

- The rate of biodegradation is mainly dependent on the physical and chemical characteristics. In particular solubility, adsorption and CMC (see Physical Chemical Properties) are key factors.
- The fate of fatty acid salts is strongly influenced by the poor water solubility of the calcium and magnesium salts.
- The rate of metabolism decreases as chain length increases.
- Unsaturation increases the rate of metabolism although the degree of unsaturation and positioning of double bonds is not highly significant.
- The available data indicate all fatty acid salt chain lengths up to and including C18 can be metabolised under aerobic conditions and can be considered to be readily biodegradable (BKH, 1994).

Loehr (1968) studied a series of fatty acid salts using the Warburg method (O2 uptake). Data from these studies indicate that oxidation exceeded 50%ThOD in many cases within 6-24 hours. The study can be summarise as follows:

i) Fatty acids sodium salts of C10-C18 can be metabolised in aerobic systems. The equivalent length calcium salts can also be metabolised, particularly if the insoluble particles are dispersed.

ii) Metabolism was influenced by solubility.

iii) The rate of metabolism decreased as chain length increased.

iv) Unsaturation increases the rate of metabolism although the degree of unsaturation and positioning of double bonds was not highly significant. This could be attributable to solubility differences between unsaturated soaps and their equivalent saturates.

Whilst solubility is a key factor when considering metabolism of materials, there has been investigation into the adaptation of respirometric methods for assessing ready biodegradability of poorly soluble materials. ECETOC (1986) reported degradation of calcium stearate under various test conditions. Results of the study to look at the influence of methods such as agitation, ultrasonic dispersion and emulsifiers/solvents for introducing the test material into the test medium indicated that the usual physical barriers preventing the assessment of poorly–solubles could be overcome. In general agitation accelerated biodegradation but overall there was no significant influence on % biodegradation. Only one combination of methods (test material adsorbed to glassfibre without agitation showed a reduced rate (Table 4).

Table 4. Summarised results for calcium stearate from the ECETOC report No. 20 (1986)

Test	Duration (days)	Agitation (Y/N)	Carrier/method	Basis of Calc.	% Degradation	Reliability
Sturm	24	N	-	CO2/ThCO2	91	2
Sturm	24	Y	-	CO2/ThCO2	99	
Sturm	24	N	Glass filter	CO2/ThCO2	55	
Sturm	20	Y	Ultrasound	CO2/ThCO2	72	
Sturm	20	Y	Glass filter	CO2/ThCO2	84	
Sturm	24	Y	Glass filter	CO2/ThCO2	88	
MITI	32	Y	-	BOD/ThOD	91	
MITI	32	Y	Nonylphenol.10EO.5PO	BOD/ThOD	93	

Very few data are available for the salts of C10, C18 (oleate) or C22 homologues. Swisher (1987) reports an overview of biodegradation data for fatty acid salts (Table 5). There are, however, several published and unpublished studies which report biodegradation of both Na and Ca salts of C18 stearate (Tables 4,5 and 6). Considering that the rate of metabolism decreases with chain length and degree of saturation, for C10 and C18 oleate, C18 (stearate) salts can be considered a worst case. As both Na and Ca salts of C18 stearate exhibit ready biodegradation all chain lengths C10 – C18 also can be assumed to be readily biodegradable. This is supported by available data for chain lengths where data exist. There is only one available value for chain lengths >C18. A mix of fatty acid chain lengths of C20/ C22 exhibited ready biodegradation (Table 6). In the absence of any other data for these longer chain lengths, this is used as evidence of ready biodegradation for C22 fatty acid salt.

Table 5. Data reported in Swisher (1987)

Substrate	Chain length	Extent (%)	Method + time	References	Reliability
Na laurate	12	58	BOD5	Marion (1966)	4
Na oleate	18	48	BOD5	Goldthorpe (1950)	4
Na stearate	18	64	BOD5	Bogan(1955)	4
Na stearate	18	48	BOD5	Goldthorpe (1950)	4
Na stearate	18	53	BOD5	Bogan (1955)	4
Na stearate	18	60	CO2 (8day)	Lotzsch (1979)	4
Tallow soap	16/18	75	BOD15	Noble (1972)	4
Na stearate	18	62	CO2 (28day)	Gerike (1984b)	4
C16-18 soap	16/18	56	CO2 (10day)	Itoh (1979)	4
Na palmitate	16	55	Warburg (2day)	Winter (1962)	4
C16-18 soap	16/18	56	CO2 (10day)	Itoh (1979)	4
Na stearate	18	62	CO2 (28day)	Gerike (1984b)	4
Na laurate	12	58	Warburg (5day)	Marion (1966)	4

Table 6. Other relevant/reliable data

Substrate	Chain length	Extent (%)	Method + time	References	Reliability
Na C18 (stearate)	18	62	CO2	Gerike (1984b)	1 / 2
Na C18 (stearate)	18	79	Sturm (28 day)	Unilever (unpublished data)	1
C20/22 fatty acid	22	89	OECD 301D BOC/COD	Henkel (unpublished data)	1
Tallow fatty acid, Ca-salt	16/18	89	OECD 301D BOC/COD	Henkel (unpublished data)	1
C12-18 fatty acid, K-salt	12-18	76	OECD 301D BOC/COD	Henkel (unpublished data)	1

Physical Chemical Properties (Appendix I)

The most important phys/chem properties for an environmental risk assessment are aqueous solubility, vapour pressure, and the octanol/water partition coefficient, or other relevant partition coefficients such as those between water and environmental matrices such as soil, sediment, or sewage sludge.

For fatty acid salts, all groups of homologues have sufficiently low predicted volatility (Appendix I) that the sensitivity of the risk assessment to the values of this parameter, other than to the order of magnitude, is negligible.

Critical Micelle Concentration (CMC)

As with all materials of surfactant nature, above a certain concentrations fatty acid salts will form micelles. CMC values are provided in Appendix Id. The low concentrations found in the environment can be considered to be well below the CMC values.

Solubility

There are few measured data for water solubility. The variation in measured solubility with chain length are not intuitive. For example the sodium salt of C16 fatty acid has a reported value of 2000mg/l (at 20^{o}C) whereas the equivalent salt of the C18 chain is reported as 50000mg/l (at 20^{o}C)(Stephen and Stephen, 1963). Intuitively these values are much higher than expected. As chain length increases one would expect solubility to decrease. For the value which exists for the sodium salt of C12 fatty acid a measured value of 22000mg/l (at 24^{o}C) is reported by the same authors. This is again not consistent with the value of 50000mg/l reported for C18 chain length.

It is possible that the effect of the Krafft point (T_K) and CMC values which explain some of these observations. The Krafft point is defined as the temperature at which the solubility of the surfactant is equal to the concentration of the micelle formulation (the CMC) and which is characterised by a rapid increase in solubility above this temperature. Krafft point values are tabulated in Appendix Id. For C12 chain length this effect would explain the high solubility observed, since the solubility was obtained at a temperature above the Krafft point of 21.5^{o}C. The high solubility values observed for the C16 and C18 chain lengths, however, cannot be explained in this way since the Krafft points for these chain lengths are 69^{o}C and 71^{o}C respectively. The presence of monovalent electrolytes such as NaCl will lower the Krafft point (Clint, 1992). It is possible that the presence an excess of such an electrolyte when tested (possibly through contamination of the tested soap with NaOH) resulted in a lowering of the Krafft point sufficiently to allow the large increase in observed solubility.

The presence of significant amounts of divalent ions (e.g. Mg and Ca) has a significant impact in raising the Krafft point. This has been observed for C12 alkyl sulphate as follows (Hato *et al*, 1979):

Krafft point [Na^{+}]: 9^{o}C
[Mg^{2+}]: 25^{o}C
[Ca^{2+}]: 50^{o}C

This effect will occurs for all anionic surfactants including fatty acid salts. Thus under environmentally relevant conditions of temperature and hardness these high solubilities will not be observed.

Data reported by other authors for the same chain lengths are also not consistent when measured at similar temperatures. Reported values for calcium salts:

- calcium salt of C16 solubilities of 28.1mg/l and 30 mg/l at 20^{o}C (Seidell, 1958):
- calcium salt of C18 oleate, solubilities of 66mg/l at 20^{o}C (Stephen and Stephen , 1963) and 400 mg/l at 25^{o}C (Seidell, 1958):

- calcium salt of C18 stearate, solubilities of 40.4mg/l at 20^{o}C (Stephen and Stephen , 1963) and 1.6mg/l at 27^{o}C (Seidell, 1958).

Laboratory measurements are also performed in conditions which are of lower hardness and higher temperature than found in the environment. Both these factors will lead to an increased solubility under laboratory conditions than in environmentally relevant conditions. Thus although the measured solubility values may be accurate, they can be considered accurate only for the conditions of hardness etc in which they were generated which are generally not consistent with environmental conditions.

Irani and Callis (1960) reported good correlation between solubility and the number of carbons in saturated fatty acid calcium salts according to the following relationship:

$-\log K_{sp} = -2.63 + 1.24C$ (Equation 1)

where C = number of carbon atoms

Ksp = solubility product = $(Ca^{++})(RCOO^{-})^{2}$

This equation allows the calculation of solubility at any specified calcium concentration and overcomes the issue of using solubility measurements generated in hardness conditions unrepresentative of the environment. Environmental concentrations of calcium are reported to vary between 0.3mmol to 3mmol (BKH review, 1994). If these two values are considered as extremes then the possible range of solubilities expected in the environment can be calculated in mg/l for each chain length when considering molarity of calcium and the relevant fatty acid. In soft water (calcium concentration = 0.3mmol) the solubility varies from 130mg/l for C10 to 0.0023mg/l for C18 and 8.5E-6mg/l for C22. For harder water (calcium concentration = 3mmol) solubility ranges from 41mg/l for C10 to 0.0007mg/l for C18 and 2.7E-6 for C22. Full values are reported in Appendix 1b.

Overall, the availability of solubility data for fatty acid salts is poor. Reliability of the available data is difficult to establish. For all solubility values, predicted values using Equation 1 are generated and used since the equation is based on measured data and also allows solubility to be predicted for environmentally realistic hardness. Solubility of the different homologues varies but is generally estimated to be low. The C18 and C22 homologues (particularly as calcium salts) will be incompletely soluble at concentrations used in ecotoxicity tests or those being present in the environment.

In the higher tier used in this risk assessment, measured values are used for removal from the aqueous phase in sewage treatment, hence, the partition coefficients based on Kow will be used only for sludge/water, soil/water and sediment/water partition. Realistic measured values for log Kow have not been reported for these materials. Therefore, all assessments based on

partitioning coefficients are based on calculated log Kow-values. The interfacial nature of surfactants give rise to a unique problem in the measurement of Kow. As such calculated values can be only considered as synonymous descriptors of log Kow and should be treated cautiously.

4.1.2. Removal

The default EUSES calculation with the SimpleTreat model has been used to estimate removal.

SimpleTreat calculation

At the first tier, a SimpleTreat calculation was used to determine removal of fatty acid salts in wastewater treatment, and their partitioning between air, water and sludge. The results are shown in Table 7. These calculations were based on the default rates assigned for readily biodegradable chemicals, and the estimated octanol-water partition coefficient of the different fatty acid salt homologues (Appendix I).

Table 7. WWTP Removal –SimpleTreat prediction. Sodium Salt

	Fraction of WWTP emission to:				Concentration on dry sewage sludge (mg/kg)
	Air	Surface water	Sludge	Degraded	
C10	7.36E-10	0.127	1.73E-4	0.873	0.0247
C12	2.27E-09	0.126	1.11E-3	0.872	5.38
C14	6.7E-09	0.126	7.13E-3	0.867	10.9
C16	5.71E-09	0.122	0.0437	0.835	98.1
C18	6.04E-08	0.106	0.185	0.709	763
C22	1.23E-11	0.0672	0.743	0.19	77.2

Due to the predominance of calcium salts in wastewater systems a more realistic removal of calcium salts was calculated using Simpletreat (Table 8) through the use of measured (where available) and predicted physical chemical parameters for the calcium salts in place of those for the sodium salts (Appendix 1a).

Table 8. WWTP Removal –SimpleTreat prediction-Calcium Salt

	Fraction of WWTP emission to:				Concentration on dry sewage sludge (mg/kg)
	Air	Surface water	Sludge	Degraded	
C10	2.17E-3	0.122	0.0306	0.845	4.37
C12	4.78E-3	0.11	0.138	0.747	668
C14	6.72E-3	0.0785	0.438	0.477	671
C16	7.2E-3	0.0647	0.703	0.225	1.58E3
C18	5.9E-3	0.0727	0.853	0.0688	3.52E3
C22	1.85E-4	0.0794	0.916	2.33E-3	95.1

Estimating the removal of fatty acid salts during the treatment process is complicated by many factors including the low solubility of the predominating calcium salts, precipitation onto suspended solids and sludge, excretion of solubilising compounds by bacteria. As with most readily biodegradable substances, the degradation values and overall removal calculated by Simpletreat in EUSES are considerable lower than reported values (Moreno *et al,* 1996; Matthijs *et al*, 1996) and can be considered unrealistically conservative. A more realistic removal of soaps may be considered using monitoring data.

Use of field monitoring data

Moreno *et al* (1996) monitored the fate of soap in a discharge point from a small town in southern Spain. Solids and aqueous samples were taken and analysed. Aqueous samples were collected in sewer and in treated effluent. Solid samples were collected from sewer, influent to and effluent from the STW and the anaerobic digestor.

Analysis of aqueous samples established concentrations <0.1ppm in all cases. This was interpreted as being due to low solubility. On suspended solids, however, soap concentrations were high and in some cases represented 15% of the total sample weight. Overall removal from the water stream during the treatment process was calculated as 99.7%.

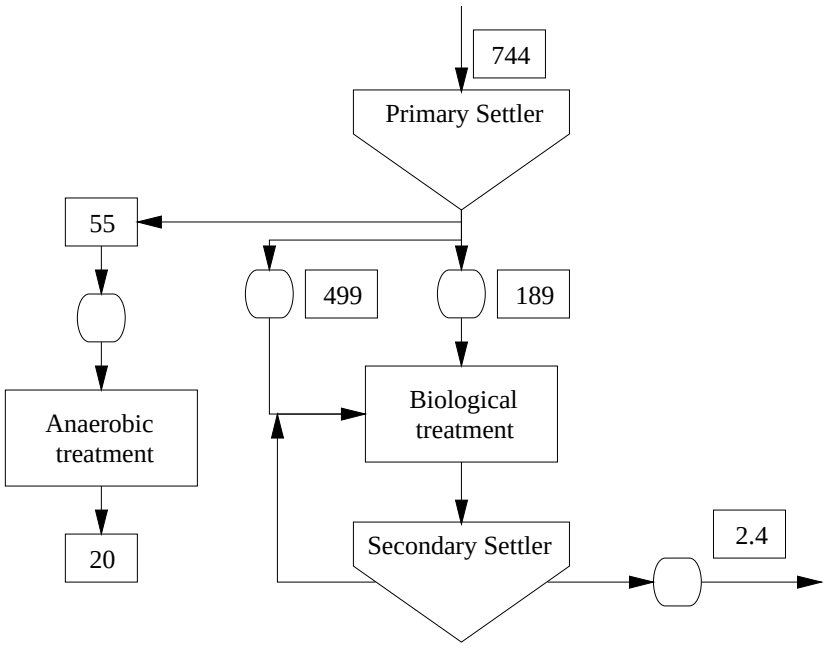
Results from analysis of samples taken from influent and effluent samples of the primary settler indicated 51% removal of suspended solids with 74% elimination of soap.

Results from analysis of samples taken from influent and effluent samples of the anaerobic digestor, indicated that the soap concentration dropped from an influent concentration of 36 g/kg dry solids to an effluent 12g/kg dry solids. This equates to a removal of soap resulting from anaerobic biodegradation of approximately 70%. This value may be considered an underestimate of removal when considering other anaerobic removal data (see ‘Degradation of anaerobic sludge digestion).

The overall mass balance measurements of soap in this study can be summarised as follows:

Fig 2. Overall mass balance for soap (kg/day) (Moreno *et al*, 1996)

The chain length distribution of the 'soap' being assessed in this study was measured at



various stages of the treatment process. The distribution in raw sewage immediately before and in the effluent after treatment is presented in Table 9. These values include removal to the anaerobic digestor and so cannot be used directly in the assessment.

Table 9. Chain length distribution in raw sewage and in treated water with calculated overall removal from water resulting from settling, aerobic and direction to the anaerobic digestor.

Chain length	Raw sewage*		Treated water*		Removal through all processes(%)
	%	Mass (kg/day)#	%	Mass (kg/day)#	
C12	6.3	47	7.0	0.17	99.6
C14	3.3	25	2.6	0.062	99.7
C16	27	200	28	0.67	99.7
C18(total)	63	470	62	1.5	99.7

* values to 2 significant figures.

values calculated from an influent value of 744kg/day and final effluent concentration of 2.4kg/day.

It is recognised that fatty acids derived from the lysis of other fatty materials will contribute to the overall measurement. Since fatty acids are formed during the sewage treatment process the reported and calculated percentage removal values for fatty acids can be considered very conservative estimate of elimination in sewage treatment plants.

Overall removal values from waste water indicated in the Moreno *et al* study (1996) (Table 9) are fairly consistent with other reported removal values for soap (Matthijs *et al*, 1996). Measured removal values for soap from the water stream during activated sludge treatment were in the range 97.7 – 99.6% (from 6 treatment plants) with an average value of 99.1%.

In the tier 2 assessment for calculation of more realistic removal and PEC values, removal values derived from measured data have been used in place of default Simpletreat values. These measured values are for soaps of unspecified chain length distribution. It is apparent from measured data that removal from the water stream is at a level of 99.1% or greater. A value of 99.1% has been used as a sensible estimate and has been applied in Simpletreat for an estimated removal from waste water of all chain lengths. Measured values do not account for differences in bioelimination (biodegradation, adsorption and precipitation) of the various chain lengths. In order to calculate the fraction of each chain length directed to sludge and the fraction degraded, the same split is assumed as calculated by Simpletreat for the calcium salts.

Table 10. WWTP Removal – Modified removal data

	Fraction of WWTP emission to:				Concentration on dry sewage sludge (mg/kg)
	Air	Surface water*	Sludge**	Degraded**	
C10	0	0.009	0.035	0.956	5
C12	0	0.009	0.154	0.837	744
C14	0	0.009	0.473	0.518	725
C16	0	0.009	0.749	0.242	1680
C18	0	0.009	0.916	0.075	3780
C22	0	0.009	0.988	0.003	103

(*) assuming 99.1% removal from waste water.

(**) assuming same split between ‘to sludge’ and ‘degraded’ as calculated by SimpleTreat

The value for fraction emission to sludge (Table 10) does not consider anaerobic degradation. Also it will not include fatty acid salts from other sources so comparison with measured sludge concentration values may be low. Therefore, this will be accounted for manually though modification of the calculated PECsoil.

Degradation in Anaerobic Sludge Digestion

Both Na and Ca salts of fatty acids (C10-C18) have been shown to exhibit significant removal through under anaerobic conditions (BKH, 1994). A number of studies have been performed for fatty acids and their salts (Tables 11 and 12).

Table 11. Anaerobic degradation of fatty acid salts

	Chain length	Test type	Test conc. (mg/l active matter)	Inoculum conc (g/l)	Test duration (days)	Result (%)	Comments	Reference
Na-Laurate	12	**Sim** - Semicontinuous	200	30 sludge	20 (retention time)	95	CH_4 measured, CO_2 calc	Mix-Spagl (1990)
Na-Laurate	12	**Screen**-ECETOC	100,200, 400		54	100 at all concs.	CH_4 and CO_2 + DIC	Varo Galvan et al (2002)
Na-Laurate	12	**Screen**-ECETOC	600		54	94	CH_4 and CO_2 + DIC	Varo Galvan et al (2002)
Na-Laurate	12	**Screen**-ECETOC	1000		54	0	CH_4 and CO_2 + DIC	Varo Galvan et al (2002)
Ca-Laurate	12	**Sim** - static	1000	30 sludge	5-6	90	CH_4 measured, CO_2 calc	Petzi (1989)
Na-palmitate	16	**Screen** - ECETOC	70	1-5 sludge	28	94	CH_4, CO_2 + DIC	Birch *et al* (1989)
Na-palm kernel	8-18	**Sim** - Semicontinuous	200	30 sludge	20 (retention time)	67	CH_4 measured, CO_2 calc	Petzi (1989)
Na-tallow	16/18	**Sim** - Semicontinuous	200	30 sludge	20 (retention time)	60	CH_4 measured, CO_2 calc	Petzi (1989)
Na-stearate	18	**Sim** - Semicontinuous	200	30 sludge	20 (retention time)	51	CH_4 measured, CO_2 calc	Mix-Spagl (1990)
Na-stearate	18	**Screen**-ECETOC	100,200, 400,600, 800		55	100 at all concs.	CH_4 and CO_2 + DIC	Varo Galvan et al (2002)
Ca-stearate	18	**Sim** - static	1000	30 sludge	10	85	CH_4 measured, CO_2 calc	Mix-Spagl (1990)
Na-oleate	18	**Sim** - Semicontinuous	200	30 sludge	20 (retention time)	69	CH_4 measured, CO_2 calc	Mix-Spagl (1990)
Na-behenate	22	**Sim** - Semicontinuous	200	30 sludge	20 (retention time)	14	CH_4 measured, CO_2 calc	Mix-Spagl (1990)
Ca-behenate	22	**Sim** - static	1000	30 sludge	10	90	CH_4 measured, CO_2 calc	Mix-Spagl (1990)

Sim: Simulation

*radiolabelled materials

Table 12. Anaerobic removal values for fatty acids

	Chain length	Test type	Test conc. (mg/l active matter)	Inoculum conc (g/l)	Test duration (days)	Result (%)	Comments	Reference
Dodecyl	12	Screen - ECETOC	20 as carbon	0.15 sludge	56	>75	Gas after acidification	Madsen et al. (1995)
	12	Screen - ECETOC	20 as carbon	4.4 freshwater swamp sediment	56	>75	Gas after acidification	Madsen et al. (1995)
	12	Screen - ECETOC	20 as carbon	0.9 organic marine sediment	96	>75	Gas after acidification	Madsen et al. (1995)
	12-18	Screen - ECETOC	18 as carbon	0.06/0.12 sludge	55	40-57	Gas after acidification	Madsen and Rasmussen (1994)
Na–C16 (U-^{14}C)*	16	**Sim** - static	-	45 sludge	28	97	$CH_4 + CO_2$	Steber and Wierich (1987)
Na–C16 (1-^{14}C)*	16	**Sim** - static	-	45 sludge	28	92	$CH_4 + CO_2$	Steber and Wierich (1987)
Na –C16 (16-^{14}C)*	16	**Sim** - static	-	45 sludge	28	97	$CH_4 + CO_2$	Steber and Wierich (1987)

The overwhelming part of the reported data from anaerobic biodegradability tests of fatty acids (C12-18) and their Na- and Ca-salts prove these substances to be very well accessible to ultimate biodegradation under anaerobic conditions. This was shown in the stringent ECETOC screening tests providing high levels of mineralisation (>75% $CH_4 + CO_2$) for C12-18 test substances. A few results with lower biodegradation levels can be explained by inhibition of biogas production at a very high test concentration (Table 11, Na-Laurate) or by an unusually low inoculum / test substance ratio (Table 12, C12/18). In addition to the screening test data, a vast majority of static and semi-static simulation studies also confirm the extensive ultimate anaerobic biodegradability (51-95% $CH_4 + CO_2$) under digester simulating conditions. A few test results contrast with this general conclusion, but this may rather be due to specific test conditions and does not pose basic biodegradability questions since the same chemical structure proved to be well biodegradable under similar test conditions (Table 11, Ca-/Na-behenate).

It should be noted the all these data refer to ultimate biodegradation based on the measurement of gas production, i.e. the final step of the anaerobic biodegradation process. The use of any of these data will lead to a conservative prediction of the removal of fatty acids and their salts in the digester as it does not take into account that the first steps of the biodegradation process (primary biodegradation) will have lead to the removal of the parent

compound.
Removal data for soaps from anaerobic digesters in practice were reported by Prats *et al* (1996). However, the values from 64-90 % removal (Table 13) from separate samples must be considered with caution since fatty acids will be formed during the digestion process from manifold chemicals from natural origin (e.g., lipids). Hence, the reported removal data will underestimate the real removal of fatty acids (C12-18) and their Na- and Ca-salts in digesters.
For a conservative estimate of the removal of fatty acids in anaerobic digesters, nevertheless, avoiding unrealistic worst case assumptions, the upper values of the removal ranges of the individual chain lengths reported by Prats *et al* (1996) were used (Table 13). For C10 and C22 where no specific biodegradation data was available, the same value as for C12 and C18, respectively, was taken.

The EUSES program does not include anaerobic degradation during sludge digestion. Instead, this process has been included in the HERA risk assessment by manual modification of the concentrations in agricultural soil calculated by EUSES.

Table 13. Values used for the estimation of removal during anaerobic digestion

	Removal (%)* reported in Prats *et al* (1996)	Removal extent (%) used in HERA assessment	Reliability
C10	-	90	2
C12	89.2 / 90.2	90	2
C14	82.5 / 77.8	82	2
C16	80.2 / 80.1	80	-
C16-1**	66.2 / 66.7	-	2
C18	89.5 / 81.0	89	2
C18-1**	70.6 / 71.5	-	-
C18-2**	64.4 / 74.1	-	-
C22	-	89	2

* Data from 2 sampling campaigns. **unsaturated fatty acids.

Degradation in Surface Water

Yoshimura *et. al.(*1984) reports 100% degradation in 20 days and degradation of various chain lengths at two starting concentrations: 7.3mg/l and 24.7mg/l. The following half lives were reported:

Table 14. Reported half lives by Yoshimura *et. al.* (1984).

Chain length	Start concentration 7.3mg/l	Start concentration 24.7mg/l
	t1/2 (hr)	t1/2 (hr)
C8	15	25
C10	24	19
C12	13	18
C14	33	47
C16	59	70
C18	62	70
C18:1	57	54
C18:2	33	42
Average	48	48

Differences in half lives between the two starting concentrations are fairly consistent between chain length. Environmental concentrations are considerably lower than the test concentrations used as part of this study. The lower of the two start concentrations is more relevant to realistic concentrations whilst still being conservative. For this reason the t1/2 values for 7.3mg/l start concentrations have been used in this assessment. These t1/2 values correspond to the degradation rates in surface water in Table 15.

Table 15. Degradation rates in surface waters.

Chain length	t1/2 as reported*	t1/2	In stream removal rate
	(hr)	(days)	(d^{-1})
C10	24	1	0.69
C12	13	0.54	1.3
C14	33	1.4	0.50
C16	59	1.2	0.58
C18	62	2.6	0.27
(C22)	-	-	0.27

*(Yoshimura *et. al*., 1984)

Worst case (C18 t1/2 of 62 hours) is assumed for all C18 chain lengths and also for C22 in the absence of other data.

Degradation in soils

Prats *et al*. (1996) report a study on the biodegradation of soaps in anaerobic digestors and in sludge amended soils. Two discrete separate rate constants were reported for the degradation of soaps in sludge amended soils from two clearly defined ‘zones’ of the degradation curve. The first of these was observed between day 0 to day 36 then a markedly slow rate from day 36 to the end of the study.

Table 16. Degradation in sludge amended soils

Zone	t1/2	k
	(d)	(d^{-1})
1	36	0.0191
2	161	0.0043

EUSES assumes that sludge is applied to agricultural land for a conservative period of 10 years and a percentage of the steady-state situation is calculated. Since the concentration of a material will be higher just after sludge application and lower at the end of the year due to removal processes, the concentration is averaged over a certain time period. For the ecosystem a period of 30 days after application is used in EUSES. For this assessment the initial rate constant of 0.0191 has been applied since the half life for this rate equates most closely to the 30 day time period.

4.1.3. Monitoring

Monitoring has been covered previously in section 4.1.2

4.1.4. PEC Calculations

EUSES was applied to calculate the regional and local exposure to fatty acid salts. Note that the resulting PECs (Predicted Environmental Concentrations) are based on the HERA tonnage (Table 3) and chain length distribution.

Local Predicted Environmental Concentrations (PECs)

The local predicted environmental concentrations (PECs), which include a regional PEC contribution, are reported below. The predicted environmental concentrations of total fatty acid salts (sum of all chain lengths) are given for information only. Note that the PECs for total fatty acid salts were not used in the risk characterisation, because a toxic units approach was used (See below).

Table 17. Local PECs for calcium salts (using tier 2 removal values)

local PEC	Water (mg/L)	Soil 30d (mg/kg)	Soil 30d * (mg/kg) (digested sludge)	Sediment (mg/kg)	STP (mg/L)
SimpleTreat					
C10	6.27E-5	5.58E-4	5.58E-5	5.12E-04	5.07E-04
C12	1.93E-3	0.833	0.0833	0.0777	0.0172
C14	6.93E-4	0.812	0.146	0.177	5.45E-03
C16	8.83E-4	1.88	0.376	1.45	7.99E-03
C18	1.15E-3	4.23	0.465	12.2	0.0147
C22	2.01E-6	0.115	0.0127	0.735	3.69E-04
Total	4.72E-03	7.87	1.08	14.6	0.0462

* taking into account chemical removal during anaerobic sludge digestion (Table 13)

Regional Environmental Concentrations

As explained in the HERA methodology document, use of production tonnage for HERA means that the losses to the region during formulation are automatically included when 100% of the production tonnage is released to the environment. The regional PECs in surface water are as follows:

Table 18. Regional PECs for calcium salts (using tier 2 removal values)

	Regional PEC water (mg/L)
C10	1.2 E-5
C12	2.2 E-4
C14	1.6 E-4
C16	1.9E-4
C18	5.4 E-4
C22	1.6 E-5
Total	1.3 E-3

Indirect Exposure to Humans

The predominance of calcium and magnesium ions in waste water leads to rapid formation and predominance of relatively insoluble Ca and Mg fatty acid salts (Swisher, 1987; Prats *et al*, 1996). Due to strong adsorption and poor water solubility of calcium salts, soaps are almost completely removed from raw sewage by normal sewage treatment plants. Any soap

remaining will be further removed by drinking water treatment processes. The amount of soap present in drinking water is likely to be insignificant. Therefore, it was felt unnecessary to calculate the indirect exposure of humans to soap via the environment.

4.2. Environmental Effects Assessment

4.2.1. Toxicity

A review of ecotoxicity data was based on NVZ Environmental data review of Soap (BKH, 1994) and on IUCLID and ECOTOX. In addition, a review of external literature was undertaken (Appendix II).

In general the availability of the data to cover all taxonomic groups at a specific chain length level is poor. Only one chronic aquatic toxicity value was found. This was for the toxicity of sodium laurate to *Danio rerio*. A number of the data are for undefined chain length distributions and have not been used for this reason although they have some limited value in supporting other data. The full data set is provided in Appendix III.

In addition all effect concentrations for chain lengths greater than C12 are above the estimated limit of solubility (Appendix 1c). Such data are not recommended for use in risk assessment (Robertson, 1995) since the observed effects are likely to be a result of such artifacts of the study as indirect physical impairment etc.. (ECETOC Technical Report No. 88). Concentrations should be based on water soluble fractions (i.e. bioavailable fractions). The use of these results in this assessment is discussed for each chain length.

Due to the absence of many complete datasets covering algae, invertebrates and fish, there is a need to fill data gaps:

1. Use of data generated for equivalent chain length fatty acids. Due to their increased lipophilicity compared to the equivalent chain length salt, data for fatty acids can be considered a conservative estimate for aquatic toxicity for the salts. This can be established when considering the data for fatty acids and fatty acid salts separately (Table 19). Data used in this comparison reflect the same chain length, test duration, endpoint and taxonomic group although species may vary.

2. Use of a QSAR to predict the toxicity of fatty acids. Equations have been derived by Onitsuka *et al* (1989) for fatty acids with *Oryzias latipes* and *Hyale plumulosa.*

Log LC50 (μM) = -0.51logKow + 3.01 (*O. latipes-freshwater*) (Equation 2)
(r=-0.996, SE=±0.49)

Log LC50 (μM) = -0.65logKow + 3.62 (*H. plumulosa*) (Equation 3)
(r=-0.999, SE=±0.22)

The study reports using measured logKow values using the OECD Guidelines for Testing of Chemicals. This is the shake-stir method. The interfacial nature of fatty acid salts makes accurate measurement of commercial materials very difficult. A more representative and consistent means of estimating a synonymous value for Kow is through a fragment approach similar to that used in EPIWIN. The use of such QSARS must be considered with caution: 1. The quality of the derived log Kow values must be considered with caution for reasons mentioned above. 2. The QSARs have been derived for these values, for a distinct range of log Kow values and for a distinct species. Their use outside this 'domain' has not been proven and, therefore, data derived using these equations should be carefully considered.

The use of reliable measured values is considered preferrable where possible even if the values are for fatty acids rather than the salts.

Table 19. Comparison of measured toxicity by chain length for fatty acids and their respective sodium salts

Chain length		Taxonomic group	Test duration (hr)	Result (mg/l)*	N	sd	Reference
C10	Fatty acid	FISH	96	20	1	-	5
	Fatty acid salt	FISH	96	54	1	-	5
C12	Fatty acid	FISH	96	8.6	1	-	8
	Fatty acid salt	FISH	96	11	1	-	5
C14	Fatty acid	No directly comparable data					
	Fatty acid salt						
C16	Fatty acid	FISH	96	12	1	-	13
	Fatty acid salt	FISH	96	150	1	-	5
C18 (oleate)	Fatty acid	FISH	96	4	8	71.5	6,7,8,9
	Fatty acid salt	FISH	96	217	1	-	5
>C18	Fatty acid	No directly comparable data					
	Fatty acid salt						

* geometric mean where n>1

Ranges in the data for any one chain length and any one taxonomic group can be considerable as indicated by the standard deviation for C18 in Table 19 (for fish). For example the data set used in calculating the geometric mean for C18 (oleate) cover a range of values from 0.1mg/l - 205mg/l.

Where recorded, most data for chain lengths C12-C18 have been generated using solvents. This makes interpretation of the data more difficult since the degree of bioavailability is unknown

Taxonomic sensitivity

Taxonomic sensitivity has been considered in the BKH review (1994). Collated data indicated that invertebrates (*Daphnia magna* and *Gammarus pulex*) were most sensitive showing a

geometric mean of EC50 = 24mg/l (s=3.9). This compared to the geometric means of the other taxonomic groups: algae EC50 = 88mg/l (s=2.4) and fish LC50 = 68mg/l (s=3.3). However, these datasets were a composite of values for both fatty acids and their salts. The conclusion drawn from this review must, therefore, be considered in parallel with other measured comparisons in this assessment.
Measured data for fatty acid salts covering all aquatic taxonomic group can only be found for C12, C18 and C16/18 chain lengths (Appendix III). These data confirm that algae are the least sensitive taxonomic group.

A number of data are available for 'soaps'. The chain length distribution of these tests is unknown and so the data have not been used specifically in this assessment. Test durations are also mostly unknown. However, if the geometric means are calculated for each taxonomic group (Table 20) a crude overview of sensitivity is in agreement with the BKH report, i.e. taxonomic sensitivity: algae<fish<invertebrates. However, when considering the standard deviations and min/max values for each group, differences in test methods etc. this overview must be considered with caution and with other data presented below (Table 21).

Table 20. Acute values for 'soap' with geometric means

	Species	EC/LC50 (mg/L)	Reference
Algae	*Chlorella vulgaris*	240	1
Geometric mean		**240 (-)**	
Aquatic Invertebrates	*Daphnia magna*	10	1
	Daphnia magna	42.3	7
Geometric mean (sd)		**20.6(22.8)**	
Fish	fish species	20	3
	Leuciscus idus melanotus	>118	10
	fish species	6.7	3
	Poecilia reticulata	423	1
	Oryzias latipes	1342	1
Geometric mean (sd)		**97.9* (562.3)**	

* taking 118mg/l as the value for >118mg/l

If specific chain lengths are considered there is no real evidence to support either invertebrates or fish being the most sensitive taxonomic group (Table 21).

Table 21. Comparison of means of toxicity values for invertebrate and fish taxonomic groups where data exist for both groups for specific chain lengths.

Chain length	Salt/ fatty acid	Taxonomic group	Geometric mean (mg/l)	Sd	N	Min	Max
C10	Fatty acid salt	INVERT	65	-	1	-	-
		FISH	54	-	1	-	-
C10	Fatty acid	INVERT	46	16	3	36	65
		FISH	44	55	2	20	95
C12	Fatty acid salt	INVERT	24	25	2	12	48
		FISH	11	-	1	-	-
C12	Fatty acid	INVERT	5.7	7.8	3	2	17
		FISH	23	39	2	8.6	63
C16/18	Fatty acid salt	INVERT	38	69	4	1.8	86
		FISH	49	19	5	26	79
C18	Fatty acid salt	INVERT	4.2	-	1	-	-
		FISH	100	72	4	44	217

For C12 chain length *D. magna* values are observed at 24 hour. At 48 hours increased toxicity would be expected. For the C10 salts and fatty acids there is no evidence to show whether invertebrates or fish are most sensitive. This is true also for the C12 fatty acid salts. For C16/18 chain length fish appear slightly more sensitive. However, when considering the standard deviation and min/max values the difference in values cannot be considered significant. Similarly for the C12 fatty acid data there are insufficient data to clearly establish which taxonomic group is most sensitive when considering the standard deviations and min/max values. For C18 the comparison is difficult since there is only one value for invertebrates.

Overall it is considered that there is insufficient evidence to establish whether invertebrates or fish are more sensitive to fatty acids and their salts and both should be considered equally when filling data gaps.

C10 Fatty Acid Salt

No salt data were found for algae for C10 chain length although one value was found for decanoic acid. A single value only was found for fish and invertebrates (96hour *Oryzias latipes* and 24hour *Daphnia magna* respectively). These values indicated similar toxicity to both species. However, the *D.magna* value was observed at 24 hour and would be expected to be less at 48 hours.

No terrestrial salt data for the fatty acid salt could be found. However, several data were found for decanoic acid. A 14 day study with *Lycopersicon esculentum* (tomato), reported values of >0.05M for leaf and stem injury and bud mortality (Tucker and Maw,1975). This value equates to a concentration of 8615mg/kg. One further study reported a 1hour ED95 of 195mg/kg decanoic acid to *Panagrellus redivius* (nematode) (Kwok *et. al.*,1992). From evidence of aquatic toxicity (Table 19), these data can be considered worst case for the

equivalent salt.

A number of studies were found for toxicity to various species of microorganisms for decanoic acid (Appendix III). Values range from a value of 43mg/l for the EC50 of the inhibition of the rate of duplication after 60 minute (*Bacillus subtilis*) (Freese *et.al*.,1971) to a value of 1016 for the 24 hour EC50 for the inhibition of acetoclastic methanogenic activity in Methanothrix (sp) (Koster and Cramer,1987). One value was found for the Potassium salt of C10 measuring EC50 using microcalorimetry. The reported EC50 value of 2377mg/l was for a range of anaerobic microorganisms (Beaubien *et. al*.,1987). The accuracy of this value has not been determined but does fit in with the overall trend that fatty acids are more toxic than the equivalent salt.
An overview of the data for the C10 fatty acid salt is provided below.

Table 22. Lowest acute ecotoxicological data for C10-Fatty acid salts

	Species	Test method	EC/LC50 (mg/L)	Reliability
Aquatic Invertebrates [16]	*D.magna*	24hr	65	2
Fish [5]	*O.latipes*	96hr days	54	2
Plants [19]	*L. esculentum*	(Fatty acid value) 48h leaf, stem injury, bud mort.	8615mg/kg	4
Terrestrial invertebrate [41]	*P. redivius*	(Fatty acid value) 1 hr immobility	ED95: 195mg/kg	4
Microorganisms [42]	*Anaerobic micro.*	Reduction in heat flux	2377	4

C12 Fatty Acid Salt

All aquatic taxonomic groups are covered by acute data for the C12 chain length. A summary of the lowest values for each taxonomic group is given below (Table 23). One value only was found for algae and fish (Huber, 1991; Onitsuka *et. al*., 1989). Algae is shown to be the least sensitive taxonomic group. Differences in sensitivity between fish and invertebrates are negligible although the *Daphnia magna* value is reported at 24 hours and not 48 hours.
One value only was found for microorganisms. A 0.5 hour EC50 value for *Photobacterium phosphoreum* indicated similar toxicity to that reported for fish and invertebrates.

One chronic value of C12 fatty acid salt (sodium) was found. The 28 day NOEC to *Danio rerio* was reported as 2mg/l (van Egmond *et al*, 1999). The value for the C12 is within the solubility for the chain length (Appendix 1b) and, therefore, can be considered representative of the true toxicity of the C12.

No terrestrial data were found for C12 fatty acids or their salts.

Table 23. Lowest acute ecotoxicological data for C12 fatty acid salt

	Species	Test method	EC/LC50 (mg/L)	Reliability
Algae [2]	*S. subspicatus*	72 hr growth inhibition	53	4
Aquatic Invertebrates [16]	*D. magna*	24 hr immobility	12	4
Fish [5]	*O. latipes*	96 hr mortality	11	2
Microorganisms [2]	*P. phosphoreum*	0.5 hr inhibition	8.8	4

Table 24. Chronic ecotoxicological data for C12 fatty acid salt

	Species	Test method	NOEC (mg/L)	Reliability
Fish [56]	*D. rerio*	28 day NOEC	2	1

C14 Fatty Acid Salt

Only limited information is available on the individual C14 homologues. Two fish studies were found which reported both LC50 and LC0 values. No values for the salts were found for either algae or aquatic invertebrates. Two values for aquatic toxicity with the fatty acid have been found for aquatic invertebrates (*Artemia salina* and *Hyale plumulosa*)(Curtis *et. al*.,1974; Onitsuka *et. al*., 1989). *A. salina* is a marine species and the relevance of the data to freshwater environments must be considered with caution. In addition it is impossible to determine a true value for the toxicity since the EC50 is reported as >27mg/l. This is particularly the case when toxicity can be observed to decrease as a result of increased salinity. This could be a result of increased amounts of non-ionised fatty acids in freshwater due to pH or due to the presence of higher concentrations of salt in marine environments leading to the less bioavailable fatty acids with divalent cations (Onitsuka *et. al.,* 1989). No toxicity was observed at saturation in the *H. plumulosa* study. Since no concentration range is reported for this study, further quantification of this value cannot be made.

The solubility of the calcium salt of C14 fatty acid is estimated as 0.57mg/l in soft water and 0.18mg/l in hard water (Appendix Ib). All observed toxicity measurements for this chain length are higher than these concentrations. The value of using measured data above the limit of solubility is questionable and not recommended for use in risk assessment (Robertson, 1995). Any observed toxicity observed above the solubility limits can be considered artifacts of the test system as discussed above.

All other data reported a value of 'greater than' with the exception of the 96hour LC50 = 118mg/l to *O. latipes* (Onitsuka *et al*, 1989). These values although not useable themselves indicate that toxicity will not manifest itself at the solubility limit and, therefore, will not manifest itself in the aquatic environment. The Onitsuka result is also artificially high when considering the solubility limit of the chain length (0.57mg/l in soft water). All values are considerably higher than the solubility limit and since the actual toxicity from tests results reported as 'greater than' cannot be determined from the published values.

One terrestrial toxicity value was found for the potassium salt to *Pseudosarcophaga affinis* (non soil dwelling arthropod). Values for 24hour and 7day indicated immobilisation at 1.7% and 3.1% respectively (House, 1967). Little information surrounds this value and so it has been treated with caution.

Only one value was found for the toxicity to an anaerobic microoganism (Methanothrix spp) for fatty acids (no fatty acid salt data were found). Two values were provided for EC50 and Minimum inhibitory concentration (MIC).

Table 25. Lowest acute ecotoxicological data for C14 fatty acid salt

	Species	Test method	EC/LC50 (mg/L)	Reliability
Aquatic Invertebrates [23]	*A.salina*	(Fatty acid value)16hr static EC50	(>)27	4
Fish [5]	O.latipes	96 hr mortality	118	2
Microorganisms [26]	*Methanothrix spp*	(Fatty acid value) 24hr growth inhibition	EC50:4.8mmol/l (1096 mg/l), MIC: 2.6mmol/l (594mg/l)	4

C16 and C18 Fatty Acid Salts

All reported values are considerably greater than the estimated solubility for C16 and C18 (solubilities of 0.037 mg/l and 0.0023 mg/l respectively in soft water and 0.012mg/l and 0.00074mg/l respectively in hard water)(Appendix Ib). Since the inherent toxicities of C16 and C18 are above their solubility limits, reported values can be expected to be higher than those reported for chain lengths where inherent toxicity is below the solubility limit (C10 and C12 chain lengths). The value of using measured data above the limit of solubility is questionable.

For the C16-18 commercial mixture, a good aquatic acute ecotox dataset is available (Appendix III). The ecotoxicity dataset for C16 individually is limited. Only one value for fish and one for microorganisms were found. One further value was found for C16 fatty acid to *Oncorhynchus kisuth.* No terrestrial data were found.

For C18 (oleate) salt homologues there are values for all taxonomic groups. However, the lowest value of 4.2mg/l for *D. magna* is of unknown quality and taken from a secondary reference only (BKH, 1994). Attempts to obtain the main reference have been unsuccessful. As such the quality of the value remains unsubstantiated and is considered unreliable. Other invertebrate data are for non standard 20 minute fertilisation endpoints with *S. purputatus* (Cherr, 1987) and as such have not been used in the derivation of a PNEC.

More reliable fish data have been found with known references. One fish LC50 value was found for C18 (stearate) salt (Onitsuka *et al*, 1989). However, the study utilised solvents to

achieve solubility. Several values were found for C18 (oleate) salt under standard test condition (96 hours) (Onitsuka *et al*, 1989; Henderson, 1959). Several other values were found for C18 (oleate) salt but these considered different end points such as biochemistry (Nakanishi *et al*, 1986). A number of test data were found for oleic, linolenic and linoleic acids (Menzie, 1979, Cherr, 1987). The majority of these demonstrated the increased toxicity of the fatty acid over the equivalent salt. However, since these observed values are above their solubility limits they should not be considered for PNEC derivation.

A number of LC50 values for oleic acid (as opposed to the salt) to *S. gairdneri* were derived from the same study with values ranging from 0.1-2.1mg/l (Menzie, 1979). This compares to an LC50 value of 205mg/l for *P. promelas* for the same test material (Matson *et al*, 1976). The values generated in the Menzie study, however, utilised solvents to aid exposure thus demonstrating the difficulties of making direct comparisons of such studies. Under environmentally realistic conditions such solvents will not be present to aid solubility and thus they are not representative of the toxicity which will be realised in the environment. The lowest value for the C18 salt which was derived from a standard test was for *P. promelas* with an LC50 = 44.1mg/l (Henderson, 1959). This test was performed in soft water. However, little information is provided in the paper to fully evaluate the result. The derivation of an aquatic PNEC for C18 chain length is discussed below.

No terrestrial data were found. One IC50 value was found for toxicity of C16 fatty acid salt to microorganisms in activated sludge.

In the absence of any invertebrate values for the C16 chain length, only fish data are available to evaluate a toxicity value. The lowest observed value of 12mg/l is for the fatty acid and not the salt. Where hardness has been reported – Onitsuka (1989) and Henkel (unpublished) (Appendix III), the studies have been performed in soft water. All results for the C16 chain length are above the limit of solubility and are thus artificially high and should not be used for use in the risk assessment. The derivation of an aquatic PNEC for C16 chain length is discussed below.

Table 26 . Lowest acute ecotoxicological data for C16 and C18 fatty acid salt

	Species	Test method	EC/LC50 (mg/L)	Reliability
C16-18 (1:2)				
Algae [2]	*S. subspicatus*	72 hr EC50	140	4
Aquatic Invertebrates [P&G]	*D. magna*	48 hr EC50	1.8	2
Fish [P&G]	*L. macrochirus*	96 hr LC50	26	2
C16				
Fish [5]	*O. latipes*	96 hr LC50	150	2
Fish [13]	*O. Kisuth*	96 hr LC50	12	2
Microorganisms [14]	*Activated sludge*	IC50	>2500	
C18 (oleate)				
Algae [2]	*S. subspicatus*	72 hr EC50	58	4
Aquatic invertebrates [2]	*D. magna*	24 hr EC50	4.2	4
Fish [50]	*P. promelas*	96 hrLC50	44.1	4
C18 (stearate) [5]	*O.latipes*	96 hr LC50	125	2

C22 Fatty Acid Salts

Only one value was found for this Chain length: 72hour EC50 to *Scenedesmus subspicatus* = 230mg/l (Huber, 1991). Counter intuitively this value is the least toxic value reported for algae of any chain length, explained by the reduction in solubility at higher chain lengths. The value is well above the solubility limit of this chain length (Appendix Ib). The derivation of an aquatic PNEC for C22 chain length is discussed below

Other trends in toxicity

In general for aliphatic chemicals, trends in toxicity are explicable in terms of physical/chemical properties. For the fatty acid salts as alkyl chain length increases toxicity increases, explaining the greater toxicity of C12 compared to C10. However, solubility decreases with increasing chain length. Although data used to determine PNEC values show a trend of increasing toxicity with increasing chain length, other data are not consistent with the expected trend. These values support the consideration that at the higher chainlengths, the concentration at which toxicity may be expected to be observed is outside the limits of solubility of these salts. In aquatic environments the low solubilities of these longer chain fatty acid salts is likely to result in toxicity less than expected from measurements of total concentration.

4.2.2. PNEC Calculations

Aquatic PNECs

For all fatty acid homologues, algae were found to be least sensitive taxonomic group. There is no clear evidence that either fish or invertebrates are most sensitive. There is no clear consistency between chain lengths e.g. for C10 96hr EC50 value to fish and the 24 hour EC50 value to *D. magna* are 54mg/l and 65mg/l respectively, whereas for C16/18, invertebrates are slightly more sensitive than fish. Neither of these comparisons are particularly significant when considering the standard deviation and min/max values (Table 21).

C10 and C12 Chain Lengths

For the PNEC calculation of salts where toxicities are within the limit of solubility (C10 and C12), where values for salts are available for a given homologue for either i) all taxonomic groups or ii) invertebrates and/or fish only, the lowest value has been used (unless there has been justification for not doing so). For C12 chain length where a reliable fish chronic NOEC value has been measured and where there is no observed difference in sensitivity between fish or invertebrate species, the NOEC value has been used to derive a more robust PNEC. The C10 and C12 chain lengths can be considered to be the only chain lengths which are sufficiently soluble to elicit a representative toxic response.

C14, C16, C18, C22 Chain Lengths

All studies for C14, C16, C18 and C22 chain lengths reported toxicity above the limit of estimated toxicity. Such observed toxicity cannot be considered to be a true representation of inherent toxicity but to be an artifact of the test system and attributable to other phenomena such as physical effects (ECETOC Technical Report No. 88). Such values are not recommended for use in risk assessment (Robertson, 1995). These chain lengths are not expected to exhibit any toxic effects in the aquatic environment due to their low solubilities. Of the two chain lengths (C10 and C12) which might be expected to exhibit aquatic toxicity, the toxicity value for C12 is the lowest (NOEC of 2mg/l). This can be expected to be the highest toxicity which would be expected to be observed for any chain length. In order to derive an aquatic PNEC for chain lengths of C14 and above, in the absence of other reliable data, a worst case approach is considered to be to use the toxicity value for the C12 chain length as an estimate for the aquatic toxicities for all these chain lengths.

Table 27. Toxicity values used for aquatic PNEC determination

	Species	Test method	Result (mg/L)	Remarks
C10	*O. latipes*	96 hour LC50	54	
C12	*D. rerio*	28 day NOEC	2	
C14	*D. rerio*	28 day NOEC	2	Value for C12 as the most toxic chain length where toxicity is oberved below the estimated solubility limit.
C16	*D. rerio*	28 day NOEC	2	Value for C12 as the most toxic chain length where toxicity is oberved below the estimated solubility limit.
C18	*D. rerio*	28 day NOEC	2	Value for C12 as the most toxic chain length where toxicity is oberved below the estimated solubility limit.
>C18 (C22)	*D. rerio*	28 day NOEC	2	Value for C12 as the most toxic chain length where toxicity is oberved below the estimated solubility limit.

PNEC determination and validation

For all fatty acid homologues, algae were generally found to be least sensitive taxonomic group. Depending on chain length invertebrates or fish generally were found to be the most sensitive. The aquatic PNEC for each chain length was determined by using an application factor (AF) of 1000 with the acute EC50 values obtained for the most sensitive taxonomic group or an AF of 100 for the chronic NOEC.

Table 28. Aquatic PNECs

Chain length	Aquatic PNEC (mg/L)
C10	0.054
C12	0.02
C14	0.02
C16	0.02
C18	0.02
C22	0.02

Solubility will strongly influence bioavailability of the fatty acids and salts and hence the realised toxicity in the environment. Values derived here are, therefore, considered to be conservative compared to the possible effects in the environment. This is particularly true for the higher chain lengths since the concentration of the bioavailable components of the fatty acids and their salts will be lower than that at which toxicity will be observed. However, the PNEC value derived in this assessment from a weighted average of chain lengths is comparable with the PNEC value of 0.027mg/l reported by Van de Plassche and Feijtel (1996). This value was for derived for a soap of unspecified chain length distribution and was based on acute toxicity data.

4.2.3 PNECs for other compartments

Sediment

Due to a general lack of data on sediment toxicity, the EUSES equilibrium partitioning method was used to derive the sediment PNECs from the corresponding aquatic PNECs. Only the C22 homologue has a log Kow > 5, and would normally qualify for an additional safety factor of 10 as specified in the EU TGD. The remaining homologues do not require this additional factor.

The results of the EUSES calculation are shown below:

Table 29. Sediment PNECs (calcium salts)

Chain length	Sediment PNEC (mg/kg)
C10	0.385
C12	0.711
C14	129
C16	53.9
C18	21.6
C22	0.879

Terrestrial

There are few data to allow full consideration of the toxicity of fatty acid salts to terrestrial organisms. The lowest reported value is 195 mg/L, for C10 *P. redivius* (nematode) although this is an EC95 value. The only data for toxicity to plants are also for the C10 homologue to *L. esculentum* (tomato) with a 48hour value for leaf and stem injury and bud mortality of 8615mg/kg, derived from application of the fatty acid directly to the plant as a mist of an aqueous solution. Both these values are for the fatty acid and are considered to be conservative.
It is felt that the available data are insufficient to justify their use in deriving a PNEC and so the EUSES equilibrium partitioning method has been used to estimate PNECs.

Table 30. Terrestrial PNECs (calcium salts)

Chain length	Terrestrial PNEC (mg/kg)
C10	0.329
C12	0.644
C14	118
C16	49.5
C18	19.8
C22	0.806

WWTP Micro-organisms

The lowest reported effect concentration is for the anaerobic microorganism Methanothrix spp. as an MIC of 594mg/l. However, the TGD indicates the use of an AF of 10 to generate a PNEC from EC50 values generated using test organisms such as *P.putida* or bacterial populations which are typical of the microorganisms present in the aerobic stage of a sewage treatment plant. A NOEC or EC10 from other test systems such as the respiration inhibition test (OECD 209) can also utilise an AF of 10. An EC50 from this test requires an AF of 100. A number of values exist for fatty acids for various studies. The only value which can be directly related to the criteria specified by the TGD is an EC10 value of 10000mg/l (conforming to OECD 209) for decanoic acid with *P. putida*. A number of growth inhibition studies have been carried out for other species. Of these the lowest EC50 value is reported as 1096mg/l for Methanothrix spp. Although not most representative of the data available this is the most conservative value and has been used for this reason. This value was applied to all chain lengths with an AF of 100 giving a PNEC of 11.0 mg/L.

Table 31. WWTP PNECs

Chain length	WWTP PNEC (mg/L)
All	11.0

Bioconcentation

There is no evidence of biocencentration in fish of the C12 fatty acid sodium salt (van Egmond *et al*, 1999). Usually metabolites are more polar than the parent material. In this case sodium laurate was observed to be extensively biotransformed probably to less polar metabolites as storage products and assimilated into growth. At the end of the 28 day exposure period an estimated bioconcentation factor of 255l/kg was derived.

With estimated logKow values of >3 for the higher chain lengths and with a measured BCF >100 for the C12 chain length, the revised TGD indicates that at least one long term study may be required for those chain lengths effected.

4.3. Environmental Risk Characterisation

In the tables below, the PEC/PNEC ratios (calculated with EUSES) are given, based on the different exposure scenarios (ie. different assumptions for removal), and PNEC derivations from acute data. The PEC/PNECs for the different chain lengths were added up to obtain a the overall PEC/PNEC for fatty acid salts(= toxic units approach).

4.3.1. Standard EUSES removal scenario

Table 32. Risk Characterisation Ratios (standard EUSES removal scenario for calcium salts)

PEC/PNEC	Water	Soil	Sediment	STP
C10	0.0164	0.0175	0.0188	7.84E-04
C12	1.33	1.38	1.50	0.0238
C14	0.309	0.502	0.344	5.40E-03
C16	0.599	1.36	0.680	6.51E-03
C18	0.451	0.262	0.509	0.0135
C22	8.35E-04	3.18E-04	9.44E-04	3.70E-04
Total	2.70	3.51	3.05	0.0503

Using SimpleTreat removal estimates and acute effects data, and not taking into account removal in anaerobic sludge digestion, leads to PEC/PNEC ratios >1 in the water, soil and sediment compartment.

4.3.2. Realistic removal scenario

The assessment can be refined by considering values generated through measured monitoring test data and by including chemical removal from sludge during anaerobic digestion, to model PEC values. Table 33 includes also the 1.25 scaling factor to account for the fact that only an estimated 80% of the HERA tonnage has been provided.

Table 33. Risk Characterisation Ratios (realistic removal scenario for calcium salts and 1.25 scaling factor)

PEC/PNEC	Water	Soil	Sediment	STP
C10	1.45E-03	2.12E-04	1.66E-03	5.76E-05
C12	0.121	0.162	0.137	1.95E-03
C14	0.0433	0.0441	0.0489	6.19E-04
C16	0.0552	0.0176	0.0623	9.08E-04
C18	0.0719	3.36E-03	0.0811	1.67E-03
C22	1.26E-04	2.66E-06	1.41E-04	4.19E-05
Total	0.293	0.227	0.331	5.25E-03

These analyses demonstrate that the fatty acid salts used in HERA products pose no environmental concerns. It must be considered that the assessment is conservative in many assumptions including the use of acute data for derivation of a PNEC for all chain lengths except C12. PEC/PNEC estimates can be expected to be considerably lower than this if further realism would be incorporated into the removal process and where more effects data become available.

4.3.3. Discussion and Conclusions

The absence of environmental concerns can be shown for current use levels fatty acid salts in HERA products. The Risk Characterisation ratios (PEC/PNEC) are below 1 for all chain lengths and environmental compartments. These ratios are considered conservative.

To demonstrate this, higher tier exposure data were used. Removal in WWTPs was determined from removal values determined through studies using measured influent and effluent fatty acid salt concentrations. Only one chronic value was found and used in the calculation of the PNEC for C12. The Predicted No Effect Concentrations were derived from measured values for the respective chain lengths for the C10 and C12 chain lengths where the toxicity values were within the limits of solubility.

Effects data for chain lengths above C12 were all observed above the limit of solubility for the respective chain lengths. As such these values were not considered acceptable to derive a reliable measure for the PNEC. Such observed values can be considered artifacts of the study rather than a true representation of the inherent toxicity of the material. In the absence of more reliable data, the aquatic toxicity value for the C12 chain length has been used for the derivation of PNECs for all chain lengths above C12. This is approach is considered conservative since the longer chain lengths (greater than C12) would not be expected to exhibit an aquatic toxic effect in the environment due to their low solubility (particularly of the calcium salt).

It is known that surfactants can be subject to high levels of in sewer removal (Matthijs *et al*, 1995) with removal values for some anionic surfactants (LAS, AS) being in excess of 50%. Although data for fatty acid salts are currently unavailable, with measured degradation in sewage treatment plants being at least as high as LAS, a high level of fatty acid salt removal can be expected in sewer systems.

The assessment for the aquatic compartment can be considered most reliable. The other compartments (terrestrial and sediment) are highly dependent on a number of assumptions. The quantification of the risks of these compartments are conservative but should be treated with some caution.

4.4. Addendum - "Total Tonnage" Scenario

4.4.1. Environmental risk characterisation

A recent value for the total fatty acid salts tonnage used in Europe has not been obtained. From literature it is estimated that the total soap useage in Europe is 701,000 tonnes/year (1988 CESIO statistics) (BKH report, 1994). An alternative more conservative exposure scenario was included in this risk assessment by assuming that this entire tonnage is disposed of down-the-drain.

The chain length distribution for the total fatty acid salts tonnage has been extrapolated from data available on 71306 tonnes of the 701000 tonnes total. Hence, the PEC/PNEC ratios for the HERA tonnage could be extrapolated to the overall tonnage by multiplying the PEC for each fatty acid salt chain length by an appropriate scaling factor, equal to the total production tonnage for this chain length divided by the HERA tonnage. This approach is valid from a mathematical point of view because of the linearity of the EUSES model.

Table 34. Risk Characterisation Ratios (advanced removal scenario)
for the total CESIO tonnage (assuming HERA chain length distribution)

PEC/PNEC	Water	Soil	Sediment	STP
C10	0.0143	2.08E-03	0.0163	5.66E-04
C12	1.19	1.59	1.34	0.0192
C14	0.426	0.433	0.481	6.09E-03
C16	0.543	0.173	0.612	8.93E-03
C18	0.707	0.0330	0.797	0.0164
C22	1.24E-03	2.61E-05	1.39E-03	4.12E-04
Total	2.88	2.23	3.25	0.0516

For the total fatty acid tonnage absence of concern for the environment could not be demonstrated. However, it must be emphasised that the approach involves a high level of conservatism due to the absence of data. The derivation of further reliable data is recommended.

5. Human Health Assessment

[CURRENTLY AS A SEPARATE DOCUMENT]

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7. Contributors to this Risk Assessment

This Risk-Assessment has been developed by Unilever. Additional input was provided by the experts of the HERA Environmental Task Force.

APPENDIX I Physical Chemical Properties – Sodium salts **(excluding solubility – see Appendix 1b)**

Chainlength : C10

Molecular weight	194.3	[g.mol-1]	
Melting point	203	[oC]	SRC
Boiling point	485	[oC]	SRC
Vapour pressure at 25 [oC]	1.1E-7	[Pa]	SRC
Octanol-water partition coefficient	0.2	[log10]	SRC

Chainlength : C12

Molecular weight	222.3	[g.mol-1]	
Melting point	217	[oC]	SRC
Boiling point	508	[oC]	SRC
Vapour pressure at 25 [oC]	2.0E-8	[Pa]	SRC
Octanol-water partition coefficient	1.2	[log10]	SRC

Chainlength : C14

Molecular weight	250.4	[g.mol-1]	
Melting point	227	[oC]	SRC
Boiling point	532	[oC]	SRC
Vapour pressure at 25 [oC]	3.9E-9	[Pa]	SRC
Octanol-water partition coefficient	2.2	[log10]	SRC

Chainlength : C16

Molecular weight	278.4	[g.mol-1]	
Melting point	238	[oC]	SRC
Boiling point	555	[oC]	SRC
Vapour pressure at 25 [oC]	7.3E-10	[Pa]	62
Octanol-water partition coefficient	3.2	[log10]	SRC

Chainlength : C18 (Stearate)

Molecular weight	306.4	[g.mol-1]	
Melting point	250	[oC]	MSDS
Boiling point	578.0	[oC]	SRC

Vapour pressure at 25 [oC]	1.3E-10	[Pa]	SRC
Octanol-water partition coefficient	4.1	[log10]	SRC

Chainlength : C18 (Oleate)

Molecular weight	304.5	[g.mol-1]	
Melting point	251	[oC]	MSDS
Boiling point	582	[oC]	SRC
Vapour pressure at 25 [oC]	1.7E-10	[Pa]	SRC
Octanol-water partition coefficient	3.9	[log10]	SRC

Chainlength : C22

Molecular weight	362.6	[g.mol-1]	
Melting point	271	[oC]	SRC
Boiling point	624	[oC]	SRC
Vapour pressure at 25 [oC]	4.5E-12	[Pa]	SRC
Octanol-water partition coefficient	6.1	[log10]	SRC

Data Sources:

SRC) SRC data are calculated by the EPIWIN programme, supplied by the Syracuse Research Corporation.

APPENDIX Ia Physical Chemical Properties – Calcium salts (excluding solubility – see Appendix 1b)

Chainlength : C10

Molecular weight	212.4	[g.mol-1]	
Melting point	68.4	[oC]	SRC
Boiling point	278	[oC]	SRC
Vapour pressure at 25 [oC]	0.32	[Pa]	SRC
Octanol-water partition coefficient	3.0	[log10]	SRC

Chainlength : C12

Molecular weight	240.4	[g.mol-1]	
Melting point	81.1	[oC]	SRC
Boiling point	308	[oC]	SRC
Vapour pressure at 25 [oC]	0.050	[Pa]	SRC
Octanol-water partition coefficient	3.9	[log10]	SRC

Chainlength : C14

Molecular weight	268.5	[g.mol-1]	
Melting point	98.9	[oC]	SRC
Boiling point	335	[oC]	SRC
Vapour pressure at 25 [oC]	7.7E-3	[Pa]	SRC
Octanol-water partition coefficient	4.9	[log10]	SRC

Chainlength : C16

Molecular weight	296.5	[g.mol-1]	
Melting point	116	[oC]	SRC
Boiling point	358	[oC]	SRC
Vapour pressure at 25 [oC]	1.4E-3	[Pa]	SRC
Octanol-water partition coefficient	5.9	[log10]	SRC

Chainlength : C18 (Stearate)

Molecular weight	324.6	[g.mol-1]	
Melting point	132	[oC]	SRC
Boiling point	382	[oC]	SRC
Vapour pressure at 25 [oC]	2.6E-4	[Pa]	SRC
Octanol-water partition coefficient	6.9	[log10]	SRC

Chainlength : C18 (Oleate)

Molecular weight	322.6	[g.mol-1]	
Melting point	132	[oC]	SRC
Boiling point	385	[oC]	SRC
Vapour pressure at 25 [oC]	2.2E-4	[Pa]	SRC
Octanol-water partition coefficient	6.7	[log10]	SRC

Chainlength : C22

Molecular weight	380.7	[g.mol-1]	
Melting point	158	[oC]	SRC
Boiling point	428	[oC]	SRC
Vapour pressure at 25 [oC]	9.9E-6	[Pa]	SRC
Octanol-water partition coefficient	8.8	[log10]	SRC

APPENDIX Ib solubility – Calcium salts

Chain length	Solubility (mg/l)		Reference
	Soft water (0.3mmol [Ca])	Hard water (3mmol [Ca])	
C10	130	41	Equation 1 (59)
C12	8.7	2.7	
C14	0.57	0.18	
C16	0.037	0.012	
C18	0.0023	0.00074	
C22	8.5E-06	2.7E-06	

APPENDIX Ic vapour pressure –fatty acids

Fatty acid chain length	Vapour pressure	units	Ref	
			secondary	primary
C10	4E-3	[Pa]	8	63
C12	2.1E-3	[Pa]	8	63
C14	4.2E-4	[Pa]	8	63
C16	2.6E-7	[Pa]	8	64
C18	9.6E-5	[Pa]	8	64

APPENDIX Id- CMC and Krafft points – sodium salts

Chain length	CMC (g/l)	Ref	Krafft point TK(^{o}C)	Ref
C12	5.8	66	21.5	65
C14	2.6	8	39	65
C16	1.1	8	69	8
C18	0.56	66	71	65

Appendix II. Literature Search

Introduction

The following search strategy was used for an external literature search. This search was used alongside both internal searches and a data request spreadsheets sent to all relevant producer and formulator companies.

Chemicals used for data searching in HERA Fatty acid salts assessment:

Chemical Name	Synonyms	Carbon Chain Length	CAS Number
Decanoic acid, sodium salt**	Capric acid, sodium salt; sodium caprate	C10	1002-62-6
Dodecanoic acid*	Lauric acid	C12	143-07-7
Dodecanoic acid, sodium salt*	Lauric acid, sodium salt; Sodium laurate	C12	629-25-4
Tetradecanoic acid***	Myristic acid	C14	544-63-8
Tetradecanoic acid, sodium salt**	Myristic acid, sodium salt; Sodium myristate	C14	822-12-8
Hexadecanoic acid***	Palmitic acid	C16	57-10-3
Hexadecanoic acid, sodium salt**	Palmitic acid, sodium salt; Sodium palmitate	C16	408-35-5
Octadecanoic acid***	Stearic acid	C18	57-11-4
Octadecanoic acid, sodium salt*	Stearic acid, sodium salt; Sodium stearate	C18	822-16-2
9-Octadecanoic acid, potassium salt*	Oleic acid, potassium salt; Potassium oleate	C18	143-18-0
9-Octadecanoic acid, sodium salt*	Oleic acid, sodium salt; Sodium oleate	C18	143-19-1
9-Octadecanoic acid (Z-) cmpd with 2-aminoethanol (1:1)*	Monoethanolamine oleate	C20	2272-11-9
Fatty acids, C10-14***	--	C10-14	90990-09-3
Fatty acids, C12-18*	--	C12-18	67701-01-3
Fatty acids, C16-18*	--	C16-18	67701-03-5
Fatty acids, C14-18 and C16-18 unsat.d*	--	C16-18	67701-06-8
Chemical Name	Synonyms	Carbon Chain Length	CAS Number
Fatty acids, C14-22*	--	C14-22	68424-37-3
Fatty acids, C8-18 and C16-18 unsatd. Sodium salts*	--	C8-18	85408-69-1
Fatty acids, rape oil*	--	C22	85711-54-2

Note:-

*These chemicals are those which are used by the formulator companies (as provided to us by AISE)

**These chemicals are salts of fatty acids within the carbon chain lengths of interest to us, that may be useful for read across.

***The chemicals are fatty acids within the carbon chain length of interest to us and may be useful for read across data.

Keywords used in Search Strategy Environmental

ENVIRONMENTAL

Ecotoxicity/ Ecotoxicology/ Ecotoxicological/ Eco toxicity/ Eco toxicology/ Eco toxicological

Effects data/Acute toxicity /aquatic and/or

LC50 / EC50 / IC50 with each of the following:

Algae, Invertebrate, Daphnia, Fish, Acute toxicity / terrestrial and/or

LC50 / EC50 / IC50 with each of the following:

Microorganism, Earthworm, Plant, Chronic toxicity / aquatic and/or

NOEC (No Observed Effect Concentration) with each of the following:

Algae, Invertebrate, Daphnia, Fish

Chronic toxicity / terrestrial and/or

NOEC (No Observed Effect Concentration) with each of the following:

Microorganism, Earthworm, Plant, Mesocosm

Bioaccumulation, Fate, Biodegradation / ready / inherent / SCAS (Semi Continuous Activated Sludge) / Zahn Wellens / MITI

Removal, Degradation, Rate constants, Aerobic, Anaerobic, Abiotic

PHYSICAL – CHEMICAL

MW / Molecular Weight/ Mp / melting point / Bp / boiling point / Vp / vapour pressure

Log P / log Kow / octanol water partition coefficient / Water solubility/ Koc – partition coefficient organic carbon water

Databases searched search sites for environmental effects and fate data:

- IUCLID CD-ROM
- http://www.epa.gov/ecotox/
- http://esc.syrres.com/efdb/TSCATS.htm
- http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB
- http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?TOXLINE.htm
- http://esc.syrres.com/efdb.htm
- http://www.msdssolutions.com/en/
- http://library.dialog.com/bluesheets/html/bl0307.html
- http://physchem.ox.ac.uk/MSDS/#MSDS

Other search sites:

- BIOSIS previews (1969-present)
- Registry of Toxic Effects of Chemical Substances.

Fatty Acids used at starting materials in the production of fatty acids salts considered in the HERA assessment

Fatty Acids			
143-07-7	Dodecanoic acid	Lauric acid	12
90990-09-3	Fatty acids, C10-14	-	10-14
67701-01-3	Fatty acids, C12-18	-	12-18
67701-03-5	Fatty acids, C16-18	-	16-18
67701-06-8	Fatty acids, C14-18 and C16-18 unsatd	-	14-18
85711-54-2	Fatty acids, rape oil	-	18-22
68424-37-3	Fatty acids C14-C22	-	14-22

Appendix III – Data (fatty acids and salts)

Effects - Aquatic

C10

Test Substance		Species	Test Method/ Endpoint	Duration (h)	Concentration (mg/l)	Secondary ref	Primary ref
Decanoic acid	ALGAE	Nitzschia closterium (marine diatom)	cell growth / EC50	72	0.3	3	34
Decanoic acid sodium salt	INVERT	Daphnia magna	Intoxication / EC50	24	65	2	16
Decanoic acid	INVERT	Artemia salina	EC50	16	36	3	23
Decanoic acid	INVERT	Daphnia magna	EC50	24	65	3	16
Decanoic acid	INVERT	Hyale plumulosa	EC50	48	41	3	5
Sodium caprate	FISH	Oryzias latipes	LC50	96	54	3	5
Decanoic acid	FISH	Leuciscus idus	DIN 38412 / LC50	48	95	3	Henkel unpublished data
Decanoic acid	FISH	Leuciscus idus	DIN 38412 / LC0	48	30	3	Henkel unpublished data
Decanoic acid	FISH	Leuciscus idus	DIN 38412 / LC100	48	300	3	Henkel unpublished data
Decanoic acid	FISH	Oryzias latipes	LC50	96	20	3	5
Decanoic acid	MICRO	Photobacterium phosphoreum	Microtox	25min	47.1-57.5 microg/l	3	35
Decanoic acid	MICRO	Bifidobacterium bifido	Growth inhibition / EC50		50mmol/l	3	36
Decanoic acid	MICRO	Bacillus subtilis	Inhibition of rate of duplication / EC50	60min	43.1	3	37
Decanoic acid	MICRO	Pseudomonas putida	DIN 38412, Teil 27 (Bacterial Oxygen consumption test) conforms to OECD 209 / EC10	30min	10000	3	Henkel unpublished data
Decanoic acid	MICRO	Bacillus megaterium	MIC	24	172.26	3	38
Decanoic acid	MICRO	Methanothrix (sp)	Inhibiition of acetoclastic methanogenic activity / EC50	24	1016	3	26
Decanoic acid	MICRO	Methanothrix (sp)	Inhibiition of acetoclastic methanogenic activity / MIC	24	448	3	26
Decanoic acid	MICRO	Streptococcus mutans	Visual determination of bacterial growth / MIC	48	>100	3	39
Decanoic acid	MICRO	Vibrio parahaemolyticus	arithmetic difference between %	9	60	3	40

			transmittance (620nm) of control and test cultures / MIC				
Decanoic acid Potassium salt	MICRO	Anerobic microorganisms	Reduction in heat flux (using flow microcalorimeter) / EC50		2377	3	42

C12

Test Substance		Species	Test Method/ Endpoint	Duration (h)	Concentration (mg/l)	Secondary ref	Primary ref
Na laurate	ALGAE	Scenedesmus subspicatus	Inhibition / EC50	72	53	1	2
Lauric acid	INVERT	Daphnia magna	Mortality / EC50	48	2	1	9
Lauric acid	INVERT	Daphnia magna		48	5.4	1	9
Natrium-laurate		Daphnia magna	Mortality / EC50		32	1	11
Na -laurate	INVERT	Daphnia magna	Immobility / EC50	24	48	1	2
Dodecanoic acid	INVERT	Daphnia magna	Immobility / EC50	48	16.9	2	15
Dodecanoic acid sodium salt	INVERT	Daphnia magna	Intoxication / EC50	24	12	2	16
C1297 lauric acid	FISH	Lepomis macrochirus	Mortality / EC50	96	63.3	1	9
Natrium – laurate	FISH	Oryzias latipes	Mortality / EC50	96	11	1	5
Sodium laurate	FISH	Danio rerio	NOEC	28 day	2		56
Na laurate	MICRO	Photobacterium phosphoreum	Inhibition / EC50	0.5	8.8	1	2
Na Talgseife	MICRO	Photobacterium phosphoreum	Inhibition / EC50	0.5	250	1	2

C14

Test Substance		Species	Test Method/ Endpoint	Duration (h)	Concentration (mg/l)	Secondary ref	Primary ref
	ALGAE						
Myristic acid	INVERT	Artemia salina	EC50	16	>27	3	23
Myristic acid	INVERT	Hyale plumosa (Gammarus)		48	no tox at saturation	3	5
Natrium – myristate	FISH	Oryzias latipes	Mortality / EC50	96	118	1	5
Myristic acid	FISH	Leuciscus idus	Mortality / LC0	48	>10000	3	20
Myristic acid (and salt)	FISH	Oncorhynchus kisuth	Mortality / LC0	96	>20	3	24
Myristic acid	MICRO	Methanothrix spp	Growth inhibition / EC50/MIC (minimum inhibitory concentration)	24	EC50:4.8mmol/l (1096 mg/l), MIC: 2.6mmol/l (594mg/l)	3	26

C12/14

Test Substance	Species	Test Method/	Duration	Concentration	Secondary	Primary ref

			Endpoint		(h)	(mg/l)	ref	
(coco)C8-1	FISH	Salmo gairdneri	Mortality EC50	/	96	42	1	8
Coco fatty acid	FISH	Trout	Mortality LC50	/	96	42 (approx)		Unilever

C16

Test Substance		Species	Test Method/ Endpoint		Duration (h)	Concentration (mg/l)	Secondary ref	Primary ref
C16	ALGAE							
Palmitoleic acid	FISH	Oncorhynchus kisuth	Mortality EC50	/		12	1	4
Natrium – palmitate		Oryzias latipes	Mortality EC50	/	2.5	150	1	5
Palmitic acid	FISH	Oncorhynchus kisuth	Mortality EC50	/	96	12		13
Hexadecanoic acid sodiumsalt	FISH	Oryzias latipes	Mortality LC50	/	96	150	3	Henkel
Sodium palmitate	MICRO	activated sludge inhibition	Inhibition LC50	/	96	>2500		14

C18

Test Substance		Species	Test Method/ Endpoint		Duration (h)	Concentration (mg/l)	Secondary ref	Primary ref
Na-Oleate	ALGAE	Scenedesmus subspicatus	Inhibition EC50	/	72	58	1	2
Na-Oleate	INVERT	Daphnia magna	Mobility EC50	/	24	4.2	1	2
Linoleic acid	INVERT	Strongylocentrotus purputatus	Fertilisation EC50	/	20min	0.3	1	12
Linolenic acid	INVERT	Strongylocentrotus purputatus	Fertilisation EC50	/	20min	1.1	1	12
Oleic acid	FISH	Salmo gairdneri	Mortality EC50	/	96	0.6	1	7
Oleic acid	FISH	Salmo gairdneri	Mortality EC50	/	96	0.1	1	7
Oleic acid	FISH	Salmo gairdneri	Mortality EC50	/	96	0.5	1	7
Oleic acid	FISH	Salmo gairdneri	Mortality EC50	/	96	2.1	1	7
Oleic acid	FISH	Lepomis macrochirus	Mortality EC50	/	96	66.6	1	12
Oleic acid	FISH	Oncorhynchus kisuth	Mortality EC50	/	33	12	1	4
Natrium – stearate (sateurated)	FISH	Oryzias latipes	Mortality EC50	/	96	125	1	5
Natrium - oleate (unsatuarted)	FISH	Oryzias latipes	Mortality EC50	/	96	217	1	5
Oleic acid	FISH	Pimphales promelas	Mortality EC50	/	96	205	1	6
Oleic acid	FISH	Salmo gairdneri	Mortality EC50	/	96	1.4	1	7
Octadecanoic acid, sodium salt	FISH	Cyprinus carpio	Biochemistry		4	6	2	17
Octadecanoic	FISH	Cyprinus carpio	Physiology		2month	10	2	18

acid, sodium salt							
Oleic acid	FISH	Trout	Mortality / LC50	96	>56		Unilever
Octadecanoic acid, sodium salt	FISH	Pimphales promelas	Mortality / LC50	96	100	3	50
Octadecanoic acid, sodium salt	FISH	Pimphales promelas	Mortality / LC50	96	44.1	3	50
Sodium Stearate sodium salt	FISH	Cyprinus carpio	Biochemistry / Change in physiochemical process, glycogen uptake, choleterol levels	0.17days	6.0mg/l	6	17

C16/C18

Test Substance		Species	Test Method/ Endpoint	Duration (h)	Concentration (mg/l)	Secondary ref	Primary ref
Sodium talgseife (tallow)	ALGAE	Scenedesmus subspicatus	Inhibition / EC50	72	190	1	2
Na-palmkernseife	ALGAE	Scenedesmus subspicatus	Inhibition / EC50	72	140	1	2
C16-18 fatty acid sodium salts	ALGAE	Scenedesmus subspicatus	Biomass DIN 38412, Teil 9 / EC50	72	190	3	Henkel unpublished data
C16/18 (Hardened Tallow/coco)	INVERT	Gammarus pulex	Mortality / EC50	72	86	1	8
Hardened tallow soap	INVERT	Gammarus pulex	Mortality / EC50	72	88	1	8
Hardened tallow soap	INVERT	Gammarus pulex	Mortality / EC50	72	160	1	8
C16-18 fatty acid sodium salts	INVERT	Daphnia magna	Biomass DIN 38412, Teil 11 / EC50	24	40	3	Henkel unpublished data
Tallow	INVERT	Daphnia magna	Immobility / EC50	48	1.8		P&G
C16/18 sodium salts	FISH	Brachydanio rerio	Mortality / LC50	96	54		Henkel unpublished data
Tallow	FISH	Lepomis macrochirus	Mortality / LC50	96	26		P&G
C16-18/C12-14 (80/20) fatty acid sodium salts	FISH	Salmo gairdneri	Mortality / LC50	96	79-118	3	Henkel unpublished data
C16-18/C12-14 (80/20) fatty acid sodium salts	FISH	Brachydanio rerio	Mortality / LC50	96	45.9	3	Henkel unpublished data
C16-18/C12-14 (80/20)	FISH	Brachydanio rerio	Mortality / LC50	96	54	3	Henkel unpublished

fatty acid sodium salts							data

SOAP (Mixed chain length distribution)

Test Substance		Species	Test Method/ Endpoint	Duration (h)	Concentration (mg/l)	Secondary ref	Primary ref
Na-behenate (C22)	ALGAE	Scenedesmus subspicatus	Inhibition / EC50	72	230	1	2
Hauslltaseife	ALGAE	Chlorella vulgaris	EC50		240	1	1
Soap	INVERT	Daphnia magna	Mobility / EC50		10	1	7
Hauslltaseife	INVERT	Daphnia magna	EC50		42.3	1	1
SOAP	FISH	fish species	Mortality / EC50		20	1	3
Soap:fatty acid, Na		Leuciscus idus melanotus	Mortality / EC50	48	>118	1	10
Soap	FISH	fish species	Mortality / EC50		6.7	1	3
Hausaltseife	FISH	Poecilia reticulata	EC50		423	1	1
Hausaltseife	FISH	Oryzias latipes	EC50		1342	1	1
Hausaltseife	MICRO	Microcystis aerugino	EC50		24	1	1
Hausaltseife	MICRO	Pseudomonas fluorescencus			134	1	1

Effects – Terrestrial

C10

Test Substance		Species	Test Method/ Endpoint	Duration	Concentration (mg/l)	Secondary ref	Primary ref
Decanoic acid	PLANT	Lycopersicon esculentum (tomato)	Leaf injury	14 days	>0.05M	2	19
Decanoic acid	PLANT	Lycopersicon esculentum (tomato)	Stem injury	14 days	>0.05M	2	19
Decanoic acid	PLANT	Lycopersicon esculentum (tomato)	Bud mortality	14 days	>0.05M	2	19
Decanoic acid	INVERT	Panagrellus redivius (nematode)	Immobility / EC95	1hr	195	3	41

C14

Test Substance		Species	Test Method/ Endpoint	Duration	Concentration (mg/l)	Secondary ref	Primary ref
myristic acid (and Potassium salt)	INVERT	Pseudosarcophaga affinis (non soil dwelling arthropod)	acute toxicity	24hour and 7day	1.7% after 24h. 3.1% after 7d	3	25

Fate

C10

Test Substance	Test Method/ Endpoint	Duration	Result	Secondary ref	Primary ref

Decanoic acid	Directive 84/449/EEC C6 Biotic degradation - closed bottle. 2mg/l. STW effluent. By analogy from octanoic acid	30 days	100-71%	3	Henkel unpublished
Decanoic acid	Warburg respirometer test. Oxygen uptake. 500mg/l. Based on data for structural similar substances. Waste water treatment: % of ThOD	1 day	23.40%	3	33
Decanoic acid	Adapted predom domestic sewage. 21+/-3oC. Adapted microbial culture (from domestic sewage)	5 days	60.90%	3	32

C12

Test Substance	Test Method/ Endpoint	Duration	Result	Secondary ref	Primary ref
C12 fatty acid Na laureate	OECD 301D, BOC/COD		87%		Henkel
	BOD5	5days	58%	1	

C14

Test Substance	Test Method/ Endpoint	Duration	Result	Secondary ref	Primary ref
Myristic acid	OECD 301D ready biodegradability testclosed bottle / aerobic Domestic sewage, STW effluent, 2mg/l test substance	30 days	85% Readily biodegradable	3	20
Myristic acid	EMPA 50mg/l related to test substance, Data extracted from graph, activated sludge, use of GC for monitoring substance.	15 days	99%	3	21
Myristic acid	Anaerobic sludge6 6.8mg/l related to Test Substance.Evolution of CO2/CH4 and disssolved inorganic carbon in % of initial organic C of test substance.	69 days	77.3 +/- 17.3%	3	20
Myristic acid	Anaerobic sludge 14C distribution - 56.6% as 14C4, 39.9% as 14CO2, 4.8% remained in sludge. 35oC, digester sludge from municipal seage treatment plant 14C evolution (CH4 + CO2)	28 days	96.5%	3	21

C12/C14

Test Substance	Test Method/ Endpoint	Duration	Result	Secondary ref	Primary ref
coco acid	Sturm		84% CO2 titration Pass		Unilever

C16

Test Substance	Test Method/ Endpoint	Duration	Result	Secondary ref	Primary ref

palmitic acid	AS	6hr	0.3% ThOD	30	33
	AS	12hr	1.0% ThOD	30	33
	AS	24hr	2.5% ThOD	30	33
Natrium - palmitate					

C18 / C16/18

Test Substance	Test Method/ Endpoint	Duration	Result	Secondary ref	Primary ref
Oleic acid	Sturm		82% CO2 titration Pass		Unilever
Sodium stearate	Sturm		79% Co2 titration (Pass)		Unilever
Sodium stearate	BOD5	5day	48%	1	
Sodium stearate	BOD5	5day	53%	1	
Sodium stearate	BOD5	5day	60%	1	
Sodium oleate	BOD5	5day	48%	1	
Sodium oleate	BOD5	5day	64%	1	
Na stearate	CO2	28day	62%	1	50
Octadecanoic acid	OECD 301D, BOC/COD		62%		Henkel
C16-18, C18-unsaturated fatty acid	OECD 301D, BOC/COD		62%		Henkel
Tallow fatty acid, Ca-salt	OECD 301D, BOC/COD		89%		Henkel

C12-18 / C22

Test Substance	Test Method/ Endpoint	Duration	Result	Secondary ref	Primary ref
C12/18 potassium salts	OECD 301D	28day	76		Henkel (unpublisted data)
			Readily biodegradable. Complete degradation in aerobic conditions.	3	51
C20/22 fatty acid	OECD 301D, BOC/COD		89%		Henkel (unpublished data)
C12-18 potassium salts	Closed bottle Directive 84/449/EEC, C6 Biotic degradation - closed bottle test.	30day	89% 2mg/l. 85-62% degradation after 30 days	3	Henkel (unpublisted data)