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

Alcohol Ethoxysulphates (AES)
Environmental Risk Assessment

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2 Executive Summary

Alcohol ethoxysulphates (AES) are a widely used class of anionic surfactants. They are used in household cleaning products, personal care products, institutional cleaners and industrial cleaning processes, and as industrial process aids in emulsion polymerisation and as additives during plastics and paint production. Uses in household cleaning products, the scope of HERA, include laundry detergents, hand dishwashing liquids, and various hard surface cleaners.

The total volume of AES surfactants used in Europe is estimated to be 276,000 tonnes/year on an active matter basis of which 108,000 tonnes/year is used in household detergents and cleaning products (CESIO, 2000).

A large environmental data set is available for AES. On the environmental fate side, this includes standard biodegradation studies, advanced simulation studies of removal in treatment systems, and field monitoring data. On the environmental effects side, acute as well as chronic single-species data are available, as well as advanced studies in micro- and mesocosm systems.

To determine the Predicted Environmental Concentration (PEC), chemical removal in wastewater treatment plants was determined from advanced simulation test data. Monitoring studies on sewage treatment plant effluents indicate that the exposure estimates in this assessment are likely to be conservative.

The Predicted No-Effect Concentration (PNEC) was based on chronic ecotoxicity data. Mesocosm studies suggest that the effects assessment based on laboratory studies is also conservative.

By means of these higher tier exposure and effects data, it could be shown that the use of AES in HERA applications (household detergents and cleaning products) results in risk characterization ratios less than one, indicating no concern, for all environmental compartments.

An additional exposure scenario was included in this risk assessment, by assuming the entire AES tonnage used in Europe is disposed of down the drain. Using the same exposure and effects assessment approach, the absence of environmental concerns can also be demonstrated for this total tonnage.

3 Substance Characterisation

Alcohol ethoxysulphates (AES) are a widely used class of anionic surfactants. They are used in household cleaning products, personal care products including toothpaste and shampoos, hand and other personal cleaning products, institutional cleaners and industrial cleaning processes, and as industrial process aids in emulsion polymerisation and as additives during plastics and paint production. Uses in household cleaning products, relevant to the HERA program of risk assessments, include laundry detergents, hand dishwashing liquids, and various hard surface cleaners.

3.1 CAS No and Grouping information

There are several CAS Numbers describing AES. A comprehensive list is presented in Annex 1 of this document. Although clearly important from a Regulatory perspective, this assessment is not based on CAS Nos., but on the environmental fate and effects of the components of the products.

3.2 Chemical structure and composition

The alcohol ethoxysulphate family is defined for HERA purposes to encompass commercial grades of linear-type primary alcohol ethoxysulphates containing AES components of basic structure $C_nH_{2n}(C_2H_4O)_mSO_4X$,) where n=12-18 and m = 0-8 and X = sodium, ammonium or triethanolamine (TEA). Sodium salts of AES are by far the most commonly used grades. Further detail on the structures included in the AES family are given in Section 3.3.

3.3 Manufacturing Route and Production/Volume Statistics

Alcohol ethoxysulphates are produced by sulphation of the ethoxylates of primary alcohols using sulphur trioxide or chlorosulphonic acid followed by immediate neutralisation with base to produce typically a sodium salt, less commonly an ammonium salt. Minor volumes are neutralised with alkanolamines, usually triethanolamine (TEA). Most commercial alcohol ethoxysulphates are produced as low or high aqueous active solutions e.g. 25-30% or 68-70%. Many grades of AES are produced commercially differing in the parent detergent alcohol, the ethoxylate (number of moles of EO), the concentration of AES active matter in water, whether shipped as a solution, a paste or in solid form. Commercial sodium AES typically contain, approximately 2-4% of unsulphated alcohol ethoxylate, 1-2% unreacted alcohol and 15-45% alcohol sulphate, and optionally trace amounts of inorganic pH buffering agents, depending on the active matter content and the degree of ethoxylation. The molecules included in the HERA AES family are ultimately derived from linear-type primary alcohols in the C_{12} to C_{18} range. As marketed, such alcohols usually contain a distribution of alkyl chain lengths.

The linear-type alcohols include those which are mixtures of entirely linear alkyl chains, and those which are mixtures of linear and mono-branched alkyl chains, though still with a linear backbone. Such alcohols and their blends are substantially interchangeable as feedstocks for AES used in the major applications falling within the scope of HERA.

The entirely-linear alcohol feedstocks include those derived from vegetable or animal sources via oleochemical processes and those derived from ethylene via Ziegler chemistry. Such alcohols contain even numbered alkyl chains only, and are produced in single carbon cuts or more usually wider cuts from C6 through C22+. C12 through C18 grades are feedstocks for HERA AES.

The essentially-linear alcohol feedstocks, also known as linear oxo-alcohols, are derived from linear higher olefins via oxo-chemistry. The feedstock linear olefins are typically derived from ethylene or normal paraffins. Such alcohols contain mixtures of even/odd or odd numbered alkyl chains depending on the feedstock olefin, and are produced in grades ranging from C7 through C15. Typically 90-40% of the carbon chains are linear, the remainder being mono-branched 2-alkyl isomers, predominantly 2-methyl. The mono-branched isomers thus have a linear backbone. C12 through C15 grades are feedstocks for HERA AES.

The principle structures present in HERA C_{12} AES for example are:

$CH_3(CH_2)_{11}O(EO)_nSO_3Na$

$$\begin{array}{l} CH_3(CH_2)_{8-m}CHCH_2O(EO)_nSO_3Na \\ \qquad\qquad\quad | \\ \qquad\quad (CH_2)_mCH_3 \end{array}$$

where n varies from 0-8 and m varies from 0-4, but is primarily 0. The average value of n is 2.7 for AES sold into household use and 2.4 for the total AES produced.

Of the AES used in consumer cleaning applications in Europe, approximately 71% is derived from even carbon numbered linear alcohols (C12-14 and C16-18), with the remaining 29% derived from odd and even carbon numbered essentially-linear oxo alcohols.

Excluded from the HERA AES family are alcohol ethoxysulphates derived from alcohols shorter than C_{12}. The tonnages of these products are very small (<1000 tonnes/year) and their toxicity is less than that of longer chainlengths. Also excluded from the family are AES with other alkyl chain structures such as multi-branched alcohols, for example commercial *iso*-tridecanols. These grades of AES are not typically used in household cleaning products. Their uses are small and specialised and they are not considered further in this assessment.

The European (EU, CH and NO) production volume of AES surfactants on an active matter basis is estimated to be 320,000 tonnes/y (CESIO statistics for 2000; CESIO = European Committee for Surfactants and their Organic Intermediates, a sector group of the European Chemical Industry Council, CEFIC). About 276,000 tonnes/y are estimated to remain in Europe, the remainder (44000 tonnes/yr) is exported. The imported volume is thought to be negligible. CESIO estimates that 39% (108,000 tonnes) of the captive use volume is used in HERA applications.

3.4 Homologue distribution in HERA applications

To determine the carbon-number distribution of 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) and companies manufacturing AES (via the CESIO Statistics Group). From the data received,

estimated distributions between carbon chain lengths have been determined. In the HERA-relevant range of C12-C18, the distribution between carbon chain lengths has been determined for 303,388 tonnes of the estimated total European AES production volume (320 000) and for 102,480 tonnes of the estimated total AES volume used in household cleaning products (108 000) (Table 1). These chainlength data are considered a reasonable representation of the distribution applicable for the marketed tonnages.

Table 1 Estimated tonnage and Chain length distribution of AES

Chain length	CESIO : Total AES Tonnage		CESIO : Estimate of Volume used in Household Cleaning Products		AISE : Estimate of Volume used in Household Cleaning Products	
	Percent	*Tonnes*	*Percent*	*Tonnes*	*Percent*	*Tonnes*
C12	60.9	184 847	57.6	59 045	46.2	32 770
C13	8.9	26 981	15.1	15 447	32.0	22 725
C14	24.8	75 315	21.6	22 145	18.2	12 894
C15	2.4	7 170	2.7	2 730	3.6	2 565
C16	2.2	6 787	2.1	2 200	-	-
C17	-	-	-	-	-	-
C18	0.8	2 288	0.9	913	-	-
ΣC_{12-18}		303 388*		102 480**		70 954**

* Compared to EU Production Tonnage of 320 000 (of which 44 000 t/a are exported)
** Compared to 108 000 t/a used in HERA applications.

CESIO estimates that 61% (168,000 tonnes) of the captive use volume is used in applications outside of the HERA scope. Second to use in household detergents and cleaning products, Personal Care applications consume the next largest volume of AES, followed by use in Industrial and Institutional cleaners and the Industrial sector (e.g. emulsion polymerisation). These applications are not considered in the body of this assessment, although an environmental assessment based on the total EU-captive tonnage is included in Annex 3.

A separate survey was performed to determine the average EO number of products used in HERA applications. The total tonnages from this survey are very similar to those from the distribution by carbon number survey. The information extracted from this EO-distribution survey is the average EO number, hence the slight difference in total tonnage will have little effect (Table 2).

Table 2 Estimated tonnage and EO distribution of AES

Commercial Product	CESIO	CESIO

AVERAGE EO	Household volume (tonnes)	AES Total tonnage (tonnes)
1	1,492	1,492
2	18,693	161,577
2.5	37,000	89,250
3	43,850	47,703
6	1,750	4,500
Total tonnage	102,785	304,522
Average EO	2.7	2.4

4 Data Search Strategy

Chemical names were extracted from the STN database, Registry file. Chemical names and CAS numbers were searched in STN database, CAPlus file and the Dialog databases BIOSIS file, Enviroline file and Pollution Abstracts file. Additional searches were made of ECOTOX (U.S. EPA) and TOMES databases.

In addition, a call-in was made for data from AISE/CESIO companies with a request for information on toxicity, fate and tonnage marketed.

5 Exposure

5.1 Tonnage

The European (EU, CH and N) production volume of AES surfactants on an active matter basis is estimated to be 320,000 tonnes/y (CESIO statistics for 2000). About 276 000 tonnes/y are estimated to remain in Europe, the remainder is exported. The imported volume is thought to be negligible. An estimated 108,000 tonnes/y is used in formulations for household use. Assessments are made based on both 108,000 for HERA applications (Section 5.2) and 276,000 tonnes for the total captive tonnage (Annex 3).

Estimates of the distribution of carbon chainlengths and EO distribution within this tonnage are shown in Table 1 and Table 2 respectively. In the following assessment it is assumed that the carbon chainlength distribution of the tonnage for which data were available is representative of the total tonnage.

5.2 Derivation of PEC

The PEC is derived on the basis of individual C# with an average EO of 2.7 for HERA applications (2.4 for total tonnage assessment, Annex 3). The only way to estimate the physchem properties of EO2.7 or EO2.4 is by interpolation of values for EO2 and EO3. Values are shown in Annex 2.

The use of individual C# is needed because there is some evidence to suggest that toxicity may show a parabolic relationship with carbon chainlength (Section 6.2.2.2). However, there appears to be an essentially linear relationship of EO and toxicity and therefore use of an average EO is justified.

5.2.1 Tonnage Scenarios

The AISE and CESIO data for tonnage in household applications differ both quantitatively and qualitatively (Table 1). The qualitatively greatest difference is that AISE attributes greater percentage tonnage to C13 and less to C12. Interpretation of this variability to estimate PEC values based on household use has been managed by scaling the highest percentage estimate to the total tonnage. For example, for C13, the AISE estimate is the highest at 32%. The sum of highest percentages for all chainlengths is 117.9%. For each carbon chainlength, the CESIO total tonnage in household use, 108,000 t/a, has been scaled by the highest percentage for that particular carbon chainlength divided by the sum percentage of the carbon chainlengths. For C13 this is 108,000 t * 32.0%/117.9% to give 29312 t/a.

The tonnages used to estimate PEC's arising from the total AES marketed in EU are derived from CESIO estimates of the C# distribution of the Total Tonnage applied to the EU captive tonnage.

Adopting this approach, the tonnages used in the PEC assessments were those shown in Table 3.

Table 3 Tonnages used in PEC assessments

	Household use		Total AES production	
	Highest estimated %	Total tonnage x Highest estimated %	CESIO estimate %	Total tonnage[1] x CESIO estimate %
C12	57.6%	52763	60.9	168160
C13	32.0%	29312	8.9	24545
C14	21.6%	19786	24.8	68516
C15	3.6%	3298	2.4	6523
C16	2.1%	1924	2.2	6174
C18	0.9%	824	0.8	2081
TOTAL	117.9%	108000	100	276000

[1]= Production tonnage minus export tonnage

5.2.2 Physico-Chemical Properties

The most important phys/chem properties for an environmental risk assessment are aqueous solubility, vapour pressure, and the octanol/water partition coefficient or other partition coefficients, for example, those between water and environmental matrices such as soil, sediment, or sewage sludge. Details of physchem properties used in modelling the PEC are shown in Annex 2.

For Alkyl Ethoxy Sulphate, all groups of homologues have sufficiently low volatility that the sensitivity of the risk assessment to the values of this parameter will be negligible.

It should be noted that for surfactants a physically meaningful log Kow cannot be measured but can be modelled from molecular structure. Therefore, all assessments based on partitioning coefficients that are not established experimentally but calculated from log Kow-values should be considered only as a first and conservative estimate

5.2.3 Removal

5.2.3.1 Biodegradation pathways

The risk assessment of a parent compound should be restricted to that compound unless the metabolites are persistent and/or more ecotoxic than the parent. There are 3 starting routes of AES degradation which all seem to occur: i) ω-/β-oxidation of the alkyl chain, ii) enzymatic cleavage of the sulphate substituent leaving an alcohol ethoxylate, iii) cleavage of an ether bond in the AES molecule producing either the alcohol (central cleavage) or an alcohol ethoxylate and an oligo(ethylene glycol) sulphate (Swisher 1987, Steber and Berger 1995). The subsequent degradation of the resulting intermediates encompasses oxidation of the alcohol to the corresponding fatty acid (itself then degraded via ß-oxidation) or degradation of the alcohol ethoxylate (via central cleavage or degradation from either end of the molecule) or degradation of the oligo(ethylene glycol) sulphate. The ultimate biodegradability of alcohol ethoxylates is well established (Swisher 1987, Holt et al. 1992) and glycol ether sulphates have also been shown to be fully degradable by mixed cultures forming inorganic sulphate and carbon dioxide (Griffith et al 1986, White and Russell 1988). The conclusion that AES degradation will not produce any recalcitrant metabolite is in line with the experimental findings on AES in the "Test for detecting recalcitant metabolites" (Gerike and Jasiak 1986). In addition, Yoshimura et al (1982) reported test data showing that the (fish) toxicity of AES decreases in the course of AES degradation. Consequently, there is no indication for the formation of persistent or markedly toxic metabolites from AES, and so primary AES removal data obtained with methods such as MBAS, LCMS and ^{14}C-radiolabelled studies are suitable for use in this assessment.

5.2.3.2 Aerobic Degradation & WWTP fate

5.2.3.2.1 Ready Biodegrability Data

Several reviews highlight that AES are readily biodegradable, with alkyl-chain length having little effect (Madsen et al 2000, BKH 1994, Painter 1992, ADL 1991).

5.2.3.2.2 Scenario I - SimpleTreat calculation

EUSES calculates degradation in a 9-box STP model ranging from 75% for C18EO2.7S to 87% for C12EO2.7S (Table 4). These calculations are based on AES being readily biodegradable.

Table 4 Fate of AES with EO2.7 in STP (fractional distribution)

C#	12	13	14	15	16	18
air	<1.0E-10	<1.0E-10	<1.0E-10	<1.0E-10	<1.0E-10	<1.0E-10
water	0.13	0.13	0.13	0.13	0.12	0.11
sludge	7.0E-4	1.8E-3	4.4E-3	1.1E-2	2.6E-2	0.14
degraded	0.87	0.87	0.87	0.86	0.85	0.75

A PEC scenario (Scenario 1) using these data is developed in Section 5.2.4.1.

5.2.3.2.3 Simulation Test Data

Information from higher tier tests was collected from producers and reported in BKH's 1994 review. Primary removal in higher tier tests is shown in Table 5.

Table 5 Primary degradation of AES in higher tier tests

C	EO	Removal %	Method	Source quoted in BKH 1994
12	2	97.2	CONF	Henkel 83
12	8	95.6	CONF	Henkel 84
12	12	95.4	CONF	Henkel 85
13.3	3.19	100	SCAS	Vista 33
12-14	2	98	CONF	Huls 111
14-15	2	98	CONF	Henkel 88
14-15	3	97.9	CONF	Henkel 89
16-18	7.8	98.6	CONF	Henkel 86
16-18	10.3	97	CONF	Henkel 87

CONF: OECD CAS test (confirmatory test)

The primary removal data listed above suggest no consistent removal trend with alkyl chainlength or degree of ethoxylation. Consequently, a geometric mean of the data (97.5% removal) has been used in subsequent analyses (Scenario II). Scaling the SimpleTreat distributions assuming 97.5% removal is shown in Table 6. These data were used to develop Scenario II shown below.

Table 6 Fate of AES with EO2.7 based on 97.5% degradation

C#	12	13	14	15	16	18
air	<1.0E-10	<1.0E-10	<1.0E-10	<1.0E-10	<1.0E-10	<1.0E-10
water	2.5E-02	2.5E-02	2.5E-02	2.5E-02	2.5E-02	2.5E-02
sludge	7.8E-04	2E-03	4.9E-03	1.2E-02	2.9E-02	0.15
degraded	0.97	0.97	0.97	0.96	0.95	0.82

It is clear from these studies that greater removal should be expected from a STP than is modelled by the default values attributed to readily biodegradable substances in the TGD by SimpleTreat.

5.2.3.3 Anaerobic Degradation

Based on the chemical structure of AES and the proven easy anaerobic biodegradability of the structurally related alcohol ethoxylates and alkyl sulphates, good anaerobic biodegradability of AES is likely (Steber and Berger, 1995). This is supported by the result from testing C12-14EO2S in a stringent anaerobic biodegradability screening test (ECETOC test) which showed a gas (CO_2 + methane) production of 75 % within the 41-day incubation period (Steber 1991). In addition, Nuck & Federle (1996) tested AES in a lab digester that simulated the situation in practice except that the system was static while real digesters are mainly run semi-continuously. Within the 17-day incubation period 88% ultimate biodegradation (based on ^{14}C-gas formation) was found for C14[^{14}C]EO3S.

Taking these mineralisation data into account it is expected that the removal of the parent AES compound under digester conditions is at least 90%. However, the organic moiety of the sewage sludge (about 50% of the sludge dry matter) is also reduced during the digestion process, typically by about 50%, suggesting a reduction in sludge volume of 25%. Scaling the reduction of AES concentration to take account of sludge volume reduces the reduction in AES concentration by a factor of 1.3 (100/75%) and consequently, AES anaerobic removal is estimated as 87 % rather than the 90% calculated when the reduction in the organic content of sludge is not taken into account.

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 (i.e. reduction by 87%) of the concentrations in agricultural soil calculated by EUSES.

5.2.3.4 Degradation in other media

Federle et al (1997) compare rate constants for 9 chems including C14-15EO2.25S in different tests. The publication doesn't give individual rates but Federle (pers. comm.) provided the following mineralization rates (1/day):

	Sturm	**Activated Sludge**	**River**	**Soil**
Mineralization rate (day^{-1})	0.18	1.79	0.48	0.29
Equivalent ½-life (days)	3.9	0.39	1.4	2.4

These data suggest that degradation will be considerably faster than assumed by the surface-water and soil rate constants used for readily biodegradable substances according to the EU-TGD (k= 0.047, t1/2 = 15 d for surface water and k=0.023, t1/2 = 30 d for soil for a substance with logKow ≤ 4.4).

Schröder (1995) investigated the half-life of AES in River water and showed a half-life of about 1 hour in a sample from the Rur river. This would be equivalent to a rate constant of 16.6 (d^{-1}).

Based on the ready biodegradability of all chainlengths of AES, it is assumed that the rate constant for degradation in bulk surface water for C14-15EO2.25S determined by Federle et al (1997) is applicable to other chainlengths. Therefore, a surface-water degradation rate of 0.48 d-1 has been applied to all chainlengths in the calculation of PEC values. The value of 0.48 d-1 indicates more rapid degradation than the default rate constant proposed in the TGD for readily biodegradable substances (0.047 d-1), but is far more conservative compared to the rate of 0.7 h-1 determined by Schröder (1995).

Lee et al (1997) report on mineralization in a stream mescosm exposed to different surfactants including C45EO2.17S and show that temperature (13-25 oC) has no effect on degradation rate.

For degradation in soil, the biodegradation kinetic obtained from the work by Federle et al (k= 0.29 d^{-1}, t1/2 = 2.4 d) was used to determine the PEC calculations instead of using the TGD default value (k = 0.023 d^{-1}, t1/2 = 30 d). Federle's figure is considered conservative because it is based on the mineralisation rate, i.e. the removal of the parent surfactant will have been much higher. Further support for the use of this figure is provided by comparing the assumed AES half life (2.4 d) with the corresponding figure for LAS which, in a field study run under realistic conditions was in the range 3-7 days (Küchler et al.,1997).

5.2.4 PEC Calculations

5.2.4.1 Local $PEC_{aquatic}$

EUSES was used to calculate local PEC based on household use tonnage which includes a contribution from the regional PEC. HERA default values were used: 7% of the continental tonnage is applied to the region and the average discharge to WWTP is increased by a factor of 1.5 to take account of local variability (HERA, 2002). The Federle et al degradation rate constants for surface water and soil were used to override the default values. The resulting PEC values are shown in Table 7.

Table 7 Simpletreat PEC estimates (Scenario I)

Carbon #	12	13	14	15	16	18
Local PEC surface water (mg/l)	5.0E-2	2.8E-2	1.9E-2	3.1E-3	1.8E-3	6.9E-4
Local PEC sediment (mg/kg wwt)	4.7E-2	3.3E-2	3.4E-2	1.0E-2	1.3E-2	2.8E-2
Local PEC agric 30 d (mg/kg wwt)	1.1E-3	1.6E-3	2.6E-2	1.1E-3	1.6E-2	3.5E-3
Local PEC agric 30 d with 87% anaerobic degradation (mg/kg wwt)	1.4 E-4	2.1E-4	3.4E-4	1.4E-4	2.1E-4	4.6E-4
PECstp microorgs (mg/l)	0.48	0.27	0.18	3.0E-2	1.7E-2	6.6E-3

Regional PEC surface water total (mg/l)	2.2E-3	1.2E-3	8.2E-4	1.4E-4	7.9E-5	3.3E-5

Simulation test degradation showed no consistent trend across carbon chainlength and an average of 97.5% degradation (Section 5.2.3.2.3). Overriding EUSES defaults to reflect the STP distribution shown in Table 6, results in the PEC values shown in Table 8.

Table 8 Simulation test PEC estimates (Scenario II)

Carbon #	12	13	14	15	16	18
Local PEC surface water (mg/l)	1.1E-02	6.3E-03	4.2E-03	7.0E-04	4.1E-04	1.8E-.04
Local PEC sediment (mg/kg wwt)	1.1E-02	7.4E-03	7.6E-03	2.3E-03	2.9E-03	7.1E-03
Local PEC agric 30 d (mg/kg wwt)	1.3E-3	1.7E-3	3.0E-3	1.2E-3	1.7E-3	3.9E-3
Local PEC agric 30 d with 87% anaerobic degradation (mg/kg wwt)	1.6E-4	2.3E-4	3.8E-4	1.6E-4	2.3E-4	5.0E-4
PECstp microorgs (mg/l)	9.5E-02	5.3E-02	3.6E-02	5.9E-03	3.5E-03	1.5E-03
Regional PEC surface water total (mg/l)	1.8E-03	9.9E-04	6.7E-04	1.1E-04	6.5E-05	2.8E-05

5.2.4.2 Indirect Exposure to Humans

As a starting point for the calculation of indirect human exposure via drinking water, the EUSES calculations for indirect uptake via regional exposure can be used (taking into account that drinking water will not be sourced immediately downstream of wastewater emissions). These are shown in Table 9 below, with the calculated uptake from a local source given for comparison. The total human uptake calculated by EUSES is also shown in the table, although known inadequacies with the current model for plant uptake mean that these calculated values will considerably overestimate the uptake from food. Thus these total regional uptake values may not be considered to be acceptably realistic for the HERA Human Health Assessment.

Table 9 AES with EO=2.7 uptake by Humans – as calculated with EUSES*

AS Fraction	Regional (mg/kg/day)		Local (mg/kg/day)	
	Drinking Water	Total Food + Water Uptake	Drinking Water	Total Food + Water Uptake
C12	5.1E-5	5.9E-5	3.2E-4	3.7E-4
C13	2.8E-5	3.8E-5	1.8E-4	2.4E-4
C14	1.9E-5	3.2E-5	1.2E-4	2.0E-4
C15	3.2E-6	7.9E-6	2.0E-5	5.0E-5
C16	1.9E-6	8.5E-6	1.2E-5	5.4E-5
C18	7.9E-7	2.0E-5	5.0E-6	1.3E-4

*EUSES defaults modified according to the HERA Detergent Scenario and taking account of 97.5% removal in STP, 87% anaerobic degradation in sludge and degradation rates in surface water and soil based on measured data.

5.2.4.3 Validation of modelling using monitoring data

STP Effluent Monitoring

Data on STP monitoring can be used to validate modelling data based on laboratory confirmatory studies and/or default values applied to laboratory screening data. Literature reports of AES monitoring generally do not distinguish between carbon chainlengths. In addition, field monitoring for AES has used analytical methods that cover C12-15 only. Therefore monitoring data have been compared with the sum of PEC values for C12-15 only. Additionally, monitoring analytical methods cannot distinguish between AS from AES and from AS itself, and therefore the sum of AES + AS will overestimate the AES PEC. Considering the tonnage of AS marketed relative to that originating from AES the error due to inclusion of AS from sources other than AES may be quite large. In addition, AES monitoring data will combine AES from detergents with that from other sources.

Comparison of monitoring and modelling data is shown in Table 10. The highest values from STP influent monitoring data are similar to EUSES estimates. EUSES estimates of STP effluent concentrations based on simulation test data are greater by more than one order of magnitude compared to the concentrations monitored in activated sludge plants. This emphasises that the aquatic PEC must be considered as a very conservative estimate. Consequently, the monitoring data suggest that a more accurate, less conservative modelling of fate in STP would lead to lower PEC values.

Table 10 Comparison of modelled PEC and field monitored concentrations

	Value	Reference	Notes	Homologues covered
C_{infl} (mg/l)	7.6	EUSES		Based on C12-15EO2.7, HERA tonnage

	0.57	Popenoe et al 1994	RBC plant	C12-15 EO0-8
	0.016 & 1.0	McAvoy et al 1998	2 act. slu. plants. 0.016 value may be particularly low due to long residence time in equalization basin before the STP	C12-15 EO0-6
	0.74	Wind pers. comm., 2002	Median value, Sum of AS+AES (approx. 90 samples) at 9 STP	C12/14 EO1-5 C12-18 AS
	3.8	Matthijs et al 1997	Average value, sum AS+AES at 7 STP	C12-15 EO0-8
	0.23 & 0.74	Schröder (1995)	Median value, Sum of AS+AES at 2 STP	C12/14 EO1-5 C12-18 AS
	0.4 - 5.1	Schröder et al 1999	Sum of AS+AES determined in 2-h composite samples (1 STP) over a 24h period	C12/14 EO1-5 C12-18 AS
C_{effl} (mg/l)	0.96	EUSES	Simpletreat defaults	Based on C12-15EO2.7, HERA tonnage
	0.19	EUSES	Using simulation test data from lab tests	Based on C12-15EO2.7, HERA tonnage
	0.004 & 0.018	McAvoy et al 1998	2 AS plants. Also 0.032-0.164 from 4 TF plants	C12-15 EO0-6
	0.012	Matthijs et al 1997	Avg, sum of AS+AES @ 7 plants	C12-15EO0-8
	<0.001	Schröder et al 1999	Sum of AS+AES determined in 2-h composite samples (1 STP) over a 24h period	C12/14 EO1-5 C12-18 AS
	0.003 & 0.008	Schröder 1995	Median value, Sum of AS+AES at 2 plants	C12/14 EO1-5 C12-18 AS
	0.002	Wind pers. comm. (2002)	Median value, Sum of AS+AES (approx. 90 samples) at 9 STP	C12/14 EO1-5 C12-18 AS
Regional PEC surface water (mg/l)	0.0044	EUSES	Simpletreat	Based on C12-15EO2.7, HERA tonnage
	0.0036	EUSES	Using simulation test data from lab tests	Based on C12-15EO2.7, HERA tonnage
	0.0103	Popenoe et al 1994	Upstream of STP	C12-15 EO0-8
	0.001	Schröder 1995	Upstream of STP	

5.2.4.4 PEC for other compartments

There are no measured concentrations of AES in sediment or soil, not even bulk AES without characterisation by C#. Local $PEC_{sediment}$ and PEC_{soil} are calculated by EUSES, although the PEC_{soil} is modified to take account of anaerobic biodegradation, and the results are included in Section 5.2.4.1.

6 Effects

6.1 Aquatic toxicity

6.1.1 Acute data

Acute toxicity data are available in several review articles (ADL 1991; BKH 1994; Madsen 2000). As a large chronic data base exists (Section 6.1.2) the acute data have not been further considered for the HERA risk assessment.

6.1.2 Chronic data

The following chronic toxicity data are available in reviews or have been identified during this HERA assessment project.

Table 11 Chronic toxicity data

Fish and other aquatic vertebrates

C#		EO#		Linearity	Species	Endpoint	Exposure	Value	Ref
Avg	Distn	Avg	Distn					(mg/l)	
12		0		?	Saccobranchus fossilis	60 d	Semi-static	>2.24	Dalela et al, 1981
?	12-13	1	?	?	P. promelas	30 d NOEC	?	0.88	BKH 1994
?	12-14	2	?	?	O. mykiss	28 d growth	flow-through	0.1	Scholz 1997
?	12-15	3	?	?	O. mykiss	28 d NOEC	flow-through Measured	0.12	BUA 1997
13.7	?	2.25	?	?	P. promelas	365 d NOEC	Measured	0.1	Maki 1979
?	14-15	2.25	?	?	P. promelas (juvenile)	45 d LC50	? (flow-through)	0.44	ADL 1991
?	14-15	2.25	?	?	P. promelas (fry)	45 d LC50	? (flow-through)	0.63	ADL 1991
?	14-15	2.25	?	?	P. promelas	45 d LC50	? (flow-through)	0.94	ADL 1991

?	14-16	2.25	?	?	P. promelas	45 d LC50	?	0.1	BKH 1994
17.3	16-18	0			Brachydanio rerio	OECD 204, NOEC		1.7	Steber et al 1988
17	?	3	?	?	P. promelas	365 d NOEC	?	0.13	BKH 1994

Invertebrates

C#		EO#		Linearity	Species	Endpoint	Exposure	Value	Ref
Avg	Dist'n	Avg	Distn						
12	99%	0	-	-	C. dubia	7 d NOEC	Flow-through	0.88	Dyer et al 1997
12	>95% Pure	1	>95% Pure	?	C. dubia	7 d NOEC	Flow-through	0.34	Dyer et al 2000
12	>95% Pure	2	>95% Pure	?	C. dubia	7 d NOEC	Flow-through	6.3	Dyer et al 2000
12	100% Pure	2	100% Pure	?	Brachionus calyciflorus	2 d EC20	Measured	0.97-1.1	Versteeg et al, 1997
12	>95% Pure	4	>95% Pure	?	C. dubia	7 d NOEC	Flow-through	2.7	Dyer et al 2000
12	99% pure	4	99% pure	?	B. calyciflorus	2 d EC20	Measured	2.3	Versteeg et al 1997
12	>90% Pure	8	>90% Pure	?	C. dubia	7 d NOEC	Flow-through	1.2	Dyer et al 2000
?	12-14	2	?	?	D. magna	21 d repro	Semi-static Nominal	0.72	Scholz 1997
?	12-14	>2	?	?	D. magna	21 d NOEC	Semi-static	0.7	BKH 1994
?	12-15	3	?	?	D. magna	21 d repro	Semi-static Measured	0.34	BUA 1997
13	>95% Pure	2	>95% Pure	?	C. dubia	7 d NOEC	Flow-through	0.28	Dyer et al 2000
13	100% pure	2	100% pure	?	B. calyciflorus	2 d EC20	Measured	0.49	Versteeg et al 1997
13.67	13-15	2.25	?	?	D. magna	21 d NOEC	Measured	0.27	Maki 1979
14	>95%	0	-	-	C. dubia	7 d NOEC	Flow-through	0.<0.062	Dyer et al 1997
14	>95% Pure	1	>95% Pure	?	C. dubia	7 d NOEC	Flow-through	0.34	Dyer et al 2000
14	>95% Pure	2	>95% Pure	?	C. dubia	7 d NOEC	Flow-through	0.31	Dyer et al 2000
14	100% pure	2	100% pure	?	B. calyciflorus	2 d EC20	Measured	0.13	Versteeg et al 1997
14	>95% Pure	4	>95% Pure	?	C. dubia	7 d NOEC	Flow-through	1.1	Dyer et al 2000

14	98% pure	4	98% pure	?	B. calyciflorus	2 d EC20	Measured	0.37	Versteeg et al 1997
?	14-15	0			C. dubia	7 d NOEC	Flow-through	0.081	Dyer et al 1997
?	14-15	2.25	?	?	D. magna	21 d NOEC	Nominal	0.18	BKH 1994
?	14-16	2.25	?	?	D. magna	21 d NOEC	?	0.27	BKH 1994
15	>95%	0	-	-	C. dubia	7 d NOEC	Flow-through	0.23	Dyer et al 1997
15	>95% Pure	1	>95% Pure	?	C. dubia	7 d NOEC	Flow-through	0.08	Dyer et al 2000
15	>95% Pure	2	>95% Pure	?	C. dubia	7 d NOEC	Flow-through	0.06	Dyer et al 2000
15	>95% Pure	4	>95% Pure	?	C. dubia	7 d NOEC	Flow-through	0.15	Dyer et al 2000
15	99% pure	4	99% pure	?	B. calyciflorus	2 d EC20	Measured	0.22	Versteeg et al 1997
15	>90% Pure	8	>90% Pure	?	C. dubia	7 d NOEC	Flow-through	5.8	Dyer et al 2000
16	>95% pure	0	-	-	C. dubia	7 d NOEC	Flow-through	0.20	Dyer et al 1997
17.3	16-18	0			D. magna	21 d NOEC		16.5	Steber et al 1988
18	>95% pure	0	-	-	C. dubia	7 d NOEC	Flow-through	0.60	Dyer et al 2000

Algae

C#		EO#		Linearity	Species	Endpoint	Exposure	Value	Ref
Avg	Dist'n	Avg	Distn						
12		0			S. capricornutum	96 h NOEC Growth inhibtion		12	Nyholm & Damgaard, 1990
12		?			River water 'community'	Chlorophyll a NOEC	3 weeks	70 mg/l (enhancement at 5 mg/l)	Drewa 1989
?	12-13	?	?	?	Selenastrum capricornutum	?	5 d NOEC	50.5	BKH 1994
?	12-14	2	?	?	Scenedesmus subspicatus	72 h NOEC AUGC	Static Nominal	0.72	Scholz 1997
?	12-14	2	?	?	Scenedesmus subspicatus	96 h NOEC	Static Nominal	0.35	BKH 1994
?	12-15	3	?	?	Scenedesmu	72 h	Static	0.9	BUA

					s subspicatus	NOEC	Measured		1997
?	14-15	?	?	?	Selenastrum capricornutum	NOEC Test duration unknown	?	21	BKH 1994
17.3	16-18	0			Scenedesmus subspicatus	72 h NOEC	Static	17	Henkel 1996

6.1.3 Mesocosm data

Several mesocosm/microcosm studies have been performed with AES.

Table 12 Mesocosm data

C#		EO#		Linearity	Species	Endpoint	Exposure	Value	Ref
Avg	Distn	Avg	Distn						
14.5	14-15	2.17	?	?	Corbicula fluminea (Asian clam)	8 weeks NOEC	Flow-through	0.075 mg/l	Belanger et al 1995a
14.5	14-15	2.17	?	?	Goniobasis spp (a snail)	8 weeks LOEC	Flow-through	>0.73 mg/l	Belanger et al 1995a
14.5	14-15	2.17	?	?	Periphyton	4 weeks NOEC	Flow-through	0.61 mg/l	Belanger et al 1996
14.5	14-15	2.17	?	?	46 invertebrate spp	8 weeks NOEC species density	Flow-through	0.25 mg/l	Belanger et al 1995b
13.2	12-15	3		80%	Fish, invertebrate and algal taxa	30 d NOEC	Flow-through	>2 mg/l	Lizotte et al 2002
?	16-18	0		?	Algae, protozoa, rotifer, bacteria spp	21 d NOEC		0.55	Steber et al 1989

6.2 $PNEC_{aquatic}$ derivation

6.2.1 Justification for PNEC based on chronic data

The abundance of chronic toxicity data is such that it is justified to base the PNEC on chronic toxicity data.

6.2.2 Trends in Toxicity/QSAR

6.2.2.1 Relative spp sensitivities,

Understanding the relative sensitivity of different taxa is important because the PNEC should be based on the most sensitive taxonomic level.

Inspection of the chronic toxicity data listed above indicates no consistent difference in the sensitivity of invertebrates and fish. For C12-14EO2S fish appear more sensitive than *D. magna* or algae, but a flow-through test was used for the fish, a semi-static for the *D. magna* and a static design for the algae. For C13.7EO2.25 fish appear 2.7 times more sensitive than D. magna based on measured concentrations, but C14-15EO2.25 appears more toxic to invertebrates, although the actual exposure concentrations were not confirmed. BKH (1994, Table 6) concluded fish were more sensitive than invertebrates to AES, but they did not take account of C#/EO#.

Lizotte et al (2002), mesocosm data suggest fish are more sensitive than periphyton/macrophytes and invertebrates. Belanger et al (1995b), mesocosm data cannot be used to determine relative sensitivity of fish compared to invertebrates and algae, because fish were not included in the experiment.

Van de Plassche et al (1999) normalised all chronic NOECs to a $C_{12.5}EO_{3.4}SO_4$ structure and showed that *B. calyciflorus* (invertebrte) is more sensitive than *P. promelas* (fish).

On the basis of this analysis, PNEC could be derived based on either fish or invertebrate data. Since the invertebrate database is more extensive than that for fish, the PNEC will be based on invertebrate data.

6.2.2.2 Justification for PNEC based on averages

Different AES homologues are expected to differ in their toxicity. In theory, a PNEC could be derived for each homologue, related to the PEC for each homologue and the resulting quotients summed to determine the risk of the AES family (a toxic units approach). However, the complexity of this approach is not warranted if the toxicity of a single structure is the same as that of a homologue distribution with an average structure equivalent to the single homologue. Choosing an average structure approach, a toxic units approach or some combination (eg consideration of individual carbon chain lengths but with average EO #) requires consideration of toxicity QSAR.

Dyer et al (2000) have developed QSAR for chronic toxicity to *Ceriodaphnia* using data on single AES homologues, including EO=0, ie AS. The chronic toxicity QSAR was based on C12-15, EO0-8 plus C16EO0 and C18EO0, but R^2 was approximately 0.7 and solubility difficulties were noted for some homologues. The QSAR developed was:

$$\log NOEC\ (mol/l) = 0.128C^2 - 3.767C + 0.152EO + 21.182$$

The QSAR estimates of toxicity are shown in Table 13.

Table 13 QSAR estimates of toxicity

	EO #

		0	1	2	3	4	5	6	7	8
	10	**53**	**88**	**140**	**230**	**360**	**570**	**880**	**1400**	**2100**
	11	**4.7**	**7.7**	**12**	**20**	**31**	**49**	**75**	**120**	**180**
	12	**0.74**	**1.2**	**2.0**	**3.1**	**4.8**	**7.5**	**12**	**18**	**27**
C #	13	**0.21**	**0.34**	**0.55**	**0.86**	**1.4**	**2.1**	**3.2**	**4.9**	**7.5**
	14	**0.11**	**0.17**	**0.28**	**0.44**	**0.68**	**1.1**	**1.6**	**2.5**	**3.7**
	15	**0.10**	**0.16**	**0.25**	**0.4**	**0.62**	**0.95**	**1.5**	**2.2**	**3.4**
	16	**0.16**	0.26	0.41	0.65	1.0	1.6	2.4	3.6	5.5
	17	**0.49**	0.78	1.2	1.9	3.0	4.5	6.9	11	16
	18	**2.6**	4.2	6.5	10	15	24	37	56	84

Values interpolated within the training set are in bold.

The chronic QSAR estimates a parabolic relationship between carbon number and toxicity with toxicity increasing from C12 to C15 and then decreasing. However, with the exception of EO0 (ie AS), the QSAR is based on an extrapolation for carbon chainlengths longer than C15. Furthermore, solubility difficulties were observed in some of the tests (C14EO1S, C15EO0S, C15EO1S, C16S and C18S). Since the Dyer et al QSAR is based on MBAS determined in samples of water from the test vessels, it may not represent the truly dissolved concentrations (bioavailable fraction) and consequently, the 'real' concentration causing effects may have been less than that reported suggesting that the QSAR is underestimating toxicity. Alternatively, the dissolution difficulties may have caused physical fouling rather than chemical toxicity. Therefore it is unclear whether the parabolic nature of the QSAR is an artifact of solubility problems (ie longer carbon chainlengths are really more toxic than predicted, the error being caused by measured concentrations overestimating the bioavailable fraction), or whether the QSAR overestimates the toxicity of the longer chainlengths due to physical fouling. Fouling would explain toxic effects, even for those carbon chainlengths for which the concentration causing effects is greater than the water solubility.

Comparison of toxicity as predicted by the chronic NOEC QSAR developed for *C. dubia* (7 d NOEC) with the observed toxicity (2 d EC20) to *B. calyciflorus* shows agreement within a factor of 3 (average 1.9) with *B. calyciflorus* being slightly more sensitive than *C. dubia*. Nevertheless the use of *C. dubia* data is favoured since *B. calyciflorus* is not a traditional test species.

Table 14 *Brachionus calyciflorus* toxicity data

Carbon chain	EO#	2 d EC20		
		Observed[1]	Predicted (QSAR)[2]	Observed / Expected
12	2	0.97-1.1	2.0	0.48-0.55
12	4	2.3	4.8	0.48
13	2	0.49	0.55	0.89
14	2	0.13	0.28	0.46

14	4	0.37	0.68	0.54
15	4	0.22	0.62	0.33

[1] Observed toxicity to *B. calyciflorus* (Versteeg et al, 1997)

[2] Toxicity predicted by QSAR for *C. dubia* 21 d NOEC (Dyer et al 2000)

The *C. dubia* chronic toxicity QSAR (Dyer et al 2000) suggests that the best fit to the data is parabolic with respect to alkyl chain length. Consequently, for chronic toxicity it is not justified to use an average structure for alkyl chain length. The effect of increasing the number of EO units is to reduce the toxicity. The effect of EO on logNOEC is essentially linear and therefore, for a single alkyl-chain length, a single homologue of EO=x will have approximately the same toxicity as a distribution of EO homologues with an average of EO=x. Consequently, a pragmatic option for development of PNEC(s) is to develop a single PNEC for each alkyl chain length, each estimated on the basis of average EO#.

Notwithstanding the parabolic nature of the chronic toxicity QSAR, there are data on the toxicity of complex structures (range of C# and EO# that can be compared with the toxicity of a single homologue as predicted by the Dyer et al (2000) QSAR. Maki (1979) published a *D. magna* 21 d NOEC for C13.67EO2.25S (average structure, C-range 13-15, EO range not known) of 0.27 mg/l while Dyer et al's QSAR would suggest a chronic NOEC for this structure of 0.34 mg/l. Belanger et al (1995b) report a mesocosm study on C14.5EO2.17S (alkyl range 14-15, EO range not known) that gave a NOEC of 0.25 mg/l. Dyer's chronic toxicity QSAR would suggest an identical NOEC for this structure (0.25 mg/l). Lizotte et al (2002) report a mesocosm study on C13.5EO2.8S (alkyl range C12-15, EO 0-10+) that gave a lowest NOEC invertebrates of 4.3 mg/l. Dyer et al's QSAR would suggest a NOEC for this structure of 0.49 mg/l.

The congruence of these data with the toxicity predicted by the Dyer et al chronic toxicity QSAR suggests that using a single PNEC for an average AES structure is justified. Nevertheless, since none of these tests used an AES that spanned the whole range of C# included in the AES family, and since the Dyer et al data suggest a parabolic relationship between toxicity and C#, separate PNEC will be determined for each C# based on the average EO# marketed.

6.2.3 $PNEC_{aquatic}$

The chronic toxicity QSAR (Dyer et al, 2000) has been used to derive PNEC values, using an application factor of 10. The application factor of 10 is justified by the taxonomic diversity of the overall dataset (Section 6.1.2). The resulting PNEC are shown in Table 15.

Table 15 $PNEC_{aquatic}$ (mg/l)

Carbon #	12	13	14	15	16	18
$PNEC_{aquatic}$ (mg/l)	0.27	0.076	0.038	0.035	0.057	0.89

6.3 Other Compartments Toxicity

6.3.1 Microbial toxicity

Goodnow & Harrison (1972) report the toxicity of AES ($C_{12}EO_3S$) to 45 isolated strains of bacteria growing in peptone medium. Growth inhibition greater than 50% was shown in 5 of the 42 strains tested at 10 mg/l but in 3 of these the AES was >90% degraded in 72 h. Only one strain tested at 100 mg/l showed complete inhibition. Lundahl et al (1973) showed a LOEC of 2 g/l for the growth of *Escherichia coli* on agar plates. Urano et al (1985) report degradation at different concentrations of C12EO5S. Degradation rate is lower at higher concentrations, but even at 100 mg/l degradation occurs. Verge et al (1996) report an OECD 209 respiration inhibition test with C12-14EO2.35 in which the 3h EC50>1600 mg/l. This last test is considered most appropriate as a basis for estimating a PNEC and consequently the microbial PNEC is set at 16 mg/l in accordance with the TGD.

6.3.2 Soil and Sediment Toxicity Data

There are no measured sediment toxicity data. Stora (1972) describes toxicity tests with a sediment dwelling polychaete, *Scololepis fuliginosa* but the exposure was in a water-only system and therefore is uninformative as to sediment toxicity.

In soil, Painter (1992) reports that 100-1000 mg AES/l gave increased germination rates and yields of soybean, pea, onion and dwarf *Coleus salicifolius.* The original reference for this work is not available, but the units of effect suggest that the exposure used a water-only system again and therefore is uninformative as to soil toxicity.

Some information is available on AS (See HERA AS assessment) and this indicates low soil toxicity. For example, the 48 h EC50 root growth inhibition of C12EO0S to *Cicer arietinum* is 361 mg/kg (Schmidt 1988) and C16-18 (avg C17.3) EO0S NOEC to 'several spp' is >1000 mg/kg (BUA 1996). It is unclear how concentrations of AES causing toxic effects would compare to AS concentrations causing effects since the more hydrophilic AES is expected to be more bioavailable but also less toxic.

Consequently it is concluded that there are no useful sediment or soil toxicity data for AES.

6.3.3 $PNEC_{sediment}$ and $PNEC_{soil}$

Since there are no measured sediment exposure data (Section 5.2.4.4) nor any sediment toxicity data, and since the logKow of none of the AES homologues exceeds logKow 5, the TGD states that the RCR for the aquatic compartment should be used for the sediment compartment. Consequently $PNEC_{sediment}$ is not calculated.

To estimate $PNEC_{soil}$ by equilibrium partitioning, the sorption behaviour of AES homologues is needed. The only sorption value found for AES was measured for $C_{12}EO_5S$ in river sediments and gave K_{oc}=1.1 (Urano et al, 1984). This compares to a K_{oc} of 2.3 calculated using the QSAR for 'Predominantly hydrophobics' from Sablijic & Gusten (1995) referenced in the TGD (logKoc=0.81 logKow + 0.1). The applicability of this QSAR to surfactants is questionable, but in the absence of other measured K_{oc} values, $PNEC_{soil}$ have been derived using this QSAR, TGD defaults for soil properties and the PNECaquatic values derived above (Table 16).

Table 16 $PNEC_{soil}$ (mg/kg)

Carbon #	12	13	14	15	16	18
$PNEC_{soil}$	3.6E-02	1.1E-02	5.6E-03	5.3E-03	9.2E-03	0.16

7 Risk Characterisation

7.1 Aquatic Compartment

RCR have been calculated using the PEC estimations, based on the household use tonnage (Table 7 and Table 8), and the PNEC derived using the *C. dubia* chronic toxicity QSAR (Table 15). The results using SimpleTreat default estimates of STP degradation (Scenario I) or primary degradation from OECD CAS or SCAS tests (Scenario II), are shown in Table 17.

Table 17 Aquatic risk quotients

PEC/PNEC (AF=10)

Carbon #	12	13	14	15	16	18	**Total RCR**
Scenario I	0.19	0.37	0.5	8.9E-02	3.2E-02	7.7E-04	1.2
Scenario II	4.1E-02	8.3E-02	0.11	2.0E-02	7.2E-03	2.0E-04	0.26

As discussed in Section 5.2.4.3, Scenario II implies a very conservative exposure estimate while Scenario I is considered to be unrealistically worst case. Consequently, the RCR based on Scenario I can be neglected.

7.2 Microbial toxicity

EUSES estimates of C_{effl} can be used as the $PEC_{micro\text{-}organisms}$. The sum of C12-18 is 0.98 mg/l. The microbial toxicity reported in Section 6.3.1 demonstrated no effect at substantially higher concentrations. Consequently, the RCR for WWTP microorganisms is <1.

7.3 Sediment Compartment

In the absence of measured data, the RCR for the sediment compartment is the same as that for the aquatic compartment.

7.4 Soil Compartment

The RCR for the soil compartment are estimated from:

- EUSES estimates of soil concentrations derived using simulation data to estimate degradation in WWTP, and 87% anaerobic degradation.

- Soil toxicity based on equilibrium partitioning.

Table 18 Soil risk quotients

Carbon #	12	13	14	15	16	18	**Total RCR**
EO=2.7	4.5E-03	2.1E-02	6.8E-02	3.0E-02	2.5E-02	3.2E-03	**0.15**

8 CONCLUSIONS

This assessment shows that the use of AES in HERA applications results in risk characterization ratios (Σ(PEC/PNEC)) less than one. To demonstrate this, higher tier exposure and effects data were needed. PEC values were estimated based on simulation test data for removal in wastewater treatment plants and receiving waters and PNEC values were based on chronic effects data.

9 CONTRIBUTORS TO THIS RISK ASSESSMENT

This risk assessment was developed by experts from the following companies: Cognis, Henkel, Procter&Gamble, and Shell Chemicals (Lead). Additional input was given by the HERA Environmental Task Force.

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11 ANNEXES

Annex 1 CAS # covered in family

CAS Number	CAS Description
27028-82-6	Ethanol, 2,2',2"-nitrilotris-, compd. with a-sulfo-w-(dodecyloxy)poly(oxy-1,2-ethanediyl) (1:1)
54116-08-4	Poly(oxy-1,2-ethanediyl), a-sulfo-w-tridecyloxy)-, sodium salt
67762-19-0	Poly(oxy-1,2-ethanediyl), a-sulfo-w-hydroxy-, C10-16-alkyl ethers, ammonium salts
68037-05-8	Poly(oxy-1,2-ethanediyl), a-sulfo-w-hydroxy-, C6-10-alkyl ethers, ammonium salts
68037-06-9	Poly(oxy-1,2-ethanediyl), a-sulfo-w-hydroxy-, C6-10-alkyl ethers
68540-47-6	Ethanol, 2,2',2"-nitrilotris-, compd. with a-sulfo-w-(tetradecyloxy)poly(oxy-1,2-ethanediyl) (1:1)
68585-34-2	Poly(oxy-1,2-ethanediyl), a-sulfo-w-hydroxy-, C10-16-alkyl ethers, sodium salts
68585-40-0	Poly(oxy-1,2-ethanediyl), a-sulfo-w-hydroxy-, C16-18-alkyl ethers, sodium salts
68891-38-3	Poly(oxy-1,2-ethanediyl), a-sulfo-w-hydroxy-, C12-14-alkyl ethers, sodium salts
96130-61-9	Poly(oxy-1,2-ethanediyl), a-sulfo-w-hydroxy-, C9-11-alkyl ethers, sodium salts
105859-96-9	Ethanol, 2,2',2"-nitrilotris-, compds. with polyethylene glycol hydrogen sulfate C11-15-sec-alkyl ether ammonium salts
125301-92-0	Poly(oxy-1,2-ethanediyl), a-sulfo-w-hydroxy-, C12-15-alkyl ethers, sodium salts
125304-06-5	Ethanol, 2,2',2"-nitrilotris-, compds. with polyethylene glycol hydrogen sulfate C16-18-alkyl ether
129783-23-9	Ethanol, 2,2'-iminobis-, compds. with polyethylene glycol hydrogen sulfate C12-15-alkyl ethers
157627-92-4	Alcohols, C10-16, ethoxylated, sulfates, mono(hydroxyethyl)ammonium salts (>1 <2.5 mol EO)
157707-82-9	Alcohols, C14-16, ethoxylated, sulfates, sodium salts (>1 <2.5 mol EO)
162201-45-8	Ethanol, 2-amino-, compds. with polyethylene glycol hydrogen sulfate C12-15-alkyl ethers

174450-50-1	Alcohol, C12-14, ethoxylated, sulfates, triisopropanolamine salts
102783-14-2	Poly(oxy-1,2-ethanediyl), a-sulfo-w-hydroxy-, C10-18-alkyl ethers, sodium salts
9004-82-4	Sodium lauryl ether sulfate
25231-22-5	Poly(oxy-1,2-ethanediyl), .alpha.-[(tridecyloxy)sulfonyl]-.omega.-hydroxy-, sodium salt
34431-25-9	Polyethylene glycol octyl ether sulfate, sodium salt
52286-19-8	Polyethylene glycol decyl ether sulfate, ammonium salt
67762-21-4	Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-, C10-16-alkyl ethers, magnesium salts
68081-91-4	Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-, C12-18-alkyl ethers, sodium salts
68184-04-3	2-Aminoethanol compd. with .alpha.-sulfo-.omega.-(dodecyloxy)poly(oxy-1,2-ethanediyl) (1:1)
68610-22-0	Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-, C12-18-alkyl ethers, ammonium salts
68891-29-2	Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-, C8-10-alkyl ethers, ammonium salts
68891-30-5	Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-, C11-15-branched alkyl ethers, ammonium salts
73665-22-2	Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-, C6-10-alkyl ethers, sodium salts
157627-95-7	Poly(1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-C16-18 and C18 unsaturated alkyl ethers, sodium salts
160104-51-8	Poly(1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-C12-14 alkyl ethers, magnesium salts
160104-52-9	Poly(1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-C16-18 and C18 unsaturated alkyl ethers, magnesium salts
67762-19-0	Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-, C10-16-alkyl ethers, ammonium salts
13150-00-0	Ethanol, 2-[2-[2-(dodecyloxy)ethoxy]ethoxy]-, hydrogen sulfate, sodium salt
32612-48-9	Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-(dodecyloxy)-, ammonium salt

Annex 2 Physchem Properties

All values estimated by interpolation of values for EO2 and EO3 calculated using SRC software

EO2.7 – Average for HERA applications

Carbon #	**12**	**13**	**14**	**15**	**16**	**18**
Molecular weight (g mol^{-1})	407	422	436	450	464	492
Melting point (°C)	298	304	309	315	320	331
Boiling point (°C)	684	695	707	719	730	754
Vapour pressure at 25°C (Pa)	1.2E-13	4.9E-14	2.1E-14	8.8E-15	3.8E-15	6.2E-16
Octanol-water partition coefficient (log_{10}) SRC	0.95	1.4	1.9	2.4	2.9	3.9
Water solubility (mg l^{-1})	425	133	41	13	4.0	0.38

EO2.4 – Average for total captive tonnage

Carbon #	**12**	**13**	**14**	**15**	**16**	**18**
Molecular weight (g mol^{-1})	394	409	423	437	451	479
Melting point (°C)	293	299	304	310	315	326
Boiling point (°C)	673	684	696	708	719	743
Vapour pressure at 25°C (Pa)	2.1E-13	8.8E-14	3.8E-14	1.6E-14	6.9E-15	1.1E-15
Octanol-water partition coefficient (log_{10}) SRC	1.0	1.5	2.0	2.5	3.0	4.0
Water solubility (mg l^{-1})	437	136	42	13	4.1	0.39

Annex 3 RCR based on Total Tonnage

PEC values have been calculated for the total EU-captive tonnage using the same assumptions as used for the HERA tonnage. Export tonnages have been omitted in estimating PEC_{local} values.

PEC - Simpletreat estimates

Carbon #	12	13	14	15	16	18
Local PEC surface water (mg/l)	0.16	2.3E-2	6.5E-2	6.1E-3	5.7E-3	1.7E-3
Local PEC sediment (mg/kg wwt)	0.16	2.9E-2	0.13	2.3E-2	4.7E-2	8.0E-2
Local PEC agric 30 d (mg/kg wwt)	4.1E-3	1.5E-3	1.1E-2	2.5E-3	5.8E-3	1.0E-2
Local PEC agric 30 d with 87% anaerobic degradation (mg/kg wwt)	5.3E-4	2.0E-4	1.4E-3	3.3E-4	7.5E-4	1.3E-3
PECstp microorgs (mg/l)	1.5	0.22	0.62	5.9E-2	5.5E-2	1.6E-2
Regional PEC surface water total (mg/l)	6.9E-3	1.0E-3	2.8E-3	2.7E-4	2.5E-4	8.3E-5

PEC - Simulation test degradation estimates

Scaling the STP fate to 97.5% degradation, as was done for the HERA tonnage, reduces the PEC values to:

Carbon #	12	13	14	15	16	18
Local PEC surface water (mg/l)	3.6E-2	5.4E-3	1.5E-2	1.4E-3	1.1E-3	4.4E-4
Local PEC sediment (mg/kg wwt)	3.5E-2	6.6E-3	2.9E-2	5.2E-3	9.1E-3	2.1E-2
Local PEC agric 30 d (mg/kg wwt)	4.6E-3	1.7E-3	1.2E-2	2.8E-3	6.5E-3	1.1E-2
Local PEC agric 30 d with 87% anaerobic degradation (mg/kg wwt)	6.0E-4	2.2E-4	1.6E-3	3.6E-4	8.4E-4	1.4E-3
PECstp microorgs (mg/l)	0.30	4.4E-2	0.12	1.2E-2	9.1E-3	3.7E-3
Regional PEC surface water total (mg/l)	5.7E-3	8.30E-4	2.3E-3	2.2E-4	2.1E-4	7.0E-5

PNEC

PNEC values (mg/l) were derived using the equation in Section 6.2.3:

	Carbon #					
	12	13	14	15	16	18
Aquatic (mg/l)	0.23	0.066	0.033	0.03	0.05	0.78
Soil (mg/kg)	3.1E-02	9.3E-03	4.9E-03	4.7E-03	8.1E-03	0.14

Indirect Exposure

AES with EO=2.4 uptake by Humans – as calculated with EUSES*

AS Fraction	Regional (mg/kg/day)		Local (mg/kg/day)	
	Drinking Water	Total Food + Water Uptake	Drinking Water	Total Food + Water Uptake
C12	1.6E-4	1.9E-4	1.0E-3	1.2E-3
C13	2.4E-5	3.3E-5	1.5E-4	2.0E-4
C14	6.6E-5	1.2E-4	4.2E-4	7.3E-4
C15	6.3E-6	1.7E-5	4.0E-5	1.1E-4
C16	5.9E-6	3.1E-5	3.2E-5	1.7E-4
C18	2.0E-6	5.8E-5	1.3E-5	3.7E-4

*EUSES defaults modified according to the HERA Detergent Scenario and taking account of 97.5% degradation in STP and 87% anaerobic degradation in sludge

RCR

Carbon #	12	13	14	15	16	18	**Total RCR**
Aquatic	0.15	8.2E-02	0.45	4.6E-02	2.2E-02	5.6E-04	0.72
Soil	1.9E-2	2.4E-2	0.31	7.7E-2	0.14	1.0E-2	0.55