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PREDICTED NO-EFFECT CONCENTRATIONS AND RISK CHARACTERIZATION OF FOUR SURFACTANTS: LINEAR ALKYL BENZENE SULFONATE, ALCOHOL ETHOXYLATES, ALCOHOL ETHOXYLATED SULFATES, AND SOAP

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Abstract—Assessment of aquatic effects requires the derivation of a predicted no-effect concentration (PNEC). In the framework of the Dutch ''Plan of Action Laundry and Cleaning Products,'' PNECs were derived for linear alkyl benzene sulfonate (LAS), alcohol ethoxylates (AE), alcohol ethoxylated sulfates (AES), and soap. All stages in an aquatic effects assessment were used: initial (assessment factors based mainly on short-term toxicity data), refined (statistical extrapolation based on long-term toxicity data), and comprehensive (field studies). Where necessary (i.e., where other structures had been tested in toxicity tests), the toxicity data were normalized to these structures using quantitative structure–activity relationships (QSARs) for short-term toxicity. Results from statistical extrapolation were compared with field no observed effect concentrations (NOECs), and a final PNEC was derived. Final PNECs for LAS, AE, AES, and soap were 250, 110, 400, and 27 μg/L, respectively. These PNECs were compared with predicted environmental concentrations (PECs) in surface water that were derived from monitoring results of removal of these surfactants in seven representative wastewater treatment plants. It is concluded that for LAS, AE, and AES, the PECs in the environment are about 50 to 100 times lower than the PNECs. The PEC for soap is about equal to the PNEC that is based on acute toxicity data. However, because the available chronic toxicity data for soap demonstrate that this substance is not more toxic than the other three surfactants, there is no reason for concern. On the basis of the results of the risk characterization, it has been concluded in the Netherlands that in properly functioning wastewater treatment plants, the risks for the aquatic compartment from the use of LAS, AE, AES, and soap are low.

Keywords—Surfactants Linear alkyl benzene sulfonate Alcohol ethoxylate Alcohol ethoxylated sulfates Soap

INTRODUCTION

Surfactants constitute one of the major groups of chemical substances that are present in consumer products. Throughout the world, about 4 to 5 million tons per year of anionic and nonionic surfactants are used in household and industrial cleaning products. Because the major part of this consumption eventually enters the environment either directly or after some sort of sewage treatment, the assessment of the risks of these substances is extremely important. The Dutch Soap Association (NVZ) and the Dutch Ministry of Housing, Physical Planning and the Environment (VROM) voluntarily agreed in 1991 on the ''Plan of Action Laundry and Cleaning Products'' [1]. The goal of this plan of action was to systematically evaluate and, if considered necessary, to reduce the environmental loading of detergent and cleaning products, taking into account minimum hygiene needs. A priority list of all detergent ingredients with a use volume of >100 tons per year was developed in 1991 by the NVZ and the National Institute of Public Health and the Environment (RIVM). The NVZ and VROM agreed to initiate the evaluation with the first four substances listed: linear alkyl benzene sulfonate (LAS), alcohol ethoxylates (AE), alcohol ethoxylated sulfates (AES), and soap. These compounds constituted about 90% of the volume of surfactants on the Dutch market.

To be able to jointly assess the environmental risks of the four ingredients, it is necessary to first agree on the risk assessment methodology that should be applied. A workshop entitled ''Environmental Risk Assessment of Detergents'' was organized on April 9, 1992, by NVZ, VROM, and RIVM, resulting in an agreed-on framework for the risk assessment of the priority surfactants [2]. In the adopted tiered approach, the risk is determined by a comparison of the predicted no-effect concentration (PNEC) to organisms in ecosystems with the predicted environmental concentration (PEC). The sequential test program or assessment proceeds further when the PEC > PNEC. This tiered approach ensures that higher-quality data are used beyond the so-called base-set data that comprise only acute toxicity data for three species and associated computer-modeled predictions.

The results of the environmental risk assessment for LAS, AE, AES, and soap were presented at an international workshop organized by the Association Internationale de la Savonnerie et de la Détergence and the Comité Européen des Agents de Surface et leurs Intermédiaires Organiques in Limelette (Belgium), November 28–29, 1995 [3]. The detailed results of the environmental monitoring and the derivation of

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PECs are described in separate papers by Matthijs et al. [4] and Feijtel et al. [5], respectively. The present paper describes the results of the derivation of the PNEC values for surface water and the risk characterization step where the comparison between the PEC and PNEC values is made.

DERIVATION OF PREDICTED NO-EFFECT CONCENTRATION

Aquatic effects assessment is a process comprising three stages: initial, refined, and comprehensive [6]. For three of the four substances considered (LAS, AE, and AES), it was possible to go through all stages of effects assessment.

Initial effects assessment

In this stage of the process, assessment factors are applied to toxicity data to derive the PNEC. The numerical value of the assessment factor depends on the number and kind of data available. The Appendix presents the assessment factors used for aquatic organisms [7].

Selection of the data for use in the calculation of the PNEC was based on the following criteria [8]. If for a single species several L(E)C50 or NOEC values were available for different effect parameters, the lowest was selected, and if for a single species several L(E)C50 or NOEC values were available for the same effect parameter, a geometric mean value was calculated.

Refined effects assessment

In this stage of the process, a statistical extrapolation method is used to derive the PNEC. In general, statistical extrapolation methods work as follows. Chronic toxicity data (NOECs) are log transformed and fitted according to a distribution function, and a prescribed percentile of that distribution is used to obtain the PNEC. To date, most authors have set this percentile at 95%. This means that for 5% of the species of the community, their NOEC may be exceeded.

Several distribution functions have been proposed. The U.S. Environmental Protection Agency (U.S. EPA) Office of Water [9] assumes a log-triangular function, Van Straalen and Denneman [10] a log-logistic function, and Wagner and Løkke [11] a lognormal function. Aldenberg and Slob [12] refined the way to estimate the uncertainty of the 95th percentile by introducing confidence levels. In the method of Aldenberg and Slob, the 95% protection level can be calculated with a 50% and 95% confidence level [12]. In the Netherlands, the PNEC is calculated as the 95% protection level with 50% confidence [8]. To indicate the uncertainty in the estimation of the PNEC, the 95% protection level with both 50 and 95% confidence is calculated.

The method uses the NOEC for the most sensitive endpoint per species as input data and is applied when at least four long-term NOEC values for different taxonomic groups are available. In the method of Aldenberg and Slob, long-term NOEC values used as input data are selected in the same way as described previously for initial effects assessment.

Comprehensive effects assessment

A wide variety of designs of laboratory and field model ecosystem studies have been developed [13]. Here the term ''field studies'' will be used for all studies that are not single-species laboratory tests. Field testing and the incorporation of the results of such tests in effects assessment is a rapidly evolving field in ecotoxicology. Several reasons can be given for field studies being carried out to refine the risk assessment [3]: to give more realistic conditions of exposure than are obtained in standard laboratory toxicity tests, to obtain effects data on a wider variety of taxa than can readily be tested in the laboratory, to allow simultaneous study of fate and effects, and to gain insight into the ecological relevance of effects.

To date, no fully elaborated strategy has been available that describes how these tests should be used in deriving PNECs. Here the following strategy was followed. A PNEC is derived on the basis of single-species toxicity data using extrapolation methods, and NOECs from field studies are compared with the PNEC from single-species studies. If the values differ significantly, possible causes of the differences should be considered and a decision made on the basis of expert judgement to derive the final PNEC. It is realized that neither PNECs from extrapolated single-species results nor those from field studies can give the exact value of a no-effect concentration for all ecosystems. Uncertainty in both PNECs is always present.

NORMALIZATION

The ecotoxicological data set for LAS, AE, and AES contains data for test compounds differing in the number of ethoxylate groups (EO) and/or alkyl chain length. As toxicity depends on these characteristics of the chemical structure, toxicity data are not always directly comparable within a surfactant group (e.g., AES). This means that for each group of surfactants, toxicity data must be normalized to a specified number of EO groups and/or a specified alkyl chain length. For each group of surfactants, the data have been normalized, where necessary, to the structures typically present in the environment. On the basis of results from the monitoring study [4] these are $C_{11.6}$ LAS, $C_{13.3}$ $EO_{8.2}$ AE, and $C_{12.5}$ $EO_{3.4}$ AES.

The normalization procedure was based on the use of quantitative structure–activity relationships (QSARs). Ideally, long-term NOECs should be normalized using QSARs for long-term toxicity. However, because no reliable long-term QSARs were available for these surfactants, QSARs for short-term toxicity were used. Normalization was carried out using the following procedure.

The log K_{ow} was calculated for the normalized structure (the specified compounds stated previously) and that for which toxicity was experimentally determined (hereafter referred to as ''tested structure''), using the Leo and Hansch method [14] with the modification for alkyl chain branching by Roberts [15], which calculates log K_{ow} values for surfactants using a position-dependent branching factor (PDBF). An increment of 0.54 is used for a CH_2 unit on the basis of the method of Leo and Hansch [14]. An increment of −0.10 is used for each EO group on the basis of the work of Roberts [15].

The EC50 values for both structures were calculated using the following QSARs for short-term toxicity:

$$\text{for AE:} \quad \log(1/\text{EC50}) = 0.87 \log K_{ow} + 1.13 \quad [16]$$

$$\text{for LAS and AES:} \quad \log(1/\text{EC50}) = 0.63 \log K_{ow} + 2.52 \quad [17]$$

The ratio between the predicted EC50s for the normalized and the tested structure was calculated. The NOEC of the tested structure was multiplied by this ratio to obtain the NOEC for the normalized structure.

For example, for a NOEC of 0.9 mg/L for $C_{12.6}$ LAS, the procedure is as follows. The calculated log K_{ow} and molecular weight for $C_{12.6}$ LAS are 3.86 and 356, respectively. Using the QSAR given previously, this leads to an EC50 of 4.0 mg/L.

Table 1. Geometric mean short term L(E)C50 values (mg/L) for species for which more than four data are available [18]

Species	Geometric mean L(E)C50 (mgL)	*n*
Daphnia magna	4.7	139
Gammarus pulex	6.2	25
Mysidopsis bahia	1.7	6
Penaeus duorarum	49	5
Carassius auratus	9.5	46
Lepomis macrochirus	3.0	88
Leuciscus idus melonatus	2.9	11
Oncorhynchus mykiss	3.0	10
Oryzias latipes	13	5
Pimephales promelas	3.2	35
Poecilia reticulata	3.8	9

For $C_{11.6}$ LAS, the calculated log K_{ow} and molecular weight are 3.32 and 342, respectively, leading to an EC50 of 8.4 mg/L. The ratio between the predicted EC50 values for $C_{11.6}$ LAS and $C_{12.6}$ LAS is 2.1. Multiplying the NOEC of 0.9 mg/L with this factor leads to a normalized NOEC of 1.9 mg/L (for $C_{11.6}$ LAS).

PNEC FOR LAS

The PNEC for LAS was derived from data collected by BKH consultants and several literature reviews on the effects of LAS on aquatic organisms: Kimerle, Painter, SDA, and IPCS [18–23].

Short-term effects

The acute toxicity data for LAS are summarized in Table 1. The intraspecies variation is almost as high as the interspecies variation [18]; for example, for *Daphnia magna* and *Pimephales promelas,* L(E)C50 values are reported to range from 0.26 to 55 mg/L and from 0.40 to 100 mg/L, respectively. These large ranges are caused by differences in the LAS tested with respect to alkyl chain length and/or phenyl isomer distribution and differences in test design. Thus, the variability of short-term data does not exclusively reflect the diversity of species sensitivity [24]. The interspecies variation decreases considerably when the geometric mean value per species is calculated.

Long-term effects

Long-term toxicity data are summarized in Table 2. Toxicity data are highly variable for algae. For example, for *Microcystis* spp. in one test an EC50 and NOEC of 0.05 and 0.09 mg/L, respectively, were obtained for $C_{11.8}$ LAS, whereas five EC50 values are reported by BKH [19]: 0.9 mg/L for $C_{11.8}$ LAS, 4.1 mg/L for $C_{11.9}$ LAS, 5.0 mg/L for $C_{13.3}$ LAS, 10 mg/L for $C_{11.6}$ LAS, and 32 mg/L for LAS (unspecified). Test durations are 72 to 120 h. To derive a NOEC for algae, the EC50 values were divided by 3 [25]. Subsequently, the NOEC values were normalized and a geometric mean was calculated for each species, including the normalized NOEC values already present.

Marine species (*M. bahia, C. virginica, M. edulis,* and *L. yokohamae*) are more sensitive than freshwater species to LAS. The average normalized NOEC for marine and freshwater species is 0.055 ± 0.045 mg/L (n = 4) and 4.0 ± 4.3 mg/L (n = 15), respectively.

Table 2. Geometric mean normalized long term no-observed-effect-concentration (NOEC) values (mg/L) for each species for linear alkyl benzene sulfonates (LAS); NOECs are normalized to $C_{11.6}$ LAS

Species	Geometric mean NOEC (mg/L)	*n*
Chlamydomonas reinhardi	12	1
Chlorella kessleri	3.5	1
Microcystus sp.	0.80	4
Plectonema boryanum	15	1
Scenedesmus subspicatus	7.7	4
Selenastrum sp.	3.8	9
Ceriodaphnia sp.	3.2	1
Daphnia magna	1.4	12
Mysidopsis bahia[a]	0.12	2
Chironomus riparius	2.8	1
Paratanytarsus parthenogenica	3.4	1
Crassostrea virginica[a]	0.025	1
Mytilus edulis[a]	0.025	1
Brachydanio rerio	2.3	1
Limanda yokohamae[a]	0.05	1
Pimephales promelas	0.87	14
Poecilia reticulata	3.2	1
Oncorhynchus mykiss	0.34	7
Tilapia mossambica	0.25	1

[a] Marine species.

Derivation of the PNEC based on single-species laboratory studies

Long-term toxicity data are available for four taxonomic groups, so the statistical method of Aldenberg and Slob [12] was applied. Input data used were the NOECs shown in Table 2. However, as marine species are clearly more sensitive to LAS than freshwater species, only data for the latter organisms were used to derive a PNEC for freshwater systems in the Netherlands. A PNEC of 320 μg/L was obtained with a 50/95 confidence ratio of 3.2. The PNEC of 320 μg/L is somewhat higher than the lowest available freshwater NOEC of 250 μg/L for *Tilapia mossambica*.

Comparison of PNEC based on single-species laboratory studies with results from field studies

The LAS has been tested extensively in field studies. Systems used varied from outdoor experimental streams and ponds to closed bottles in lakes to indoor systems containing aquaria with or without sediment. Although no internationally agreed protocols exist for the design of field studies, some quality criteria were defined [18], such as the presence of a clear concentration-effects relationship and continuous or frequent dosing together with analytical verification of the test concentrations. Results from field studies with LAS are summarized in Table 3 [18, 26].

The NOECs derived from field studies with microorganisms vary from 0.09 to 20 mg/L. The value of 0.09 mg/L for photosynthetic response of phytoplankton is considered an outlier, as the LOEC in the study of Lewis and Hamm [27] was 0.87 mg/L, and all other field studies in which phytoplankton was included resulted in NOEC values higher than 0.24 mg/L. The NOECs derived from ecosystem studies—having a higher degree of realism than the field studies with microorganisms and phytoplankton—varied from <0.25 to 3.5 mg/L. From all studies it was judged that the lower limit of NOECs from field studies with higher and lower taxonomic groups is 0.25 to 0.50 mg/L for C_{12} LAS.

Table 3. Results from field studies with linear alkyl benzene sulfonates

Taxonomic groups	No-observed-effect-concentration (mg/L)	Reference
Multispecies studies with microorganisms		
Bacteria	0.5	[53]
Bacteria	>5.0	[53]
Bacteria	20	[53]
Phytoplankton	0.09	[27]
Phytoplankton	0.24	[28]
Periphyton	1.1	[54]
Periphyton	9.8	[54]
Bacteria, algae, protozoans	0.3	[55]
Ecosystem studies		
Bacteria, periphyton, crustaceans, insects, fish	1.0	[531
Bacteria, plants, crustaceans, insects, fish	0.2–0.5	[53]
Phytoplankton, rotifers, chironomids, zooplankton	<0.25	[29]
Periphyton, invertebrates, snails, amphipods, fish	<0.36	[30]
Phytoplankton, plants, cyclopodia, cladocera	3.5	[56]
Phytoplankton, zooplankton, periphyton, (Macro) invertebrates, fish	0.12	[26]

The PNEC value of 0.32 mg/L, based on single-species laboratory test results, is in good agreement with the NOEC from field studies of 0.25 to 0.50 mg/L. Several field studies showed minor effects at concentrations at the lower limit of this range: Lewis [28], NOEC of 0.24 mg/L for relative abundance of phytoplankton; Lewis and Hamm [27], NOEC of 0.09 mg/L for photosynthetic response of phytoplankton; Chattopadhyay and Konar [29], NOEC <0.25 mg/L for number and wet weight of chironomids; Fairchild et al. [30], NOEC <0.36 mg/L for fish growth and survival; and Tattersfield et al. [26], NOEC of 0.12 mg/L. Thus, a final PNEC of 0.25 mg/L, equal to the lower limit of the field NOECs, is derived for $C_{11.6}$ LAS.

PNEC FOR AE

Short-term effects

A large database is available on the short-term effects of AE on bacteria, algae, diatoms, worms, insects, mollusks, crustaceans, fish, and aquatic plants (freshwater as well as marine organisms). For $C_{12–15}$ $EO_{3–10}$ AE, these data are taken from BKH [31] and are summarized in Table 4.

As for LAS, intra- and interspecies variability is large, especially for algae. One reason is the chemical heterogeneity of AE, which in commercial applications is a mixture of varying alkyl chain and EO groups. Also, most commercial products consist of mixtures of homologues; especially the number of EO groups can vary over a broad range. A further complication is the presence of about 2 to 5% of nonethoxylated alcohol and 0.5 to 2.0% polyethyleneglycol.

Long-term effects

Long-term toxicity data are available for several taxonomic groups: blue algae, diatoms, green algae, rotifers, crustaceans, mollusks, fish, and worms (Table 5). As for LAS, the toxicity data for algae and especially for *Selenastrum capricornutum* vary greatly. For the latter, EC50 values range from 0.09 to 10 mg/L, whereas NOEC values range from 0.60 to 1.9 mg/L. A statistical analysis showed no clear relationship between alkyl chain length, number of EO groups, and toxicity [31]. Explanations have already been mentioned, including variability in test design. The static test design of the algal test can be added as another confounding factor.

Marine species (*C. sapidus, P. duorarum, M. edulis,* and *F. heteroclitus*) appear somewhat less sensitive than freshwater species. On the basis of the original data, the average NOECs for marine and freshwater species are 3.3 ± 4.5 mg/L and 0.71 ± 0.71 mg/L, respectively. Both species were used to derive a PNEC from single-species tests.

Derivation of PNEC based on single-species laboratory studies

As long-term data are available for more than four taxonomic groups, the statistical method of Aldenberg and Slob [12] was applied. Using normalized NOEC values, the PNEC of 110 μg/L was obtained using data for freshwater as well as marine species. The 50/95 confidence ratio is 3.7.

Comparison of PNEC based on single-species laboratory studies with results from field studies

Several field studies were available for AE. All were ecosystem studies. Results are presented in Table 6. Normalized field NOECs vary from 42 to 380 μg/L. Critical endpoints were density of the (macro)invertebrates *Gammarus pulex* [32,33], *Simuliidae* [34–37], and *Simulium* spp. [38]; reproduction of *Pimephales promelas* [34,39]; and leaf processing rate [34,35].

The PNEC of 110 μg/L, based on single-species data, is in agreement with the field NOECs presented in Table 6. The field NOEC of 42 μg/L is more than a factor of two lower than the single-species PNEC. However, in this test an AE with a relatively short alkyl chain was tested, and normalization was over three alkyl chain units from $C_{9/11}$ to $C_{13.3}$, which is considered less reliable. Thus, 110 μg/L was confirmed as the final PNEC for $C_{13.3}$ $EO_{8.2}$ AE.

PNEC FOR AES

Compared to the ecotoxicological databases for LAS and AE, the one for the effects of AES on aquatic organisms is relatively small. Most of the data are on short-term effects [40]. The interpretation of tests with commercial products must be done with care because these products may contain other constituents in significant amounts, such as unsulfated alkyl ethoxylates and alkyl sulfate, and biodegradation of the parent compound may have occurred, as most of the tests were static without analysis of the test substance.

Table 4. Short-term data for $C_{12–15}$ $EO_{3–10}$ alcohol ethoxylates [31]

Taxonomic group	Species	Chain length	EO	L(E)C50 (mg/L)	*n*
Bacteria	*Photobacterium phosphoreum*	13.4	9	1.5	1
Algae	*Mycrocystis aeruginosa*	13–15	6–9	0.6–30	3
	Navicula pelliculosa	15	6	0.28	1
	Navicula seminulum	15	7	1.34	1
	Nitzschia fonticola	13	9	0.2	1
	Scenedesmus subspicatus	15	10	1.53	1
	Selenastrum capricornutum	13–15	4–9	0.09–10	10
Crustaceans	*Asellus* sp.	15	7	6.2	1
	Callinectes sapidus	15	7	30.9	1
	Crangon crangon	14	3–7	1.4–4.8	2
	Ceriodaphnia dubia	15	7	0.66	1
	Daphnia magna	13–15	3–10	0.41–4.17	17
	Daphnia sp.	13–14	6–9	0.76–13	5
	Gammarus sp.	15	7	1.4	1
	Mysidopsis bahia	13–15	7-10	0.2–2.24	2
	Penaeus duorarum	15	7	0.98	1
Insects	*Culex pipiens*	12–15	3–9	5–44	5
	Paratanytarsus parthenogenica	15	7	5	1
Molluscs	*Biomophalaria glabrata*	14	9	11	1
	Mytilus edulis	14	9	0.11	1
	Crassostrea virginica	14	9	0.11	1
Worms	*Dero* sp.	15	7	2.6	1
	Dugesia gonocephala	15	6	1	1
	Oligochaeta sp.	15	7	2.6	1
	Planaria sp.	15	7	1	1
	Rhabditis sp.	15	7	6.8	1
Fish	*Brachydanio rerio*	13–15	4–10	1.2–2.3	5
	Carassius auratus	13–14	6–9	1.4–5.1	4
	Ictalurus punctatus	14	9	1.2	1
	Lepomis macrochirus	13–15	3–9	0.7–4.8	4
	Leuciscus idus melonatus	13–15	3–10	0.9–3.5	8
	Limanda limanda	14	3	1.8	1
	Oryzias latipes	12	3–8	2.4–3.5	4
	Oncorhynchus mykiss	13–15	3–10	0.78–2.4	7
	Pimephales promelas	13–15	3–9	0.84–7.7	11
	Rasbora heteromorpha	13	8	1.2	1
	Salmo salar	12	4	1.5	1
	Salmo trutta	13	8	0.8	1
Plants	*Lemna minor*	15	7	1.9	1

Table 5. Geometric mean normalized long-term no-observed-effect-concentration (NOEC) values (mg/L) for each species for alcohol ethoxylates; NOECs are normalized to $C_{13.3}$ $EO_{8.2}$ AE

Species	Normalized NOEC (mg/L)	*n*
Microcystis aeruginosa	1.9	1
Navicula pelliculosa	0.93	1
Navicula seminulum	8.7	3
Selenastrum capricornutum	0.74	3
Scenedesmus subspicatus	1.3	6
Chlorella vulgaris	0.20	2
Brachionus calyciflorus	1.3	1
Callinectes sapidus	48	1
Ceriodaphnia dubia	0.86	4
Daphnia magna	0.59	13
Penaeus duorarum	2.7	1
Mytilus edulis	5.5	1
Brachydanio rerio	1.5	2
Fundulus heteroclitus	4.8	1
Pimephales promelas	0.72	5
Dugesia gonocephala	0.17	1
Navicula humilis	0.17	1

Short-term effects

Results from the short-term tests are summarized in Table 7. Results from short-term tests are available for green algae, crustaceans, and fish. The L(E)C50 values are 3.5 to 10, 4.2 to 350, and 0.39 to 94.4 mg/L for algae, crustaceans, and fish, respectively. High L(E)C50 values are found for AES with a short alkyl chain length: LC50 values below 1 mg/L are reported for *Cyprinodon variegatus* (C_{14}–C_{16} $EO_{2.25}$ AES) and *Pimephales promelas* (C_{16} $EO_{2.4}$ AES and C_{14}–C_{16} $EO_{2.25}$ AES). On the basis of the short-term data, fish seem to be more susceptible to AES than other taxonomic groups.

Long-term effects

Long-term test results are available for green algae, rotifers, crustaceans, and fish (Table 8).

Derivation of PNEC based on single-species laboratory

As long-term data are available for more than four taxonomic groups, the statistical method of Aldenberg and Slob [12] was applied. Using normalized NOEC values, the PNEC is 650 μg/L with a 50/95 confidence ratio of 3.4. The PNEC is somewhat higher than the low short-term LC50 values for *Cyprinodon variegatus* and *Pimephales promelas*. However, these LC50 values were obtained for compounds with an alkyl

Table 6. Results from field studies with alcohol ethoxylates; no-observed-effect-concentrations (NOECs) are normalized to $C_{13.3}$ $EO_{8.2}$ AE

Ecosystem study type	Test substance	Normalized NOEC (μg/L)	Reference
Outdoor artificial streams	$C_{12–15}$ EO_7	70–100	[32,33]
Stream mesocosms	$C_{9–11}$ EO_6	42	[34,39]
Experimental streams	$C_{14–15}$ EO_7	380	[34,35]
Stream mesocosm	$C_{12–13}$ $EO_{6.5}$	<200	[36,37]
Outdoor artificial streams	$C_{12–15}$ EO_9	68	[41]

chain length of C_{14} to C_{16} and C_{16}, whereas the PNEC has been derived for $C_{12.5}$.

Comparison of PNEC based on single-species laboratory studies with results from field studies

Several field studies are available for AES. Belanger and Rupe tested $C_{14–15}$; $EO_{2.17}$ to *Goniobasis* spp. and *Corbicula fluminea* in an experimental stream mesocosm for 8 weeks [41,42]. Five concentrations were tested, ranging from 14 to 730 μg/L. No effects were observed on survival, shell length, and growth of clams up to a measured concentration of 730 μg/L (normalized value 4.4 mg/L). For snails a NOEC of 75 μg/L, based on weight gain, was derived (normalized value 0.48 mg/L). Belanger et al. tested $C_{14–15}$ $EO_{2.17}$ AES to acclimated and unacclimated periphyton communities in laboratory microcosms for 28 d [42–44]. The main objective of the study was the validation of a periphyton community bioassay. Test concentrations were 54 and 608 μg/L. Significant acclimation effects were observed. On the basis of five community-level responses and 13 population endpoints, a NOEC of 608 μg/L was established (normalized value 3.7 mg/L). Belanger et al. tested $C_{14–15}$ $EO_{2.17}$ AES in a model stream ecosystem for 8 weeks [42–46]. Five concentrations were tested, ranging from 13 to 730 μg/L. One mayfly taxon, *Tricorythodes,* had a NOEC of 31 μg/L for density, whereas the one for biomass was 251 μg/L (normalized values 190 μg/L and 1.5 mg/L, respectively). Fifteen other invertebrate populations had NOECs of 251 μg/L or higher.

The tests with *Goniobasis* spp. and *Corbicula fluminea* can in fact be regarded as single-species tests. The NOECs from these studies are measured total concentrations in natural waters, whereas the NOECs from laboratory single-species studies are dissolved concentrations. As the difference between total and dissolved concentrations will be small because of minor sorptive losses for this surfactant, the normalized NOEC values of 4.4 and 0.48 mg/L are included in the data set used for the calculation of the PNEC, leading to a value of 400 μg/L with a 50/95 confidence ratio of 3.9.

The results from the field studies are in reasonable agreement with the normalized PNEC of 400 μg/L obtained from single-species tests. It must be stated that all field studies were carried out with $C_{14–15}$ $EO_{2.17}$ AES, whereas a variety of compounds were used in the single-species tests, differing not only in their alkyl chain length and number of EO groups but also in alkyl sulfate content. Also, the field study results were normalized from $C_{14–15}$ to $C_{12.5}$, leading to a considerable increase of the field NOECs by a factor of about six.

Field study results are both higher and lower than the normalized PNEC of 400 μg/L from single-species tests. The NOEC of 190 μg/L for *Tricorythodes* is somewhat lower, whereas the NOEC of 3.7 mg/L for periphyton is considerably higher. Clearly, endpoints in the periphyton community bioassay were less susceptible than effects on other taxonomic groups. As the model stream ecosystem study [44–46] is the most extensive one with respect to taxonomic groups and endpoints studied, comparison with this study is most appropriate. Considering this, there seems to be no reason to either lower or raise the PNEC on the basis of single-species toxicity data. Thus, 400 μg/L was confirmed as the final PNEC for $C_{12.5}$ $EO_{3.4}$ AES.

According to BKH [40], commercial AES contains 20 to 50% alkyl sulfates (AS). The PNEC is based on single-species toxicity tests performed with commercial AES. This means that measured concentrations for AES cannot be compared directly with the PNEC. Because AS has a different toxicity compared to AES, in principle the PNEC must be corrected; AES is less lipophilic than AS because of the presence of several EO groups, so AES is probably less toxic than AS with corresponding alkyl chain length. According to IPCS [23], the toxicity of AS is comparable to that of other anionic surfactants, such as LAS. This means that the comparison of the PEC for AES with the PNEC of 400 μg/L for AES may lead

Table 7. Short-term data for alcohol ethoxylated sulfates (mg/L) [40]

Test species	L(E)C50(mg/L)	*n*
Selenastrum capricornutum	3.5–10	2
Daphnia magna	4.2–72	9
Daphnia pulex	20.2	1
Penaeus duorarum	350	1
Crassostrea virginica	9	1
Brachydanio rerio	1.9–3.1	3
Carassius auratus	2.1–3.8	3
Cichlasoma nigrofasciatum	2.5–3.1	3
Cyprinodon variegatus	0.39–25	5
Lepomis macrochirus	1.11–74.5	4
Leuciscus idus melonatus	4.5–10	2
Oncorhynchus mykiss	1.9–94.4	9
Oryzias latipes	10–68	3
Pimephales promelas	0.7–13	8
Poecilia reticulata	2.1–2.4	3
Rasbora heteromorpha	3.9	1
Salmo trutta	1.5–1.6	2

Table 8. Geometric mean normalized long-term no-observed-effect-concentration (NOEC) values (mg/L) for each species for alcohol ethoxylated sulfate; NOECs are normalized to $C_{12.5}$ $EO_{3.4}$ AES [40]

Species	NOEC (mg/L)	*n*
Scenedesmus subspicatus	2.4	3
Selenastrum capricornutum	2.4	2
Brachionus calyciflorus	0.80	3
Daphnia magna	1.6	3
Pimephales promelas	1.2	2

Table 9. Ecotoxicological data for soap (mg/L) [47,49]

Unspecified alkyl chain length	
Short-term data for L(E)C50	
Pseudomonas fluorescens	134
Chlorella vulgaris	53
Microcystus aeruginosa	24
Daphnia magna	10, 42
Aedes aegyptii	4,233
Oryzias latipes	1,342
Poecilia reticulata	423
Fish (unknown species)	20
Carassius auratus	6.7
Xenopus laevis	423
Long-term data for NOEC	
Algae (unknown species)	10
Daphnia magna	10
Alkyl chain length of C_{12}–C_{14}	
Short-term data for L(E)C50	
Photobacterium phosphoreum	8.8
Scenedesmus subspicatus	53
Daphnia magna	3.3, 32, 48
Oryzias latipes	11, 118
Lepomis macrochirus	63
Oncorhynchus mykiss	42
Long term data: NOEC	
Brachydanio rerio	3.7
Alkyl chain length of C_{16}–C_{18}	
Short-term data for L(E)C50	
Photobacterium phosphoreum	250
Scenedesmus subspicatus	58, 140, 190
Daphnia magna	4.2, 25, 40
Gammarus pulex	88, 160
Oncorhynchus mykiss	0.6
Oncorhynchus kisuth	12, 12
Lepomis macrochirus	67
Oryzias latipes	125, 150, 217
Pimephales promelas	205

to an overestimation of the risk. A separate environmental risk assessment for AS should be carried out.

PNEC FOR SOAP

Short- and long-term effects

The database for ecotoxicological effects of soap on aquatic organisms is small. Most of the data are on short-term effects [47]. No clear conclusions can be drawn with respect to interspecies variation in the toxicity for soap and the influence of the alkyl chain length. The outcome of the tests seems to be highly influenced by test conditions, such as use of solvents, water hardness (possible formation of insoluble calcium and magnesium salts), and type of soap [47]. Actual concentrations were not measured in any of the tests.

BKH divided the data into three groups [47]: soaps with unspecified alkyl chain length (referred to as ''soap'' in the study), soaps with an alkyl chain length of C_{12} to C_{14} (Na-laurate, lauric acid, and Na-myristate), and soaps with an alkyl chain length of C_{16} to C_{18} (Na-oleate, oleic acid, palmitoleic acid, Na-palmitate, and hardened tallow soap). Results for these groups are presented in Table 9.

Short-term L(E)C50 values range from 6.7 to 4233 mg/L for unspecified alkyl chain length. Some values are clearly above the water solubility of the tested substance. The lowest value of 6.7 mg/L is not valid for prediction of effects in natural waters, as water hardness is reported as 0 mg $CaCO_3$/L [47]. The only long-term data available were a 96-h NOEC for algae and a 21-d NOEC for *Daphnia magna* determined by Canton and Slooff [48]. Short-term L(E)C50 for alkyl chain length C_{12} to C_{14} values range from 3.3 to 118 mg/L for bacteria, green algae, crustaceans, and fish. The lowest EC50 is for lauric acid tested on *Daphnia magna*. The only available long-term NOEC is from a 28-d growth test with sodium laurate, resulting in 3.7 mg/L for *Brachydanio rerio* [49].

Only short-term data are available for alkyl chain length C_{16} to C_{18}. The L(E)C50 values range from 0.6 to 250 mg/L for bacteria, green algae, crustaceans, and fish. The lowest value of 0.6 mg/L for *Oncorhynchus mykiss* is very low compared to the LC50 values for the other fish species. In contrast to the other values, a solvent was used in this test. However, no details on the amount used are available. In the only marine test available, using the sea urchin sperm toxicity test for *Strongylocentrolus purpuratus,* a solvent was also used [50]. Low EC50 values of 0.28 and 1.07 mg/L for linoleic and linolenic acid, respectively, for effects on fertilization are determined in this test. Ethanol was the solvent, but no adverse effects are reported for the solvent control. These low values are probably the result of the specific sensitivity of the test rather than the use of ethanol as a solvent, although evidence to the contrary is not available. Several L(E)C50 values are less reliable because precipitation was observed [47].

Derivation of PNEC based on single-species laboratory studies

Not enough long-term data are available to apply the statistical extrapolation method. Thus, assessment factors were used to derive a PNEC. This leads to the following values for the three groups. (1) Unspecified chain length: The lowest L(E)C50 value of 6.7 mg/L is considered invalid because of the low water hardness and thus is not used. The second-lowest value is an EC50 of 10 mg/L for *Daphnia magna*. There is also another short-term EC50 of 42 mg/L and a NOEC from a long-term study of 10 mg/L for this species. Because the test compound is not specified in the test, no geometric mean EC50 is calculated. Thus, the EC50 value of 10 mg/L was divided by 100, leading to a PNEC of 100 μg/L. (2) Alkyl chain length C_{12} to C_{14}: The lowest L(E)C50 value of 3.3 mg/L for crustaceans divided by 100 gives a PNEC of 33 μg/L. (3) Alkyl chain length C_{16} to C_{18}: The lowest L(E)C50 value is 0.6 mg/L for fish, leading to a PNEC of 6 μg/L, applying a factor 100.

The difference between the PNEC for an alkyl chain length of C_{16} to C_{18} and the other two PNEC values are a factor of 5.5 and 15. It is unclear whether the low value for C_{16} to C_{18} is caused by an outlier due to the use of a solvent. In theory, using a solvent does not increase the toxicity but leads to a maximum bioavailability of the test compound [51]. As in several other tests, some precipitation was observed; it may well be that the LC50 value of 0.6 mg/L is the ''true'' toxicity of oleic acid to *Oncorhynchus mykiss*. On the other hand, all other short-term values show a much lower toxicity of soap to aquatic organisms. On the basis of these considerations, the geometric mean of the three individual PNEC values was used to obtain a final PNEC of 27 μg/L.

FINAL PNECs

Final PNECs for the four surfactants are summarized in Table 10 together with the results from extrapolation methods and field studies. The value for soap must be considered an indicative value, as short-term toxicity results represent most of the data.

Table 10. Final predicted no-effect concentrations (PNEC) and negligible concentrations (NC) (μg/L, expressed as dissolved concentrations) and uncertainty factors for linear alkyl benzene sulfonate (LAS), alcohol ethoxylate (AE), alcohol ethoxylated sulfates (AES), and soap

Surfactant	PNEC based on single species data	Range of field NOECs	Final PNEC	NC	Uncertainty factor
$C_{11.6}$ LAS	320	250–500	250	2.5	2
$C_{13.3}$ $EO_{8.2}$ AE	110	42–380	110	1.1	5
$C_{12.5}$ $EO_{3.4}$ AES	400	190–3,700	400	4.0	5
Soap	27	—	27	0.27	10

It is concluded that for the discussed surfactants, PNECs calculated with the statistical extrapolation method of Aldenberg and Slob are in good agreement with results from field studies. The PNECs and underlying ecotoxicological data for LAS, AE, and AES show that these surfactants have a comparable toxicity. The PNEC for soap is a factor 4 to 15 lower than the others. This is due to the use of a high assessment factor: Comparing the short- and long-term toxicity data available for soap with the data for LAS, AE, and AES, it cannot be concluded that soap is the most toxic. On the contrary, the long-term data available for three species for soap show NOECs of 3.7 to 10 mg/L being higher than most NOECs for the other surfactants.

It is realized that extrapolated single-species NOECs as well as multispecies mesocosm NOECs can provide only estimates of a no-effect concentration for all ecosystems. Uncertainty is always present in both. For LAS, the uncertainty is considered to be low because of the presence of an extensive data set from laboratory short-term studies through to multispecies studies under more realistic conditions. For the other compounds, the uncertainty will be higher, especially for soap, as only short-term data are available. On the basis of the number and variation in results from short-term, long-term, and field studies and using expert judgment, the uncertainty in the PNEC values presented in Table 10 is estimated to range from a factor of 2 for LAS to a factor of 10 for soap.

In the Netherlands, the setting of quality objectives or standards for the environment is based on a risk policy. The policy document ''Premises for Risk Management'' [52] provides the basis for setting standards for the concentration of a substance or a group of substances in the environmental compartments. For all environmental compartments, substance concentrations can be calculated above which the risk on adverse effects is considered unacceptable: the maximum permissible concentration (MPC). In addition, the concentration at which the occurrence of adverse effects is considered to be negligible can be calculated: the negligible concentration (NC). Between these two risk limits is a so-called gray area where reduction of the risks is desirable. Normally, the NC is a fixed factor of 100 lower than the MPC so that the possible effects of mixtures of substances that are present in the environment can be taken into consideration. In general, the MPC is equivalent to the previously mentioned PNEC.

RISK CHARACTERIZATION

Risk characterization is the step where PEC and PNEC values are compared. The results of the comparison of the PNEC values for the four priority substances with the PEC values using different values for the in-stream removal in the river, as derived by Feijtel et al. [5], are shown in Table 11. From this comparison, it can be concluded that for LAS, AE, and AES, the estimated concentrations in the environment are close to or below the negligible concentrations. The situation for soap is different. The estimated concentrations in the environment are close to or somewhat higher than the PNEC. In the judgment of the acceptability of the PEC/PNEC ratios, it is very useful to take into account the uncertainty in both parameters. This uncertainty analysis may help in deciding whether and what type of subsequent policy action must be taken. Figure 1 shows PEC, PNEC, and NC values for the four substances, including their uncertainty ranges. The PEC values with an in-stream removal of 0.14/d are used, which probably still represents a worst-case situation [5]. From Figure 1 it can be seen that even when the highest PEC and the lowest PNEC are compared, the risks for LAS, AE, and AES are very low. Again, for soap risks are higher, but the uncertainty in the risk quotient is much larger because of the lack of chronic data for this substance.

On the basis of the results of the risk characterization, it has been concluded in the Netherlands that in properly functioning wastewater treatment plants, the risks for LAS, AE, and AES for the aquatic compartment are low. Concentrations are close to or below the negligible concentration. When in-stream removal is taken into account, the PEC for soap is about equal to the PNEC on the basis of acute toxicity data. However, because the available chronic toxicity data for soap demonstrate that this substance is not more toxic than the other three surfactants, and because of the uncertainties in the actual PEC for soap, it has been decided that no further risk reduction measures are needed.

Table 11. Predicted environmental concentration/predicted no-effect concentration (PEC/PNEC) and PEC/NC ratios for four surfactants assuming three different in-stream removal rates

	$k = 0$ d^{-1}		$k = 0.14$ d^{-1}		$k = 0.7$ d^{-1}	
Surfactant	PEC/PNEC	PEC/NC	PEC/PNEC	PEC/NC	PEC/PNEC	PEC/NC
LAS $C_{11.6}$	0.037	3.7	0.026	2.6	0.015	1.5
AE $C_{13.3}$ $EO_{8.2}$	0.012	1.2	0.008	0.8	0.005	0.5
AES $C_{12.5}$ $EO_{3.4}$	0.007	0.7	0.005	0.5	0.003	0.3
Soap	1.9	190	1.3	130	0.74	74

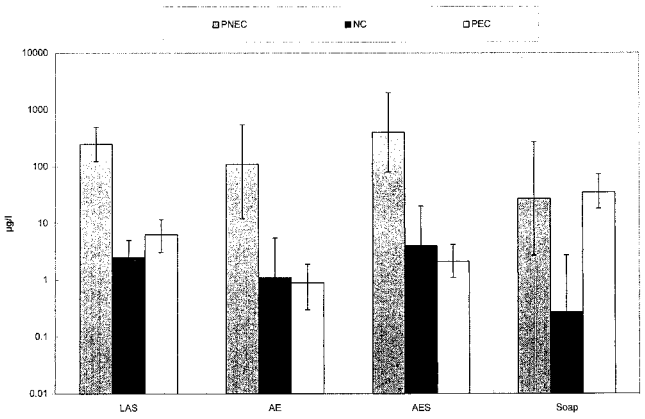

Fig. 1. PEC, PNEC, and NC values with uncertainty ranges for LAS $C_{11.6}$, AE $C_{13.3}$ $EO_{8.2}$, AES $C_{12.5}$ $EO_{3.4}$, and soap. All values in µg/L. See text for abbreviations.

DISCUSSION

It is recognized that the data used in the risk assessment inherently contain uncertainty and variability, which are sometimes referred to together as uncertainty. Uncertainty represents measurement error, for example, in a physical or chemical parameter that is used to predict the fate and exposure concentration for the substance of interest. Variability represents ranges in environmental characteristics (e.g., dilution factors in water bodies in which effluent, treated or untreated, is discharged or ranges in temperature, organic carbon, or moisture in soils to which sludge or gray water containing a substance are discharged). These uncertainties and variabilities can have important consequences on both the final risk quotient and the certainty that this risk quotient and the decision regarding safety or lack thereof is accurate. It has been suggested that the assessments should move from numerical quotients or point estimates (PEC/PNEC values) to true risk assessments where measures of the probability and severity of an adverse effect are given, characterized in terms of a statistical distribution with a most probable value for the risk and some confidence interval instead of a single number. This approach has not yet been applied to the data presented in this study. However, the numerical comparison of the PEC/PNEC values, together with their uncertainty ranges as shown in Figure 1, was considered suitable to sufficiently underpin the risk management decisions.

Validation of the PNECs derived in this study by monitoring actual effects in the field is difficult and probably impossible because in practice these substances are released through sewage treatment plant effluents that consist of complex mixtures of anthropogenic and natural substances with a different toxicological profile. In general, it can be stated that it is difficult to predict effects that might occur in the field on the basis of ecotoxicological data collected in the laboratory. Some features will tend to make laboratory tests overestimate effects in the field, whereas for other features the reverse may be the case. Overestimation of the toxic effects in the field occurs, for example, because in natural waters concentrations of dissolved organic matter (e.g., humic acids) and suspended solids may reduce the bioavailability as a result of complexation or adsorption. In addition, in laboratory tests rigorous efforts are made to maintain exposure concentrations, whereas in most field situations exposure will vary over time, and degradation rates are likely to be higher. Underestimation of toxic effects in the field may occur because in the laboratory, especially in longer-term tests, efforts are made to optimize conditions for the test organism (remove stressors other than the substance under test). In the field, nonchemical stressors (e.g., temperature, concentration of dissolved oxygen, or disease) may increase the susceptibility to a substance above that found in laboratory tests.

Whether the species used in the PNEC derivation for the four surfactants (either in laboratory studies or in field studies) are also representative for other aquatic ecosystems is a difficult question to answer. Relatively few species are used to produce laboratory toxicity data, and it would be unrealistic to assume that they will always encompass the most susceptible species in the field. In addition, it is recognized that the test species that are normally used in standard ecotoxicity testing are not representative for the biodiversity in a river ecosystem. On the other hand, it must be recognized that a total of 750 LAS records, 388 AE records, 91 AES records, and 47 soap records were analyzed, including data from cold- and warm-water species and fresh and marine water species. This analysis showed that (1) the toxicity range for different species is rather narrow and does not indicate a specific mode of action and that (2) because of intrinsic test, laboratory, and other variability, no specific underlying trends in species sensitivity can be observed [18,19,31,40,47]. Furthermore, effects of temperature, water hardness, and ionic strength seem to be minor as compared to the variability in species sensitivity. Thus, it can be expected that the PNECs derived for LAS, AE, AES, and soap account for these uncertainties, and extrapolation of these PNECs to other systems is judged feasible.

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APPENDIX

Assessment factors used in initial effects assessment for aquatic organisms [7]

Available information[a]	Assessment factor
Lowest short-term L (E)C50 or QSAR estimate for short-term toxicity	1,000
Lowest short-term L (E)C50 or QSAR estimate for short-term toxicity For at least representatives of algae, crustaceans, and fish	100
Lowest long-term NOEC or QSAR estimate for long-term toxicity For at least representatives of algae, crustaceans, and fish	10

[a] QSAR estimates (if available) are used if a group of structure related substances is considered. If the required information is only partly present (e.g., two short-term LC50s and one long-term NOEC), the lowest value upon application of the various assessment factors (10, 100, or 1,000) to the information concerned is considered to be the PNEC.