

RIVM report 711701 020

**Ecotoxicological Serious Risk Concentrations
for soil, sediment and (ground)water: updated
proposals for first series of compounds**

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Abstract

The Intervention Value for Soil/sediment and for Groundwater is based on the integration of a separately derived human toxicological serious risk concentration or SRC_{human} , and an ecotoxicological serious risk concentration or SRC_{eco} . This report presents a technical evaluation of the SRC_{eco} and proposals for updated SRC_{eco} for the first series of compounds. The evaluation considered the underlying data as well as the methodology used to derive SRCs. The compounds considered are heavy metals, cyanides, aromatic compounds, PAHs, chlorinated hydrocarbons (such as alkanes, benzenes, phenols and PCBs), pesticides, and other compounds such as phthalates. Over 100 individual compounds are considered, sum-values for isomers or compound classes are proposed when appropriate. Together with the derivation of the SRC_{eco} , also new Maximum Permissible Concentrations (MPCs) are derived. The information in this report is used in RIVM report 711701 023, 'Technical evaluation of Intervention Values for Soil/sediment and Groundwater'.

Preface

This report contains results for the evaluation of the ecological serious risk concentrations obtained in the framework of the project 'Risks in relation to soil quality'. The results have been discussed in the expert group on ecotoxicological risk assessment ('Setting Integrated Environmental Quality Standards Advisory Group'), who are acknowledged for their contribution. The members are J. Van Wensem (TCB), D.T.H.M. Sijm and T.P. Traas (RIVM-CSR), J. Appelman (CTB), T. Brock (Alterra), S. Dogger (Gezondheidsraad), J.H. Faber (Alterra), K.H. den Haan (VNO/NCW-BMRO), M. Koene (Stichting Natuur en Milieu), A.M.C.M. Peijnenburg (RIKZ), E. Sneller (RIZA), and W.J.M. van Tilborg (VNO/NCW-BMRO). D. Sijm and T. Traas (both RIVM-CSR) are acknowledged for critically reviewing earlier versions of this report. The co-workers on the project of the evaluation of the Intervention Values, A.J. Baars, P.F. Otte, M. Rikken and F.A. Swartjes (all RIVM), are acknowledged for their contribution to the discussions. We are indebted to J. Lijzen for his contributions to this report as primary RIVM-responsible for the technical evaluation of the Intervention Values.

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Samenvatting

In 1990 is de eerste tranche van ecotoxicologisch onderbouwde 'Serious Risk Concentration' (SRC_{eco} , voorheen aangeduid als ECOTOX-SCC) afgeleid voor de compartimenten bodem en sediment. Deze waarden dienden als basis voor de Interventiewaarden zoals in 1994 vastgesteld door het ministerie van VROM. Bodem/sediment of grondwater wordt als ernstig verontreinigd beschouwd, wanneer deze waarde wordt overschreden. Dit rapport betreft een evaluatie van de SRC_{eco} voor de stoffen uit deze 1e tranche, en nieuwe waarden worden voorgesteld voor de compartimenten bodem, sediment en grondwater. De stoffen uit de 1e tranche zijn zware metalen en cyanide, aromatische verbindingen, PAKs, pesticiden, ftalaten, en gechloreerde verbindingen zoals alkanen, benzenen, fenolen en PCBs. Het rapport maakt deel uit van een project waarin de technische basis van de Interventiewaarden zal worden geëvalueerd. Naast de ecotoxicologische afleiding zoals beschreven in dit rapport zijn de volgende onderwerpen beschouwd: humane risico niveaus (Baars et al., 2001, RIVM rapport 711701 025), model concepten voor de humane blootstelling (Rikken et al., 2001, RIVM rapport 711701 022), en invoerparameters voor deze modellen (Otte et al., 2001, RIVM rapport 711701 021). Deze ingrediënten leiden tot voorstellen voor geïntegreerde SRCs, gebaseerd op zowel humaan-toxicologische als ecotoxicologische SRCs (SRC_{human} en SRC_{eco}) (Lijzen et al., 2001, RIVM rapport 711701 023).

Aquatische en terrestrische toxiciteitsgegevens die zijn verzameld in het kader van het project 'Integrale Normstelling Stoffen' (INS) voor de afleiding van Maximaal toelaatbare risiconiveaus (MTR_{eco}) en streefwaarden, zijn gebruikt om de nieuwe SRC_{eco} waarden af te leiden. Voor stoffen waarvoor nog geen MTR_{eco} is afgeleid, zijn nieuwe gegevens gezocht en geëvalueerd. Voor alle stoffen is naast een SRC_{eco} ook een nieuwe MTR_{eco} voorgesteld. Alle terrestrische toxiciteitsgegevens zijn omgerekend naar standaardbodem, met een vast percentage lutum en organisch stof. Bij gebrek aan experimentele toxiciteitsgegevens, en in sommige gevallen als controle van de experimentele toxiciteitsgegevens, zijn kwantitatieve structuur-activiteit relaties (QSARs) gebruikt. De sorptie coëfficiënten voor bodem en sediment, en octanol-water partiticoëfficiënten -gebruikt als invoer voor QSARs- zijn overgenomen uit RIVM rapport 711701 021.

De methodiek voor afleiding van de SRC_{eco} is waar mogelijk in overeenstemming met die voor de afleiding van de MTR_{eco} en streefwaarden. De SRC_{eco} is gebaseerd op de HC50, dit is de concentratie waarbij voor 50% van de soorten of processen een ongewenst effect op de populatie is te verwachten. De HC50 kan worden beschouwd als een robuust getal, omdat het ongevoelig is voor de spreiding in de data. De MTR_{eco} is gebaseerd op de HC5, de concentratie waarbij voor 95% van de soorten of processen geen ongewenst effect wordt verwacht. Beide risiconiveau's worden afgeleid met behulp van de statistische extrapolatie ('refined risk assessment') of, bij onvoldoende gegevens, met 'preliminary risk assessment'. De SRC_{eco} wordt bij preliminary risk assessment afgeleid uit het geometrisch gemiddelde van de NOECs of de L(E)C50s/10 (extrapolatiefactoren 1 en 10). Voor de MTR_{eco} worden voor preliminary risk assessment extrapolatiefactoren variërend van 10 tot 1000 gebruikt. Doorvergiftiging is niet meegenomen in de afleiding van de SRC_{eco} , verondersteld is dat doorvergiftiging van minder belang is daar de ernstig verontreinigde situatie doorgaans een beperkt oppervlak beslaat.

Er zijn een aantal veranderingen in de afleiding van de SRC_{eco} ten opzichte van de in 1990 afgeleide waarden die de vigerende Interventiewaarden onderbouwen:

- De dataset voor toxiciteitgegevens, sorptiecoëfficiënten en octanol/water partiticoëfficiënten is herzien.
- De SRC_{eco} voor grondwater is gebaseerd op data voor oppervlaktewater.
- De SRC_{eco} voor sediment wordt separaat afgeleid, en niet meer automatisch gelijkgesteld aan de SRC_{eco} voor bodem.
- Omdat voor metalen de achtergrondconcentratie aanzienlijk is ten opzichte van de HC50 en niet opgenomen in de toxiciteitsgegevens, is de toegevoegde risicobenadering toegepast om de SRC_{eco} af te leiden. Dit is in lijn met de afleiding van MTR_{eco} en streefwaarden voor metalen.
- Terrestrische processen zijn meegenomen in de afleiding van de SRC_{eco} .
- LC50s en EC50s zijn niet gescheiden.
- Soorten worden gebruikt als invoer in de risicobeoordeling in plaats van taxonomische groepen.
- De eisen om statistische extrapolatie toe te passen zijn minder streng, en de statistische extrapolatiemethode is veranderd van een log-logistische naar een log-normale verdeling (m.n. van belang voor de MTR_{eco}).
- Bij weinig data ('preliminary risk assessment') is de SRC_{eco} gebaseerd op de laagste waarde van ofwel het geometrisch gemiddelde van chronische toxiciteitsgegevens ofwel van acute gegevens gedeeld door 10 ofwel evenwichtspartitie.

Over het algemeen zijn de SRC_{eco} waarden voor bodem gebaseerd op een beperkte hoeveelheid gegevens, met uitzondering van de metalen. Voor alle metalen, en 24 organische stoffen, werd de SRC_{eco} afgeleid op basis van terrestrische toxiciteitgegevens. Voor meer dan de helft van de organische stoffen waren geen terrestrische gegevens beschikbaar, en werd SRC_{eco} voor de bodem afgeleid op basis van uitsluitend aquatische toxiciteitgegevens en partiticoëfficiënten. Voor alle metalen, met uitzondering van nikkel, en voor pentachloorfenol kon statistische extrapolatie worden toegepast.

De SRC_{eco} voor sediment is afgeleid met behulp van evenwichtspartitie. De meeste toxiciteitsgegevens zijn beschikbaar voor aquatische soorten. Voor meer dan een derde van de stoffen was een statistische extrapolatie mogelijk voor het aquatisch milieu.

SRC_{eco} van organische stoffen afgeleid uit terrestrische toxiciteitsgegevens of op basis van evenwichtspartitie blijken onderling consistent. Verder blijken de MPCs zoals verkregen met extrapolatiefactoren goed aan te sluiten bij de resultaten na statistische extrapolatie. Voor cyaniden zijn geen bruikbare terrestrische toxiciteitsgegevens beschikbaar en ook partiticoëfficiënten ontbreken. Daarom zijn voor de verschillende vormen van cyanide alleen een SRC_{eco} voor grondwater afgeleid. Er is geen SRC_{eco} afgeleid voor minerale olie.

De resulterende SRC_{eco} waarden zijn niet altijd direct te vergelijken met de oude ECOTOX-SCCs die de vigerende Interventiewaarden onderbouwden, omdat destijds voor minder individuele congeneren risiconiveau's zijn afgeleid. Daar waar een direct vergelijk mogelijk is, zijn de nieuwe SRC_{eco} gemiddeld ongeveer gelijk aan de oude ECOTOX-SCC waarden. Dit verschil is hetzelfde voor de metalen als voor de meeste organische verbindingen. Er zijn slechts enkele gevallen waarin de oude en nieuw voorgestelde ecotoxicologische risiconiveau's meer dan een orde-grootte verschillen. Het gaat dan om dichloormethaan, trichlooretheen, hexachloorbenzeen, drins, carbaryl en carbofuran, waarvoor in alle gevallen de oude ECOTOX-SCC meer dan een orde-grootte hoger lag dan de nieuw voorgestelde SRC_{eco} . Voor de zware metalen zijn de nieuw voorgestelde waarden maximaal een factor 3,6

hoger (Hg) en maximaal een factor 2,1 lager (Ni). De veranderingen in SRC_{eco} waarden kunnen zowel het gevolg zijn van verschillen in de methodiek als veranderingen in de gegevens omtrent toxiciteit en partiticoëfficiënten.

Veel van de in dit rapport afgeleide MTR_{eco} zijn lager dan de huidige waarden. De op een log-normale distributie gebaseerde statistische extrapolatie, gebruikt in dit rapport, leidt tot vrijwel dezelfde MTR_{eco} als de log-logistische extrapolatie. Extrapolatiefactoren volgens de EU/TGD resulteren in MTR_{eco} die gemiddeld een factor 2 lager zijn dan de voorheen toegepaste 'aangepaste EPA' methode.

Summary

In 1990 the first series of ecotoxicological ‘Serious Risk Concentration’ (SRC_{eco} , formerly denoted as ECOTOX-SCC) were derived for the compartments soil and sediment. These values served as ecotoxicological basis for the proposed Intervention Values for Soil/sediment, which were established in 1994 by the Dutch Ministry of Housing, Spatial Planning and the Environment (Ministry of VROM). Soil/sediment or groundwater is considered as seriously contaminated, if the Intervention Value is exceeded. This report concerns an evaluation of the SRC_{eco} for the compounds from the first series, and new values are proposed for the compartments soil, sediment and groundwater. The compounds from the first series are heavy metals, cyanides, aromatic compounds, PAHs, pesticides, phthalates and chlorinated hydrocarbons such as alkanes, benzenes, phenols and PCBs. The report is part of a project in which the technical basis of the current Intervention Values for Soil/sediment and Groundwater are evaluated. Besides the ecotoxicological derivation which is described in the current report, the following issues are considered: human risk levels (Baars et al., 2001, RIVM report 711701 025), model concepts for human exposure (Rikken et al., 2001, RIVM report 711701 022), and input parameters for these models (Otte et al., 2001, RIVM report 711701 021). These ingredients lead to new proposals for SRCs, based on both human-toxicological and ecotoxicological SRCs (SRC_{human} and SRC_{eco}) (Lijzen et al., 2001, RIVM report 711701 023).

Aquatic and terrestrial toxicity data which are collected in the framework of the project ‘Setting Integrated Environmental Quality Standards’ (INS) for the derivation of Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) are used to derive the new SRC_{eco} values. For compounds for which no MPCs have been derived yet, new data are collected and evaluated. Besides an SRC_{eco} also a new MPC is derived for all compounds. All terrestrial toxicity data are recalculated into a standard soil, with a fixed clay and organic matter content. When experimental toxicity data are lacking, and in some cases as a check of the experimental toxicity data, quantitative structure activity relationships (QSARs) are used. Sorption partition coefficients for soil and sediment, and octanol-water partition coefficients which are used as input for QSARs, are adopted from the RIVM report 711701 021.

The methods for deriving SRC_{eco} is where possible in agreement with the methods for the derivation of the MPCs and NCs. The SRC_{eco} is based upon the HC50, which is the concentration at which for 50% of the species or processes adverse effects on the population can be expected. The HC50 can be considered as a robust value, as it is insensitive to the scatter in the data. The MPC is based on the HC5, the concentration at which for 95% of the species or processes no adverse effects are expected. Both risk limits are derived by either statistical extrapolation (refined risk assessment) or in the case of little data by preliminary risk assessment. The SRC_{eco} is in the case of preliminary risk assessment derived from the geometric mean of the NOECs or the L(E)C50s/10 (extrapolation factors 1 and 10). For the MPC, in case of preliminary risk assessment, extrapolation factors are used ranging from 10 to 1000. Biomagnification throughout the food-chain is not considered in the derivation of the SRC_{eco} , as seriously contaminated situations are generally restricted to a limited surface area. There are few changes in the derivation of the SRC_{eco} compared to the values derived in 1990 which are underpinning the current Intervention Values:

- The data for toxicity, sorption coefficients and octanol/water partition coefficients are revised.

- The SRC_{eco} for groundwater is based upon toxicity data for surface water.
- As for metals the background concentrations are substantial compared to the HC50 and not included in the toxicity data, the added risk approach is used to derive the SRC_{eco} . This is in line with the derivation of MPCs and NCs for metals.
- Terrestrial processes are included in the derivation of the SRC_{eco} .
- LC50s and EC50s are considered in conjunction.
- Species are used as input in the ecotoxicological risk assessment instead of taxonomic groups.
- The requirements to use statistical extrapolation techniques are less stringent, and the extrapolation method assumes a log-normal instead of log-logistic distribution (influences mainly the MPC).
- If little data are available ('preliminary risk assessment') the SRC_{eco} is based on the lowest value from the geometric mean of chronic toxicity data *or* from acute toxicity data divided by 10 *or* from equilibrium partitioning.

In general SRC_{eco} values for soil are based on a limited amount of data, with metals as an exception. For all metals and 24 organic compounds, the SRC_{eco} was directly based on terrestrial toxicity data. No terrestrial data were available for more than half of the organic compounds, the SRC_{eco} for soil was then derived solely based upon aquatic toxicity data and partition coefficients. For all metals, with the exception of nickel, and for pentachlorophenol statistical extrapolation could be applied. The SRC_{eco} for sediment was derived by applying equilibrium partitioning. Most toxicity data are available for aquatic species. For more than a third of the compounds, refined risk assessment was possible for the aquatic environment.

SRC_{eco} for organic chemicals derived based on terrestrial toxicity data or based on equilibrium partitioning appear mutually consistent. For MPCs, results after using the assessment factors for preliminary risk assessment fit well with MPCs obtained after statistical extrapolation

For cyanides no usable terrestrial toxicity data are available, nor sorption coefficients. Therefore only SRC_{eco} values for groundwater are derived for cyanides. No SRC_{eco} is derived for mineral oil.

The resulting SRC_{eco} values cannot always directly be compared with the values that are underpinning the current Intervention Values (ECOTOX-SCCs), as formerly risk levels were derived for less individual congeners. Where direct comparison is possible, the newly derived SRC_{eco} are on average approximately equal to the old ECOTOX-SCC values. This difference is the same for metals and most of the organic compounds. There are only few cases in which the old and newly proposed ecotoxicological risk limits differ more than an order of magnitude. This considers dichloromethane, trichloroethene, hexachlorobenzene, dieldrin, carbaryl and carbofuran for which the old ECOTOX-SCCs are more than an order of magnitude higher than the newly proposed SRC_{eco} . For the heavy metals the newly proposed values are maximally a factor 3.6 higher (Hg) and a factor 2.1 lower (Ni). Changes in SRC_{eco} values may both be the result of differences in both methodology and changes in data on toxicity and partition coefficients.

Most of the MPCs derived in this report are lower than the current values. The statistical extrapolation method based on a log-normal distribution as used in this report results in almost the same MPCs as the log-logistic extrapolation. Extrapolation factors according to

the EU/TGD result in MPCs that are on average a factor of 2 lower than the previously used 'modified EPA' method.

1 Introduction

Intervention Values are generic risk limits for soil/sediment and groundwater quality. When exceeding these values, historical contamination is classified as seriously contaminated. In 1994 Intervention Values for the first series of seventy compounds (Van den Berg and Roels, 1991) have been implemented (VROM, 1994). In 1997 24 new Intervention Values or Indicative Levels for serious soil contamination were implemented (VROM, 1997), based on the second series of proposals for Intervention Values (Van den Berg et al., 1994) and the third series of proposals for Intervention Values (Kreule et al., 1995). Another set of 15 compounds or groups followed in 2000 (Ministry of VROM, 2000) based on proposals for the fourth series (Kreule and Swartjes, 1998).

This report is part of the technical evaluation of the Intervention Values from the first series of compounds. The project contains evaluations of the following subjects: human toxicology (Baars et al., 2001), model concepts for human exposure (Rikken et al., 2001), input parameters for these models (Otte et al., 2001) and ecotoxicology (this report). The Intervention Value is based on an integration of human-toxicological and ecotoxicological criteria (Van de Berg 1991/1994); the human toxicological serious risk concentrations or SRC_{human} and ecotoxicological serious risk concentration or SRC_{eco} (see Figure 1.1). These values were previously referred to as serious soil contamination concentration (SCC), the HUM-TOX SCC and ECOTOX-SCC for human toxicological and ecotoxicological risks respectively.

In 1990 SRC_{eco} values were proposed for the first series of compounds (Denneman and Van Gestel, 1990). These were based on the concentration that leads to adverse effects in 50% of the tested species (HC50), or the geometric mean of the available toxicity data. Adverse effects due to accumulation in the food-chain were not taken into account.

In this report proposals for updated SRC_{eco} are presented, based on the new information that has become available in recent years. Some of the compounds considered in this report have been evaluated in the context of the project 'Setting Integrated Environmental Quality Standards' to derive Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs). For substances for which MPCs/NCs have been derived between 1990 and now, the same underlying data and information is used to derive the SRC_{eco} . The compounds of concern are listed in Table 1.1, together with the RIVM report in which these MPCs/NCs are published. The underlying data can be found in the cited reports as well. Only for the substances for which new data have been searched for, these underlying data are incorporated in the annex to this report. The selected data for the derivation of the SRC_{eco} are reported in the appendices of this report. These data are single species toxicity data for terrestrial and aquatic organisms and effect data on terrestrial processes. All toxicity data on aquatic and terrestrial organisms refer to effects that may affect the species at the population level.

The methodology for deriving SRCs is adapted; log-normal distributions are used instead of log-logistic distributions for refined ecotoxicological risk assessment (Aldenberg and Jaworska, 2000). For preliminary risk assessment also modifications are applied; the SRC_{eco} is determined by the minimum value of 1) the geometric mean of NOECs and 2) $L(E)C50s/10$. The added-risk approach is applied to derive the SRC_{eco} for metals (Crommentuijn et al., 2000), because the background concentration is not included in the nominal concentrations from the underlying toxicity tests. For this purpose a general background concentration is used (Van den Hoop, 1995; Crommentuijn et al., 1997a).

Secondary poisoning is not included in the derivation of the SRC_{eco} , because the SRC_{eco} is proposed for limited areas of highly contaminated soil.

Together with the SRC_{eco} proposals for MPCs are given. There are two reasons to this. First, for several compounds no MPCs were derived yet in the framework of the project 'Setting Integrated Environmental Quality Standards' and for other compounds additional data were searched for. Second, the methodology to derive MPCs has been changed recently (see Chapter 2 and Traas, 2001). For compounds for which MPCs were derived with inclusion of secondary poisoning, the newly derived MPC is always compared with the old value for secondary poisoning. Because the air was not taken into account, the same reasoning applies to the harmonisation with the air compartment.

No ecotoxicological risk limits for total petroleum hydrocarbon (TPH or mineral oil) has been derived in this report. Main problem was that in most studies the composition of the mineral oil in the test medium was unknown. New data and methods will be taken into account in a separate study.

For the derivation of the SRC_{eco} partition coefficients between soil/sediment and water are used. The K_{ps} used in this report are taken from Otte et al. (2001).

In chapter 2 a summary of the methodology used to derive the SRC_{eco} is given in detail. The methodology is also described in the 'Guidance document on the derivation of ecotoxicological risk limits' (Traas, draft), and is based on the procedures described by Denneman and van Gestel (1990, 1991), Slooff et al., (1992), Crommentuijn et al. (1994), and taking into account the comments of the Technical Soil Protection Committee on the results for the second, third and fourth series of compounds (TCB, 1997, 1998). Chapter 3 presents the proposals for the SRC_{eco} and MPCs together with the underlying data. A summary of the new proposals and old values for the SRC_{eco} , the MPC and the discussion on the results is presented in chapter 4.

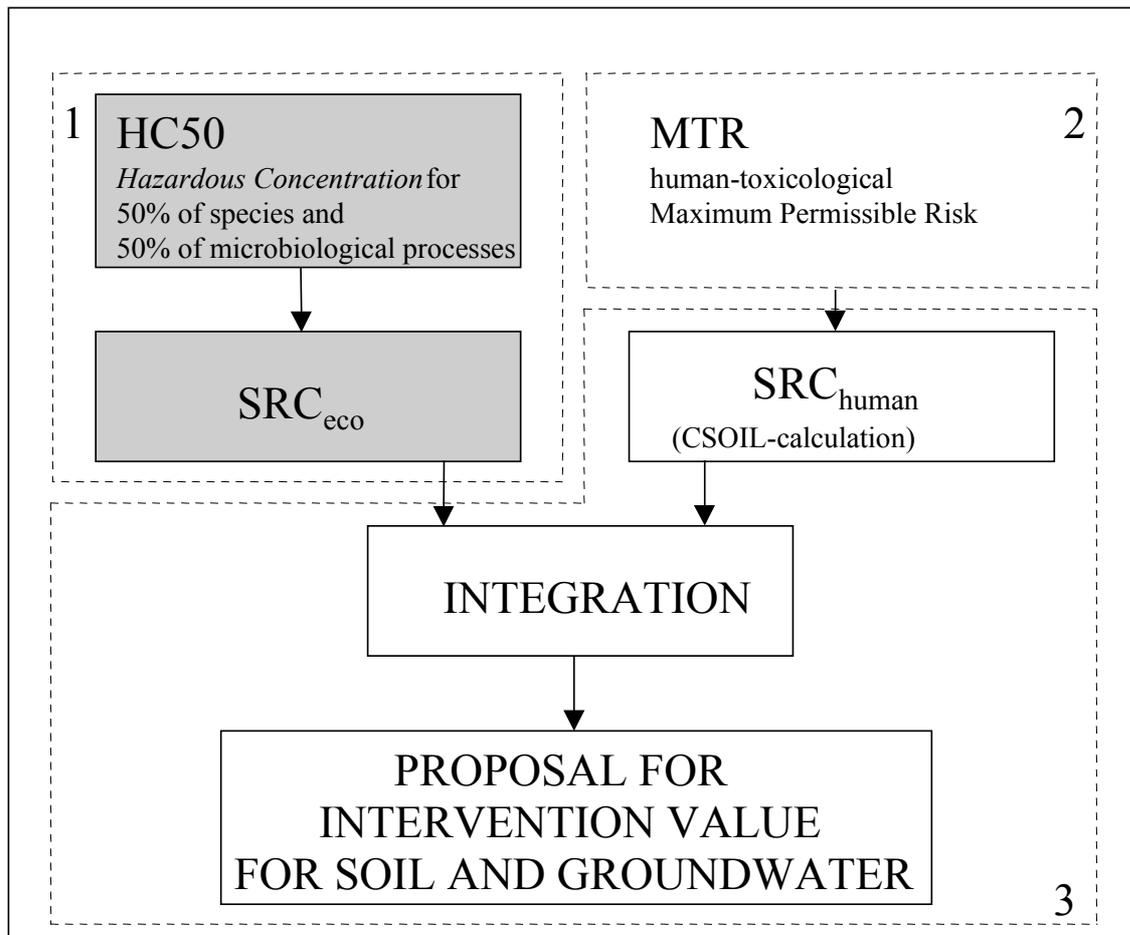


Figure 1.1: Outline of the Intervention Value for soil, sediment and groundwater. 1 is the SRC_{eco} (this report), 2 is the MTR_{human} (Baars et al., 2001) and 3 is SRC_{human} and the integration of these two, the proposal for the Intervention Value for soil, sediment and groundwater (report number 711701 023).

Table 1.1: List of compounds considered in this report and reports where underlying data can be found.

Compound	Underlying data	compound	underlying data
I Metals		V Chlorinated aliphatic hydrocarbons	
Arsenic	Crommentuijn et al., 1997a	1,2-Dichloroethane	Van de Plassche et al., 1993
Barium	Van de Plassche et al., 1992	Dichloromethane	Van Apeldoorn et al., 1988; Van de Plassche et al. 1993
Cadmium	Crommentuijn et al., 1997a	Tetrachloromethane	Van de Plassche et al., 1993
Chromium	Crommentuijn et al., 1997a	Tetrachloroethene	Van de Plassche et al., 1993
Cobalt	Van de Plassche et al., 1992	Trichloromethane	Van de Plassche et al., 1993
Copper	Crommentuijn et al., 1997a	Trichloroethene	Van de Plassche et al., 1993
Mercury	Slooff et al., 1995	Vinylchloride	Van de Plassche et al., 1993
Lead	Janus et al., 2000; Crommentuijn et al., 1997a		
Molybdenum	Van de Plassche et al., 1992	VI Chlorinated aromatic hydrocarbons	
Nickel	Van de Meent et al., 1990	Chlorobenzenes	Hesse et al., 1991; Van de Plassche et al., 1993
Zinc	Janus, 1993; adapted Janus et al., 1996; Crommentuijn et al., 1997a	Chlorophenols	Janus et al., 1991; new data, annex to this report
		Chloronaphthalenes	new data, annex to this report
II Inorganic compounds		PCBs	Van Wezel et al., 1999a
Cyanides	new data, annex to this report	VII Pesticides	
Thiocyanates	new data, annex to this report	DDT/DDE/DDD	Van de Plassche et al., 1994
Cyanide complexes	new data, annex to this report	Aldrin	Van de Plassche et al., 1994
III Aromatic compounds		Dieldrin	Van de Meent et al., 1990
Benzene	Van de Plassche et al., 1993; Knaap et al., 1988	Endrin	Van de Plassche et al., 1994
Toluene	Van de Plassche et al., 1993; Van der Heijden et al., 1988	HCH-isomers	Van de Plassche et al., 1994
Ethylbenzene	Van de Plassche et al., 1993	Carbaryl	Crommentuijn et al. 1997c
Xylenes	Van de Plassche et al., 1993	Carbofuran	Van de Plassche et al., 1994
Styrene	Van de Plassche et al., 1993	Maneb	Crommentuijn et al. 1997c
Phenol	new data, annex to this report	Atrazine	Crommentuijn et al. 1997c
Cresols	new data, annex to this report	VIII Miscellaneous compounds	
Catechol	new data, annex to this report	Cyclohexanone	new data, annex to this report
Resorcinol	new data, annex to this report	Phthalates	Van Wezel et al. 1999b; new data, annex to this report
Hydroquinone	new data, annex to this report	Pyridine	new data, annex to this report
IV PAHs		Tetrahydrofuran	new data, annex to this report
Naphthalene	Kalf et al., 1995	Tetrahydrothiophene	new data, annex to this report
Anthracene	Kalf et al., 1995		
Phenanthrene	Kalf et al., 1995		
Fluoranthene	Kalf et al., 1995		
Benzo[<i>a</i>]anthracene	Kalf et al., 1995		
Chrysene	Kalf et al., 1995		
Benzo[<i>k</i>]fluoranthene	Kalf et al., 1995		
Benzo[<i>a</i>]pyrene	Kalf et al., 1995		
Benzo[<i>ghi</i>]perylene	Kalf et al., 1995		
Indeno[1,2,3- <i>cd</i>]pyrene	Kalf et al., 1995		

2 Methodology

Figure 2.1 presents a schematic outline of the methodology to derive Ecotoxicological Risk Limits (ERLs), consisting of 4 different steps. The steps 1 to 4 in Figure 1 are followed for each substance or for a group of substances when MPCs/NCs and $SRCs_{eco}$ are derived. Step 4 is followed for the derivation of ERLs for sediment and, in the case that the toxicity data for terrestrial species are limited, for soil too. These steps are described in the sections below.

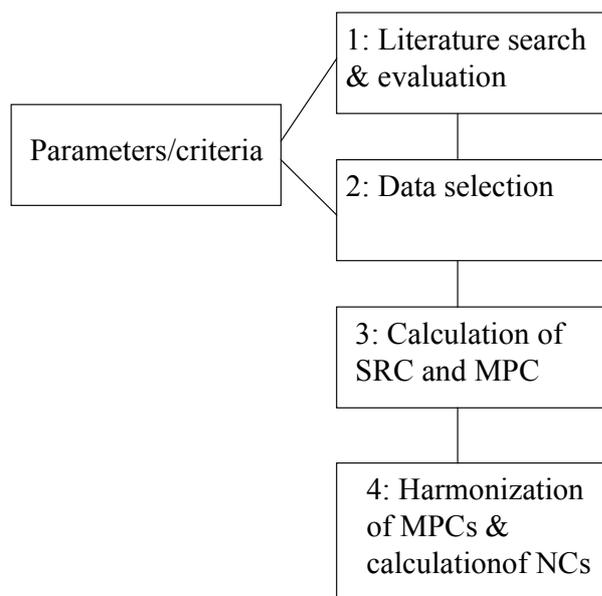


Figure 2.1: Schematic outline of methodology to derive Ecotoxicological Risk Limits for soil.

2.1 Literature search and evaluation

Sources used for the collection of single-species toxicity data and data on soil/water and sediment/water partition coefficients are both in-house and external documentation centres and libraries, and bibliographic databases. A detailed description of the parameters searched for and criteria applied when performing the literature search and evaluation is described in Traas (2001). A summary is given below.

Toxicological criteria for aquatic and terrestrial organisms, which may affect the species at the population level are taken into account. In general these are survival, growth and reproduction and are commonly expressed as an L(E)C50 (short-term tests) or NOEC (long-term tests, covering a complete or partial life cycle, including a sensitive life stage or reproduction cycle). Besides this, effect data on microbiological processes and enzymatic activity are searched for, commonly expressed as a NOEC or ECx value. Sometimes also other toxicological criteria are taken into account. This is the case when the criteria in question are considered ecologically relevant, e.g. histopathological effects on reproductive organs of a species.

Contaminants accumulating through the food chain may exert toxic effects on birds and mammals. From physicochemical parameters like $\log K_{ow}$ and water solubility an indication can be obtained for the bioaccumulative potential of the substance in question. If there is a positive indication, also data on the sensitivity of birds and mammals and BCFs for worms, fish and mussel have to be searched for deriving an MPC/NC. The substances for which this step is considered are organic substances with a $\log K_{ow} > 5$ and a molecular weight < 600 .

For metals this is considered case by case. However, for the derivation of SRCs this process of secondary poisoning is considered to be of minor importance, because these $SRC_{S_{eco}}$ are proposed for limited areas of highly concentrated contaminated soil. Therefore, secondary poisoning is not included in the derivation of the $SRC_{S_{eco}}$.

For a proper evaluation of the toxicity studies the reliability of the study has to be taken into account. A study is considered reliable if the design of the experiment is in agreement with international accepted guidelines such as the OECD guidelines (OECD, 1984).

Tables for chronic and acute toxicity data are given in the appendices of this report. The results of terrestrial tests are given in $mg/kg_{d.w.}$ of the soil and separate tables for species and processes are given. For soil, only studies in which the humus or organic matter content or organic carbon content is reported are taken into account. In all tables the results are shown together with the experimental conditions.

Not all the tests described in the literature are performed under the same conditions.

Therefore normalisation of terrestrial test results was proposed by Denneman and Van Gestel (1990). All data on the sensitivity of species are recalculated for a standard soil containing 10% organic matter and 25 % of clay. For metals the following equation is used:

$$ECx_{(soil)} = ECx_{(exp)} \frac{R_{(soil)}}{R_{(exp)}} \quad (1)$$

in which: $ECx_{(soil)}$ = Effect Concentration; normalised NOEC or LC50 for standard soil,
 $ECx_{(exp)}$ = Effect Concentration; NOEC or LC50 for soil as used in the experiment,
 $R_{(soil)}$ = Reference-value for standard soil,
 $R_{(exp)}$ = Reference-value for soil used in experiment.

The Reference values for soil are based on the reference-lines. For all metals these so-called reference lines were derived by correlating measured ambient background concentrations (total concentrations in the soil-matrix) at a series of remote rural sites in the Netherlands to the percentage clay and the organic matter content of these soils (see Edelman (1984) and De Bruijn and Denneman (1992) and Van den Hoop (1995) for calculating the Reference-values; values given in section 3.1.12). The reference line corresponds to the 90th percentile of the background concentrations. At present, the correction of the test concentration in laboratory tests to standard soil in the described manner is subject to debate. However, the values for metals presented here are still corrected in this way.

For organic substances the following equation is used:

$$ECx_{(soil)} = ECx_{(exp)} \frac{H_{(soil)}}{H_{(exp)}} \quad (2)$$

in which: $ECx_{(soil)}$ = Effect Concentration: normalised NOEC or LC50 for standard soil,
 $ECx_{(exp)}$ = Effect Concentration: NOEC or LC50 for soil as used in the experiment,
 $H_{(soil)}$ = Organic matter content of standard soil (10%),
 $H_{(exp)}$ = Organic matter content of soil used in experiment.

Considering Eq. 2 for organic substances: if $H < 2\%$ the percentage is set to 2%, if $H > 30\%$ the percentage is set to 30%. For PAHs the lower limit of 2% is set to 10% in actual risk assessment (Stuurgroep Integrale Normstelling Stoffen, 1999). However, in the derivation of MPCs the lower limit of 2% was used (Kalf et al., 1995). Organic carbon content is derived from the organic matter content by dividing it by 1.7.

2.2 Data selection

This step will result in a selection of the toxicity data to be used in the extrapolation. The aim of selecting toxicity data is first to select reliable toxicity data and second, to select one single toxicity value for each compound and species. One parameter per species is necessary as input in the extrapolation methods. Therefore chronic as well as acute toxicity data are weighed as follows (Slooff, 1992):

- If for one species several toxicity data based on the same toxicological endpoint are available, these values are averaged by calculating the geometric mean.
- If for one species several toxicity data based on different toxicological endpoints are available, the lowest value is selected. The lowest value is determined on the basis of the geometric mean, if more than one value for the same parameter is available (see above).
- In some cases data for effects of different life-stages are available. If from these data it becomes evident that a distinct life-stage is more sensitive, this result may be used in the extrapolation by selecting the most sensitive life-stage.

Further, from one study NOEC or EC_x values for different exposure times might be given. In general the most commonly used exposure time is selected, e.g. for acute tests with fish 96 h, for *Daphnia* species 48 h and for *Vibrio fischeri* 15 min. In some cases, especially when the effect parameter is growth, an effect may decrease after longer exposure times. In this case, the shortest exposure time is selected, e.g. for *Lactuca sativa*: 7 d, and for algae ≤ 48 h.

For soil, toxicity data on terrestrial species as well as for microbial and enzymatic processes may be available. The latter are in principle summed parameters expressing the performance of a process. The process in question may be performed by more than one species and under toxic stress, the functioning of the process may be taken over by less sensitive species. From the foregoing it may be clear that effects on species and effects on processes are quite different. According to Van Beelen and Doelman (1996) the results of ecotoxicological tests with microbial processes can not be used together with single species tests in a single extrapolation, because of the difference between them. Therefore these data are not combined and both data for species and processes are selected separately.

In contrast with the selection of data for terrestrial species, for the data on microbial processes and enzymatic activity more than one value per process is included in the extrapolation method. As mentioned above NOECs for the same process but using a different soil as substrate are regarded as NOECs based on different populations of bacteria and/or microbes. Therefore these NOECs are treated separately. Only if values are derived from a test using the same soil, one value is selected/calculated.

For water, toxicity studies are collected for both fresh water and marine species. For the calculation of the ERLs these data are combined if there are no significant differences between the two sets. In this report, this is tested for all compounds with an unpaired T-test. Prior to this, differences in variance are tested by an F-test. However, the kind or number of toxicity data that are available for both groups can cause differences. If for example for fresh water species data are available for algae, crustaceans and fish and for marine species only for algae, differences in variance can be expected. To account for these differences in variance, the T-test is performed with a Welch correction. If the sets are significantly different, it is

examined whether this can be caused by differences in available data, such as the presence of other species in the fresh and salt water data sets. If it can be concluded that differences between fresh water and marine species are most likely due to differences in sensitivity, for example caused by differences in bioavailability, the data sets are not combined.

2.3 Calculating Ecotoxicological Risk Limits

In the Netherlands the extrapolation methods used for risk assessment are the refined risk assessment (section 2.3.1) and the preliminary risk assessment (section 2.3.2). The first one is applied if chronic data for 4 or more different taxonomic groups or different processes are available. The second one if less chronic data or only acute data are available. For metals, having a natural background concentration, the Added Risk Approach is applied (section 2.3.3). For substances tending to bioaccumulate besides the ERL for direct exposure, based on single-species toxicity data, also an MPC/NC for Secondary Poisoning is derived applying the Secondary Poisoning Approach. For the derivation of the Intervention Values secondary poisoning is not included. In case, for the terrestrial environment no toxicity data are available, ERLs are derived on the basis of aquatic toxicity data and applying the Equilibrium Partitioning Method or EqP-method (section 2.3.4).

The SRC_{eco} for groundwater is based on toxicity data for surface water.

2.3.1 Refined risk assessment

The refined risk assessment or statistical extrapolation method is based on the assumption that the sensitivities of species in an ecosystem can be described by a statistical frequency distribution. This statistical frequency distribution describes the relationship between the concentration of the substance in a compartment and a certain percentage of species unprotected. The method is applied if at least 4 NOEC values of species from different taxonomic groups or for 4 different terrestrial processes are available. For a detailed overview of the theory and the statistical adjustments since its introduction, it is referred to the original literature (Kooijman, 1987; Van Straalen and Denneman, 1989; Wagner and Løkke, 1991; Aldenberg and Slob, 1993; Aldenberg and Jaworska, 2000).

The concentration corresponding with a 50% protection level, which is the same as a Potentially Affected Fraction of all species of 50% or PAF = 0.5, is the HC50 (hazardous concentration to 50% of the species). This HC50 serves as basis for the ecotoxicological Serious Risk Concentration (SRC_{eco}) and can be derived from the same sensitivity distribution as is used for deriving the MPC or from the geometric mean of the underlying data.

The aim of the MPC is that it protects all species in an ecosystem. However, in order to be able to use extrapolation methods like the one of Aldenberg and Slob (1993), a 95% protection level is chosen for the MPC as a sort of cut-off value (VROM, 1989). This HC5 (hazardous concentration to 5% of all species) can be derived using statistical extrapolation methods.

Until now, the method of Aldenberg and Slob (1993) was used for deriving MPCs if NOECs for four or more different taxonomic groups or different processes are available. This method assumes that the NOECs used for estimating the distribution fit the log-logistic distribution. Another method to determine the HC5 of HC50 is the use of a log-normal (Gaussian) instead of a log-logistic distribution. Numerically, the differences between these two distribution are marginal. The method described by Aldenberg and Jaworska (2000) is used in this report to evaluate the data. The advantage of the log-normal distribution is that it underlies many of the

most common statistical tests, such as the T-test for testing differences of the mean between data sets and the F-test for testing differences in variance. Also a normality test (Kolmogorov-Smirnov) to test whether the data follow the assumed normal distribution, can be easily performed.

The HC5 and HC50 can be derived by (Aldenberg and Jaworska, 2000):

$$\log HC_x = \bar{x} - k \cdot s \quad (3)$$

in which:

- \bar{x} = mean of the log-transformed data
- k = extrapolation constant, which is dependent on the number of data and the protection level (HC5 or HC50)
- s = standard deviation of the log-transformed data

Another advantage of the method as described by Aldenberg and Jaworska (2000) is that it presents extrapolation factors to calculate the 5% and 95% confidence limit of the HC5 and HC50 values.

2.3.2 Preliminary risk assessment

2.3.2.1 Assessment factors for the SRC_{eco}

If chronic NOECs are available for less than 4 taxonomic groups, preliminary risk assessment is applied, in which assessment factors are applied to the chronic or acute toxicity data. The factors and conditions used for deriving SRC_{eco} are shown in Table 2.1. In principle, to the acute toxicity data an acute-to-chronic ratio (ACR) of 10 is always applied to compare acute L(E)C50s with chronic NOECs. In future, one may deviate from this factor of 10 if more information of the ACR for the specific compound or endpoint can be involved. The data for the terrestrial compartment are always compared with those derived from the SRC_{eco} for the aquatic compartment by equilibrium partitioning.

Table 2.1: Assessment factors used to derive the SRC_{eco} for the aquatic and terrestrial compartment.

Available data	Additional criteria	MPC based on	Assessment factor	Tag
only L(E)C50s and no NOECs		geometric mean of L(E)C50s	10	a
≥ 1 NOECs available*	geometric mean of L(E)C50s / 10 < geometric mean of NOECs	geometric mean of L(E)C50s	10	b
	geometric mean of L(E)C50s / 10 \geq geometric mean of NOECs	geometric mean of NOECs	1	c

* this value is subsequently compared to the extrapolated value based on acute L(E)C50 toxicity values. The lowest one is selected

2.3.2.2 Assessment factors for the MPC

The magnitude of the assessment factors for the MPC depends on the number and kind of these toxicity data. The method used until 1999 for deriving MPCs in the framework of the project 'Setting Integrated Environmental Quality Standards' is often referred to as the modified EPA-method (Van de Meent et al., 1990). The factors and conditions used in this method for deriving MPCs from aquatic and terrestrial studies and from secondary poisoning are shown in Table 2.2 - Table 2.4, respectively. In the derivation of the MPCs the minimum value (indicated by min in the tables) of the NOECs or L(E)C50s for aquatic or terrestrial

species (indicated by aqua or terr in the tables) or birds and mammals (indicated by bird or mam in the tables) is used as a starting point.

Table 2.2: Modified EPA assessment factors for aquatic organisms.

Available data	Additional criteria	MPC based on	Assessment factor
L(E)C50 or QSAR estimate	$L(E)C50_{aqua_{min}}/1000 < NOEC_{aqua_{min}}/10$	$L(E)C50_{aqua_{min}}$	1000
L(E)C50 or QSAR estimate for minimal algae/crustaceans/fish	$L(E)C50_{aqua_{min}}/100 < NOEC_{aqua_{min}}/10$	$L(E)C50_{aqua_{min}}$	100
NOEC or QSAR estimate	$L(E)C50_{aqua_{min}}/1000 (100) \geq NOEC_{aqua_{min}}/10$	$NOEC_{aqua_{min}}$	10*
NOEC or QSAR estimate for minimal algae/crustaceans/fish		$NOEC_{aqua_{min}}$	10

* this value is subsequently compared to the extrapolated value based on acute L(E)C50 toxicity values. The lowest one is selected

Table 2.3: Modified EPA assessment factors for terrestrial organisms.

Available data	Additional criteria	MPC based on	Assessment factor
L(E)C50 or QSAR estimate	$L(E)C50_{terr_{min}}/1000 < NOEC_{terr_{min}}/10$	$L(E)C50_{terr_{min}}$	1000
L(E)C50 or QSAR estimate for minimal three representatives of microbe-mediated processes, earthworms or arthropods and plants	$L(E)C50_{terr_{min}}/100 < NOEC_{terr_{min}}/10$	$L(E)C50_{terr_{min}}$	100
NOEC or QSAR estimate	$L(E)C50_{terr_{min}}/1000 (100) \geq NOEC_{terr_{min}}/10$	$NOEC_{terr_{min}}$	10*
NOEC or QSAR estimate for minimal three representatives of microbe-mediated processes, earthworms or arthropods and plants		$NOEC_{terr_{min}}$	10

* this value is subsequently compared to the extrapolated value based on acute L(E)C50 toxicity values. The lowest one is selected

Table 2.4: Modified EPA assessment factors for birds and mammals.

Available information	Additional criteria	MPC based on	Assessment factor
less than 3 L(E)C50 values	$L(E)C50_{bird/mam_{min}}/1000 < NOEC_{bird/mam_{min}}/10$	$L(E)C50_{bird/mam_{min}}$	1000
at least 3 L(E)C50 values	$L(E)C50_{bird/mam_{min}}/100 < NOEC_{bird/mam_{min}}/10$	$L(E)C50_{bird/mam_{min}}$	100
less than 3 NOECs	$L(E)C50_{bird/mam_{min}}/1000 (100) \geq NOEC_{bird/mam_{min}}/10$	$NOEC_{bird/mam_{min}}$	10*
3 NOECs		$NOEC_{bird/mam_{min}}$	10

* this value is subsequently compared to the extrapolated value based on acute L(E)C50 toxicity values. The lowest one is selected

In this report the use of quantitative structure-activity relationships (QSARs) is restricted to those cases, in which the experimental data for organic chemicals exceed the QSAR data for narcosis. Because these QSARs represent the minimum toxicity caused by narcosis, this can be regarded as the upper limit for the HC5 or HC50.

In 1999, it was decided to use the assessment factors from the Technical Guidance Document of the European Union (EU/TGD), because of the harmonisation of the project ‘Setting Integrated Environmental Quality Standards’ with the framework of admission of plant protection products and biocides (Kalf et al., 1999). The scheme with assessment factors used are shown in Table 2.5 for the aquatic compartment and in Table 2.6 for the terrestrial compartment. Some modifications have been applied to the original schemes for the purpose of the project ‘Setting Integrated Environmental Quality Standards’.

- First, the classification in taxonomic groups is used instead of the original classification in trophic levels, because this classification is used throughout the whole derivation of MPCs.
- Second, for terrestrial data a comparison with equilibrium partitioning is made in all cases of preliminary risk assessment (see section 2.3.4).
- A third minor modification is that as input for one species the geometric mean of several toxicity data based on the same toxicological endpoint is taken instead of the arithmetic mean.

Table 2.5: EU/TGD assessment factors for aquatic organisms.

Available data	Additional criteria	MPC based on	Assessment factor	Tag #
L(E)C50s for algae, <i>Daphnia</i> and fish (base set)		L(E)C50 _{aqua_min}	1000	a
Base set + 1 NOEC (not algae)	NOEC from same taxonomic group as L(E)C50 _{aqua_min} (fish or <i>Daphnia</i>)? Yes	NOEC _{aqua_min}	100	b
	No. L(E)C50 _{aqua_min} /1000 < NOEC _{aqua_min} /100	L(E)C50 _{aqua_min}	1000	c
	No. L(E)C50 _{aqua_min} /1000 ≥ NOEC _{aqua_min} /100	NOEC _{aqua_min}	100	d
Base set + 2 NOECs	NOEC from same taxonomic group as L(E)C50 _{aqua_min} ? Yes	NOEC _{aqua_min}	50	e
	No	NOEC _{aqua_min}	100	f
Base set + 3 NOECs	NOECs for Algae, <i>Daphnia</i> and fish? Yes	NOEC _{aqua_min}	10	g
	No. NOEC from same taxonomic group as L(E)C50 _{aqua_min}	NOEC _{aqua_min}	10	h
	No. NOEC not from same taxonomic group as L(E)C50 _{aqua_min}	NOEC _{aqua_min}	50	i

For the aquatic compartment it is required that the base set is complete, i.e. acute toxicity studies for algae, *Daphnia* and fish. However, for more hydrophobic compounds ($\log K_{ow} \geq 3$) short term toxicity data may not be representative, since the time span of an acute test may be too short to reach a toxic internal level. In those cases, the completeness of the base set is not demanded and an assessment factor of 100 may be applied to a chronic test, which should not be an alga test if this is the only chronic test available.

In case the base set is incomplete, a factor 100 and/or 1000 will be applied to the lowest NOEC and/or L(E)C50, respectively, to derive the MPC. In Kalf et al. (1999) it is stated that

the modified EPA method should be used in such a case. However, according to this method an assessment factor of only 10 should be applied to the lowest NOEC, while the highest assessment factor in the EU/TGD method to apply to a chronic NOEC is 100. If data are available for terrestrial species as well as processes, the data are considered separately and MPCs are derived for both.

Table 2.6: EU/TGD assessment factors for terrestrial species/processes.

Available data	Additional criteria	MPC based on	Assessment factor	Tag #
≥ 1 L(E)C50		L(E)C50terr _{min}	1000	a
1 NOEC, no L(E)C50s		NOECterr _{min}	100	b
1 NOEC, ≥ 1 L(E)C50s	L(E)C50terr _{min} /1000 < NOECterr _{min} /100	L(E)C50terr _{min}	1000	c
	L(E)C50terr _{min} /1000 \geq NOECterr _{min} /100	NOECterr _{min}	100	d
2 NOECs	NOEC from same taxonomic group as L(E)C50terr _{min} ? Yes	NOECterr _{min}	50	e
	No	NOECterr _{min}	100	f
3 NOECs	NOEC from same taxonomic group as L(E)C50terr _{min} ? Yes	NOECterr _{min}	10	g
	No	NOECterr _{min}	50	h

2.3.3 Added risk approach

The added risk approach, which was modified from Struijs et al. (1997) by Crommentuijn et al. (1997a), is used to calculate risk limits for the different environmental compartments. The approach starts with calculating an addition (SRA_{eco}, MPA or NA instead of SRC_{eco}, MPC or NC, respectively) on the basis of available data from laboratory toxicity tests in the same way as described in the previous sections. The effect concentrations from these laboratory toxicity tests are expressed in (nominal) concentrations added to the test soil. The specific ERL (SRC_{eco}, MPC or NC) consists of this added part, which may be related to anthropogenic activities, and the background concentration (C_b):

$$\text{SRC}_{\text{eco}} = C_b + \text{SRA}_{\text{eco}}, \quad \text{MPC} = C_b + \text{MPA}, \quad \text{NC} = C_b + \text{NA} \quad (4)$$

The negligible addition (NA) is equal to MPA/100, in which the factor 100 is a safety factor, to take into account combination toxicity (VROM, 1989). It must be noted that the background concentration and the SRC_{eco} or MPA are independently derived values. The theoretical description of the added risk approach as described by Struijs et al. (1997) includes bioavailable fractions of the background concentrations that can vary between 0% and 100%. For the purpose of deriving environmental risk limits this approach has been worked out by assuming that the bioavailable fraction of the background concentration is zero ($\varphi = 0$) (Crommentuijn et al., 1997a). This was done because from a policy point of view the effects of the natural background concentration may be considered desirable. Furthermore, at this moment not enough information is available to derive the bioavailability of the background concentrations for metals and it was shown by Crommentuijn et al. (2000) that the resulting MPCs are not much different by assuming different bioavailability. With regard

to the bioavailable fraction of the metals and metalloids in laboratory tests, it is assumed here that the added metals and metalloids to the test medium are completely bioavailable, i.e. the bioavailable fraction of the added metal and metalloid in the laboratory tests is 100%.

2.3.4 Equilibrium partitioning method

In case no data on terrestrial/sediment species are available, the Equilibrium Partitioning method or EqP-method is applied to derive ERLs for soil. Besides the EqP-method is used for harmonisation (see section 2.3.5) of ERLs (MPCs and SRC_{s_{eco}}). Three assumptions are made when applying this method. First of all, it is assumed that bioavailability, bioaccumulation and toxicity are closely related to the pore water concentrations. Second, it is assumed that sensitivities of aquatic organisms are comparable with sensitivities of organisms living in the sediment. Third, it is assumed that an equilibrium exists between the chemical sorbed to the particulate sediment organic carbon and the pore water and that these concentrations are related by a partition coefficient (K_{oc}).

Soft-bodied terrestrial organisms like earthworms and enchytraeids, will be mainly exposed via the pore water. The amount of a compound available in the pore water depends strongly on soil characteristics such as pH for metals and organic matter content for both organic compounds and metals. Relationships between the accumulation of metals by invertebrates and soil characteristics have been found (reviewed in Van Gestel et al., 1995). Also some relationships between toxicity and soil characteristics have been found like for instance for cadmium and earthworms (Van Gestel and Van Dis, 1988) and between chlorobenzenes and earthworms (Belfroid et al., 1994). However, for hard-bodied organisms this assumption of uptake via the pore water phase is questionable and it is unclear whether or not equilibrium partitioning gives a good estimate of the toxicity for these type of organisms. This topic is a point under discussion at this moment.

To be able to apply the EqP-method data on partition coefficients are required. In the framework of the evaluation of Intervention Values, a protocol has been developed for the derivation of sorption coefficients for organic substances normalised to organic carbon (K_{oc}) and values have been calculated for all compounds considered in this report (Otte et al., 2001). These sorption coefficients are used for the derivation of the SRC_{eco}. According to this protocol, the mean of all reliable experimental data and one calculated value is taken. The calculated log K_{oc} can be estimated using the regression equations described by Sabljic et al. (1995). These are empirical formulas from which a log K_{oc} can be derived using a log K_{ow} . The log K_{ow} is derived from the MEDCHEM database; the star values from this database (MlogP) are preferred. If not available the value calculated on the basis of the ClogP method is used which is also given in the MEDCHEM data base.

From the K_{oc} s partition coefficients for standard soil and sediment (K_{ps}) are calculated. Standard soil and sediment contains 10% organic matter and therefore the K_{oc} s are divided by 10·1.7 to obtain K_{ps} .

$$K_{p \text{ (standard soil)}} = K_{oc} \cdot f_{oc} \quad (5)$$

in which: $K_{p \text{ (standard soil)}}$ = partition coefficient for standard soil in l/kg
 K_{oc} = organic carbon normalised partition coefficient in l/kg
 f_{oc} = fraction organic carbon of standard soil (=0.0588)

The risk limit for terrestrial/sediment species using equilibrium partitioning is calculated using the following equation:

$$ERL(\text{sed} / \text{soil}_{EP}) = ERL(\text{water}) * K_{P(\text{standard soil/sed})} \quad (6)$$

in which: $ERL(\text{sed}/\text{soil}_{Eqp}) =$ Risk Limit for terrestrial species using the equilibrium partition method
 $ERL(\text{water}) =$ Risk Limit for aquatic species
 $K_{p(\text{standard soil/sed})} =$ partition coefficient for standard soil or standard sediment in l/kg

2.3.5 Deriving Negligible Concentrations

The Negligible Concentration (NC), in contrast to the MPC, is not based on a fraction of species protected and is derived by dividing the MPC by a factor 100. This factor is applied to take into account combination toxicity (VROM, 1989).

2.4 Harmonisation of independently derived ERLs

When independently derived ERLs for water and sediment/soil are available, these have to be harmonised with those for water. This is done by calculating the ERL for sediment or soil from the ERL for water and applying the equilibrium partition method as described in section 2.3.4. In principle the lowest value of the ERL derived directly from the terrestrial data and the ERL resulting from Eq. 8 is then taken as the harmonised ERL. This is done for the MPC as well as for the SRC_{eco} .

However, the uncertainties in both ERLs and the partition coefficient are taken into account. If statistical extrapolation can be applied to the terrestrial data (species or processes), the MPC and SRC_{eco} are derived directly from the terrestrial toxicity data and no comparison with equilibrium partitioning is made. If not enough terrestrial data are available and preliminary risk assessment is applied, a comparison with equilibrium partitioning is always made for the derivation of the SRC_{eco} . From this comparison the minimum value is chosen as SRC_{eco} . Mostly, the derivation of the MPC is done in the same way. However, some exceptions to this rule were made in the framework of 'Setting Integrated Environmental Quality Standards' because of expert judgement. In view of the status of the SRC_{eco} the minimum value is always selected as a precaution principle.

In Figure 2.2 an overview is given how the aspects discussed in 2.3.1, 2.3.2, and 2.3.4 lead to the proposed SRC_{eco} . As basis for the SRC_{eco} the HC50 is taken. The HC50 for water is derived directly from the aquatic toxicity data, either by refined or preliminary risk assessment. For soil the same approach is followed. Only if not enough data are available to perform refined risk assessment, harmonisation with the water compartment is completed by means of equilibrium partitioning. It should be noted that the HC50 for sediment is almost always derived by equilibrium partitioning, because data for sediment-dwelling organisms are seldom available, and that the SRC_{eco} for groundwater is not harmonised with soil.

Harmonisation of ERLs may be necessary because e.g. releases of chemicals to water and soil can, after volatilisation, lead to deleterious effects in the air. Multimedia fate models have been proposed (Van de Meent and De Bruijn, 1995) to harmonise independently derived ERLs. In these models, the environmental compartments are represented by boxes. Steady state intermedia concentrations that are expected to be the result of long term management policy are calculated. Comparison of the computed intermedia concentration with the proposed quality guidelines is carried out to check whether coexistence of these guidelines is possible.

In the case of the Intervention Values, the derived $SRCS_{eco}$ are compared with the human-toxicological risk limits. These limits are obtained by recalculating the MPC for human toxicology into a corresponding concentration in soil, water or sediment by means of the exposure model CSOIL (Van den Berg, 1995) or SEDISOIL (Bockting et al., 1996).

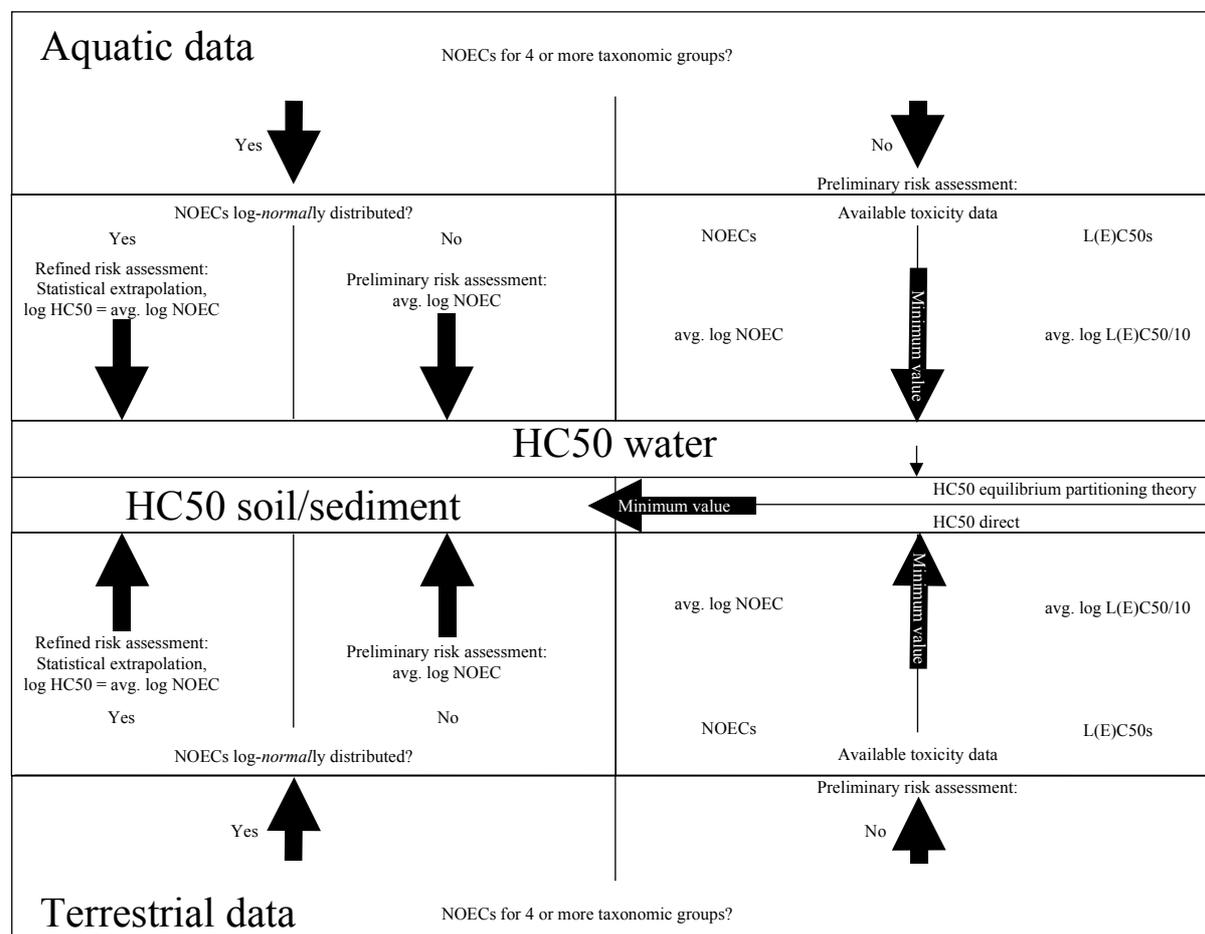


Figure 2.2: Schematic outline of the derivation of the $SRCS_{eco}$

2.5 Mixture toxicity: sum values and toxic units

For some groups of similar compounds, it will be desirable to take into account the combined toxic effects. A requirement for the implementation of risk limits for groups of compounds is that the compounds considered have the same mode of toxic action and their effects are additive. To deal with the combined effects of different compounds there are two possibilities.

First, a sum value can be derived for a group of chemicals. The sum of the concentrations of the individual compounds from the group as measured in the field is compared with this ERL for the whole group, which can be derived by taking the geometric mean of the individual values for the single compounds. An additional condition in this case is that the effect concentrations of the individual compounds are similar. The use of one value for the sum of similar compounds has the advantage that influences of uncertainties in the derivation of the ERLs for individual compounds are decreased.

Accumulation in organisms from soil and sediment is more or less independent of the physicochemical properties of the individual compounds. Sorption to soil and sediment and bioconcentration of organic compounds are almost equally dependent on hydrophobicity,

which results in more or less constant ratios between the concentrations in sediment and soil on the one hand and the concentration in organisms on the other, the biota-to-sediment/soil-accumulation-factors (BSAFs) (Hendriks et al., 1998; Tracey and Hansen, 1996). If compounds have the same intrinsic toxicity (mode of toxic action) this will also result in almost constant effect concentration in soil or sediment. For compounds with different physicochemical properties, a sum value can be derived for soil and sediment only if these BSAF values of the individual compounds are comparable, otherwise the effect concentrations will be different.

Because no information is available for these BSAF values, sum values are only derived in this report for isomers of compounds, for which it is assumed that they have similar physicochemical behaviour. These isomers are xylenes, cresols, dihydroxybenzenes, isomers of chlorophenols and chlorobenzenes, monochloronaphthalenes and hexachlorocyclohexanes (HCHs). Sum values are also derived for the structural similar groups of the drins. For pragmatic reasons a sum value for polychlorinated biphenyls (PCBs) is derived. In section 4.3.4, the outlook of deriving a sum value in the future for compounds that act mainly by narcosis is discussed.

Second, mixture toxicity can also be captured by working with toxic units. In this case, the compounds are assumed to have the same mode of toxic action and their effect concentrations are additive. In this approach the ratios of the concentration and the ERL of compounds from the same group are summed. The ERL for the sum of these compounds is exceeded if the sum of these ratios exceeds the value of one. An advantage of working with toxic units is that for each single compound the ERL is not averaged with that of other compounds. Consequently, differences in toxicity between the individual constituents in a group of compounds that are considered to have the same mode of action are still present in the calculation of the combined toxic pressure. In this way, mixture toxicity can also be taken into account for compounds with different physicochemical behaviour. For the water compartment, this is the only way to take into account mixture toxicity for most groups of compounds, because the individual compounds differ in their accumulation in aquatic species and therefore also in their toxicity.

For groups of compounds with a similar toxic mode of action but with different environmental behaviour, such as the chlorobenzenes, this approach is proposed. For the groups of PAHs, chlorinated aliphatic hydrocarbons, chlorophenols, and phthalates the mode of toxic action is not the same for all compounds. Some of the compounds in these groups exhibit only an a-specific mode of action, while others have besides this narcotic effect also a more specific mode of action to a part of the species. Therefore, no toxic unit approach or sum values for these groups of compounds are proposed in this report. Nevertheless, it may be desirable to take into account mixture toxicity for these groups. This topic of mixture toxicity will be addressed in a separate project within the framework of 'Setting Integrated Environmental Quality Standards'.

2.6 Methodology to determine reliability of SRCs_{eco}

To denote the SRCs_{eco} as reliable, they should meet the following criteria, according to the Technical Soil Protection Committee (TCB, 1997):

- at least four toxicity data should be available for as much as possible different taxonomic groups,
- for metals all toxicity data should be based on the terrestrial compartment,
- for organic substances not more than two data should be based on equilibrium partitioning.

Applying these criteria means that an SRC_{eco} for metals can be classified reliable only if toxicity data for the terrestrial compartment are available.

In this report three classes of reliability are introduced for the SRC_{eco}: high, medium and low.

- SRCs_{eco}(soil) for both metals and organic substances are assigned a high reliability if the SRC is completely based on terrestrial toxicity studies. This means that for a high reliability score the SRC_{eco} must be based on refined risk assessment for terrestrial data. This requires the presence of chronic toxicity studies for at least 4 taxonomic groups or terrestrial processes.
- A medium reliability score is assigned if preliminary risk assessment is applied to terrestrial data, i.e. some terrestrial toxicity studies are available. For organic substances a further possibility for a medium reliability score is, when the aquatic SRC_{eco} is based on refined risk assessment and equilibrium partitioning is applied, provided that a reliable partition coefficient is available.
- A low reliability score is assigned to metals and organic substances if no terrestrial data are available, with the exception for organic substances mentioned above.

For sediment the same criteria are applied. This means that SRC_{eco}(sediment) for metals will always have a low reliability, due to the absence of sediment toxicity studies. For organic substances, the reliability may be medium or low, depending on the number of aquatic toxicity studies.

For water the reliability is considered high if statistical extrapolation can be applied. If both chronic and acute toxicity studies are available the reliability has a medium score. If only acute or chronic toxicity studies are available the reliability is low. A low reliability score is also assigned to the SRC_{eco} if only QSAR estimates are used for the derivation. If QSARs are applied as a comparison for the experimental toxicity data, the reliability score is based on the number of experimental data and not on the QSARs.

2.7 Differences with former methodology

The ecotoxicological basis of the first series of Intervention Values was completed by Denneman and van Gestel in 1990. The methodology that was used to derive these Serious Soil Contamination Concentrations is slightly different from the methodology used in this report. In this report the methodology largely follows that of the project 'Setting Integrated Environmental Quality Standards'. A summary of the differences with the methodology used by Denneman and van Gestel is given below.

- The SRC_{eco} for groundwater is based upon toxicity data for surface water. The former SRCs were derived by equilibrium partitioning from the integrated SRC values.
- As for metals the background concentrations are substantial compared to the HC50 and not included in the toxicity data, the added risk approach is used to derive the SRC_{eco}. This is in line with the derivation of MPCs and NCs for metals.

- Terrestrial processes are included in the derivation of the SRC_{eco} , while in principle, processes were used by Denneman and van Gestel as a verification of the data on single species.
- LC50s and EC50s are considered in conjunction, the ACR applied to both values is 10, while Denneman and van Gestel treated these values separately, with ACRs of 10 and 5, respectively.
- Species are used as input in the ecotoxicological risk assessment instead of taxonomic groups. Denneman and van Gestel used the geometric mean of the data for each taxonomic group as entry.
- The requirements to use statistical extrapolation techniques are less stringent, and is applied if NOECs are available for at least 4 taxonomic groups. Statistical extrapolation was only applied by Denneman and van Gestel if there were toxicity data for at least five taxonomic groups from at least three representative groups for that compartment (e.g. algae, crustaceans and fish for water).
- Statistical extrapolation is only used on chronic data, in the past also extrapolation on LC50s and EC50s was applied.
- The extrapolation method assumes a log-normal instead of log-logistic distribution.
- If few data are available ('preliminary risk assessment') the SRC_{eco} is based on the lowest value from the geometric mean of chronic toxicity data *or* from the geometric mean of acute toxicity data divided by 10 *or* from equilibrium partitioning. In the methodology of Denneman and van Gestel, the number of data was the first discriminating factor to base the HC50 upon and thereafter the type of data: 4 NOECs, 4 EC50s, 4 LC50s, ... , 1 NOEC, 1 EC50, 1 LC50, EqP.

3 Results

In this chapter proposals for SRC_{eco} are given for compounds belonging to the different groups (see Table 1.1). For the compounds that have been evaluated in the framework of the project 'Setting Integrated Environmental Quality Standards' the same data have been used to derive the proposals. The selected data used for the extrapolations are shown in the Appendices.

If at least 4 NOECs for species belonging to different taxonomic groups and/or at least 4 NOECs for different processes are available, the data and the estimated sensitivity curves are presented in a figure. In these figures the x-axis presents the sensitivity in categories (width 0.5 log(NOEC) units) and the y-axis the frequency of experimental data within a category. This frequency is obtained by dividing the amount of data in a certain category by the total number of data. The estimated curve is scaled on the same y-axis as the experimental data. In case no experimental data for terrestrial species and processes are available, the SRC_{eco} for soil is based on equilibrium partition method or EqP-method (see 2.3.4). The SRC_{eco} for sediment are all based on the EqP-method, as no relevant data are available yet, except for diethylhexyl phthalate.

3.1 Proposal SRA_{eco} for metals

Metals occur naturally in the environment. However, the risk limits are based on the added amount of the metal and not on the total amount of metal present in the soil. All ERLs derived below are based on the added fraction. Therefore, the HC50 serves not as basis for the Serious Risk Concentration (SRC) but for a Serious Risk Addition (SRA). The proposed values for the SRC_{eco} are based on this SRA and a background concentration, similar to the MPC and MPA:

$$SRC = SRA + C_b \quad (7)$$

For the purpose of intervention values, a generic background concentration or for some metals a location specific background concentration might be derived, by relating the background concentration to fraction clay and humus of the soil (Edelman, 1984; De Bruijn and Denneman, 1992). The total concentration of the metal in soil has to be compared to the SRC, which is derived by adding the background concentration to the SRA.

For barium, cobalt and molybdenum the toxicity data as presented by van de Plassche (1992) are used to derive the SRA_{eco} . The toxicity data as presented by Crommentuijn et al. (1997a) are used to derive SRA_{eco} for arsenic, cadmium, chromium, copper, mercury, lead, nickel and zinc. The data were used to derive MPCs and the information on the ecotoxicity tests can be found in the mentioned reports. The proposals for the SRA_{eco} are included on the following pages. Because the used data are expressed as added concentration in first instance the HC50 is calculated as an added concentration. The selected data used for extrapolation are included in Appendix 2. For cadmium, chromium, nickel, and zinc an European evaluation (EU commission regulation 1488/94) will be available on a short term.

When evaluating partition coefficients for soil and sediment it was decided that different values should be used for soil and sediment. The partition coefficients that are used in this report to derive the SRA are presented by Otte et al. (2001). Consequently, for metals always a different SRA for soil and sediment is derived. Most of the SRA_{eco} for soil are derived directly from terrestrial toxicity data. SRA_{eco} for sediment are derived by equilibrium

partitioning for all metals. Therefore, the choice of the $\log K_p$ has a major influence on the derived $\text{SRC}_{\text{eco}}(\text{sediment})$, in view of the large variance in $\log K_p$ values from literature (Otte et al., 2001).

All the proposed SRAs_{eco} are summarised in Table 3.2 together with the generic background concentrations, old values as proposed by Denneman and van Gestel (1990) and MPAs/MPCs as proposed by Crommentuijn et al. (1997a).

3.1.1 SRA_{eco} for arsenic

For terrestrial species only three NOECs for two taxonomic groups are available, 2 for plants and one for a worm (Appendix 2, Table A2. 1). The geometric mean of these values is calculated for deriving the $\text{HC50}(\text{species})$ of 56 mg/kg. Enough experimental data are available for microbial and enzymatic processes to estimate a sensitivity distribution (Figure 3.1, data in Table A2. 2). The HC50 from this sensitivity distribution is $1.6 \cdot 10^2$ mg/kg (90% CI: $1.1 \cdot 10^2 - 2.5 \cdot 10^2$ mg/kg). The lowest of these two is selected as the proposal for the SRA_{eco} for soil: **56 mg/kg** based on species.

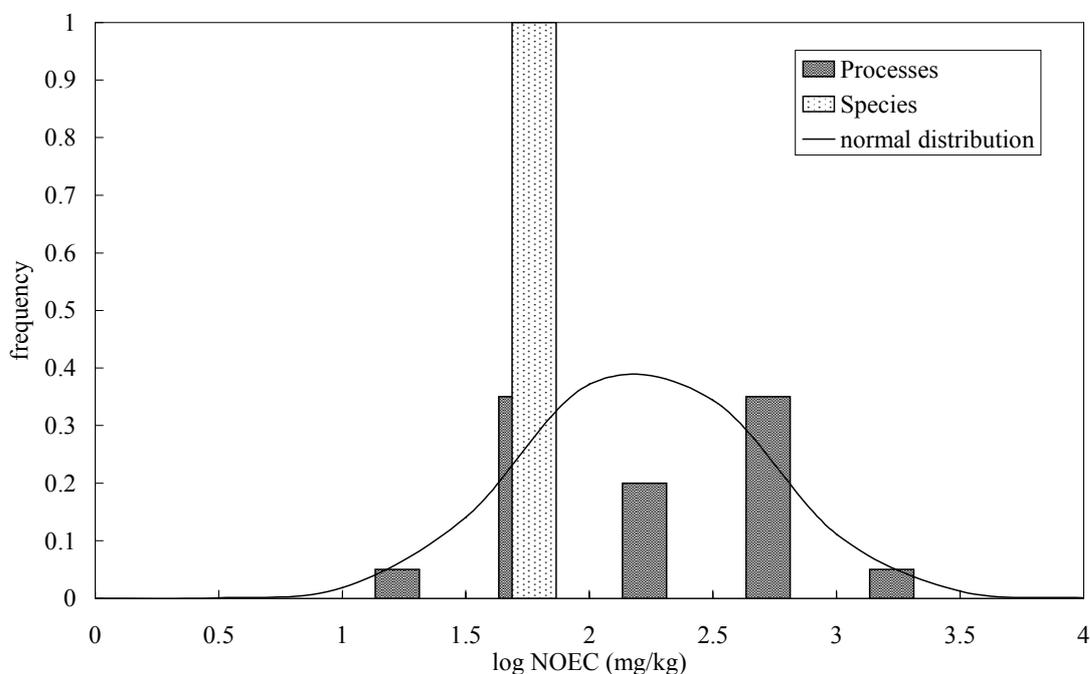


Figure 3.1: Arsenic: Distribution of chronic toxicity data for terrestrial species and processes. The estimated curve is based on the data for processes ($n = 20$, $\bar{x} = 2.21$, $s = 0.49$).

The HC5 derived from the distribution of processes is 25 mg/kg (90% CI: 11 – 44 mg/kg). The MPA(terrestrial species) of 4.5 mg/kg was derived by applying a safety factor of ten to the lowest NOEC for species according to the modified EPA method (Crommentuijn et al., 1997a). With the assessment factors of the EU/TGD a factor of 50 is applied if 3 NOECs are available. In this case, the resulting MPA is 0.90 mg/kg.

For fresh water 15 NOECs for species of 6 taxonomic groups are available. For the marine environment 2 NOECs for a macrophytic algae and a crustacean are available. Freshwater and marine data (selected data presented in Appendix 2, Table A2. 3 and Table A2. 4) are not significantly different ($P = 0.38$) and lumped to derive the $\text{HC50}(\text{aquatic species})$. From these data a log-normal frequency distribution can be estimated (Figure 3.2). The $\text{HC50}(\text{aquatic species})$ is $8.9 \cdot 10^2$ $\mu\text{g/l}$ (90% CI: $3.6 \cdot 10^2 - 22.1 \cdot 10^2$ $\mu\text{g/l}$). The HC5 of this log-normal

distribution is $24 \mu\text{g/l}$ (90% CI: 4 - 77 $\mu\text{g/l}$). With the log-logistic distribution a similar value of 25 $\mu\text{g/l}$ was derived (Crommentuijn et al., 1997a).

For sediment the SRA_{eco} is derived by applying the equilibrium partitioning method (EqP-method). The $\log K_{\text{p}(\text{sed/w})}$ is 3.82 resulting in an SRA_{eco} for sediment of $5.9 \cdot 10^3 \text{ mg/kg}$ and an MPA of $1.6 \cdot 10^2 \text{ mg/kg}$. The $\log K_{\text{p}(\text{soil/w})}$ is 3.26 resulting in corresponding values for $\text{SRA}(\text{EqP})$ and $\text{MPA}(\text{EqP})$ for soil of $1.6 \cdot 10^3$ and 44 mg/kg , which are higher than the SRC_{eco} derived directly from terrestrial toxicity data.

For soil as well as for sediment a background concentration of 29 mg/kg (van den Hoop, 1995) is assumed. For water a background concentration of 0.77 $\mu\text{g/l}$ (Crommentuijn et al., 1997a) is assumed.

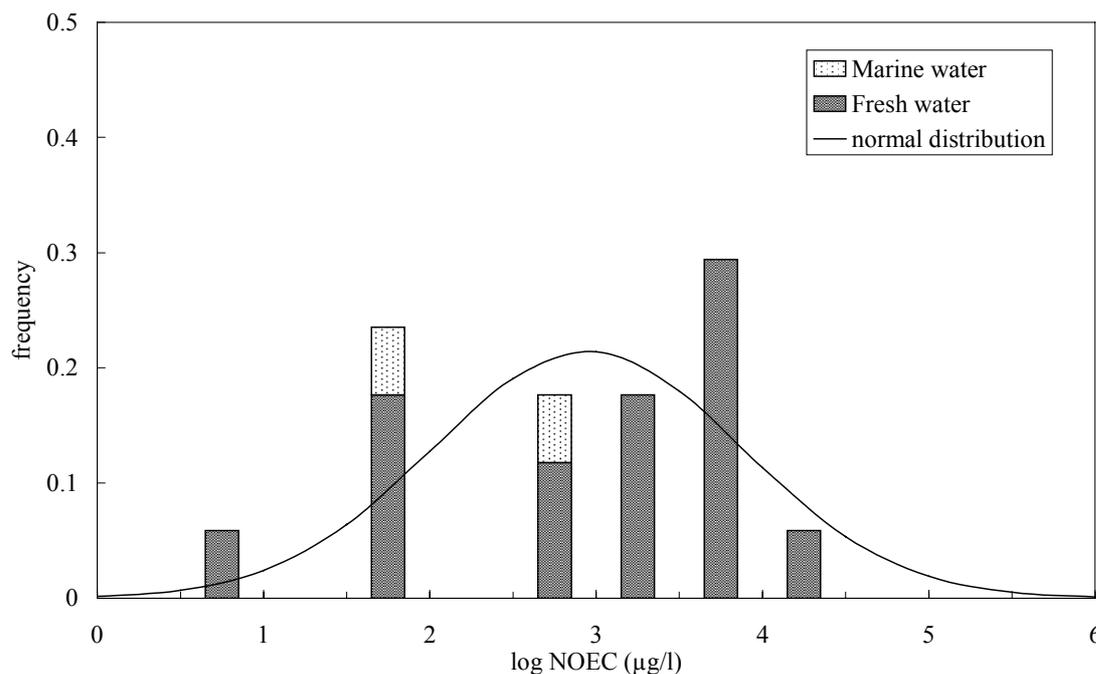


Figure 3.2: Arsenic: Distribution of chronic toxicity data for aquatic species. The estimated curve is based on the combined set of fresh water and marine toxicity data ($n = 20$, $\bar{x} = 2.95$, $s = 0.93$).

3.1.2 SRA_{eco} for barium

No ecotoxicological data on terrestrial species are available for barium. Selected data on terrestrial processes are listed in Table A2. 5. The distribution of these data is shown in Figure 3.3. The HC50 of this distribution is $7.3 \cdot 10^2 \text{ mg/kg}$ (90% CI: $5.0 \cdot 10^2 - 10.1 \cdot 10^2 \text{ mg/kg}$).

The HC5 of this distribution is $1.8 \cdot 10^2 \text{ mg/kg}$ (90% CI: $0.9 \cdot 10^2 - 2.9 \cdot 10^2 \text{ mg/kg}$). These data have not been included in the derivation of the MPA. The MPA of 9.0 mg/kg for soil was derived by equilibrium partitioning with a $\log K_{\text{p}}$ of 1.78 l/kg from the MPA for water (Crommentuijn et al., 1997a).

The selected data for aquatic species are shown in Appendix 2, Table A2. 6. For barium, only data for the sensitivity of freshwater species are available. On the basis of the NOEC data an HC50(aquatic species) of $7.0 \cdot 10^3 \mu\text{g/l}$ is derived. Applying an ACR of 10 to the geometric mean of the L(E)C50 values yields a slightly higher value of $9.3 \cdot 10^2 \mu\text{g/l}$. The MPA for water was derived by the modified EPA method (Crommentuijn et al., 1997a). Because acute toxicity data are available for crustaceans (*Daphnia*) and fish and a chronic toxicity study shows that algae are not more sensitive, a safety factor of 100 is applied to the lowest

L(E)C50. The resulting MPA for barium was $1.5 \cdot 10^2 \mu\text{g/l}$ (Crommentuijn et al., 1997a). According to the EU/TGD method, a safety factor of 100 is applied to the lowest NOEC in this case, resulting in an MPA of **29** $\mu\text{g/l}$.

The $\log K_{p(\text{soil/w})}$ used here is 3.40 and the $\log K_{p(\text{sed/w})}$ 3.00. Applying equilibrium partitioning results in an SRA_{eco} of $7.0 \cdot 10^3 \text{ mg/kg}$ for sediment. The MPA for sediment derived by equilibrium partitioning is **29** mg/kg (Crommentuijn et al., 1997a). The $\log K_{p(\text{soil/w})}$ results in values for $\text{SRA}(\text{EqP})$ and $\text{MPA}(\text{EqP})$ of $1.8 \cdot 10^4$ and 73 mg/kg , which is much higher than the value derived from the terrestrial toxicity data in the case of the SRA.

For soil as well as for sediment a background concentration of 155 mg/kg (van de Plassche and de Bruijn, 1992) is assumed.

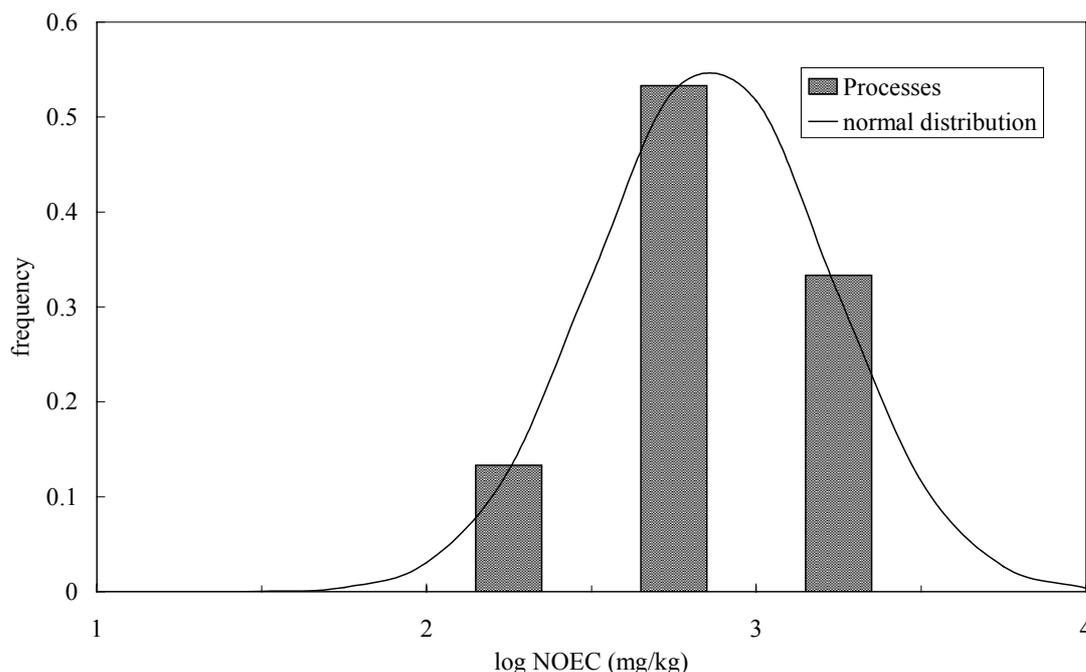


Figure 3.3: Barium: Distribution of chronic toxicity data for terrestrial processes and estimated sensitivity distribution ($n = 15$, $\bar{x} = 2.86$, $s = 0.36$).

3.1.3 SRA_{eco} for cadmium

For cadmium enough experimental NOECs are available for species as well as processes to estimate sensitivity distributions (Figure 3.4). The data used for extrapolation are shown in Appendix 2, Table A2. 7 and Table A2. 8. For species an HC50 of 12 mg/kg (90% CI: $5 - 27 \text{ mg/kg}$) and for processes an HC50 of $1.2 \cdot 10^2 \text{ mg/kg}$ (90% CI: $0.9 \cdot 10^2 - 1.5 \cdot 10^2 \text{ mg/kg}$) is derived. The lowest of the two is selected as the proposal for the SRA_{eco} for soil: **12** mg/kg based on species.

For species the HC5 of this distribution is 0.79 mg/kg (90% CI: $0.16 - 2.10 \text{ mg/kg}$) and for processes the HC5 is 15 mg/kg (90% CI: $10 - 21 \text{ mg/kg}$) is derived. The lowest of the two is selected as the proposal for the MPA for soil: **0.79** mg/kg based on species (similar to the MPA of 0.76 mg/kg derived by the log-logistic distribution; Crommentuijn et al., 1997a).

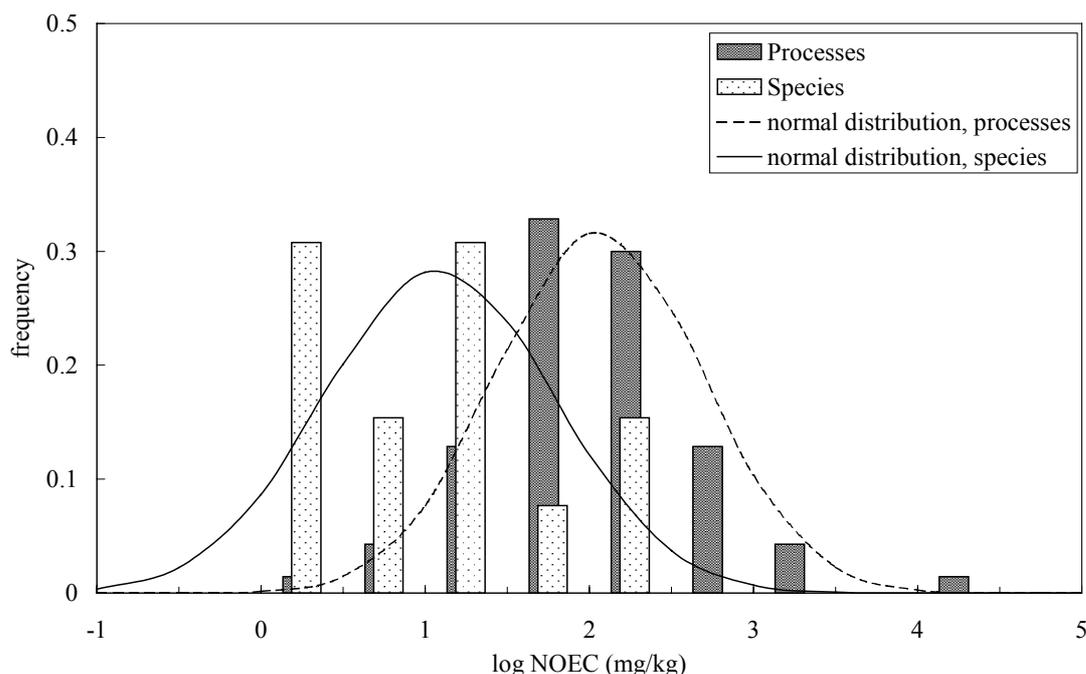


Figure 3.4: Cadmium: Distribution of chronic toxicity data for terrestrial species and processes and estimated sensitivity distributions for terrestrial species ($n = 13$, $\bar{x} = 1.08$, $s = 0.70$) and processes ($n = 70$, $\bar{x} = 2.08$, $s = 0.54$).

For cadmium NOECs for fresh water species and marine species are available (selected data presented in Appendix 2, Table A2. 9 and Table A2. 10). Fresh water and marine data are treated separately to derive the HC50s for aquatic species (Figure 3.5), because differences in the distributions were significant ($P = 0.042$, Welch-corrected). This is possibly caused by differences in bioavailability due to other complexation behaviour in a saline environment. The HC50(aquatic species) is **9.6** $\mu\text{g/l}$ (90% CI: 6.1 – 15.2 $\mu\text{g/l}$) for fresh water and **27** $\mu\text{g/l}$ (90% CI: 14 – 55 $\mu\text{g/l}$) for marine water.

The HC5 of these distributions are 0.42 $\mu\text{g/l}$ (90% CI: 0.19 – 0.79 $\mu\text{g/l}$) and 0.34 $\mu\text{g/l}$ (90% CI: 0.10 – 0.88 $\mu\text{g/l}$). From these values it is apparent that one MPA for both fresh water and marine water might be derived as well. This HC5 from the combined sets of data is **0.34** $\mu\text{g/l}$ (90% CI: 0.17 – 0.61 $\mu\text{g/l}$). With the log logistic distribution the same MPA was derived (Crommentuijn et al., 1997a).

For sediment the SRA_{eco} is derived by applying the equilibrium partitioning method (EqP-method). The $\log K_{\text{p(sed/w)}}$ is 4.93, resulting in SRAs_{eco} of **$8.2 \cdot 10^2$** mg/kg for fresh water sediment and **$2.3 \cdot 10^3$** mg/kg for marine sediment. It should be noted that this partition coefficient is not derived for marine water. The MPA of **29** mg/kg for sediment is derived from the MPA for water.

For soil as well as for sediment a background concentration of 0.8 mg/kg (van den Hoop, 1995) is assumed. For water, background concentrations are assumed of 0.08 $\mu\text{g/l}$ for fresh water (Crommentuijn et al., 1997a) and 0.025 $\mu\text{g/l}$ for marine water (Van den Hoop, 1995).

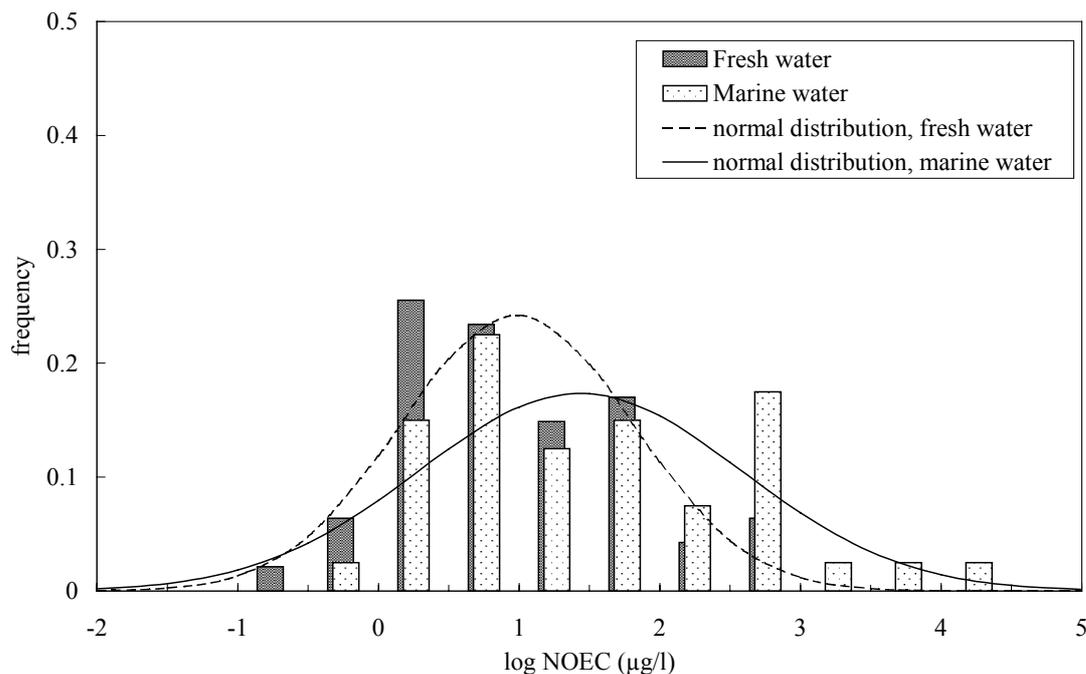


Figure 3.5: Cadmium: Distribution of chronic toxicity data for aquatic species and estimated sensitivity distributions for fresh water species ($n = 47$, $\bar{x} = 0.98$, $s = 0.82$) and marine species ($n = 40$, $\bar{x} = 1.43$, $s = 1.15$).

3.1.4 SRA_{eco} for chromium

Cr(III) is the most common stable form in soil. Most of the Cr(VI) present in soil is directly reduced to Cr(III). Only in oxygen rich soils, containing almost no organic matter and in which manganese oxide is present as an oxidant, Cr(III) is oxidised to Cr(VI) (Slooff et al., 1990).

Most toxicity tests in soil are for Cr(III), the most stable form (Appendix 2, Table A2. 11 and Table A2. 12). A statistical comparison between the data for Cr(III) and Cr(VI) is not very meaningful because of the limited data set for chromium(VI). The NOECs for chromium(VI) are within the range of the toxicity data for chromium(III) ($P = 0.28$, Table A2. 13). Still, SRA_{eco} are derived for both Cr(III) and Cr(VI).

- Chromium(III) in soil: NOECs are available for plants and earthworms resulting in an $HC50(\text{species})$ of $1.2 \cdot 10^2$ mg/kg. With two NOECs available the MPA according to the EU/TGD method would be 0.38 mg/kg. For microbe-mediated processes an $HC50(\text{processes})$ of $1.3 \cdot 10^2$ mg/kg (99% CI: $0.8 \cdot 10^2 - 2.1 \cdot 10^2$ mg/kg) is derived (Figure 3.6), almost equal to the $HC50$ for species. The $HC5$ from this distribution is 8.5 mg/kg (90% CI: 3.8 – 15.9 mg/kg).
- Chromium(VI) in soil: For chromium(VI) only two experimental data are available for processes, resulting in an $HC50(\text{processes})$ of $9.8 \cdot 10^2$ mg/kg. The MPA derived from these data according to the EU/TGD method is 6.8 mg/kg.

The lowest value is selected to be the SRA_{eco} : $1.2 \cdot 10^2$ mg/kg based on the $HC50(\text{species})$ for Cr(III). The MPA of 3.8 mg/kg for chromium was the lowest value for chromium(III) derived with the modified EPA method (Crommentuijn et al., 1997a). With the EU/TGD assessment factors this MPA is **0.38** mg/kg.

To derive an SRA_{eco} for sediment the EqP-method is applied using aquatic toxicity data. In water the distribution between Cr(III) and Cr(VI) depends on environmental circumstances,

for instance pH, redox potential and total chromium concentration (Schmidt, 1984). Cr(III) and Cr(VI) can be interconverted depending on environmental conditions. However in surface water, especially marine surface water, either Cr(III) or Cr(VI) can be stable.

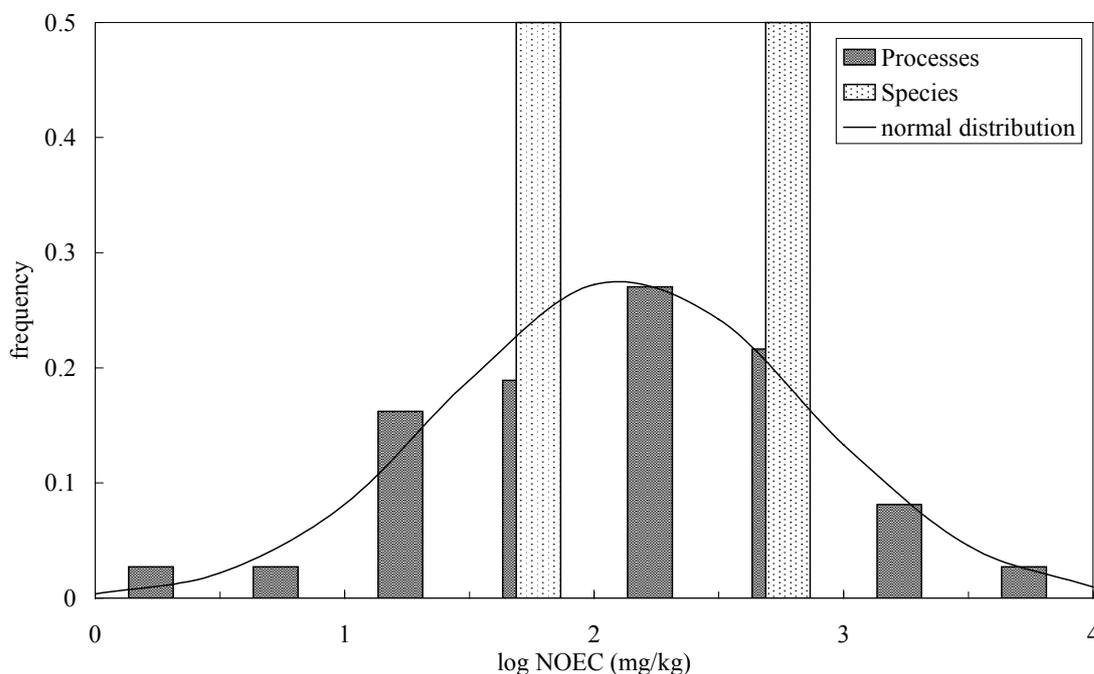


Figure 3.6: Chromium(III): Distribution of chronic toxicity data for terrestrial species and processes. The estimated curve is based on the data for processes ($n = 37$, $\bar{x} = 2.13$, $s = 0.72$).

According to Nriagu and Nieboer (1988), Cr(VI) is more toxic than Cr(III) for most organisms. On the basis of the data presented in Table A2. 14 - Table A2. 16, it can be concluded that there is less variation in the NOECs for chromium(III) than for chromium(VI) but no differences in sensitivity of the combined sets (fresh water and marine species) between Cr(III) and Cr(VI) were proven. This comparison is however based on a smaller amount of data for Cr(III) ($n=7$) than for Cr(VI) ($n=55$). Therefore, HC50s(aquatic species) are derived for both Cr(III) and Cr(VI) and toxicity data are not combined.

- Chromium(III) in water (Figure 3.7). For aquatic species only data on fresh water species are available (Table A2. 14). The HC50(aquatic species) is $2.2 \cdot 10^2 \mu\text{g/l}$ (90% CI: $1.0 \cdot 10^2 - 4.8 \cdot 10^2 \mu\text{g/l}$). The HC5 from this distribution is $36 \mu\text{g/l}$ (90% CI: $6 - 85 \mu\text{g/l}$).
- Chromium(VI) in water (Figure 3.8). One protozoan species is very sensitive compared to other species for Cr(VI) (Table A2. 15). For the marine environment only data for three taxonomic groups are available (Table A2. 16). The data for fresh water and marine species are not significantly different ($P = 0.84$) and therefore both sets of data are combined. The HC50(aquatic species) is $2.6 \cdot 10^2 \mu\text{g/l}$ (90% CI: $1.6 \cdot 10^2 - 4.0 \cdot 10^2 \mu\text{g/l}$). The HC5 from this distribution is $8.7 \mu\text{g/l}$ (90% CI: $4.0 - 16.4 \mu\text{g/l}$).

If both sets for chromium(III) and chromium(VI) are combined the resulting HC50(aquatic species) is equal to $2.5 \cdot 10^2 \mu\text{g/l}$. This value is of course largely dominated by the data for chromium(VI).

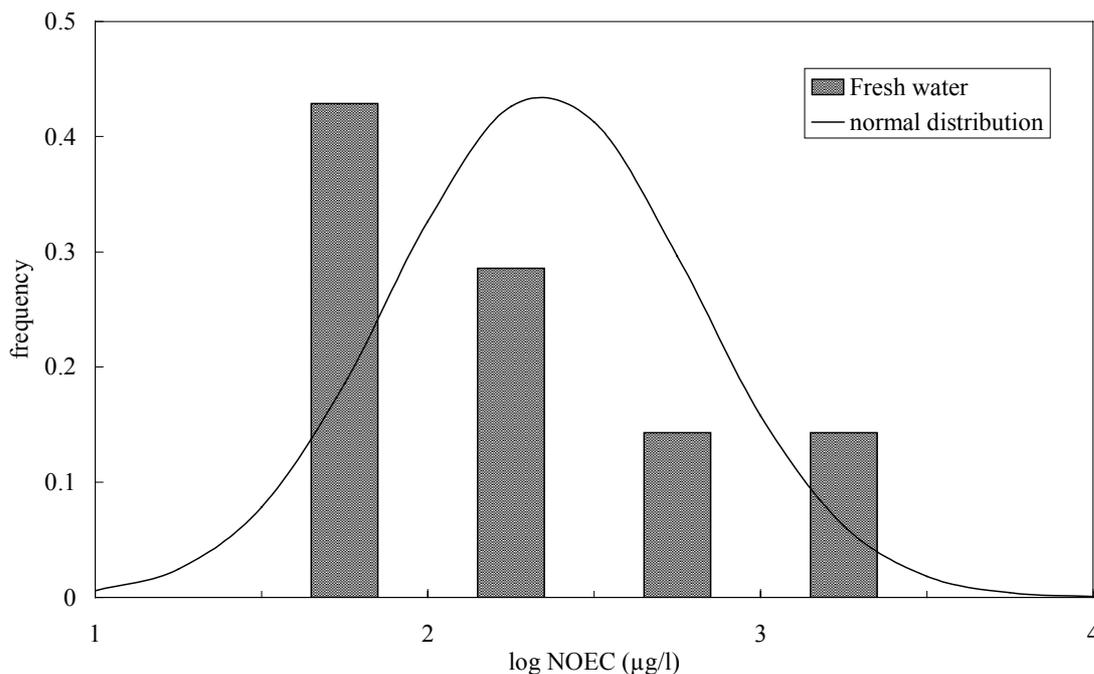


Figure 3.7: Chromium(III): Distribution of chronic toxicity data for aquatic species and estimated sensitivity distribution curve ($n = 7$, $\bar{x} = 2.35$, $s = 0.46$).

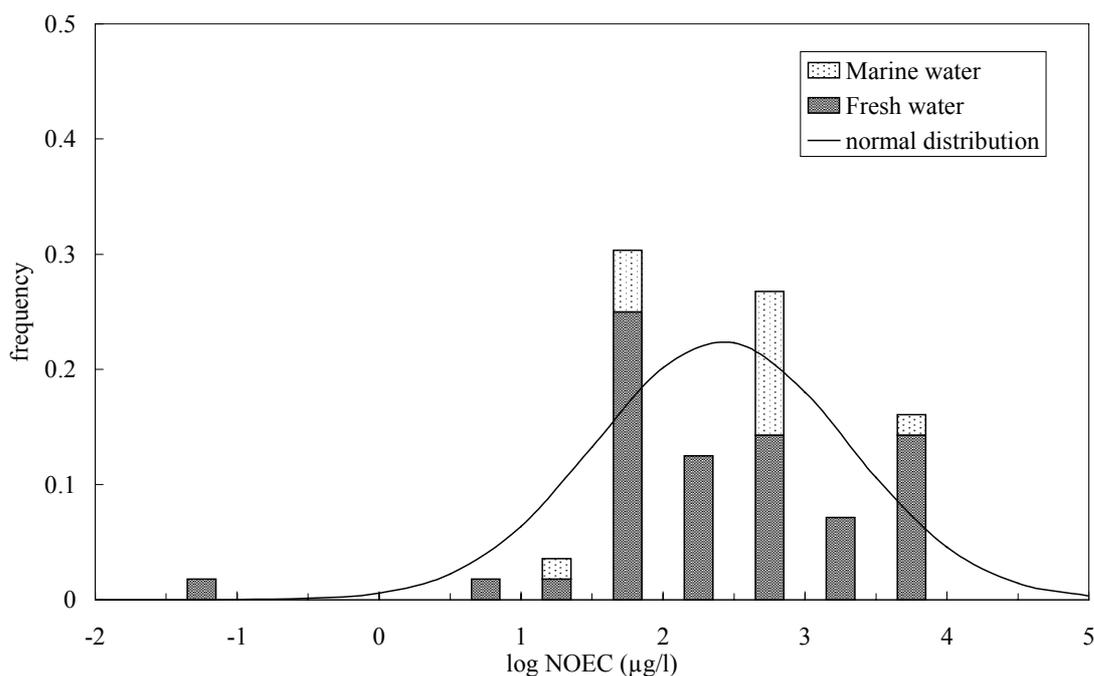


Figure 3.8: Chromium(VI): Distribution of chronic toxicity data for aquatic species. The estimated curve is based on the combined set of fresh water and marine toxicity data ($n = 56$, $\bar{x} = 2.41$, $s = 0.89$).

The HC50(aquatic species) for chromium(III) of $2.2 \cdot 10^2$ µg/l is selected to be used when applying an SRA_{eco} for sediment. The MPA for chromium(VI) is lower than that for chromium (III). This MPA is 8.7 µg/l (similar to the MPA of 8.5 µg/l for chromium derived from the log-logistic distribution; Crommentuijn et al., 1997a).

The log $K_{p(\text{sed/w})}$ 5.28 resulting in an SRA_{eco} for sediment of $4.2 \cdot 10^4$ mg/kg. With the MPA of $8.7 \mu\text{g/l}$ for water the MPA for sediment is $1.7 \cdot 10^3$ mg/kg. The log $K_{p(\text{soil/w})}$ of 3.68 results in values for $\text{SRA}(\text{EqP})$ and $\text{MPA}(\text{EqP})$ of $1.2 \cdot 10^3$ and 42 mg/kg, which are higher than the values derived from the terrestrial toxicity data. For soil as well for sediment a background concentration of 100 mg/kg (van den Hoop, 1995) is assumed.

3.1.5 SRA_{eco} for cobalt

For cobalt one NOEC of 240 mg/kg for earthworms is available (Table A2. 17). Data on processes are presented in Table A2. 18. The distribution of the terrestrial toxicity data is shown in Figure 3.9.

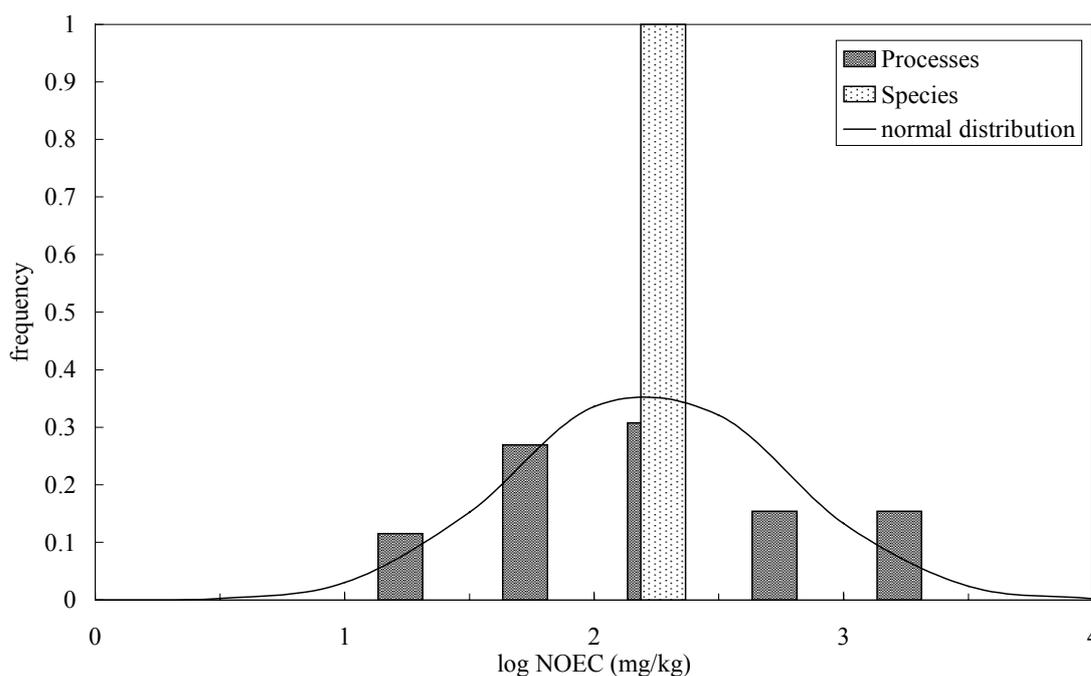


Figure 3.9: Cobalt: Distribution of chronic toxicity data for terrestrial species and processes. The estimated curve is based on the data for processes ($n = 26$, $\bar{x} = 2.22$, $s = 0.55$).

From this distribution an HC50 of $1.7 \cdot 10^2$ mg/kg is derived (90% CI: $1.1 \cdot 10^2 - 2.5 \cdot 10^2$ mg/kg). The HC5 is equal to 21 mg/kg (90% CI: 10 – 36 mg/kg). The lowest value for the HC50 of $1.7 \cdot 10^2$ mg/kg for processes is proposed as SRA_{eco} for soil. The MPA of 24 mg/kg for soil was derived from the NOEC for species by the modified EPA method (Crommentuijn et al., 1997a). With the EU/TGD assessment factor of 100 to the lowest NOEC an MPA of 2.4 mg/kg is derived. Because enough data are available for terrestrial processes, no comparison with equilibrium partitioning is made. The lowest of the MPAs for species and processes is selected as the MPA for cobalt: **2.4 mg/kg**.

For aquatic species data on freshwater and marine species are available. The selected data for aquatic species used in the extrapolation are shown in Appendix 2, Table A2. 19 and Table A2. 20. The data on NOECs for fresh water ($n=3$) and marine species ($n=5$) are significantly different, with the median NOEC for marine species being almost two orders of magnitude higher. Even the median L(E)C50 for marine species ($n=4$) is lower than the median NOEC for marine species, while the L(E)C50 for fresh water species is higher than that for marine species (Appendices 2 and 3 in van de Plassche et al. 1992). Probably, there is no real difference between the fresh water and marine species and the statistical analysis is strongly affected by the small number of data. Therefore, fresh water and marine data were combined.

The distribution of the combined data for fresh water and marine species is shown in Figure 3.10. An HC50(aquatic species) of $8.1 \cdot 10^2 \mu\text{g/l}$ is derived (90% CI: $0.9 \cdot 10^2 - 71.1 \cdot 10^2 \mu\text{g/l}$). The HC5 from this distribution is $3.0 \mu\text{g/l}$ (90% CI: $0.03 - 35.8 \mu\text{g/l}$). With the log-logistic distribution the derived MPA was $2.6 \mu\text{g/l}$ (Crommentuijn et al., 1997a).

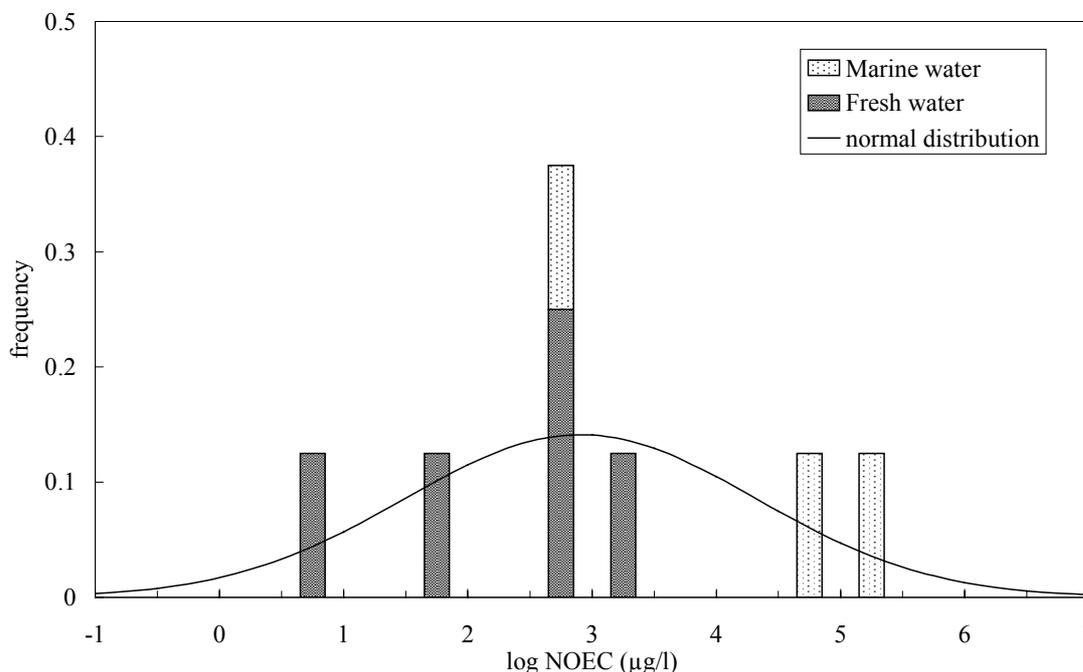


Figure 3.10: Cobalt: Distribution of chronic toxicity data for aquatic species. The estimated curve is based on the combined set of fresh water and marine toxicity data ($n = 8$, $\bar{x} = 2.91$, $s = 1.41$).

Using the HC50(aquatic species) of $8.1 \cdot 10^2 \mu\text{g/l}$ and applying the EqP-method with a log $K_{p(\text{soil/w})}$ of 2.08, an $\text{SRA}_{\text{eco}}(\text{EqP})$ of 97 mg/kg and an MPA(EqP) of 0.36 mg/kg are derived, about 2 and 7 times lower than the values derived from the terrestrial toxicity data. The log $K_{p(\text{sed/w})}$ is 3.60 resulting in an SRA_{eco} for sediment of $3.2 \cdot 10^3 \text{ mg/kg}$ and an MPA of 12 mg/kg. For soil as well for sediment a background concentration of 9.0 mg/kg (van de Plassche and De Bruijn, 1992) is assumed.

3.1.6 SRA_{eco} for copper

For copper enough experimental data are available to estimate sensitivity distributions for both species and processes (Table A2. 21 and Table A2. 22). However, the data for microbe-mediated processes are not log-logistically nor log-normally distributed ($P = 0.031$). This deviation from these distribution is caused by the fact that 19 out of the 59 NOECs are for the same process but different soils from the same study. These data for ethylene production are all located at the lower end of the distribution (without correction for standard soil all NOECs are 10 mg/kg). From the distributions an HC50(species) of $3.0 \cdot 10^2 \text{ mg/kg}$ (90% CI: $1.4 \cdot 10^2 - 6.6 \cdot 10^2 \text{ mg/kg}$) is derived and an HC50(processes) of 60 mg/kg is calculated as the geometric mean of the data. The lowest of these two is selected to be the SRA_{eco} for soil: **60 mg/kg** based on the HC50(processes).

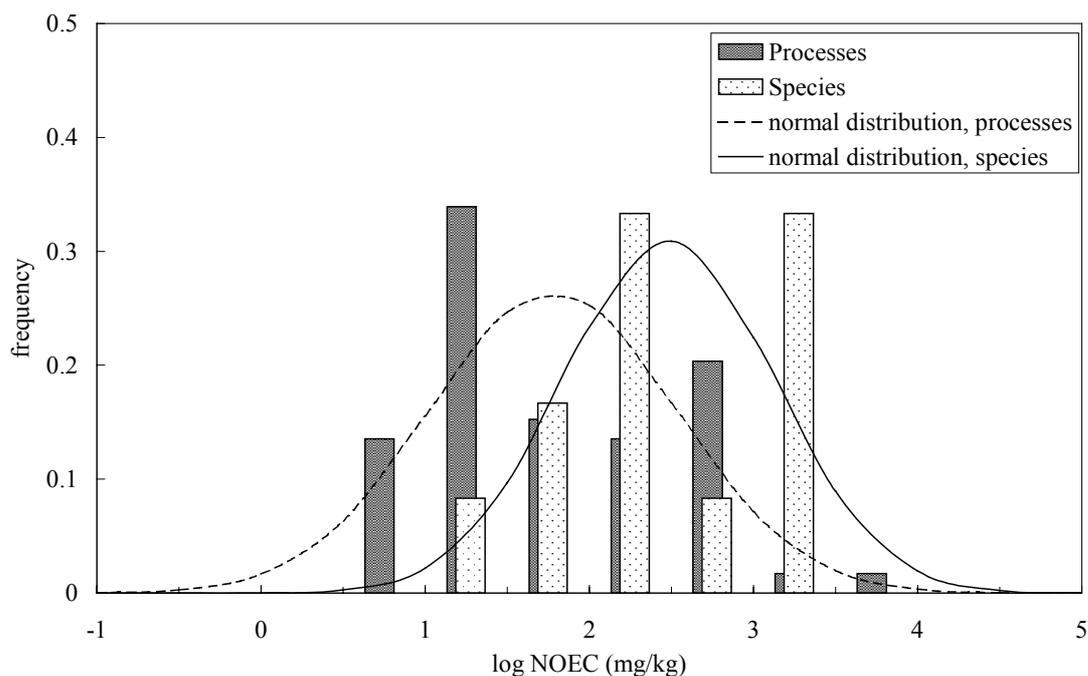


Figure 3.11: Copper: Distribution of chronic toxicity data for terrestrial species and processes. The estimated sensitivity distribution is based on the data for terrestrial species ($n = 12$, $\bar{x} = 2.48$, $s = 0.65$).

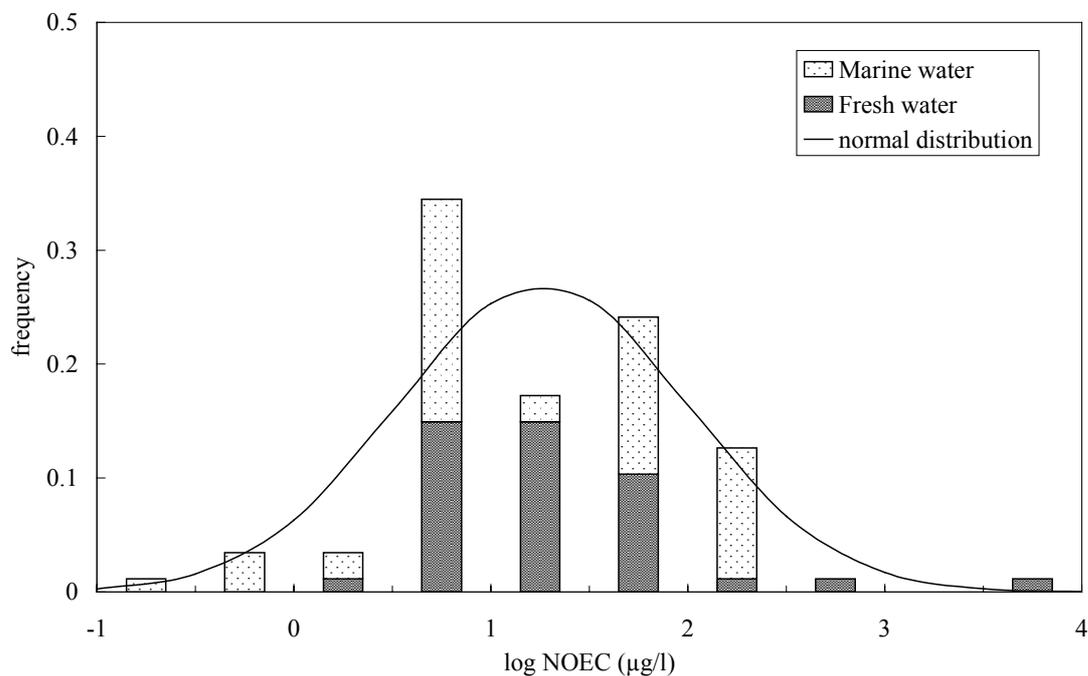


Figure 3.12: Copper: Distribution of chronic toxicity data for aquatic species. The estimated curve is based on the combined set of fresh water and marine toxicity data ($n = 87$, $\bar{x} = 1.26$, $s = 0.74$).

The HC5 from the estimated distribution for species is 25 mg/kg (90% CI: 5 – 63 mg/kg). If statistical extrapolation is applied to the data on processes, regardless whether it is log-normally distributed or not, the resulting HC5 is much lower **3.4 mg/kg** (90% CI: 1.8 – 5.7 mg/kg). The value of 3.5 mg/kg derived from the log-logistic distribution is set as the current

MPA for soil (Crommentuijn et al., 1997a). The 90% confidence interval of the HC50 would be 41 – 87 mg/kg.

The fresh water and marine data sets (Table A2. 23 and Table A2. 24) are not significantly different ($P = 0.61$). The combined data sets are log-normally distributed (Figure 3.12). On the basis of these data an HC50(aquatic species) of $18 \mu\text{g/l}$ (90% CI: 14 - 25 $\mu\text{g/l}$) is derived. The HC5 from this distribution is $1.1 \mu\text{g/l}$ (90% CI: 0.7 – 1.7 $\mu\text{g/l}$) equal to the current MPA for the log-logistic distribution.

To derive an SRA_{eco} for sediment the EqP-method is applied. Applying a log $K_{\text{p(sed/w)}}$ of 4.53, an SRA_{eco} of $6.2 \cdot 10^2 \text{ mg/kg}$ is derived. The MPA for sediment derived by equilibrium partitioning is 36 mg/kg. For soil as well as for sediment a background concentration of 36 mg/kg (Van den Hoop, 1995) is assumed.

3.1.7 SRA_{eco} for lead

The selected terrestrial data from Janus et al. (2000) are taken, where information on the ecotoxicity tests and selection of data used for extrapolation can be found (Table A2. 25 and Table A2. 26). The distribution of the available experimental NOECs for lead (species as well as processes) is shown in Figure 3.13. NOECs for species of six taxonomic groups are available ranging from 40 mg/kg to 1500 mg/kg. For processes NOECs for 12 different processes are available ranging from 15 to 7700 mg/kg. On the basis of these data an HC50(species) of $4.9 \cdot 10^2 \text{ mg/kg}$ (90% CI: $2.7 \cdot 10^2 - 8.9 \cdot 10^2 \text{ mg/kg}$) and an HC50(processes) of $5.2 \cdot 10^2 \text{ mg/kg}$ (90% CI: $3.6 \cdot 10^2 - 7.5 \cdot 10^2 \text{ mg/kg}$) are derived resulting in an SRA_{eco} for soil of $4.9 \cdot 10^2 \text{ mg/kg}$.

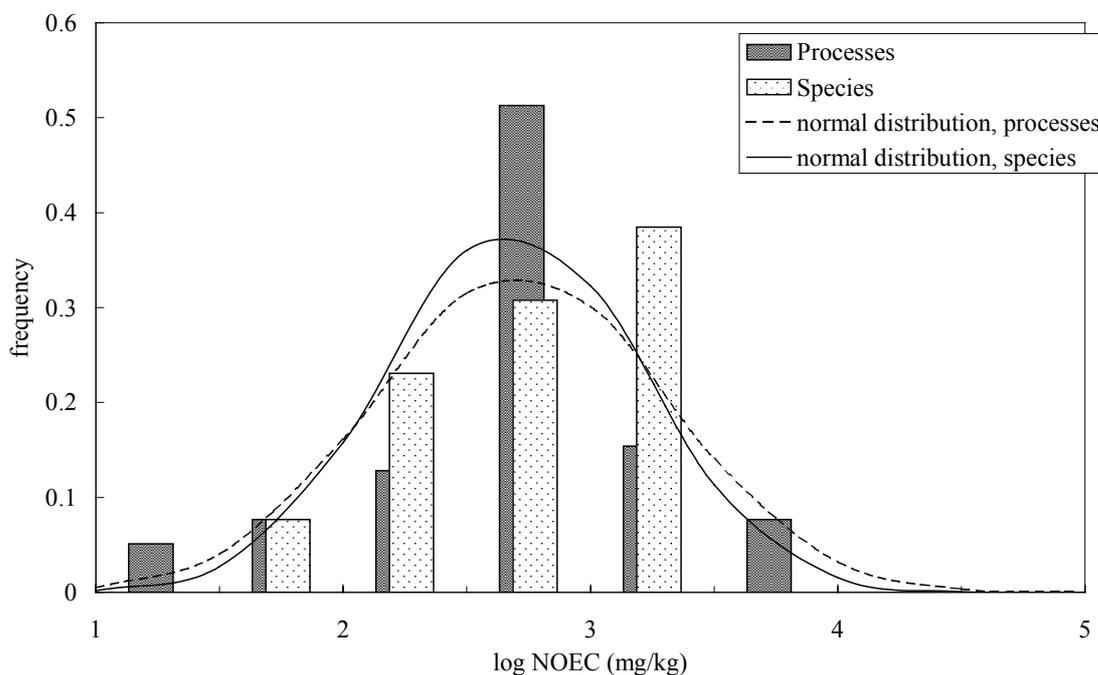


Figure 3.13: Lead: Distribution of chronic toxicity data for terrestrial species and processes and estimated sensitivity distributions for terrestrial species ($n = 13$, $\bar{x} = 2.69$, $s = 0.52$) and processes ($n = 39$, $\bar{x} = 2.72$, $s = 0.59$).

The HC5 for from the statistical extrapolations are 66 mg/kg (90% CI: 20 – 136 mg/kg) for species and 55 mg/kg (90% CI: 29 – 90 mg/kg) for processes. The latter value was also derived from the log-logistic distribution and is the current value for the MPA (Crommentuijn et al., 1997a).

For sediment the equilibrium partitioning theory is used to derive an SRA_{eco} , based on aquatic data. The selected aquatic data from Janus et al. (2000) are taken, where information on the ecotoxicity tests and selection of data used for extrapolation can be found (Appendix 2, Table A2. 27 and Table A2. 28). The same as for mercury, lead can occur in a methylated form (D'Itri, 1990). However not enough information is available from the results of the toxicity tests to discriminate between different forms. The data for fresh water and marine species are not significantly different ($P = 0.63$). The distribution of the available aquatic experimental NOECs for lead on species is shown in Figure 3.14. An HC50(aquatic species) of $1.5 \cdot 10^2 \mu\text{g/l}$ is derived (90% CI: $1.0 \cdot 10^2 - 2.2 \cdot 10^2 \mu\text{g/l}$). The HC5 from this distribution is $11 \mu\text{g/l}$ (90% CI: $5 - 18 \mu\text{g/l}$). This is also the current value for the MPA (Crommentuijn et al., 1997a).

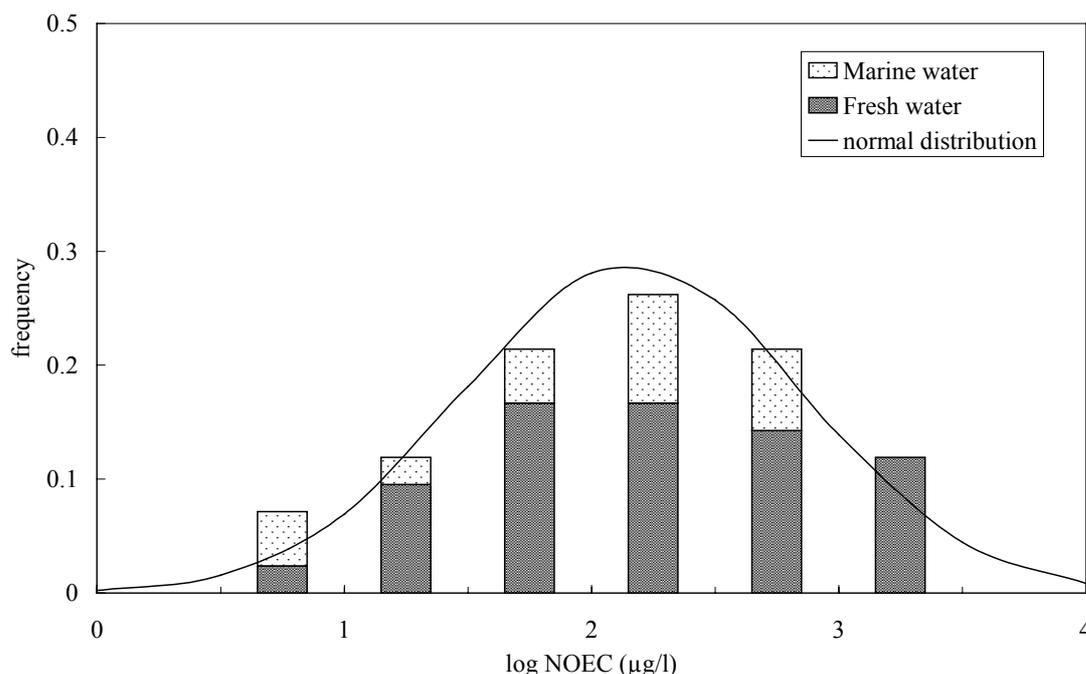


Figure 3.14: Lead: Distribution of chronic toxicity data for aquatic species. The estimated curve is based on the combined set of fresh water and marine toxicity data ($n = 42$, $\bar{x} = 2.17$, $s = 0.69$).

The $\log K_{p(\text{sed/w})}$ for calculating the SRA_{eco} for sediment is 5.63 resulting in a value of $6.3 \cdot 10^4 \text{ mg/kg}$. With this K_p a value of $4.5 \cdot 10^3 \text{ mg/kg}$ is derived for the MPA. The background concentration for soil and sediment is 85 mg/kg (Van den Hoop, 1995).

3.1.8 SRA_{eco} for mercury

Slooff et al. (1995) state that although methylation of inorganic mercury primarily occurs in sediments, it may also occur in soils. However, hardly any data are available for soils. Based on the scarce data available Slooff et al. (1995) assume that mercury in soil mainly occurs as inorganic mercury. However, as methyl-mercury in soil organisms has been demonstrated an SRA_{eco} for organic (methyl-mercury) as well as inorganic mercury is derived.

- Inorganic mercury: For inorganic mercury enough data on processes are available to apply statistical extrapolation (Figure 3.15 and Appendix 2, Table A2. 29). The HC50 of this distribution is 36 mg/kg (90% CI: $17 - 73 \text{ mg/kg}$). The HC5 is 1.9 mg/kg (90% CI: $0.5 - 4.8 \text{ mg/kg}$). No data on species are available.

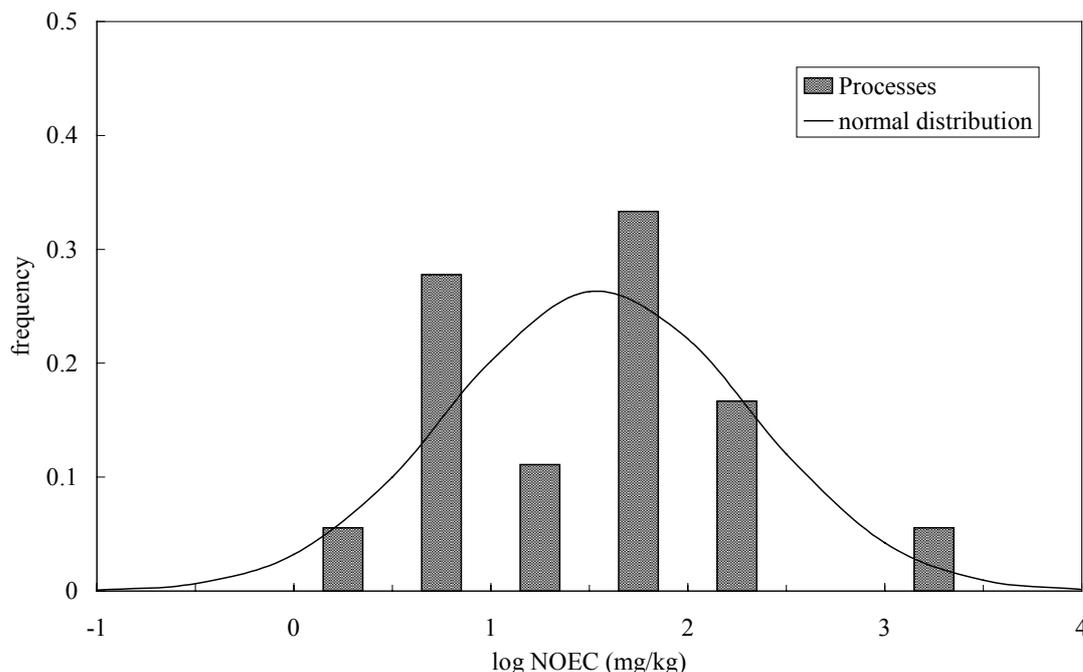


Figure 3.15: Inorganic mercury: Distribution of chronic toxicity data for terrestrial processes and estimated sensitivity distribution ($n = 18$, $\bar{x} = 1.55$, $s = 0.76$).

- Methyl-mercury: Only one NOEC of **3.7** mg/kg is available for methyl-mercury (Appendix 2, Table A2. 30). With the modified EPA method the MPA from this NOEC is 0.37 mg/kg (Crommentuijn et al., 1997a). Using the assessment factor of 100 according to the EU/TGD this MPA becomes **0.037** mg/kg.

To derive an SRA_{eco} for sediment the EqP-method is applied. In natural water systems inorganic mercury is continuously methylated into its organic form, methyl-mercury. This transformation is carried out by micro-organisms in the water column and in anoxic sediment (Korthals and Winfrey, 1987). However, a highly significant difference is found between the toxicity of inorganic and organic mercury ($P = 0.0001$), when comparing the fresh water or the combined data sets. Separate SRA_{eco} for inorganic and organic mercury in surface water are derived below and included in the table.

- Inorganic mercury: Highly significant differences ($P = 0.0099$) in sensitivity between freshwater species and marine species are found (Appendix 2, Table A2. 31 and Table A2. 32), and therefore, separate HC50 are derived for fresh water and marine water. The data for both fresh water and marine species are log-normally distributed. The HC50(aquatic species) is **14** $\mu\text{g/l}$ for fresh water (90% CI: 6 – 30 $\mu\text{g/l}$) and **2.7** $\mu\text{g/l}$ for marine water (90% CI: 1.4 – 5.1 $\mu\text{g/l}$). The HC5s of these distributions are 0.43 $\mu\text{g/l}$ for fresh water (90% CI: 0.10 – 1.20 $\mu\text{g/l}$) and 0.21 $\mu\text{g/l}$ for marine water (90% CI: 0.06 – 0.046 $\mu\text{g/l}$). These HC5s are in the same range and therefore one HC5 for inorganic mercury can be derived as well: **0.23** $\mu\text{g/l}$ (90% CI: 0.09 – 0.49 $\mu\text{g/l}$).
- Methyl-mercury: For marine organisms only one NOEC of 0.3 $\mu\text{g/l}$ is available (Table A2. 34). This NOEC falls well ($P = 47\%$) within the range of the freshwater NOEC values (Table A2. 33). The HC50(aquatic species) is derived using statistical extrapolation, combining the data sets: **0.36** $\mu\text{g/l}$ (90% CI: 0.12 – 1.11 $\mu\text{g/l}$). The HC5 from this distribution is **0.011** $\mu\text{g/l}$ (90% CI: 0.001 – 0.042).

Just as for soil, methyl-mercury is most toxic in surface water.

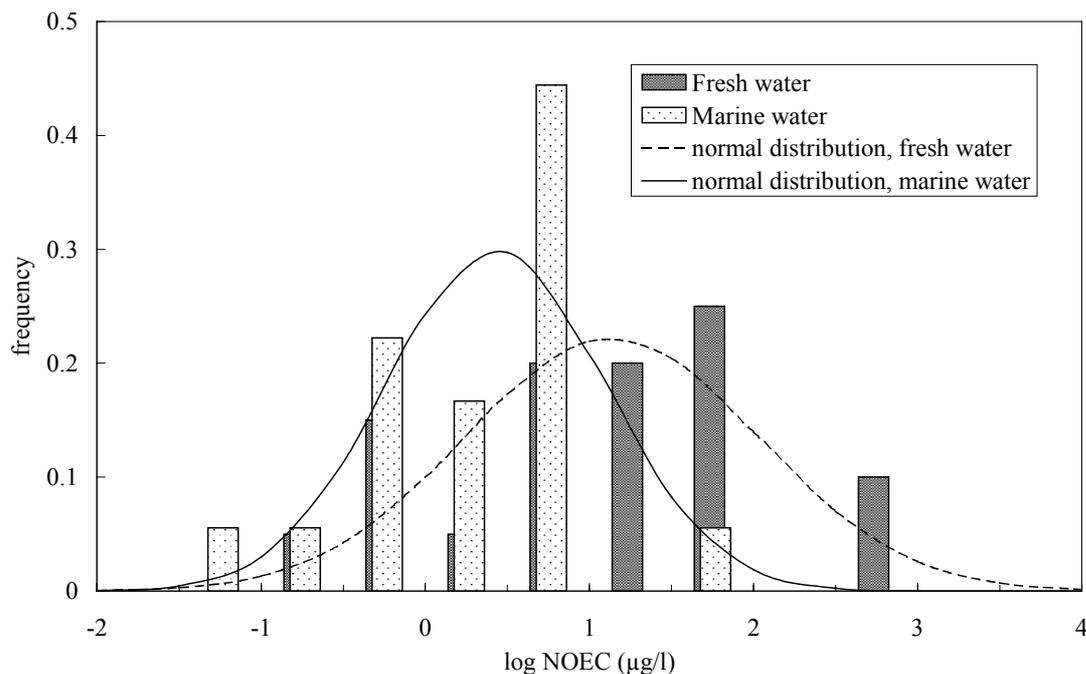


Figure 3.16: Inorganic mercury: Distribution of chronic toxicity data for aquatic species. The estimated curves are based on the separate sets of fresh water ($n = 20$, $\bar{x} = 1.14$, $s = 0.90$) and marine toxicity data ($n = 18$, $\bar{x} = 0.43$, $s = 0.67$).

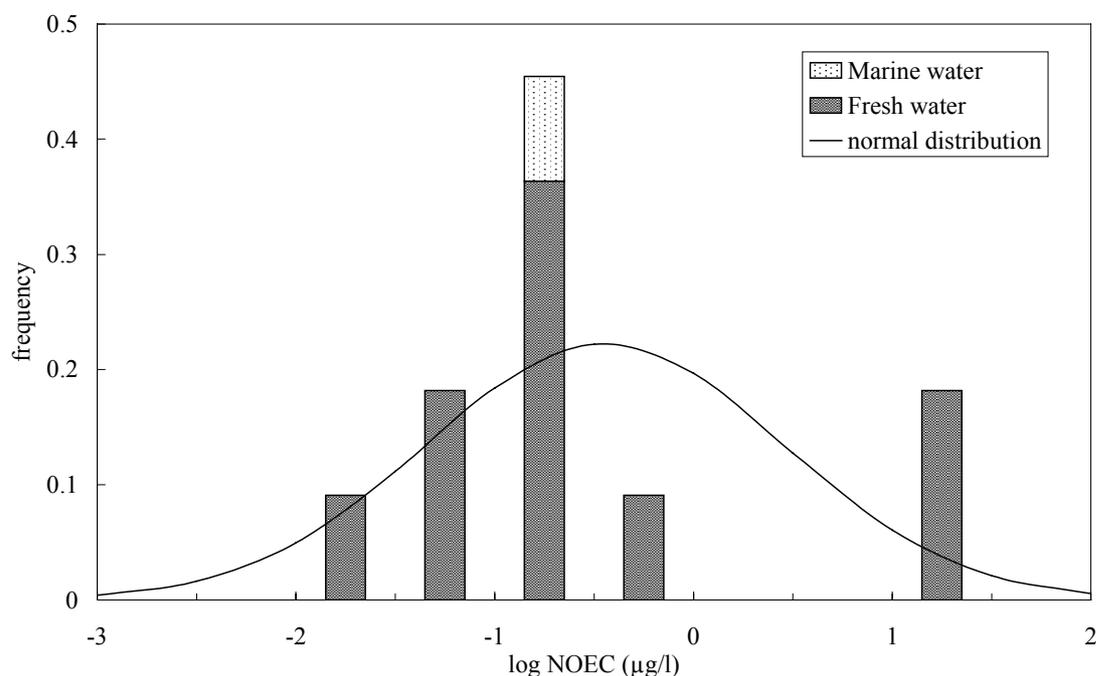


Figure 3.17: Methyl mercury: Distribution of chronic toxicity data for aquatic species. The estimated curve is based on the combined set of fresh water and marine toxicity data ($n = 11$, $\bar{x} = -0.45$, $s = 0.90$).

The $\log K_{p(\text{sed/w})}$ for mercury is 5.05 (Otte et al., 2001). This value refers to anorganic mercury. It is not clear whether or not this value is applicable for methyl-mercury. Therefore, no ERLs for methyl-mercury are derived by equilibrium partitioning, and consequently no

SRC_{eco} for sediment is given. For anorganic mercury the SRC_{eco} fresh water sediment are $1.5 \cdot 10^3$ mg/kg. The SRC_{eco} for marine sediment is $3.0 \cdot 10^2$ mg/kg. The MPA for both sediments is 26 mg/kg. The $\log K_{p(\text{soil/w})}$ is 3.88. With equilibrium partitioning an HC50 for soil of $1.0 \cdot 10^2$ mg/kg is derived for anorganic mercury. This value is almost three times higher than the value from the terrestrial toxicity data. The MPA calculated by means of equilibrium partitioning is almost the same as the value derived from terrestrial toxicity data: 1.7 mg/kg.

For soil as well as for sediment a background concentration of 0.3 mg/kg (van den Hoop, 1995) is assumed. This background is based on a total concentration without discrimination between organic and inorganic mercury.

3.1.9 SRA_{eco} for molybdenum

Only data on terrestrial on processes are available for molybdenum (Table A2. 35). The sensitivity distribution of these data is shown in (Figure 3.18). The HC50(terrestrial processes) is $1.9 \cdot 10^2$ mg/kg (90% CI: $1.4 \cdot 10^2 - 2.7 \cdot 10^2$ mg/kg). The HC5 from this distribution is 39 mg/kg (90% CI: 21 – 60 mg/kg).

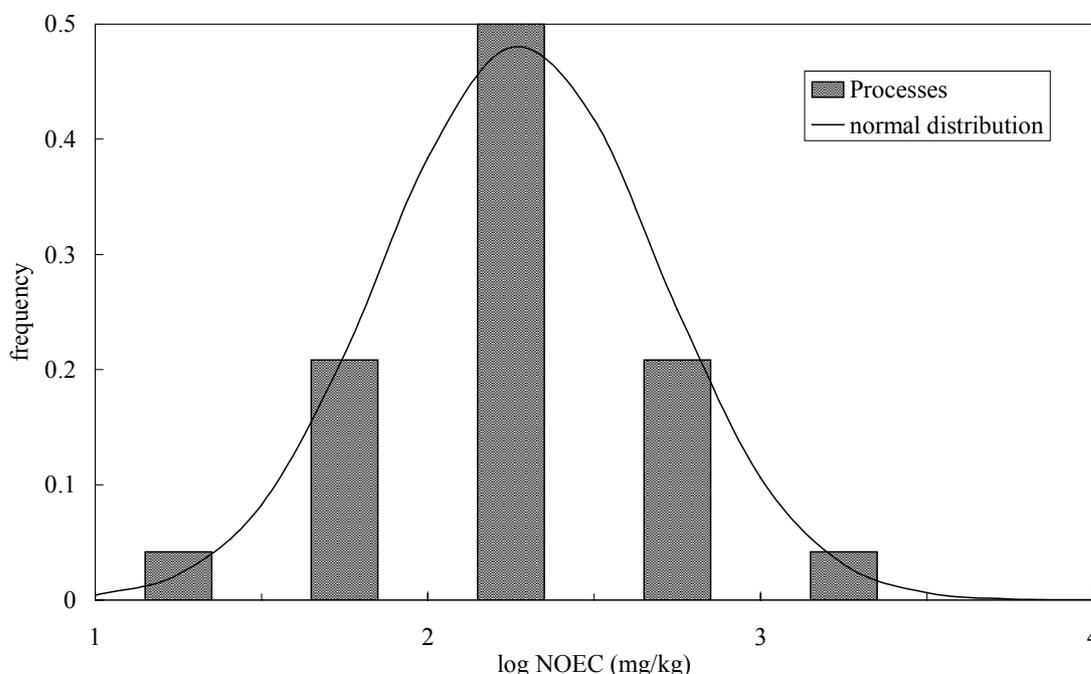


Figure 3.18: Molybdenum: Distribution of chronic toxicity data for terrestrial processes and estimated sensitivity distribution ($n = 24$, $\bar{x} = 2.28$, $s = 0.41$).

The selected data for aquatic species are shown in Appendix 2, Table A2. 36 and Table A2. 37. Only one NOEC of 27 mg/l is available. L(E)C50 data are available for both freshwater species and marine species. On the basis of these data, no significant differences in sensitivity between fresh water and marine species are observed ($P = 0.57$). By applying a safety factor of 10 to the median L(E)C50 of the combined sets, an HC50 of 68 mg/l is derived. The proposed SRA_{eco} for aquatic species is therefore 27 mg/l. No acute toxicity data are available for either *Daphnia* species or algae. Therefore, no MPA can be derived according to the EU/TGD method. Therefore, a maximum assessment factor of 100 or 1000 is used for the lowest NOEC or L(E)C50, respectively. The resulting MPA is 29 µg/l. Acute toxicity data are available for other crustaceans and one chronic study is available for algae, which presents a NOEC that is almost equal to the lowest L(E)C50. Therefore, the MPA according to the

modified EPA method was derived by applying a factor of 100 to the lowest L(E)C50. The resulting MPA was $2.9 \cdot 10^2 \mu\text{g/l}$ (Crommentuijn et al., 1997a).

The SRA_{eco} for sediment is based on aquatic data and applying the EqP-method. The log $K_{\text{p(sed/w)}}$ is 2.93 resulting in an SRA_{eco} of **23** g/kg and an MPA of **25** mg/kg. With a log $K_{\text{p(soil/w)}}$ of 1.60, an $\text{SRA}_{\text{eco}}(\text{EqP})$ of $1.1 \cdot 10^3$ mg/kg is derived for soil. This value is markedly higher than the value of $1.9 \cdot 10^2$ mg/kg from the terrestrial processes, which is proposed as SRA_{eco} for soil. The MPA(EqP) of 1.2 mg/kg is lower than the HC5 from the statistical extrapolation. For soil as well as for sediment a background concentration of 0.5 mg/kg (van den Hoop, 1995) is assumed.

3.1.10 SRA_{eco} for nickel

For nickel the HC50(terrestrial species) is based on the NOEC of 65 mg/kg that was available for earthworms (Table A2. 38). Two NOECs for microbe-mediated processes are available (Table A2. 39), resulting in an HC50(processes) of $1.2 \cdot 10^2$ mg/kg. The lowest of these two is selected to be the SRA_{eco} for soil: 65 mg/kg based on the HC50(terrestrial species).

According to the modified EPA method a safety factor of 10 is applied to the lowest NOEC of 26 mg/kg for urease resulting in an MPA for soil of 2.6 mg/kg. With the safety factors of the EU/TGD an MPA for species of 0.65 mg/kg is derived and 0.26 mg/kg for processes. Both MPA-values are derived by preliminary risk assessment and therefore a comparison with equilibrium partitioning is made.

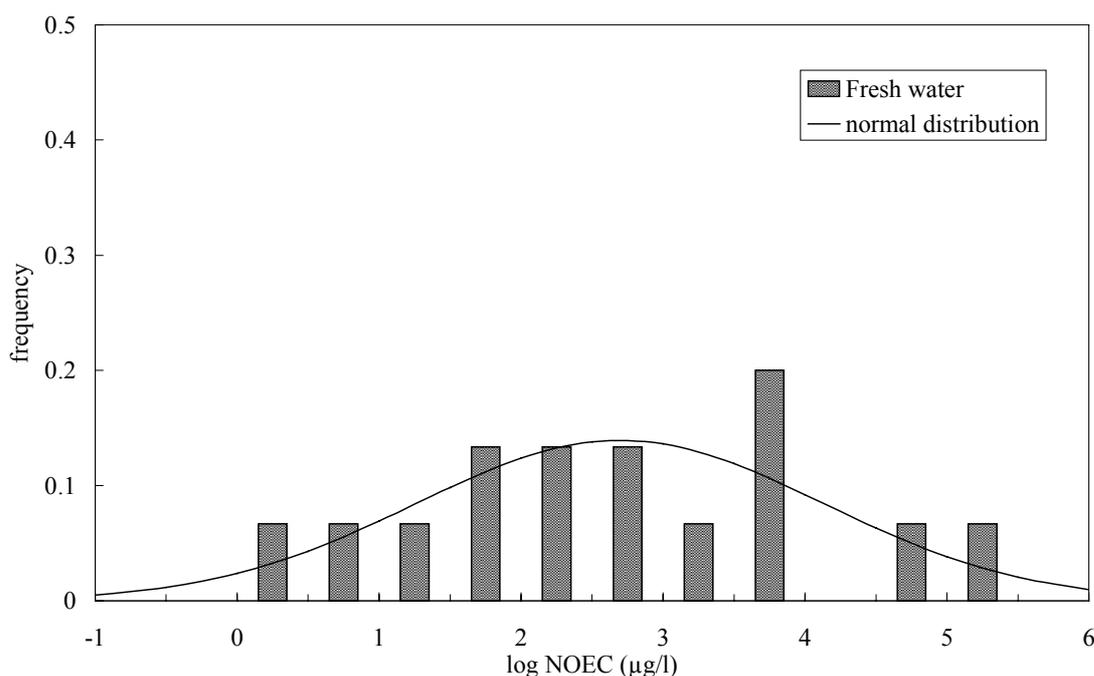


Figure 3.19: Nickel: Distribution of chronic toxicity data for aquatic species and estimated distribution ($n = 15$, $\bar{x} = 2.70$, $s = 1.43$).

For sediment the equilibrium partitioning theory is used to derive an SRA_{eco} , based on aquatic data. The selected aquatic data from van de Meent et al. (1990) are taken (Appendix 2, Table A2. 40). The distribution of the available aquatic experimental NOECs for nickel on species is shown in Figure 3.19. NOECs are available for species of six taxonomic groups. An HC50(aquatic species) of $5.0 \cdot 10^2 \mu\text{g/l}$ is derived (90% CI: $1.1 \cdot 10^2 - 22.2 \cdot 10^2 \mu\text{g/l}$). The HC5 from this distribution is **1.9** $\mu\text{g/l}$ (90% CI: 0.1 – 12.6 $\mu\text{g/l}$).

Because of the limited terrestrial data for nickel, a comparison with equilibrium partitioning is made. The $\log K_p$ for soil is 3.30. With the HC50(aquatic species) of $5.0 \cdot 10^2 \mu\text{g/l}$, the resulting value for the HC50(EqP) is $9.9 \cdot 10^2 \text{ mg/kg}$. This value is higher than the HC50 of 65 mg/kg derived directly from the terrestrial toxicity data. The final proposal for the SRA_{eco} is thus **65 mg/kg**. Also the MPA for soil calculated from the HC5 for water by equilibrium partitioning is higher than the MPA derived from the terrestrial toxicity data. The MPA is therefore derived from the terrestrial data: **0.26 mg/kg**.

The $\log K_p$ for sediment is 3.72 resulting in an SRA_{eco} of **$2.6 \cdot 10^3 \text{ mg/kg}$** and an MPA of **10 mg/kg**. The background concentration for soil and sediment is 35 mg/kg (Van den Hoop, 1995).

3.1.11 SRA_{eco} for zinc

For zinc the selected terrestrial data from Janus (1993) are taken (Table A2. 41 and Table A2. 42). The distributions of the available experimental NOECs for zinc are shown in Figure 3.20. On the basis of these data an HC50(species) of $3.9 \cdot 10^2 \text{ mg/kg}$ (90% CI: $2.5 \cdot 10^2 \text{ mg/kg} - 6.0 \cdot 10^2 \text{ mg/kg}$) and an HC50(processes) of $2.1 \cdot 10^2 \text{ mg/kg}$ (90% CI: $1.2 \cdot 10^2 \text{ mg/kg} - 3.4 \cdot 10^2 \text{ mg/kg}$) are derived resulting in an SRA_{eco} for soil of **$2.1 \cdot 10^2 \text{ mg/kg}$** . The HC5 for species is $1.4 \cdot 10^2 \text{ mg/kg}$ (90% CI: $0.5 \cdot 10^2 \text{ mg/kg} - 2.2 \cdot 10^2 \text{ mg/kg}$). For processes this value is much lower: **16 mg/kg** (90% CI: 6 – 31 mg/kg).

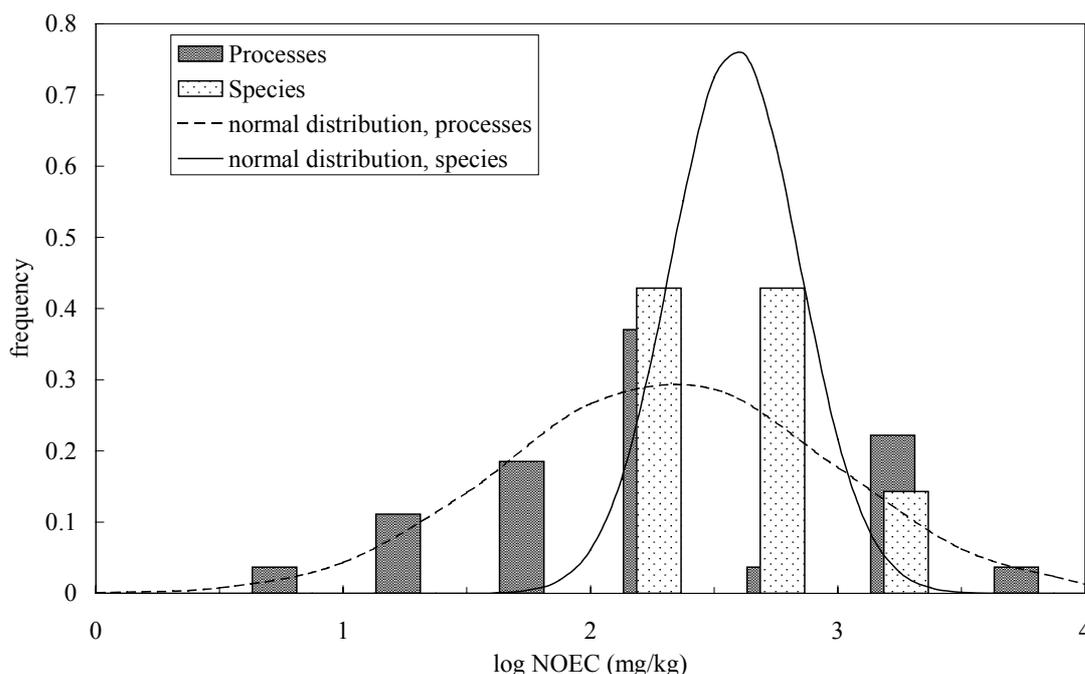


Figure 3.20: Zinc: Distribution of chronic toxicity data for terrestrial species and processes and estimated sensitivity distributions for terrestrial species ($n = 7$, $\bar{x} = 2.59$, $s = 0.26$) and processes ($n = 27$, $\bar{x} = 2.32$, $s = 0.67$).

For sediment the equilibrium partition theory is used to derive an SRA_{eco} , based on aquatic data. The selected aquatic data from Janus (1993) are taken, where information on the ecotoxicity tests and selection of data used for extrapolation can be found (Appendix 2, Table A2. 43 and Table A2. 44). Fresh water and marine species are not significantly different ($P = 0.63$). The distribution of the available aquatic experimental NOECs for zinc on species is shown in Figure 3.21. An HC50(aquatic species) of **89 $\mu\text{g/l}$** is derived (90% CI: 62 - 127 $\mu\text{g/l}$). The HC5 is **7.3 $\mu\text{g/l}$** (90% CI: 3.9 – 11.9 $\mu\text{g/l}$). The $\log K_p$ for sediment is 4.86 resulting

in an SRA_{eco} of $6.4 \cdot 10^3$ mg/kg and an MPA of $5.3 \cdot 10^2$ mg/kg. The background concentration for soil and sediment is 140 mg/kg (Van den Hoop, 1995).

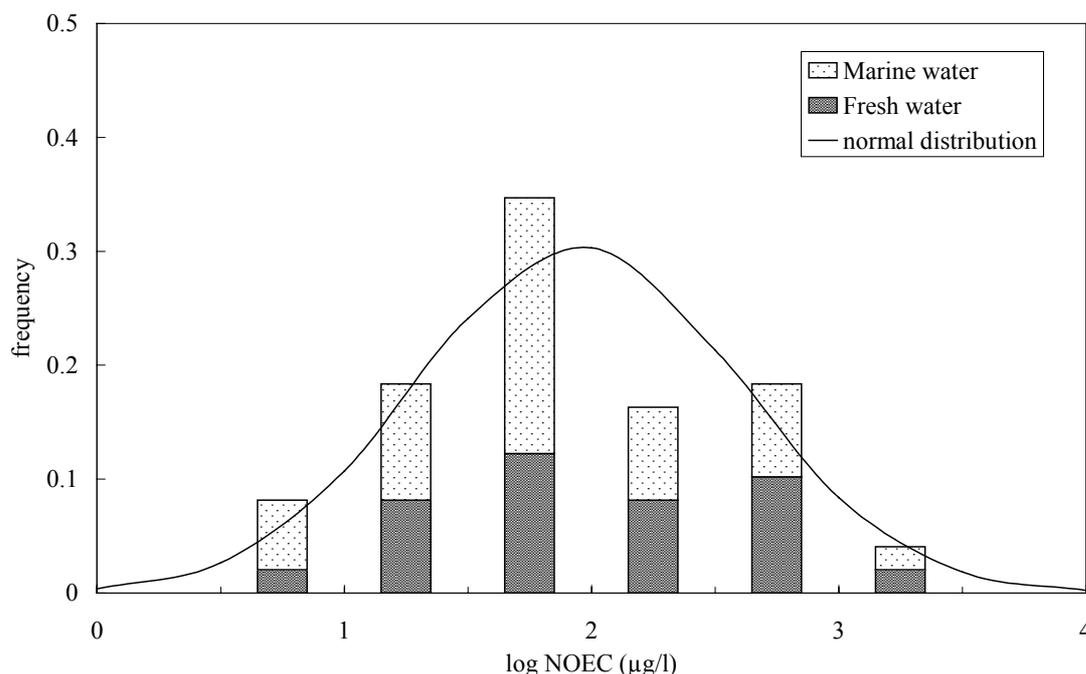


Figure 3.21: Zinc: Distribution of chronic toxicity data for aquatic species. The estimated curve is based on the combined set of fresh water and marine toxicity data ($n = 49$, $\bar{x} = 1.95$, $s = 0.66$).

3.1.12 Summary and comparison with old values and MPCs

In Table 3.2 the SRA_{eco} for metals in soil and sediment are summarised. Besides the values derived in the present report also the old values derived in Denneman and Van Gestel (1990) and the background concentrations and MPA values as derived in the context of the project ‘Setting Integrated Environmental Quality Standards’ (Van de Plassche and De Bruijn, 1992; Crommentuijn et al., 1997a) are presented. For each metal and compartment the reliability of the SRC is indicated.

To illustrate the influence of the $\log K_p$ on the SRA_{eco} and MPCs, values for soil and sediment derived with equilibrium partitioning and the values for soil derived directly from terrestrial toxicity data are included in Table 3.1. For comparison, both the $\log K_p$ values used in the context of the project ‘Setting Integrated Environmental Quality Standards’ (INS, data from Bockting et al., 1992 in Crommentuijn et al., 1997) and those used here in the context of the project 711701 to derive the new SRC values (IW, data from Sauvé et al., 2000 in Otte et al., 2001). Most of the SRCs derived by equilibrium partitioning are in the same order of magnitude as the values derived directly from terrestrial data (< factor of 10). However, it is clear that large differences exist between the two sets for $\log K_p$. Therefore, the use of $\log K_p$ to derive ERLs for metals by equilibrium partitioning introduces large uncertainties. The ERLs for sediment are all based on equilibrium partitioning. The data set of Stortelder et al. (1989) for $\log K_p$ of sediment is used for this purpose. Because of the crucial role of $\log K_p$ in the derivation of the ERLs for sediment, these ERLs should be considered uncertain as far as metals are concerned. For mercury it is not clear whether the partition coefficients may be applied to the values for methyl-mercury.

Table 3.1: SRA_{eco} and MPA for metals in soil or sediment derived directly from terrestrial toxicity data, or by equilibrium partitioning (EqP) from the soil/sediment-water partition coefficients (K_p) used in the framework of the projects 'Setting Integrated Environmental Quality Standards' (INS) and 'Technical evaluation of Intervention Values for soil/sediment and groundwater' (IW)

Compound	Compartment	SRA_{eco} [mg/kg]	MPA [mg/kg]	$\log K_p$
arsenic	soil, direct	56	0.90	
	soil, EqP K_p INS	170	4.7	2.28
	soil, EqP K_p IW	1600	44	3.26
	sediment, EqP	5900	160	3.82
barium	soil, direct	730	180	
	soil, EqP K_p INS	420	1.7	1.78
	soil, EqP K_p IW	18000	73	3.40
	sediment, EqP	7000	29	3.00
cadmium	soil, direct	12	0.79	
	soil, EqP K_p INS	1.9	0.068	2.30
	soil, EqP K_p IW	25	0.87	3.41
	sediment, EqP	820	29	4.93
	marine sediment, EqP	2300		4.93
chromium ^a	soil, direct	120	0.38	
	soil, EqP K_p INS	24	0.95	2.04
	soil, EqP K_p IW	1100	42	3.68
	sediment, EqP	42000	1700	5.28
cobalt	soil, direct	170	2.4	
	soil, EqP K_p INS	32	0.12	1.60
	soil, EqP K_p IW	97	0.36	2.08
	sediment, EqP	3200	12	3.60
copper	soil, direct	60	3.4	
	soil, EqP K_p INS	18	1.0	2.99
	soil, EqP K_p IW	39	2.2	3.33
	sediment, EqP	620	36	4.53
mercury	soil, direct	36	1.9	
	soil, EqP K_p INS	2.3	0.040	2.23
	soil, EqP K_p IW	100	1.7	3.88
	sediment, EqP	1500	26	5.05
lead	marine sediment, EqP	300		5.05
	soil, direct	490	55	
	soil, EqP K_p INS	280	20	3.28
	soil, EqP K_p IW	5300	380	4.56
	sediment, EqP	63000	4500	5.63
molybdenum	soil, direct	190	39	
	soil, EqP K_p INS	24000	25	2.94
	soil, EqP K_p IW	1100	1.2	1.60
	sediment, EqP	23000	25	2.93
nickel	soil, direct	65	0.26	
	soil, EqP K_p INS	60	0.23	2.08
	soil, EqP K_p IW	990	3.9	3.30
	sediment, EqP	2600	10	3.72
zinc	soil, direct	210	16	
	soil, EqP K_p INS	14	1.2	2.20
	soil, EqP K_p IW	230	19	3.41
	sediment, EqP	6400	530	4.86

a Based on data for Cr(III), MPAs derived by equilibrium partitioning based on Cr(VI).

It should be noted that for comparison with the old data from Denneman and van Gestel (1990) the background concentration has to be summed to SRA_{eco} . For the purpose of Intervention Values the use of a location specific background concentration may be suitable.

With the reference lines for the metals and the known composition of the soil (% organic matter (H) and % clay (L)) this background concentration can be calculated and added to the SRA to obtain a location specific Intervention Value.

In Table 3.3 the $SRAs_{eco}$ for metals in water are listed. Further, information on the MPA and background concentrations as derived in the project 'Setting Integrated Environmental Quality Standards' is given. The $SRAs_{eco}$ in fresh surface water serve as the basis for the Intervention Values in groundwater. To the $SRAs_{eco}$ and MPC the dissolved background concentrations should be added. Also fresh, marine and groundwater these background concentrations are listed in the table. In most cases background concentrations for water are almost negligible compared to the $SRAs_{eco}$.

Table 3.2: Summary of new SR_{eco} values for metals in soil and sediment, values as derived by Denmeman and van Gestel (1990), MPA and background values with reference lines as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and revised MPA values derived in this report. Values are given as concentrations in mg/kg standard soil/sediment (soil and sediment containing 10% organic matter (H) and 25% clay (L), sediment containing 10% organic matter and 25% clay).

Compound	Compartment	SR_{eco} [mg/kg]	Method* / reliability score	Denmeman and van Gestel (1990) [mg/kg]	MPA this report [mg/kg]	Method*	MPA INS [mg/kg]	C_b [mg/kg]	C_b reference line [mg/kg]
arsenic	soil	56	1 c sp.<ref. pr. / high	40	0.90	50 h sp.<ref. pr.	4.5	29	15 + 0.4·(L + H)
	sediment	5900	EqP / low		160	EqP	160	29	15 + 0.4·(L + H)
barium	soil	730	ref. pr. / high	650	180	ref. pr.	9.0	155	30 + 5·L
	sediment	7000	EqP / low		29	EqP	150	155	30 + 5·L
cadmium ^d	soil	12	ref. sp.<ref. pr. / high	12	0.79	ref. sp.<ref. pr.	0.76	0.8	0.4 + 0.007·(L + 3·H)
	sediment	820	EqP / low		29	EqP	29	0.8	0.4 + 0.007·(L + 3·H)
chromium ^{a,d}	marine sediment	2300	EqP / low			EqP			
	soil	120	1 c sp.<ref. pr. / high	230	0.38	100 f sp.<100 f pr.	3.8	100	50 + 2·L
cobalt	sediment	42000	EqP / low		1700	EqP	1620	100	50 + 2·L
	soil	170	ref. pr.<1 c sp. / high	120	2.4	100 f sp.<ref. pr.	24	9.0	2 + 0.28·L
copper	sediment	3200	EqP / low		12	EqP	10	9.0	2 + 0.28·L
	soil	60	ref. pr.<ref. sp. / high	190	3.4	ref. pr.<ref. sp.	3.5	36	15 + 0.6·(L + H)
mercury	sediment	620	EqP / low		36	EqP	37	36	15 + 0.6·(L + H)
	soil	36	ref. pr. / high	10	1.9	ref. pr.	1.9	0.3	0.2 + 0.0017·(2·L + H)
methyl-mercury ^b	sediment	1500	EqP / low		26	EqP	26	0.3	0.2 + 0.0017·(2·L + H)
	marine sediment	300	EqP / low			EqP			
lead	soil	3.7	1 c sp. / medium		0.037	100 b sp.	0.37	0.3	0.2 + 0.0017·(2·L + H)
molybdenum	soil	490	ref. sp.<ref. pr. / high	290	55	ref. pr.<ref. sp.	55	85	50 + L + H
	sediment	63000	EqP / low		4500	EqP	4700	85	50 + L + H
nickel ^d	soil	190	ref. pr. / high	<480°	39	ref. pr.	253	0.5	0.5
	sediment	23000	EqP / low		25	EqP	250	0.5	0.5
zinc ^d	soil	65	1 c sp.<1 c pr. / medium	210	0.26	100 f pr.<100 b sp.	2.6	35	10 + L
	sediment	2600	EqP / low		10	EqP	9.4	35	10 + L
zinc ^d	soil	210	ref. pr.<ref. sp. / high	720	16	ref. pr.<ref. sp.	16	140	50 + 1.5·(2·L + H)
	sediment	6400	EqP / low		530	EqP	480	140	50 + 1.5·(2·L + H)

- * For the SRA_{eco} and the MPA the abbreviation ref. is used in case of refined risk assessment. EqP (equilibrium partitioning) or the assessment factor together with the designation according to Table 2.1 and Table 2.6 is given in case of preliminary risk assessment. Whether the SRA_{eco} or the MPA is based on species or processes is indicated by the abbreviation sp. and pr.
- a Based on data for Cr(III), MPAs derived by equilibrium partitioning based on Cr(VI).
 - b It is not clear to what extent the partition coefficients are usable for methyl-mercury
 - c Value for 'minimal soil' (=soil containing 2% organic matter and 5% clay), for standard soil no value has been derived.
 - d For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

Table 3.3: Summary of new SRA_{eco} values for metals in water, MPA and background values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and revised MPA values derived in this report. Values are given as concentrations in $\mu\text{g/l}$ water.

Compound	Compartment	SRA_{eco} [$\mu\text{g/l}$]	Method* / reliability score	MPA this report [$\mu\text{g/l}$]	Method*	MPA INS [$\mu\text{g/l}$]	C_b fresh water, dissolved [$\mu\text{g/l}$]	C_b marine water, dissolved [$\mu\text{g/l}$]	C_b groundwater, dissolved [$\mu\text{g/l}$]
arsenic	surface water	890	ref. / high	24	ref.	24	0.77	-	7.0
barium	surface water	7000	1 c / medium	29	100 f	150	73	-	197
cadmium ^b	fresh water	9.6	ref. / high	0.34	ref.	0.34	0.08	-	0.06
	marine water	27	ref. / high					0.025	
chromium ^{a,b}	surface water	220	ref. / high	8.7	ref.	8.5	0.17	-	2.4
cobalt	surface water	810	ref. / high	3.0	ref.	2.6	0.20	-	0.63
copper	surface water	18	ref. / high	1.1	ref.	1.1	0.44	0.25	1.3
mercury	fresh water	14	ref. / high	0.23	ref.	0.23	0.01	-	-
	marine water	2.7	ref. / high					0.0025	
methyl- mercury	surface water	0.36	ref. / high	0.011	ref.	0.01	0.01	0.0025	-
lead	surface water	150	ref. / high	11	ref.	11	0.15	0.02	1.6
molybdenum	surface water	27000	1 c / medium	29	100 incompl.	290	1.4	-	0.69
nickel ^b	surface water	500	ref. / high	1.9	ref.	1.8	3.3	-	2.1
zinc ^b	surface water	89	ref. / high	7.3	ref.	6.6	2.8	0.35	24

* For the SRA_{eco} and the MPA the abbreviation ref. is used in case of refined risk assessment. The assessment factor together with the designation according to Table 2.1 and Table 2.5 is given in case of preliminary risk assessment. An incomplete base set is indicated by the abbreviation incompl.

a SRA based on data for Cr(III), MPA based on data for Cr(VI).

b For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

3.2 Proposals for SRC_{eco} for cyanides

For free cyanide (CN⁻), thiocyanate (SCN⁻) and complex cyanides ([CN⁻]_x) no data have been collected in the framework of the project ‘Setting Integrated Environmental Quality Standards’. Therefore, a literature search was performed for cyanides. These data are presented in the annex to this report. Because no risk limits have been derived for cyanides, also the MPC and NC are derived for these compounds besides the HC50. For none of the three groups distribution coefficients between soil and water are available at this time. Further, no suitable ecotoxicological data for soil or sediment were found. Therefore, it was decided to base the SRC_{eco} on concentrations in groundwater. All selected data are presented in Appendix 3. The derived risk limits are summarised in 3.2.4

3.2.1 SRC_{eco} for free cyanide

For free cyanide data are available for six taxonomic groups (Table A3. 1 and Table A3. 2). Therefore, statistical extrapolation can be applied. Only one study is performed with marine species, which fits well into the overall log-normal distribution (P = 54%). Therefore, the fresh and marine data are grouped together. The statistical extrapolation is shown in Figure 3.22. The HC50(aquatic species) is **31** µg/l (90% CI: 7 – 134 µg/l). The MPC is equal to the HC5 estimate of **0.23** µg/l (90% CI: 0.01 – 1.33 µg/l).

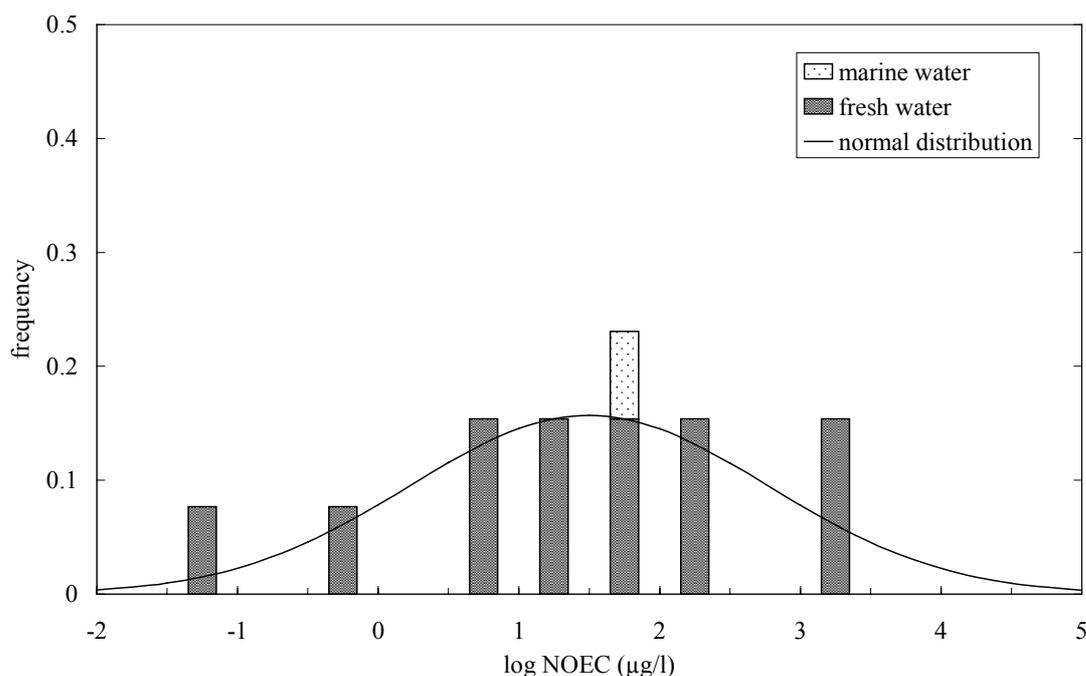


Figure 3.22: Free cyanide: Distribution of chronic toxicity data for aquatic species. The estimated curve is based on the combined set of fresh water and marine toxicity data ($n = 13$, $\bar{x} = 1.50$, $s = 1.27$).

3.2.2 SRC_{eco} for thiocyanate

For thiocyanate one LC50 for a terrestrial species is available (Table A3. 3). This value of $6.2 \cdot 10^3$ mg/kg could be used for the derivation an SRC_{eco} for soil. With an assessment factor of 10 the resulting SRC_{eco} is $6.2 \cdot 10^2$ mg/kg. Application of an assessment factor of 1000 results in an MPC of **6.2** mg/kg. However, no comparison is possible with equilibrium

partitioning due to the lack of distribution coefficients. For aquatic species, chronic and acute studies are available for fresh water species only (Table A3. 4). From the chronic toxicity studies an HC50 of $1.0 \cdot 10^4$ $\mu\text{g/l}$ is derived. With an ACR of 10, the HC50 derived from acute data is $1.9 \cdot 10^4$ $\mu\text{g/l}$. The lower value of **$1.0 \cdot 10^4$** $\mu\text{g/l}$ is selected as the HC50(aquatic species). For thiocyanate neither chronic nor acute data for algae are available. Therefore, the MPC is based on a comparison between chronic and acute data, according to the modified EPA method. Applying a safety factor of 10 to the lowest chronic NOEC gives a value of 36 $\mu\text{g/l}$. However, applying a safety factor of 1000 to the lowest acute study gives a lower value of 5.9 $\mu\text{g/l}$, which is proposed as MPC. The EU/TGD method could not be used to derive an MPC because the base set of data is not complete. Therefore, a maximum assessment factor of 100 or 1000 is used for the lowest NOEC or L(E)C50, respectively. The resulting MPC is **3.6** $\mu\text{g/l}$.

3.2.3 SRC_{eco} for cyanide complex

For three cyanide complexes data were found in literature: $\text{Na}_3[\text{Cu}(\text{CN})_4]$ for fresh water species and $\text{K}_3\text{Fe}(\text{CN})_6$ and $\text{K}_4\text{Fe}(\text{CN})_6$ for marine species (Table A3. 5 and Table A3. 6). The values are expressed as CN^- . On the basis of acute data an HC50 of 65 $\mu\text{g/l}$ is derived and from the chronic studies 29 $\mu\text{g/l}$. The HC50(aquatic species) of **29** $\mu\text{g/l}$ is almost equal to the value for free cyanides and consequently, no separate value is necessary for these types of cyanide complexes.

For cyanide complexes, a safety factor of 10 applied to the lowest NOEC according to the modified EPA method returns a value of 2.6 $\mu\text{g/l}$. However, chronic studies are available for only algae. Therefore, a comparison is made with acute toxicity data. Acute toxicity data are available for algae, crustaceans (no *Daphnia*) and fish. Therefore, a safety factor of 100 is applied to the lowest acute value, which leads to an MPC of 1.3 $\mu\text{g/l}$. Because no complete base set is available, no MPC can be derived according to the EU/TGD method. Therefore, a maximum assessment factor of 100 or 1000 is applied to the lowest NOEC or L(E)C50, respectively. The resulting MPC is **0.13** $\mu\text{g/l}$.

3.2.4 Summary

No risk limits have been derived formerly, neither as Intervention Value nor in the context of the project 'Setting Integrated Environmental Quality Standards'. For free and complex cyanides, no suitable terrestrial toxicity data are available. Information on the partitioning between soil and water is also missing and therefore, the equilibrium partitioning theory cannot be applied. For these reasons, only SRC_{eco} for free and complex cyanides are derived for groundwater. These values are based on the SRC_{eco} for surface water and are listed in Table 3.4, together with the values for thiocyanate.

Table 3.4: Summary of new SRC_{eco} values and MPC/NC values for cyanides.

Compound	Compartment	SRC _{eco} [$\mu\text{g/l}$]	Method* / reliability score	MPC [$\mu\text{g/l}$]	Method*	NC [$\mu\text{g/l}$]
free cyanide (CN^-)	surface water	31	ref. / high	0.23	ref.	0.0023
thiocyanate (SCN^-)	surface water	$1.0 \cdot 10^4$	1 c / medium	3.6	1000 incompl.	0.036
cyanide complexes (CN^-)	surface water	29	1 c / medium	0.13	100 incompl.	0.0013
		[mg/kg]		[mg/kg]		[mg/kg]
thiocyanate (SCN^-)	soil	620	10 a sp. / low	6.2	1000 a sp.	0.062

* For the SRC_{eco} and the MPC the abbreviation ref. is used in case of refined risk assessment. The assessment factor together with the designation according to Table 2.1, Table 2.5, and Table 2.6 is given in case of preliminary risk assessment. An incomplete base set is indicated

by the abbreviation incompl. Whether the SRC_{eco} or the MPC for soil is based on species or processes is indicated by the abbreviation sp. and pr.

For the type of cyanide complexes considered here, both the SRC_{eco} and MPC are almost equal to that for free cyanides. Therefore, a separate SRC or MPC is not necessary. For thiocyanate one terrestrial toxicity study is available besides the aquatic toxicity data. Based on this study, an SRC_{eco} of 620 mg/kg and an MPC of 6.2 mg/kg could be derived. For comparison with the ERLs concentrations in water should be measured as CN⁻ or SCN⁻.

3.3 Proposals for SRCs_{eco} for non-halogenated monocyclic aromatic hydrocarbons

For the BTEX (benzene, toluene, ethylbenzene and *o*-, *m*-, and *p*-xylene) compounds, the data presented by van de Plassche and Bockting (1993) are used to derive the SRC_{eco} values, for toluene together, with the data from van der Heijden et al. (1988). For phenol, *o*-, *m*-, and *p*-cresol and the dihydroxybenzenes (catechol, resorcinol and hydroquinone) new data have been collected. For benzene, toluene, ethylbenzene, styrene, and phenol an European evaluation (EU commission regulation 1488/94) will be available on a short term.

The proposed SRCs_{eco} are summarised in 3.3.9 together with old values as proposed by Denneman and van Gestel (1990) and MPCs as proposed by van de Plassche and Bockting (1993). The selected data used for extrapolation are included in Appendix 4.

3.3.1 SRC_{eco} for benzene

For benzene chronic NOECs are available for more than four taxonomic groups (Table A4. 1 and Table A4. 2). The differences between fresh water and marine species are significant ($P < 0.05$), even after Welch-correction for differences in variance. It should be noted that the taxonomic groups are dissimilar for fresh water and marine species. Further, the only chronic study with a fresh water alga (*Selenastrum capricornutum*) is about one order of magnitude higher than the chronic toxicity data for marine algae, and still higher than the acute algae toxicity studies. Moreover, both sets of data are very small (6 and 4) and therefore, it was decided to combine the chronic data for fresh water and marine species (Figure 3.23). The HC50(aquatic species) from this distribution is 41 mg/l (90% CI: 8 – 211 mg/l).

Compared with the acute toxicity data, the chronic NOECs for fresh water species seem to be very high, maybe because of the taxonomic groups (bacteria, algae, protozoa and nematoda). Both sets of acute toxicity data are not significantly different ($P = 0.40$) and the geometric mean of 61 mg/l is only slightly higher than that of the chronic NOECs for fresh water species or the combined sets of data.

Therefore, the HC50(aquatic species) is also derived from QSAR estimates (data in Table A4. 3) with the same set of QSARs as used by Van de Plassche et al. (1993). The log K_{ow} used for the QSAR estimates is taken from Otte et al. (2001). Because a comparison with experimental data is made no additional safety factor is applied to the geometric mean of these values. The resulting HC50 is 30 mg/l (90% CI: 17 – 53 mg/l).

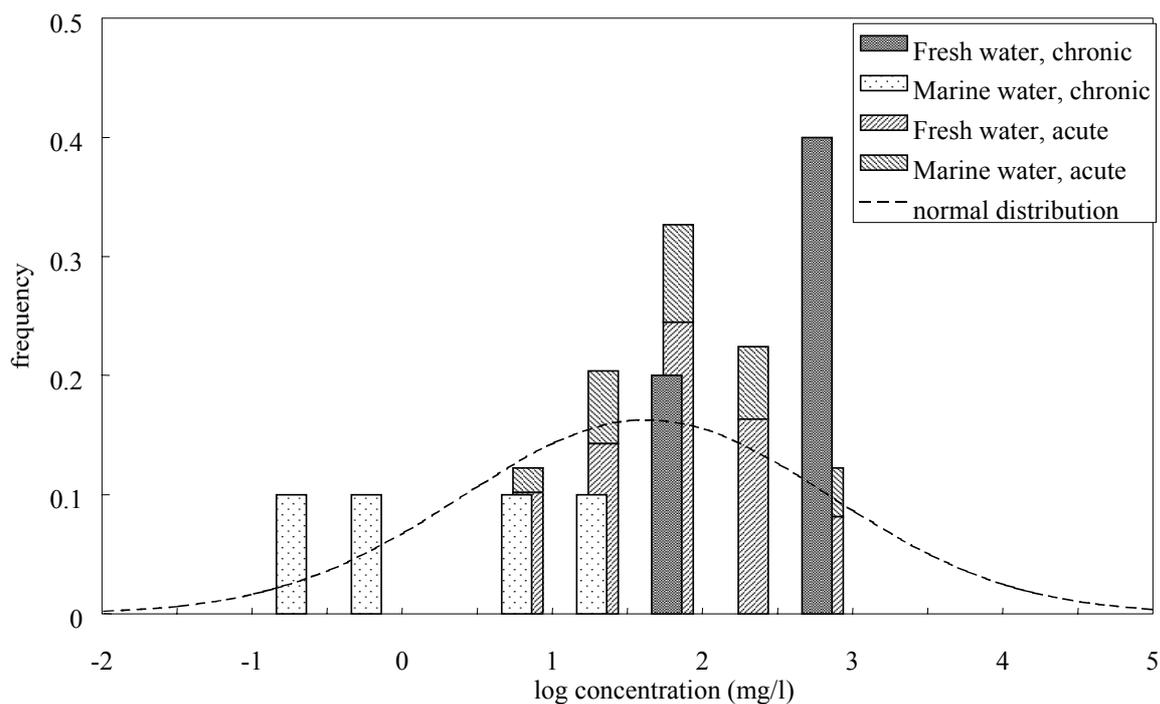


Figure 3.23: Distribution of chronic and acute toxicity data for benzene. The estimated curve is based on the combined sets of chronic toxicity data ($n = 10$, $\bar{x} = 1.61$, $s = 1.22$).

The current MPC of $2.4 \cdot 10^2$ $\mu\text{g/l}$ for surface water is based on QSARs and statistical extrapolation (van de Plassche et al., 1993) and an extra safety factor of 10 for the harmonisation with the air compartment (van de Plassche and Bockting, 1993). From the statistical extrapolation of the experimental data a similar value of $3.4 \cdot 10^2$ $\mu\text{g/l}$ is derived (90% CI: 0.01 – 2.34 $\mu\text{g/l}$), while the QSAR estimates without a factor of 10 give rise to a substantially higher HC5 of 2.8 mg/l (90% CI: 0.9 – 5.7 mg/l). The lower HC5 from the experimental data is caused by a higher variance in these data.

No studies for terrestrial species are available for benzene. Therefore, the HC50(soil) is derived by equilibrium partitioning. The log K_p for standard soil and sediment is 0.64. The corresponding HC50 for soil and sediment is $1.3 \cdot 10^2$ mg/kg. By multiplying the MPC for surface water with this K_p of benzene, an MPC in soil and sediment of 1.0 mg/kg is obtained.

3.3.2 SRC_{eco} for toluene

For toluene chronic aquatic toxicity data are available for bacteria, cyanophyta, protozoa, algae and fish (Table A4. 5 and Table A4. 6). The fresh water and marine data are not significantly different ($P = 0.32$, Welch-corrected) and therefore both sets are combined. The sensitivity distribution of these data is shown in Figure 3.24. The HC50 of the statistical extrapolation is 13 mg/l (90% CI: 6 – 27 mg/l).

The majority of the acute toxicity data are for crustaceans and fish. For comparison, these acute toxicity data are almost as low as the chronic toxicity data, which are dominated by lower organisms. For the acute toxicity data, marine and fresh water species are not significantly different ($P = 0.48$). The geometric mean of the acute toxicity data is 27 mg/l, whereas the geometric mean of the chronic toxicity data is 16 mg/l.

Because the chronic toxicity data for toluene are relatively high, the derived HC50(aquatic species) is compared with QSAR estimates (data in Table A4. 7). The log K_{ow} value used for

these estimates is 2.73 (Otte et al., 2001) The value derived from QSARs is slightly lower. The resulting HC50(aquatic species) is **11 mg/l** (90% CI: 6 – 20 mg/l).

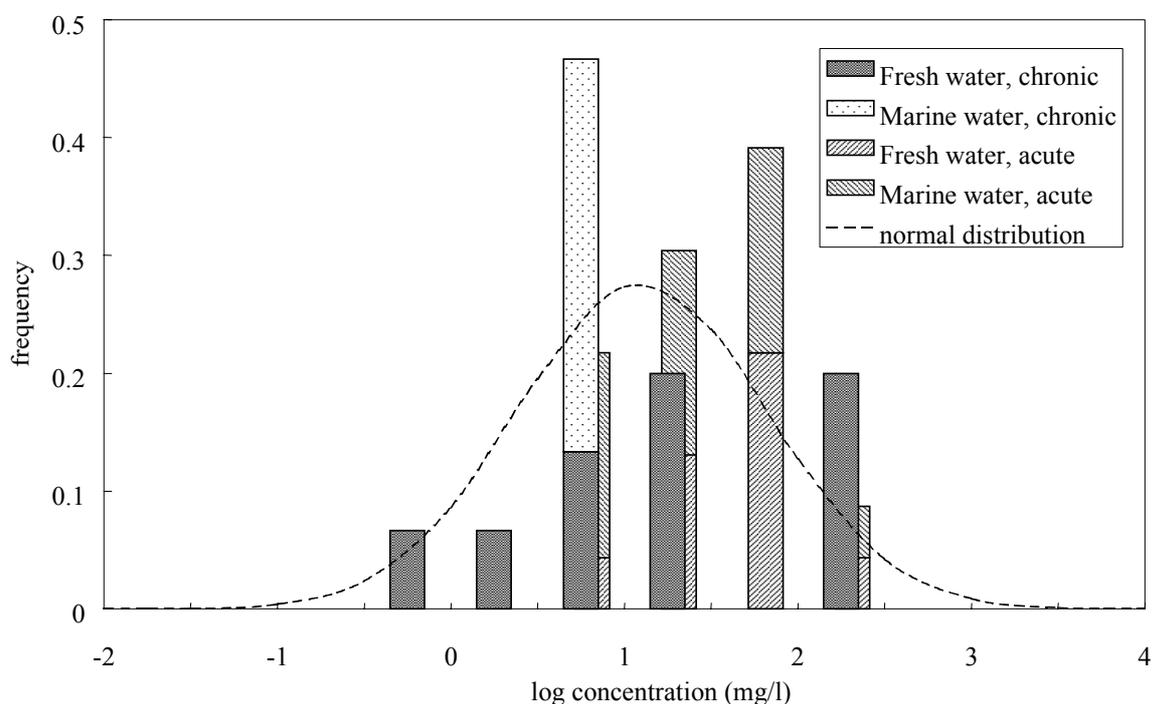


Figure 3.24: Toluene: Distribution of chronic and acute toxicity data. The estimated curve is based on the chronic toxicity data ($n = 15$, $\bar{x} = 1.10$, $s = 0.72$).

Statistical extrapolation from the chronic toxicity data yields an HC5 of $7.7 \cdot 10^2 \mu\text{g/l}$ (90% CI: $1.8 \cdot 10^2 - 19.8 \cdot 10^2 \mu\text{g/l}$). The current MPC of $7.3 \cdot 10^2 \mu\text{g/l}$ derived from QSARs and statistical extrapolation is slightly lower (van de Plassche et al., 1993). With the same set of QSARs and the log K_{ow} value from Otte et al. (2001), the HC5 of the log-normal distribution is $8.5 \cdot 10^2 \mu\text{g/l}$ (90% CI: $2.7 \cdot 10^2 - 18.5 \cdot 10^2 \mu\text{g/l}$). The HC5 from the chronic toxicity data can therefore, be regarded as MPC in surface water for toluene.

For toluene, two chronic toxicity studies for terrestrial species are available (Table A4. 4). The geometric mean of these values is 47 mg/kg. For toluene the log K_p for standard soil and sediment is 0.86. This leads to an HC50(EqP) of 79 mg/kg. The lowest value, 47 mg/kg, is chosen as the HC50(soil). For sediment the HC50 is equal to the value of 79 mg/kg derived with equilibrium partitioning.

The lowest NOEC for soil is 14 mg/kg. According to the modified EPA method the MPC for soil would be 1.4 mg/kg. A factor of 100 is applied according to the EU/TGD leading to an MPC of 0.14 mg/kg. Applying equilibrium partitioning to the MPC of $7.7 \cdot 10^2 \mu\text{g/l}$ yields an MPC for sediment of 5.6 mg/kg.

3.3.3 SRC_{eco} for ethylbenzene

For ethylbenzene NOECs are available for four taxonomic groups (bacteria, cyanophyta, algae and protozoa, Table A4. 8). The HC50 derived from statistical extrapolation (see Figure 3.25) is 20 mg/l (90% CI: 1 – 319 mg/l). These taxonomic groups seem to be rather insensitive, compared with the acute toxicity data. The acute toxicity data for fresh water and marine species are not significantly different ($P = 0.46$). The geometric mean of the acute toxicity data is equal to that of the chronic data (Table A4. 8 and Table A4. 9): 20 mg/l.

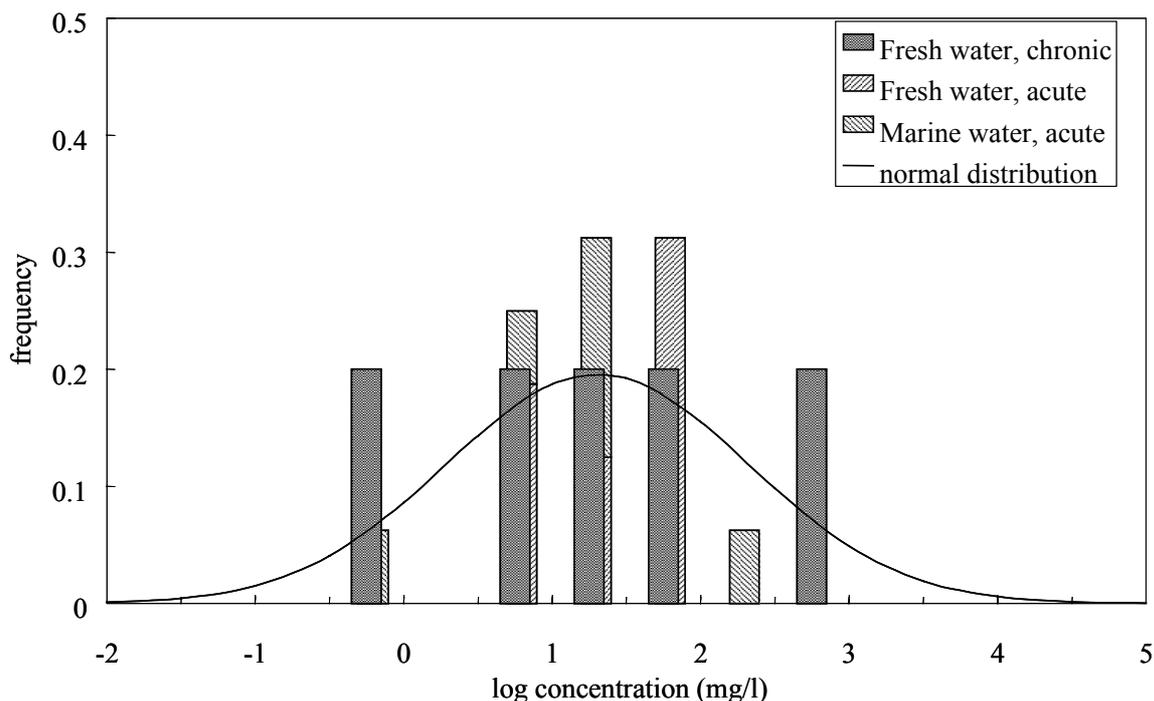


Figure 3.25: Distribution of chronic and acute toxicity data for ethylbenzene. The estimated curve is based on the chronic toxicity data ($n = 5$, $\bar{x} = 1.31$, $s = 1.02$).

Because the chronic toxicity data for ethylbenzene are relatively high, the HC50(aquatic species) is also derived from QSAR estimates (data in Table A4. 10) with the same set of QSARs as used by Van de Plassche et al. (1993). The log K_{ow} used for the QSAR estimates is taken from Otte et al. (2001). Because experimental data are available no additional safety factor is applied to the geometric mean of these values. The resulting HC50 is **5.5 mg/l** (90% CI: 2.9 – 10.5 mg/l).

It has to be noted that the HC5 derived from the chronic toxicity data by statistical extrapolation is slightly lower than the HC5 derived from QSARs: **$3.1 \cdot 10^2$** versus $3.8 \cdot 10^2$ $\mu\text{g/l}$, but the uncertainty in this estimate is large (90% CI: 1 – 2970 $\mu\text{g/l}$) in comparison with that of the HC5 estimated from QSARs (90% CI: $1.1 \cdot 10^2$ – $8.5 \cdot 10^2$ $\mu\text{g/l}$). Less variation is observed for the QSAR estimates than for the experimental toxicity data.

For ethylbenzene no terrestrial studies are available. Therefore, the HC50(soil) is derived by equilibrium partitioning. The log K_p for standard soil and sediment is 1.30. The resulting value of the HC50 for soil and sediment is **$1.1 \cdot 10^2$** mg/kg. Applying the equilibrium theory to the HC5 of 310 $\mu\text{g/l}$ for surface water gives an MPC for soil and sediment of **6.2 mg/kg**.

3.3.4 SRCs_{eco} for xylenes

For xylenes the three isomers are considered separately. Thereafter it is considered whether a combined risk limit can be derived or not.

3.3.4.1 SRC_{eco} for *o*-xylene

For *o*-xylene two chronic NOECs are available for fresh water species (Table A4. 11). The geometric mean of these data is 3.0 mg/l. The acute toxicity data for fresh water and marine species (Table A4. 11 and Table A4. 12) are not significantly different ($P = 0.23$) and therefore, both sets are combined. Applying an ACR of 10 to the geometric mean of both sets, gives an HC50 of **1.0 mg/l**.

The MPC of 380 µg/l for *o*-xylene was derived from QSARs and statistical extrapolation (Van de Plassche et al., 1993). This value is very close to the HC50 derived from the experimental data. Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. The lowest L(E)C50 is 1.3 mg/l for a crustacean. NOECs are available for algae and protozoa. The lowest NOEC is 1.0 mg/l. Applying the modified EPA method leads to an MPC of 13 µg/l. The assessment factors for aquatic toxicity data following EU/TGD yield a similar value of **10** µg/l. Both values are well below the current MPC.

No terrestrial toxicity data are available for the *o*-xylene isomer. With the log K_p for standard soil and sediment of 0.95 an HC50(soil/sediment) of **9.3** mg/kg is derived. Applying equilibrium partitioning to the value of 10 µg/l from the EU/TGD method yields a value of **0.089** mg/kg.

3.3.4.2 SRC_{eco} for *m*-xylene

The same type of information as for *o*-xylene is available for *m*-xylene. The acute toxicity studies for fresh water and marine species (Table A4. 13 and Table A4. 14) are not significantly different ($P = 0.55$). The geometric mean of the chronic toxicity data is 4.4 mg/l and that of the acute toxicity data 12 mg/l. This leads to an HC50(aquatic species) of **1.2** mg/l.

The lowest NOEC is 0.7 mg/l and the lowest L(E)C50 is 1.6 mg/l with studies available for algae, crustaceans (a.o. *Daphnia*) and fish. The MPC according to the modified EPA method is 16 µg/l. With the EU/TGD method an MPC of **7.0** µg/l is derived. The current MPC for *m*-xylene based on QSARs and statistical extrapolation is 380 µg/l. This value is much higher than the values based on the experimental toxicity data and is close to the HC50.

The log K_p for standard soil and sediment is 1.18. Applying the equilibrium theory leads to an HC50(soil/sediment) of **18** mg/kg. With the aquatic MPC from the EU/TGD method an MPC of **0.11** mg/kg is derived for soil and sediment.

3.3.4.3 SRC_{eco} for *p*-xylene

The derivation of the risk limits for *p*-xylene follows the same route as for *o*-xylene and *m*-xylene. The acute toxicity studies for fresh water and marine species (Table A4. 15 and Table A4. 16) are not significantly different ($P = 0.21$). The geometric mean of the chronic toxicity data is 2.8 mg/l and that of the acute toxicity data 11 mg/l. This leads to an HC50(aquatic species) of **1.1** mg/l.

The lowest NOEC is 0.9 mg/l and the lowest L(E)C50 is 1.6 mg/l with studies available for algae, crustaceans (a.o. *Daphnia*) and fish. The MPC according to the modified EPA method is 16 µg/l. With the EU/TGD method the MPC becomes **9.0** µg/l. The current MPC for *p*-xylene is based on QSARs and statistical extrapolation is 380 µg/l, which is close to the HC50. The MPC derived from the experimental data is much lower.

The log K_p for standard soil and sediment is 1.43. Applying the equilibrium theory gives an HC50(soil/sediment) of **30** mg/kg. With the EU/TGD method an MPC of **0.24** mg/kg is derived for soil and sediment.

3.3.4.4 Combined values for the three xylene isomers

The three isomers of xylene seem to be very similar to each other, both in terms of physico-chemical properties and toxicity. From the HC50s(aquatic species) of the three isomers of xylene a geometric mean of **1.1** mg/l is calculated as SRC_{eco} in surface water. The MPC for surface water for the sum of xylenes, calculated as the geometric mean of the MPC values from the EU/TGD method, is **8.6** µg/l. For soil and sediment the geometric mean of the

SRC_{eco} is **17 mg/kg** and that of the MPC **0.13 mg/kg**. The experimental concentrations of the three isomers should be summed when comparing with these ERLs.

3.3.5 SRC_{eco} for styrene

For styrene data are available for both fresh water and marine species (Table A4. 17 and Table A4. 18). The geometric mean of the acute toxicity data is lower than that of the chronic data and therefore the HC50 is based on the acute toxicity data. The fresh water and marine data are not significantly different ($P = 0.67$, Welch-corrected) and therefore both sets of data are combined. After application of an ACR of 10 the HC50(aquatic species) is **3.8 mg/l**. The lowest L(E)C50 is 9.1 mg/l. With the modified EPA method, the MPC for surface water is **9.1 μ g/l**. The current MPC for styrene of 570 μ g/l is based on QSARs and statistical extrapolation. No data are available for algae and therefore no MPC according to the EU/TGD protocol can be derived.

No terrestrial data for styrene are available. Consequently, the HC50 for soil and sediment is derived by equilibrium partitioning. The log K_p for standard soil and sediment is 1.35. The resulting HC50 is **86 mg/kg**. With the MPC derived by the modified EPA method, the MPC for soil and sediment is **0.20 mg/kg**.

3.3.6 SRC_{eco} for phenol

For phenol enough data are available for statistical extrapolation (Table A4. 20 and Table A4. 21). The data follow the log-normal distribution (Figure 3.26). One NOEC for a marine algae falls well within the log-normal distribution for all aquatic species ($P = 60\%$) and therefore, the fresh water and marine data are combined. The HC50(aquatic species) is **7.0 mg/l** (90% CI: 2.0 – 24.0 mg/l). The MPC is based on the HC5 estimate of **0.10 mg/l** (90% CI: 0.01 – 0.47 mg/l).

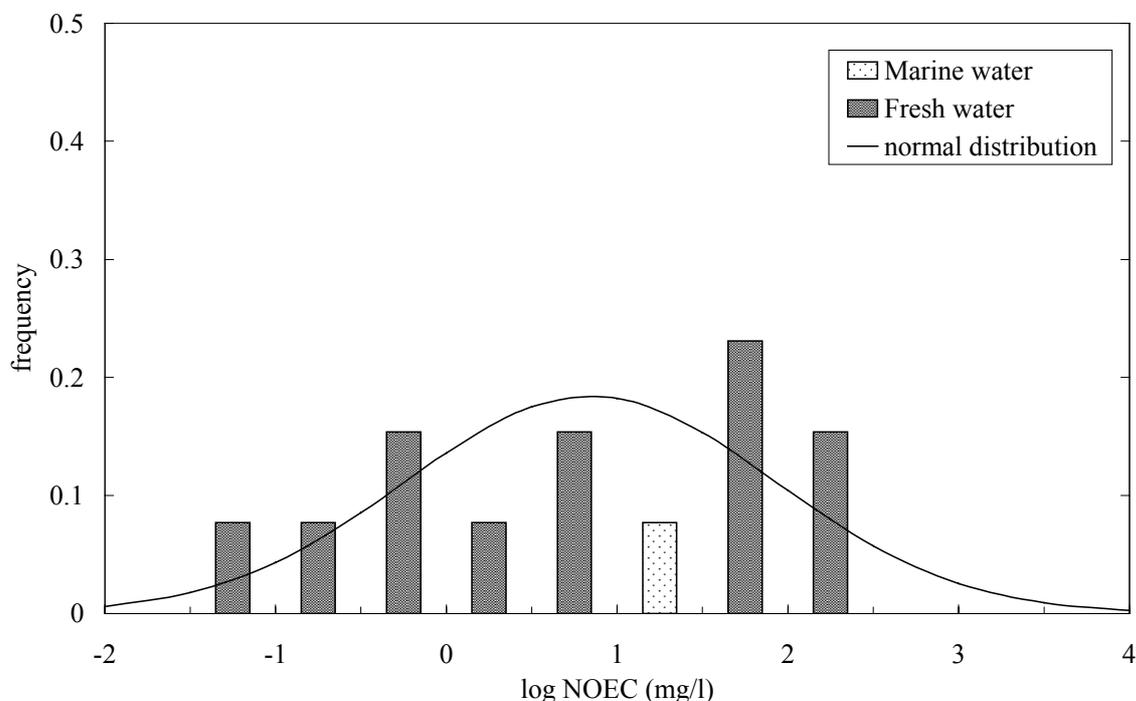


Figure 3.26: Phenol: Chronic toxicity for fresh water and marine species. The estimated distribution is based on the combined sets ($n = 13$, $\bar{x} = 0.84$, $s = 1.08$).

For terrestrial species both a chronic as well as an acute study is available (Table A4. 19). However, both studies concern the same species, which is the macrophyt *Lactuca sativa*. For this reason the HC50(terrestrial species) is based on the NOEC of 160 mg/kg. Because of the limited number of data, a comparison is made with a value derived from equilibrium partitioning. The $\log K_p$ for standard soil and sediment is 0.29 for phenol. The resulting HC50(EqP) of 14 mg/kg is used as the HC50(soil/sediment).

The MPC for terrestrial organisms, directly calculated from the chronic toxicity for *Lactuca sativa*, is compared with equilibrium theory. According to the modified EPA method or the EU/TGD method a safety factor of 1000 is applied to the lowest L(E)C50 of 400 mg/kg. This value is lower than the NOEC value of 160 mg/kg divided by 10 or 100, according to the modified EPA or EU/TGD method, respectively. In the framework of the project 'Setting Integrated Environmental Quality Standards' this MPC is harmonised with the water compartment by equilibrium partitioning. The HC5 for aquatic species multiplied by the K_p for standard soil leads to an MPC for soil and sediment of 0.20 mg/kg.

3.3.7 SRC_{eco} for cresols

Data for *o*, *m*, and *p*-cresol have been collected and are presented in the annex to this report. In first instance, risk limits are derived individually. Afterwards it was examined if an HC50 for the sum of the three isomers could be determined.

3.3.7.1 SRC_{eco} for *o*-cresol

NOECs are available for the same taxonomic groups as in the case of ethylbenzene (Table A4. 23). Statistical extrapolation is used to derive an HC50(aquatic species) of 29 mg/l (90% CI: 17 – 50 mg/l). The HC5 of this distribution is 6.3 mg/l (90% CI: 1.9 – 11.9 mg/l). Again, the taxonomic groups for which chronic toxicity data are available seem to be not very sensitive. The acute toxicity data for fresh water and marine species (Table A4. 23 and Table A4. 24) are not significantly different ($P = 0.14$). The geometric mean of the combined sets of acute toxicity data (30 mg/l) is almost equal to that of the chronic toxicity data.

Although *o*-cresol is not a nonpolar chemical, a comparison is made with QSAR estimates (Table A4. 25) because of the relatively high chronic NOECs. The HC50 derived from these QSARs is slightly higher than that from the experimental data 59 mg/l (90% CI: 34 – 104 mg/l). However, the HC5 of 5.7 (90% CI: 2.0 – 11.6 mg/l) is slightly lower than the HC5 from the experimental values. Therefore, this HC5 of 5.7 mg/l is proposed as MPC.

Acute toxicity data are available for crustaceans (*Daphnia*) and fish but not for algae. From the chronic toxicity data it appears that algae are not more sensitive to *o*-cresol than crustaceans or fish. Therefore, if the modified EPA method is used a safety factor of 100 is applied to the lowest L(E)C50 value. This would lead to an MPC for surface of 84 µg/l. With the EU/TGD method a safety factor of 50 is applied to the lowest NOEC leading to an MPC of $1.4 \cdot 10^2$ µg/l. It is apparent that the MPC derived by statistical extrapolation is rather high. For *o*-cresol one terrestrial NOEC of 50 mg/kg is available (Table A4. 26). Therefore both the HC50 and the MPC are derived by comparison with equilibrium theory. The $\log K_p$ of *o*-cresol for standard soil or sediment is 0.36. The resulting HC50(EqP) for soil and sediment is 66 mg/kg and the MPC(EqP) is 14 mg/kg. The value of 50 mg/kg is proposed as SRC_{eco} for soil. For sediment the value of 66 mg/kg derived by equilibrium partitioning is proposed as SRC_{eco}. The safety factors for the derivation of the MPC are 10 and 100 with the modified EPA method and the EU/TGD method, respectively. The proposed MPC for soil is the value of 0.5 mg/kg derived with the EU/TGD method. For sediment the MPC derived by equilibrium partitioning is 13 mg/kg.

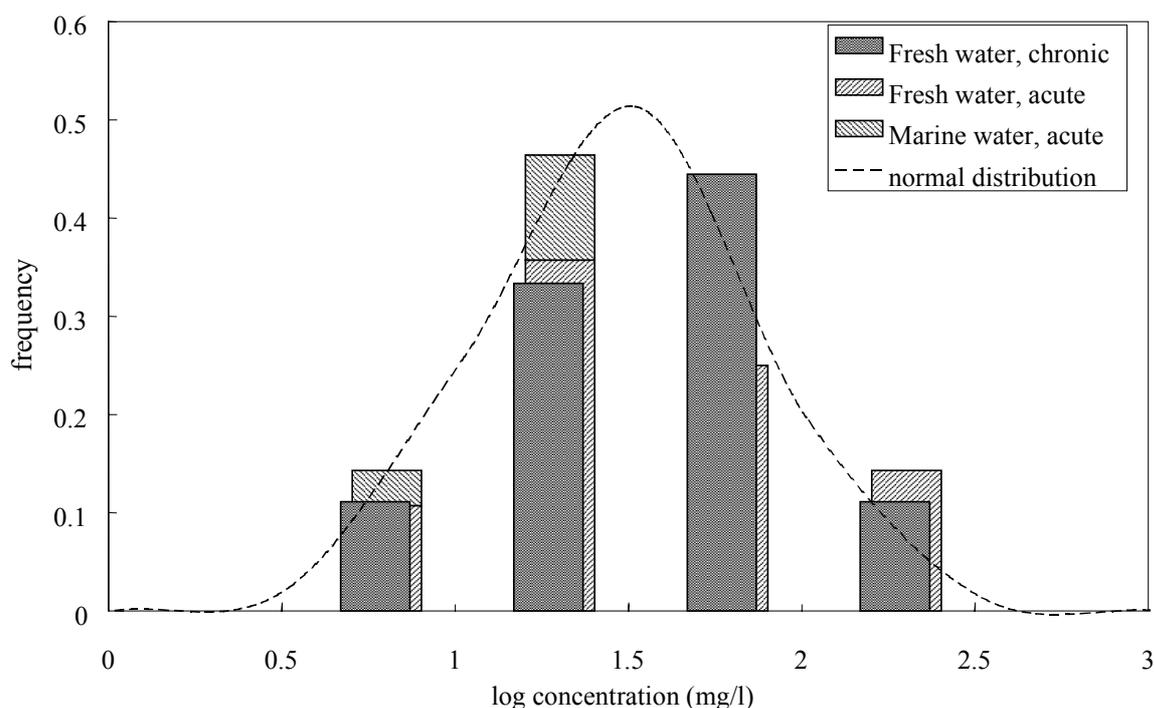


Figure 3.27: *o*-Cresol: Distribution of chronic and acute toxicity data. The estimated curve is based on the chronic toxicity data ($n = 9$, $\bar{x} = 1.46$, $s = 0.39$).

3.3.7.2 SRC_{eco} for *m*-cresol

For *m*-cresol the derivation of the HC50s and MPCs can be motivated in exactly the same way as for *o*-cresol. The chronic toxicity data for the same taxonomic groups are not very sensitive again (Figure 3.28, compare with Figure 3.27). The HC50 from this distribution is **36 mg/l** (90% CI: 18 – 72 mg/l). The acute toxicity data for fresh water and marine species (Table A4. 27 and Table A4. 28) can be combined ($P = 0.52$) and have a lower geometric mean of 23 mg/l. The HC5 derived by statistical extrapolation from the chronic toxicity data is 8.3 mg/l (90% CI: 1.6 – 17.3 mg/l).

Because of the relatively high values for the chronic NOECs also for *m*-cresol a comparison with QSAR estimates is made (Table A4. 29). Also in this case the HC50 from the QSAR estimates is slightly higher than that from the experimental data: 58 mg/l (90% CI: 53 – 102 mg/l) However, the HC5 is slightly lower and this value is proposed as MPC: **5.5 mg/l** (90% CI: 1.9 – 11.3 mg/l).

Using the modified EPA method with a safety factor of 100, an MPC for surface water is derived of 75 µg/l. According to the EU/TGD method a safety factor of 50 is applied to the lowest NOEC in this case. This results in an MPC of $2.6 \cdot 10^2$ µg/l. Also for *m*-cresol, the MPC derived by statistical extrapolation is rather high.

One terrestrial NOEC of 16 mg/kg is available (Table A4. 26). With the log K_p of 0.49 and equilibrium partitioning, an HC50 of $1.1 \cdot 10^2$ mg/kg and an MPC of 17 mg/kg. For soil the NOEC of **16 mg/kg** is proposed as SRC_{eco}. For sediment this value is $1.1 \cdot 10^2$ mg/kg derived by equilibrium partitioning. Applying the modified EPA method to the terrestrial toxicity data gives an MPC of 0.48 mg/kg (factor of 1000 to the lowest L(E)C50). According to the EU/TGD method a factor of 100 is applied to the lowest NOEC because this values is lower than 0.48 mg/kg. The resulting MPC for soil is **0.16 mg/kg**. For sediment the value derived by equilibrium partitioning of **17 mg/kg** is suggested as MPC.

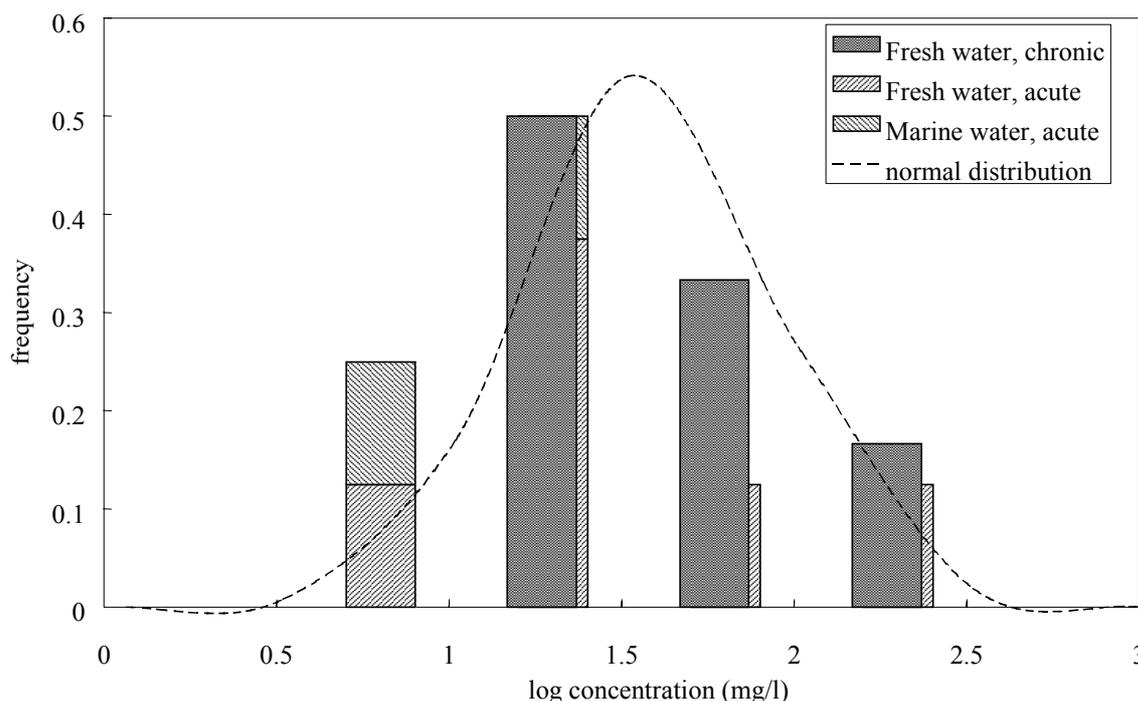


Figure 3.28: *m*-Cresol: Distribution of chronic and acute toxicity data. The estimated curve is based on the chronic toxicity data ($n = 6$, $\bar{x} = 1.56$, $s = 0.36$).

3.3.7.3 SRC_{eco} for *p*-cresol

For *p*-cresol only one chronic NOEC is available for *Daphnia magna* (Table A4. 30). The HC50 from the geometric mean of the combined sets of acute toxicity data for fresh water and marine species ($P = 0.25$, Table A4. 30 and Table A4. 31) is 1.7 mg/l after application of an ACR of 10. The NOEC of 1 mg/l is lower than this value. The HC50(aquatic species) is therefore **1.0 mg/l**.

The lowest value for acute toxicity of 2.0 mg/l is for the bacteria *Vibrio fisheri*. Because data are available for algae, crustaceans (a.o. *Daphnia*) and fish, a safety factor of 100 can be applied to the lowest L(E)C50 according to the modified EPA method. This leads to an MPC for surface water of 20 µg/l. With the EU/TGD method the factors applied to the NOEC and the L(E)C50s are 10 times as much in this case. This results in an MPC of **2.0 µg/l**.

No terrestrial data are available for *p*-cresol. Therefore both the HC50(soil) and the MPC are derived from equilibrium partitioning. With the log K_p of 0.41 for standard soil and sediment, the resulting values are **2.6 mg/kg** and **0.051 mg/kg**.

3.3.7.4 Combined values for the three cresol isomers

The three isomers of cresol seem to be very similar to each other, both in terms of physico-chemical properties and toxicity. The values for HC50 and MPC are very different values. This is the result of the different methods used to derive the ERLs. For both *o*- and *m*-cresol the values for surface water are derived by statistical extrapolation. The NOECs for bacteria, cyanophyta, protozoa and algae seem to be rather insensitive. For *p*-cresol not enough data were available for statistical extrapolation. The acute studies for the three isomers show very similar values. However, the only NOEC for *p*-cresol, which is for a crustacean in this case, is much lower than the NOECs for the other two.

From the HC50s(aquatic species) for the three isomers of cresol a geometric mean of **10 mg/l** in surface water is calculated as SRC_{eco}. The MPC for surface water for the sum of cresols is

$4.0 \cdot 10^2$ µg/l. The SRC_{eco} for the sum of cresols are **13** mg/kg for soil and **27** mg/kg for sediment and the MPCs are **0.16** mg/kg for soil and **1.0** mg/kg for sediment. The experimental concentrations of the three isomers should be summed when comparing with these ERLs.

3.3.8 SRC_{eco} for dihydroxybenzenes

Data for catechol, resorcinol and hydroquinone (*o*-, *m*-, and *p*-dihydroxybenzene) have been collected and are presented in the annex to this report. In first instance, risk limits are derived individually. Afterwards it is examined if an HC50 for the sum of the three isomers could be determined.

3.3.8.1 SRC_{eco} for catechol

For catechol no chronic toxicity data are available. The only study for marine species fits within the log-normal distribution of all acute aquatic toxicity data ($P = 89\%$). The geometric mean of the acute aquatic toxicity studies for fresh water and marine species (Table A4. 32 and Table A4. 33) is $6.3 \cdot 10^3$ µg/l. With an ACR of 10 an HC50(aquatic species) of $6.3 \cdot 10^2$ µg/l is derived. The MPC is derived by the modified EPA. The lowest L(E)C50 is 0.77 mg/l. The corresponding MPC is **0.77** µg/l. Because the base set is not complete no MPC according to the EU/TGD procedure can be derived.

No terrestrial data are available. Therefore, the HC50(soil) is derived by equilibrium partitioning. The log K_p for standard soil and sediment is 0.62. Applying the equilibrium theory leads to an HC50(soil/sediment) of **2.6** mg/kg and an MPC of **0.0032** mg/kg.

3.3.8.2 SRC_{eco} for resorcinol

For resorcinol two chronic studies for fish are available (Table A4. 34) with a geometric mean of 5.7 mg/l. The acute toxicity data for fresh water and marine species (Table A4. 34 and Table A4. 35) are not significantly different ($P = 0.22$). The geometric mean of the acute data is 98 mg/l. Therefore the HC50(aquatic species) is **5.7** mg/l.

The lowest NOEC is 1 mg/l. No data for algae are available. The lowest L(E)C50 is 42 mg/l. With the modified EPA method the MPC is **42** µg/l. Because the base set is not complete no MPC according to the EU/TGD procedure can be derived.

No terrestrial data are available for resorcinol. Therefore, equilibrium partitioning is applied. The log K_p for standard soil and sediment is -0.09 . The resulting HC50 for soil and sediment is **4.6** mg/kg. The MPC is equal to **0.034** mg/kg.

3.3.8.3 SRC_{eco} for hydroquinone

For hydroquinone chronic toxicity studies are available for bacteria, cyanophyta, protozoa and algae (Table A4. 37). Also in this case the geometric mean of the acute toxicity data is lower than the geometric mean of the chronic data (Table A4. 37, Table A4. 38 and Figure 3.29).

Statistical extrapolation of the chronic toxicity data gives an HC50 of **8.2** mg/l (90% CI: 2.0 – 33.2 mg/l) and an MPC of $4.1 \cdot 10^2$ µg/l (90% CI: $0.1 \cdot 10^2$ – $18.4 \cdot 10^2$ µg/l).

The acute toxicity studies for fresh water and marine species are not significantly different ($P = 0.72$) and therefore, both sets of data are combined. The geometric mean of both sets is 3.5 mg/l, lower than the HC50 from the chronic toxicity data. For acute toxicity, data for algae, crustaceans (a.o. *Daphnia*) and fish are available. With the modified EPA method application of a factor of 100 to the lowest L(E)C50 of 44 µg/l gives an MPC of 0.44 µg/l. The MPC according to the EU/TGD method is in this case derived by applying a factor of 50 to the

lowest NOEC. The resulting MPC is 19 µg/l. It is obvious that the HC5 from the statistical extrapolation of the chronic toxicity data is rather high compared with these MPCs.

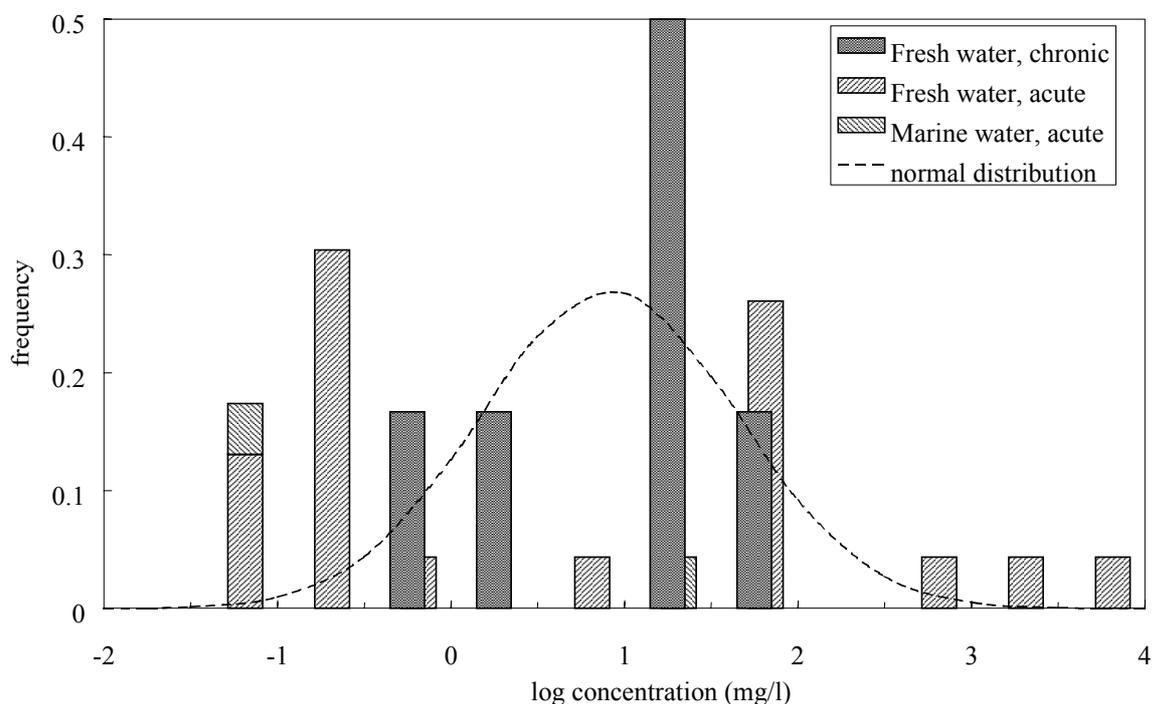


Figure 3.29: Hydroquinone: Distribution of chronic and acute toxicity data. The estimated curve is based on the chronic toxicity data ($n = 6$, $\bar{x} = 0.91$, $s = 0.74$).

For hydroquinone two terrestrial NOECs are available for plants (Table A4. 36). The geometric mean of these NOECs is $8.2 \cdot 10^2$ mg/kg. With the modified EPA method the MPC is 76 mg/kg derived by applying a factor of 10 to the lowest NOEC. The EU/TGD method results in a lower value of 7.6 mg/kg because of a factor of 100. The $\log K_p$ for standard soil and sediment is 0.72. Applying equilibrium partitioning results in an HC50 for soil and sediment of 43 mg/kg. The MPC for both compartments is equal to 2.2 mg/kg.

3.3.8.4 Combined values for the three dihydroxybenzene isomers

The three isomers of dihydroxybenzene have similar physico-chemical properties. However, the differences in toxicity are remarkable with hydroquinone being the most toxic isomer, if toxicity data for the same species are considered (e.g. see acute toxicity data for fish and *Vibrio fisheri*). On the other hand, because of the differences in the derivation of the ERLs, the HC50 and MPC for hydroquinone are the highest of all three isomers. Therefore, combined values can be derived for the three dihydroxybenzene isomers to minimise variation caused by differences in available data. For surface water the geometric mean of the three isomers for the SRC_{eco} is $3.1 \cdot 10^3$ µg/l and for the MPC 24 µg/l. For soil and sediment the combined SRC_{eco} is 8.0 mg/kg and the MPC 0.063 mg/kg. The experimental concentrations of the three isomers should be summed when comparing with these ERLs.

3.3.9 Summary and comparison with old values and MPCs

In Table 3.5 the SRC_{eco} for non-halogenated monocyclic aromatic hydrocarbons are summarised. Also included in this table are the few old values derived in Denneman and Van

Gestel (1990) and the MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (Van de Plassche and Bockting, 1993).

The SRCs for surface water are listed in Table 3.6. These values are the basis for SRCs for groundwater. For 6 compounds chronic toxicity data were available for bacteria, cyanophyta, protozoa and algae. The derived ERLs from statistical extrapolation are rather high in these cases, when compared with acute toxicity data. Therefore, a comparison with QSAR estimates was made.

Table 3.5: Summary of new SRC_{eco} values for monocyclic non-halogenated aromatic hydrocarbons in soil or sediment, values as derived by Denneman and van Gestel (1990), MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report. Values are given as concentrations in mg/kg standard soil/sediment (soil containing 10% organic matter and 25% clay, sediment containing 10% organic matter and 25% clay).

Compound	Compartment	SRC _{eco} [mg/kg]	Method* / reliability score	Denneman and van Gestel (1990) [mg/kg]	MPC this report [mg/kg]	Method*	MPC ^a INS [mg/kg]
benzene ^d	soil	130	EqP / medium	25	1.5	EqP	0.95^b
	sediment	130	EqP / medium	-	1.5	EqP	0.95
toluene ^d	soil	47	1 c sp. / medium	150	0.14	100 f sp.	1.4 ^c
	sediment	79	EqP / medium	-	5.6	EqP	4.2
ethylbenzene ^d	soil	110	EqP / medium	-	6.2	EqP	3.1
	sediment	110	EqP / medium	-	6.2	EqP	3.1
o-xylene	soil	9.3	EqP / low	-	0.089	EqP	-
	sediment	9.3	EqP / low	-	0.089	EqP	-
m-xylene	soil	18	EqP / low	-	0.11	EqP	-
	sediment	18	EqP / low	-	0.11	EqP	-
p-xylene	soil	30	EqP / low	-	0.24	EqP	-
	sediment	30	EqP / low	-	0.24	EqP	-
sum xylenes	soil	17	EqP / low	-	0.13	EqP	14
	sediment	17	EqP / low	-	0.13	EqP	14
styrene ^d	soil	86	EqP / low	-	0.20	EqP	25
	sediment	86	EqP / low	-	0.20	EqP	25
phenol ^d	soil	14	EqP < 1 c sp. / medium	40	0.20	EqP < c sp.	-
	sediment	14	EqP / medium	-	0.20	EqP	-
o-cresol	soil	50	1 c sp. / medium	150	0.50	100 b sp.	-
	sediment	66	EqP / medium	-	13	EqP	-
m-cresol	soil	16	1 c sp. / medium	15	1.6	100 d sp.	-
	sediment	110	EqP / medium	-	17	EqP	-
p-cresol	soil	2.6	EqP / low	-	0.0051	EqP	-
	sediment	2.6	EqP / low	-	0.0051	EqP	-
sum cresols	soil	13	EqP / low	50	0.16	EqP	-
	sediment	27	EqP / low	-	1.0	EqP	-
catechol	soil	2.6	EqP / low	-	0.0032	EqP	-
	sediment	2.6	EqP / low	-	0.0032	EqP	-
resorcinol	soil	4.6	EqP / low	-	0.034	EqP	-
	sediment	4.6	EqP / low	-	0.034	EqP	-

<i>Compound</i>	<i>Compartment</i>	<i>SRC_{eco}</i> [mg/kg]	<i>Method* / reliability score</i>	<i>Denneman and van Gestel (1990)</i> [mg/kg]	<i>MPC this report</i> [mg/kg]	<i>Method*</i>	<i>MPC^a INS</i> [mg/kg]
hydroquinone	soil	43	EqP<1 c sp. / medium	-	2.2	EqP<f sp.	-
	sediment	43	EqP / medium	-	2.2	EqP	-
sum dihydroxybenzenes	soil	8.0		-	0.062		-
	sediment	8.0		-	0.062		-

* For the SRC_{eco} and the MPC, EqP (equilibrium partitioning) or the assessment factor together with the designation according to Table 2.1 and Table 2.6 is given. Whether the SRC_{eco} or the MPC is based on species or processes is indicated by the abbreviation sp. and pr.

a MPC for water is derived from QSARs for narcotics, whereupon statistical extrapolation on these data is performed (Van de Plassche et al., 1993). The MPC for soil is derived from these values with equilibrium partitioning and comparison with soil toxicity data and harmonisation with the air compartment (Van de Plassche and Bockting, 1993).

b MPC for water is harmonised with the air compartment; bold value indicates that no update of the MPC is proposed.

c Based on terrestrial toxicity data.

d For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

Table 3.6: Summary of new SRC_{eco} values for monocyclic non-halogenated aromatic hydrocarbons in surface water, MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report from experimental studies.

Compound	Compartment	SRC _{eco} [µg/l]	Method* / reliability score	MPC this report [µg/l]	Method*	MPC ^b INS [µg/l]
benzene ^c	surface water	30000	QSAR / ref. / high	340	ref.	240^b
toluene ^c	surface water	11000	QSAR / ref. / high	770	ref.	730
ethylbenzene ^c	surface water	5500	QSAR / ref. / high	310	ref.	370
<i>o</i> -xylene	surface water	1000	10 b / medium	10	100 f	-
<i>m</i> -xylene	surface water	1200	10 b / medium	7.0	100 f	-
<i>p</i> -xylene	surface water	1100	10 b / medium	9.0	100 f	-
sum xylenes	surface water	1100		8.6		380
styrene ^c	surface water	3800	10 b / medium	9.1	1000 incompl.	570
phenol ^c	surface water	7000	ref. / high	100	ref.	-
<i>o</i> -cresol	surface water	29000	ref. / high	5700	QSAR / ref.	-
<i>m</i> -cresol	surface water	36000	ref. / high	5500	QSAR / ref.	-
<i>p</i> -cresol	surface water	1000	1 c / medium	2.0	1000 c	-
sum cresols	surface water	10000		400		-
catechol	surface water	630	10 a / low	0.77	1000 incompl.	-
resorcinol	surface water	5700	1 c / medium	42	1000 incompl.	-
hydroquinone	surface water	8200	ref. / high	410	ref.	-
sum dihydroxybenzenes	surface water	3100		24		-

* For the SRC_{eco} and the MPC the abbreviation ref. is used in case of refined risk assessment. QSAR (QSAR estimates) or the assessment factor together with the designation according to Table 2.1 and Table 2.5 is given in case of preliminary risk assessment. An incomplete base set is indicated by the abbreviation incompl.

- a MPC is derived from QSARs for narcosis, whereupon statistical extrapolation on these data is performed (Van de Plassche et al., 1993).
b MPC is harmonised with the air compartment; bold value indicates that no update of the MPC is proposed.
c For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

3.4 Proposals for SRC_{eco} for PAHs

For polycyclic aromatic hydrocarbons (PAHs) the data as presented by Kalf et al. (1995) are used to derive the SRC_{eco}. These data were used in the mentioned report to derive MPCs and the information on the ecotoxicity tests can be found there. Only for anthracene, benzo(a)anthracene and benzo(a)pyrene experimental terrestrial data are available and SRC_{eco} for soil are based on terrestrial experimental data. SRC_{eco} for soil for the other PAHs as well as SRC_{eco} for sediment for all PAHs are based on aquatic data and application of the EqP-method. For naphthalene and anthracene an European evaluation (EU commission regulation 1488/94) will be available on a short term.

Kalf et al. (1995) evaluated log K_{oc} values for soil and sediment and compared the experimental data with estimated values. Because of the large variation in experimental values it was decided to use estimated values using the regression equation proposed by DiToro et al. (1991) for extrapolation. In this report, log K_{oc} values are used that were derived in the framework of the project 'Intervention values for soil clean-up' (Otte et al., 2001). These log K_{oc} values are the average value of experimental values extended with one value calculated according to Sabljic et al. (1995). The proposals for the SRC_{eco} are included on the following pages and summarised in paragraph 3.4.11. The selected data used for extrapolation are included in Appendix 5.

3.4.1 SRC_{eco} for naphthalene

For naphthalene no terrestrial data are available. The HC50 for soil and sediment is therefore based on aquatic data to which the EqP-method is applied. The variance of the L(E)C50 data for fresh and marine water are significantly different (Table A5. 1 and Table A5. 2).

However, this is probably caused by the differences in taxonomic groups and geometric means are not significantly different ($P = 0.49$, Welch-corrected). Therefore, data for both fresh and marine water are combined. For the chronic data no significant differences were observed ($P = 0.21$). On the basis of the selected data an HC50(aquatic species) of $2.9 \cdot 10^2$ µg/l is derived from chronic as well as from acute data.

The MPC for naphthalene was derived by the modified EPA method (Kalf et al., 1995). An assessment factor of 100 was applied to the lowest L(E)C50 because data are available for algae, crustaceans (a.o. *Daphnia*) and fish. This resulted in an MPC of 1.2 µg/l. According to the EU/TGD method an assessment factor of 10 can be applied to the lowest NOEC because more than 3 NOECs are available, including the same taxonomic group as the lowest L(E)C50. This results in an MPC of 2.1 µg/l

The log K_p for standard soil and sediment is 1.76 resulting in an HC50 for soil and sediment of 17 mg/kg. Applying equilibrium partitioning to the MPC for surface water derived by the EU/TGD method gives an MPC for soil and sediment of 0.12 mg/kg.

3.4.2 SRC_{eco} for anthracene

For anthracene two L(E)C50s for plants are available, 150 mg/kg and 3600 mg/kg (Table A5. 3). From these data an HC50(terrestrial species) of 73 mg/kg is derived. According to both the modified EPA and the EU/TGD method an assessment factor of 1000 is applied to the lowest value in this case. The MPC derived from these terrestrial data is 0.15 mg/kg.

The median value of the aquatic NOEC data is 12 µg/l (Table A5. 4). However, applying an ACR of 10 to the median of the aquatic L(E)C50 data results in an HC50(aquatic species) of 1.4 µg/l.

Chronic toxicity are available for algae, crustaceans (*Daphnia*) and an acute toxicity study for fish. Because the chronic toxicity data for algae and crustaceans are comparable in effect concentration as the acute toxicity study with fish, a factor of 100 was applied to the lowest L(E)C50 according to the modified EPA method. The resulting MPC was 0.07 µg/l (Kalf et al., 1995). With the EU/TGD method, a similar reasoning can be used for the base set of toxicity data. Moreover, the requirement for a complete base set doesn't hold because anthracene has a log K_{ow} value higher than 3. With three NOECs but not for the same taxonomic group as the lowest acute data, the assessment factor applied to the lowest NOEC is 50. This results in an MPC of **0.034** µg/l.

The log K_p for standard soil and sediment is 3.06 resulting in an HC50(EqP) of 1.6 mg/kg. From comparison of the terrestrial toxicity data with the HC50(EqP) and from the aquatic toxicity data alone, it appears that macrophyta probably are a taxonomic group that is relatively insensitive to anthracene. Consequently, the HC50 for soil and sediment is equal to **1.6** mg/kg. With the MPC for 0.034 µg/l, an MPC for soil and sediment of **0.039** mg/kg is derived by equilibrium partitioning.

3.4.3 SRC_{eco} for phenanthrene

For phenanthrene no terrestrial data are available. The SRC_{eco} is therefore based on aquatic data and application of the EqP-method. The acute studies for fresh water and marine species (Table A5. 5 and Table A5. 6) are not significantly different ($P = 0.24$) and also the only chronic study for a marine species fits well into the overall log-normal distribution ($P = 65\%$). On the basis of the selected data HC50s of 94 and 30 µg/l are derived, on the basis of chronic and acute data respectively. The HC50(aquatic species) of **30** µg/l is used to derive an HC50(EqP).

The MPC for phenanthrene was derived using the modified EPA method (Kalf et al., 1995). Acute toxicity data are available for crustaceans (a.o. *Daphnia*) and fish but not for algae. The used assessment factor was 100 because it appeared from deviating tests that algae are not more sensitive. The resulting MPC was 0.3 µg/l. With the EU/TGD method an assessment factor of 10 can be applied to the lowest NOEC, because more than three NOECs are available also for the same taxonomic group as the lowest L(E)C50. The resulting MPC is **3.2** µg/l.

The log K_p for soil and sediment is 3.01, resulting in an HC50 for soil and sediment of **31** mg/kg. The MPC for soil and sediment is **3.3** mg/kg.

3.4.4 SRC_{eco} for fluoranthene

For fluoranthene no terrestrial data are available. The proposed SRC_{eco} is therefore based on aquatic data and application of the EqP-method. On the basis of the limited data for aquatic species (Table A5. 7 and Table A5. 8), HC50s of 49 and 30 µg/l are derived from chronic and acute data, respectively. The HC50(aquatic species) of **30** µg/l is used to derive an HC50(EqP).

The MPC for fluoranthene of 0.3 µg/l was derived with the modified EPA method by applying an assessment factor of 1000 to the lowest L(E)C50 (Kalf et al., 1995). According to the EU/TGD method the base set of acute toxicity data is not required if the compound has a log K_{ow} value higher than three. This is the case for fluoranthene. With two NOECs the applied assessment factor is 100. The resulting MPC is **0.12** µg/l.

The log K_p for soil and sediment is 3.93, resulting in an HC50 for soil and sediment of **2.6·10²** mg/kg. The MPC for soil and sediment calculated by equilibrium partitioning from the value of 0.12 µg/l is **1.0** mg/kg.

3.4.5 SRC_{eco} for benzo[a]anthracene

For benzo[a]anthracene one NOEC for an isopod is available, 2.5 mg/kg (Table A5. 9). The MPC derived from this study is 0.25 mg/kg according to the modified EPA method (Kalf et al., 1995). With the EU/TGD method an assessment factor of 100 is applied, resulting in an MPC of 0.025 mg/kg. Because these values are based on only one study, also an HC50 and MPC on the basis of the EqP-method are derived.

From one acute aquatic study (Table A5. 10) an HC50(aquatic species) of **1.0** µg/l is derived after application of an ACR of 10. The MPC derived from this study by means of the modified EPA method is **0.01** µg/l (Kalf et al., 1995). No MPC can be derived with the EU/TGD method because too few data are available.

The log K_p for soil and sediment is 4.69 resulting in an HC50(EqP) of 49 mg/kg. On the basis of this information an SRC_{eco} of **2.5** mg/kg is proposed for soil and **49** mg/kg for sediment. The MPC for soil is **0.025** mg/kg. With equilibrium partitioning an MPC for sediment of **0.49** mg/kg is calculated.

3.4.6 SRC_{eco} for chrysene

For chrysene no terrestrial and no aquatic data are available. The aquatic MPC was derived using QSARs and applying an extra safety factor of 10 (Kalf et al., 1995). The QSAR values used here are shown in Table A5. 11. The log K_{ow} used for these QSAR estimates is 5.81 (Otte et al., 2001). This value is slightly higher than that of 5.73 used by Kalf et al. (1995). For the aqueous solubility the value of 8.8 µg/l from Kalf et al. (1995) was used. If also for the solubility of chrysene the value of 1.8 µg/l from Otte et al. (2001) is chosen, only 5 QSAR estimates are remaining. On the basis of the 11 QSARs an HC50(aquatic species) of **1.2** µg/l is derived after application of a safety factor of 10 (90% CI: 0.8 – 2.0 µg/l). The MPC derived in this way is **0.28** µg/l (90% CI: 0.11 – 0.50 µg/l). Due to the limited scatter of the 11 QSAR data that are not higher than 10 times the maximum water solubility, the MPC is rather high compared to the HC50. The log K_p for soil and sediment is 4.46 resulting in an HC50 for soil and sediment of **35** mg/kg and an MPC of **8.1** mg/kg.

3.4.7 SRC_{eco} for benzo[k]fluoranthene

For benzo[k]fluoranthene no terrestrial data are available. The SRC_{eco} is therefore based on aquatic data and application of the EqP-method. On the basis of one NOEC for fish (Table A5. 12) an HC50(aquatic species) of 0.36 µg/l is derived. According to the modified EPA method the MPC derived from this value is 0.04 µg/l (Kalf et al., 1995). With the EU/TGD method this MPC is a factor of 10 lower: **0.0036** µg/l. The log K_p for soil and sediment is 5.02 resulting in an SRC_{eco} for soil and sediment of **38** mg/kg and an MPC of **0.38** mg/kg.

3.4.8 SRC_{eco} for benzo[a]pyrene

For benzo[a]pyrene four NOECs for terrestrial species are available (Table A5. 13). On the basis of these NOECs an HC50(terrestrial species) of 7.0 mg/kg is derived. The MPC of 0.26 was derived from these terrestrial data with the modified EPA method (Kalf et al., 1995). According to the EU/TGD an assessment factor of 50 is applied in this case. The resulting

MPC is **0.052** mg/kg. Because these values are based on two taxonomic groups only, also an HC50 and MPC on the basis of the EqP-method are derived.

One NOEC of 6.3 µg/l for a fish species is available (Table A5. 14). On the basis of three acute data an HC50(aquatic species) of 0.72 µg/l is derived. Data for algae, crustaceans (*Daphnia*) and fish (chronic study) are available. The MPC for benzo[*a*]pyrene of 0.05 µg/l was derived by the modified EPA method, using an assessment factor of 100 for the lowest L(E)C50 (Kalf et al., 1995). With one NOEC available according the EU/TGD method a comparison is made between the acute and chronic toxicity as well. The MPC of **0.0050** µg/l is calculated from the lowest L(E)C50 with an assessment factor of 1000.

The log K_p for soil and sediment is 4.59 resulting in an HC50(EqP) of 28 mg/kg and an MPC(EqP) of 0.19 mg/kg. On the basis of this information an HC50 of **7.0** mg/kg for soil and an HC50 of **28** mg/kg for sediment are derived. The MPC for soil is **0.052** mg/kg and the MPC for sediment **0.19** mg/kg.

3.4.9 SRC_{eco} for benzo[*ghi*]perylene

For benzo[*ghi*]perylene no terrestrial and no aquatic data are available. The aquatic MPC was derived using QSARs and applying an extra safety factor of 10 (Kalf et al., 1995). The QSAR values used here are shown in Table A5. 15. All data were calculated with a log K_{ow} value of 6.22 (Otte et al., 2001) instead of 6.63. Then, only three QSARs estimates remain, which are less than 10 times the maximum water solubility of 0.26 µg/l. If also for the solubility of benzo[*ghi*]perylene the value of 0.19 µg/l from Otte et al. (2001) is chosen, only 1 QSAR estimate is left.

On the basis of the QSARs and after application of a safety factor of 10 an HC50(aquatic species) of **0.18** µg/l is derived. Too few data are available for statistical extrapolation. Therefore, the MPC is derived by preliminary risk assessment. With the modified EPA method an assessment factor of 10 is applied leading to an MPC of 0.016 µg/l after application of an extra safety factor of 10 for the QSAR estimates. With the EU/TGD assessment factor of 50 this MPC is **0.0031** µg/l. The log K_p for soil and sediment is 5.26 resulting in an HC50 for soil and sediment of **33** mg/kg and an MPC of **0.57** mg/kg.

3.4.10 SRC_{eco} for indeno[*1,2,3-cd*]pyrene

For indeno[*1,2,3-cd*]pyrene no terrestrial and no aquatic data are available. The QSAR approach was not applied because all QSAR estimates are more than ten times the aqueous solubility (Kalf et al., 1995). With the higher log K_{ow} of 6.87 (Otte et al., 2001), 3 QSAR estimates (Table A5. 16) are within 10 times the maximum water solubility of 0.05 µg/l from Kalf et al. (1995). If the solubility of 1.5 µg/l (Otte et al., 2001) is used, this number of QSAR estimates is even 12. The derivation of the HC50 and the MPC is done in the same way as for benzo[*ghi*]perylene. For surface water, the HC50 and the MPC are **0.036** and **0.00061** µg/l, respectively. The log K_p for soil and sediment is 5.26 resulting in an SRC_{eco} for soil and sediment of **1.9** mg/kg and an MPC of **0.031** mg/kg.

3.4.11 Summary and comparison with old values and MPCs

In Table 3.7 the SRC_{eco} for PAHs in soil and sediment are summarised. Besides the values derived in the present report also the old values derived in Denneman and Van Gestel (1990) and the MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (Kalf et al., 1995) are presented. In Table 3.8 the SRC values for surface water are presented, which form the basis for the SRC for groundwater.

PAHs are compounds that may have both a natural or an anthropogenic source (Kalf et al., 1995). Nevertheless, background concentrations are assumed to be negligible when compared to the proposed $SRC_{S_{eco}}$. It should be noted that the old intervention value for PAHs of 40 mg/kg is a risk limit for the summed concentrations of the 10 PAHs. However, there is no scientific consensus whether the PAHs are concentration additive and whether they act by the same mode of action or not (Kalf et al. 1995). Some of the PAHs can have a strong photoinduced toxicity (see e.g. Mekenyan et al., 1994). Because of these uncertainties no sum value, nor a toxic unit approach are proposed for PAHs.

Nevertheless, in the framework of the intervention values a risk limit for soil and sediment for the sum of the 10 PAHs might be a useful alternative to the separate values for the single compounds. Except from anthracene, which shows somewhat higher toxicity, and the higher deviating value of fluoranthene, the derived $HC50s$ (aquatic species) seem to be related to their hydrophobicity, while the $HC50s$ for soil derived by equilibrium partitioning are less different and are not dependent on hydrophobicity (Figure 3.30). Also it cannot be excluded that due the limited number of toxicity studies the outliers are generated by chance.

The geometric mean of the $HC50s$ (soil) of the 7 PAHs for which experimental data are available, is 15 mg/kg. This value is about ten times the $HC50$ (soil) of anthracene, which has the lowest value. Because not all polycyclic aromatic hydrocarbons have the same molecular weight, this value can better be expressed in terms of moles instead of grams. The resulting value of the geometric mean of the $HC50$ for soil is 73 $\mu\text{mol}/\text{kg}$. For sediment the geometric mean of the $HC50$ is 27 mg/kg or $1.4 \cdot 10^2 \mu\text{mol}/\text{kg}$.

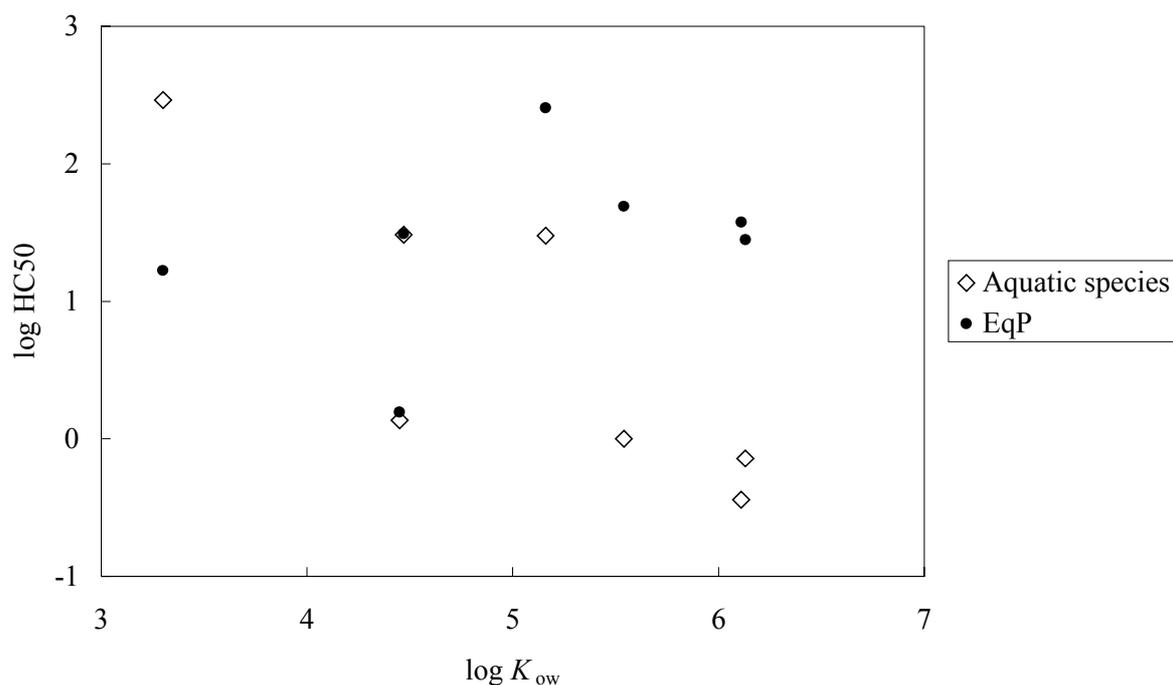


Figure 3.30: $HC50$ values for PAHs for aquatic species, derived from experimental data, and for soil, derived from equilibrium partitioning.

Table 3.7: Summary of new SRC_{eco} values for PAHs in soil or sediment, values as derived by Denneman and van Gestel (1990), MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report. Values are given as concentrations in mg/kg standard soil/sediment (soil containing 10% organic matter and 25% clay, sediment containing 10% organic matter and 25% clay).

Compound	Compartment	SRC _{eco} [mg/kg]	Method ^a / reliability score	Denneman and van Gestel (1990) [mg/kg]	MPC this report [mg/kg]	Method ^a	MPC INS [mg/kg]
sum PAHs	soil	-		40	-		-
naphthalene ^b	soil	17	EqP / low	30	0.12	EqP	0.14
	sediment	17	EqP / low	-	0.12	EqP	0.14
anthracene ^b	soil	1.6	EqP < 1 c sp. / medium	-	0.039	EqP < a sp.	0.12
	sediment	1.6	EqP / low	-	0.039	EqP	0.12
phenanthrene	soil	31	EqP / low	100	3.3	EqP	0.51
	sediment	31	EqP / low	-	3.3	EqP	0.51
fluoranthene	soil	260	EqP / low	-	1.0	EqP	2.6
	sediment	260	EqP / low	-	1.0	EqP	2.6
benzo[<i>a</i>]anthracene	soil	2.5	1 c sp. / medium	-	0.025	100 b sp.	0.25
	sediment	49	EqP / low	-	0.49	EqP	0.36
chrysene ^a	soil	35	EqP / -	-	8.1	EqP	10.7
	sediment	35	EqP / -	-	8.1	EqP	10.7
benzo[<i>k</i>]fluoranthene	soil	38	EqP / low	-	0.38	EqP	2.4
	sediment	38	EqP / low	-	0.38	EqP	2.4
benzo[<i>a</i>]pyrene	soil	7.0	1 c sp. / medium	-	0.052	50 h sp.	0.26
	sediment	28	EqP / low	-	0.19	EqP	2.7
benzo[<i>ghi</i>]perylene ^a	soil	33	EqP / -	-	0.57	EqP	7.5
	sediment	33	EqP / -	-	0.57	EqP	7.5
indeno[1,2,3- <i>cd</i>]pyrene ^a	soil	1.9	EqP / -	-	0.031	EqP	5.9
	sediment	1.9	EqP / -	-	0.031	EqP	5.9

* For the SRC_{eco} and the MPC, EqP (equilibrium partitioning) or the assessment factor together with the designation according to Table 2.1 and Table 2.6 is given. Whether the SRC_{eco} or the MPC is based on species or processes is indicated by the abbreviation sp. and pr.

a Derived from QSARs for aquatic species with equilibrium partitioning with a safety factor of 10.

b For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

Table 3.8: Summary of new SRC_{eco} values for PAHs in surface water, MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report.

Compound	Compartment	SRC_{eco} [$\mu\text{g/l}$]	Method / reliability score	MPC this report [$\mu\text{g/l}$]	Method	MPC INS [$\mu\text{g/l}$]
naphthalene ^b	surface water	290	10 b / 1 c / medium	2.1	10 h	1.2
anthracene ^b	surface water	1.4	10 b / medium	0.034	50 i	0.07
phenanthrene	surface water	30	10 b / medium	3.2	10 h	0.3
fluoranthene	surface water	30	10 b / medium	0.12	100 f	0.3
benzo[<i>a</i>]anthracene	surface water	1.0	10 a / low	0.010	1000 incompl.	0.01
chrysene ^a	surface water	1.2	QSAR/10 / -	0.28	QSAR/10 / ref.	0.34
benzo[<i>k</i>]fluoranthene	surface water	0.36	1 c / low	0.0036	100 d	0.04
benzo[<i>a</i>]pyrene	surface water	0.72	10 b / medium	0.0050	1000 c	0.05
benzo[<i>ghi</i>]perylene ^a	surface water	0.18	QSAR/10 / -	0.0031	QSAR/10 / 50 i	0.03
indeno[1,2,3- <i>cd</i>]pyrene ^a	surface water	0.036	QSAR/10 / -	0.00061	QSAR/10 / 50 i	0.04

* For the SRC_{eco} and the MPC, QSAR (QSAR estimates) or the assessment factor together with the designation according to Table 2.1 and Table 2.5 is given in case of preliminary risk assessment. An incomplete base set is indicated by the abbreviation incompl.

a Derived from QSARs with a safety factor of 10.

b For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

3.5 SRC_{eco} for halogenated aliphatic hydrocarbons

For chlorinated aliphatic hydrocarbons the data collected in the framework of the project 'Setting Integrated Environmental Quality Standards' have been used. The selected data used for extrapolation are included in Appendix 6. For trichloromethane (chloroform), trichloroethene, and tetrachloroethene an European evaluation (EU commission regulation 1488/94) will be available on a short term.

3.5.1 SRC_{eco} for 1,2-dichloroethane

Chronic toxicity data for aquatic species were found for seven taxonomic groups (bacteria, cyanophyta, algae, protozoa, annelids, crustaceans and fish; Table A6. 1 and Table A6. 2). The only value for marine species fits well in the overall log-normal distribution ($P = 62\%$). Therefore, both sets are combined and statistical extrapolation can be performed (Figure 3.31). The HC50 of this distribution is $1.3 \cdot 10^2$ mg/l (90% CI: $0.5 \cdot 10^2 - 3.2 \cdot 10^2$ mg/l). For comparison the acute toxicity data are added to this figure. The geometric mean of the combined sets of fresh and marine acute toxicity data ($P = 0.92$, after Welch-correction), which includes partly the same taxonomic groups, is slightly higher than the geometric mean of the chronic toxicity data: $1.8 \cdot 10^2$ mg/l. Although for this type of compounds that mainly act by narcosis the ACR will generally not be that large, the data for *Daphnia magna* differ between acute and chronic toxicity by almost a factor of 30.

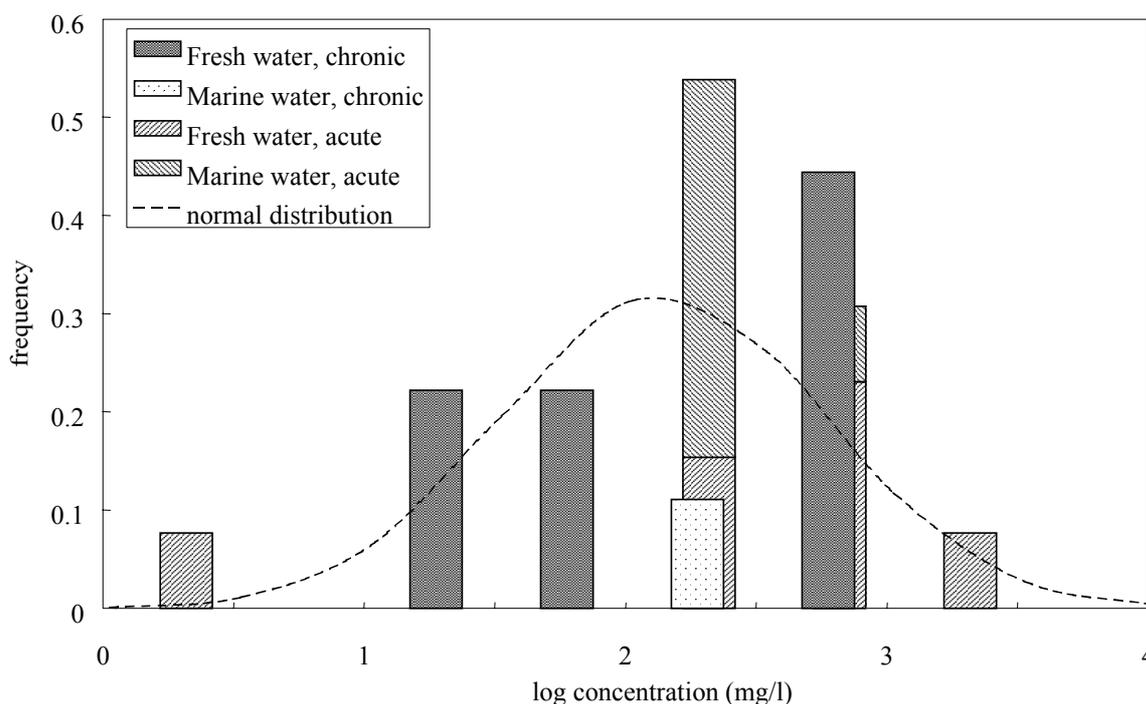


Figure 3.31: 1,2-Dichloroethane: Distribution of chronic and acute toxicity data for aquatic species. The estimated curve is based on the chronic toxicity data ($n = 9$, $\bar{x} = 2.12$, $s = 0.61$).

Because of the relatively high values for chronic toxicity, a comparison with QSAR estimates is made. A log K_{ow} value of 1.47 is used for 1,2-dichloroethane (Otte et al., 2001). The QSAR estimates are shown in Table A6. 3. The HC50 from the statistical extrapolation is $1.4 \cdot 10^2$ mg/l (90% CI: $0.8 \cdot 10^2 - 2.4 \cdot 10^2$ mg/l). This value is also slightly higher than that from the experimental data. The HC50 for surface water is also $1.3 \cdot 10^2$ mg/l.

The HC5 from the log-normal distribution of the chronic toxicity data is 11 mg/l (90% CI: 2 – 32 mg/l). The MPC of 14 mg/l was derived from QSARs for narcosis, to which statistical extrapolation was applied (Van de Plassche et al., 1993) However, after harmonisation with the air compartment, this MPC was adjusted downwards by a factor 20 to 0.70 mg/l. No terrestrial data are available for 1,2-dichloroethane. Therefore, the HC50(soil) is derived by equilibrium partitioning. The log K_p for soil and sediment is 0.26 resulting in an HC50 for soil and sediment of $2.4 \cdot 10^2$ mg/kg. Applying equilibrium partitioning to the MPC of 0.70 mg/l, gives an MPC for soil of **1.3** mg/kg.

3.5.2 SRC_{eco} for dichloromethane

For dichloromethane no chronic aquatic toxicity data are available. Therefore, the HC50 has to be based on the acute aquatic toxicity data (Table A6. 5 and Table A6. 6). One marine species fits well into the overall log-normal distribution and therefore (P = 45%), both data sets are combined. The geometric mean of these data is $4.0 \cdot 10^2$ mg/l. With an ACR of ten this leads to a HC50(aquatic species) of **40** mg/l. The MPC for dichloromethane of 20 mg/l was derived by QSARs for narcosis and statistical extrapolation (Van de Plassche et al., 1993), which is higher than the lowest L(E)C50. Acute toxicity data are available for algae, crustaceans (*Daphnia*) and fish. With the modified EPA method the MPC would be 0.18 mg/l, after application of a factor 100 to the lowest L(E)C50 value. According to the EU/TGD method a factor of 1000 is applied to the lowest L(E)C50 value if the base set is complete. This results in an MPC of **18** µg/l.

For dichloromethane also data for processes are available (Table A6. 4), which were not included in the derivation of the MPC. Although 5 NOECs for different processes are available, it is impossible to apply statistical extrapolation. All processes are from one study and have the same value. These data for terrestrial processes are not suitable to base the MPC upon. However, the HC50 terrestrial processes can be derived from these data. The proposed SRC_{eco} for soil is **3.9** mg/kg. The log K_p for soil and sediment is -0.01 resulting in an HC50 for sediment of **40** mg/kg. From the MPC for surface water an MPC in soil and sediment of **0.018** mg/kg can be derived in this way.

3.5.3 SRC_{eco} for trichloromethane (chloroform)

For trichloromethane no terrestrial data are available. For aquatic species, there are chronic toxicity data for 4 taxonomic groups (bacteria, cyanophyta, algae and crustaceans; Table A6. 7 and Table A6. 8). The study with the marine species fits well in the overall log-normal distribution (P = 73%) and both sets are combined. The HC50 of this distribution is 99 mg/l (90% CI: 34 – 283 mg/l). However, compared to the acute toxicity data these taxonomic groups are rather insensitive (Figure 3.32). The geometric mean of the acute toxicity data is 99 mg/l too. Further, the data for *Daphnia magna* show that there is a substantial difference between acute and chronic toxicity, with an ACR of more than 7. The acute toxicity data are represented by algae, crustaceans and fish.

Therefore, a comparison is made with QSAR estimates, which are presented in Table A6. 9. For the calculations a log K_{ow} value of 1.97 is used (Otte et al., 2001). The HC50 from these QSAR estimates is slightly lower than that of the experimental data: 63 mg/l (90% CI: 36 – 110 mg/l). For surface water this value of **63** mg/l is proposed as SRC_{eco}.

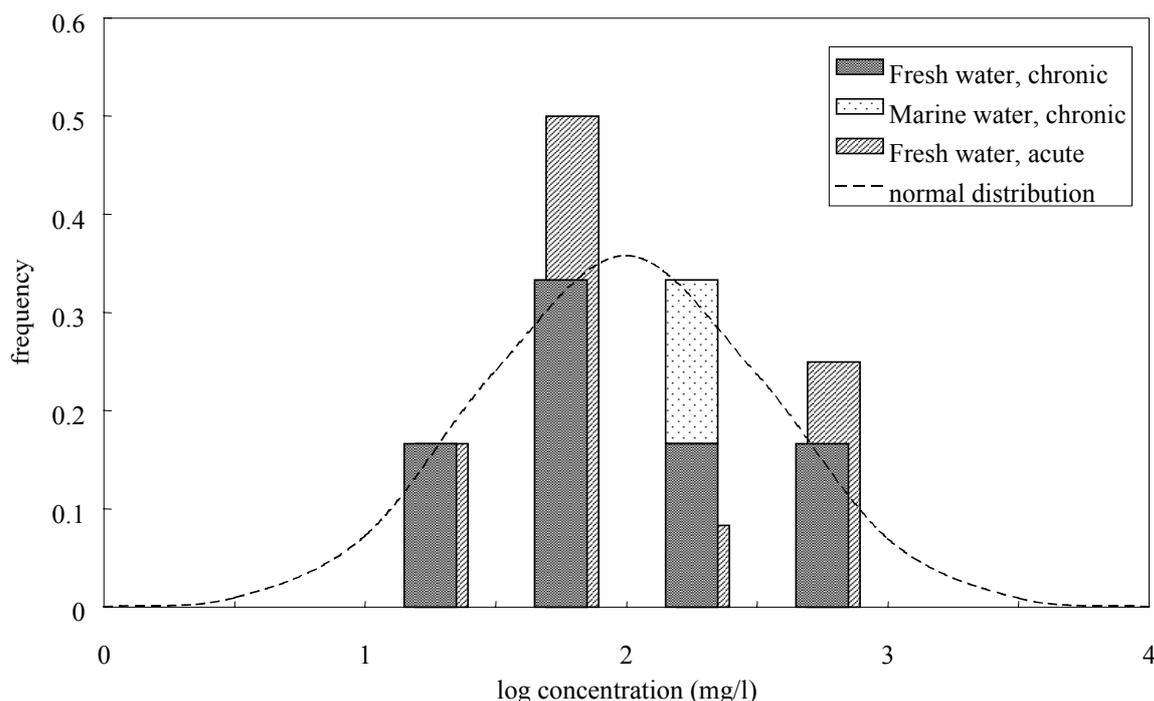


Figure 3.32: Trichloromethane: Distribution of chronic and acute toxicity data for aquatic species. The estimated curve is based on the chronic toxicity data ($n = 6$, $\bar{x} = 1.99$, $s = 0.56$).

The MPC of 5.9 mg/l for trichloromethane was derived from chronic QSARs for narcosis to which statistical extrapolation was applied (Van de Plassche et al., 1993). This MPC was adjusted by a factor 10 to 0.59 mg/l after harmonisation with the air compartment. The HC5 from the log-normal distribution of the chronic toxicity data is 10 mg/l (90% CI: 1 – 32 mg/l). The log K_p for soil and sediment is 0.43 resulting in an HC50 for soil and sediment of $1.7 \cdot 10^2$ mg/kg. With an MPC for surface water of 0.59 mg/l, the MPC for soil and sediment derived by equilibrium partitioning is 1.6 mg/kg.

3.5.4 SRC_{eco} for tetrachloromethane

The only data available for tetrachloromethane are for two marine species (Table A6. 10). The geometric mean of these data is 87 mg/l. With an ACR of ten this leads to a HC50 (aquatic species) of 8.7 mg/l. The MPC for dichloromethane of 1.1 mg/l was derived by QSARs for narcosis and statistical extrapolation (Van de Plassche et al., 1993). The modified EPA method results in a value of 50 µg/l. No MPC can be derived according to the EU/TGD method, because the base set is not complete. The log K_p for soil and sediment is 0.52 resulting in an HC50 for soil and sediment of 29 mg/kg. The MPC for soil and sediment is 0.17 mg/kg.

3.5.5 SRC_{eco} for vinylchloride (chloroethene)

For vinylchloride no terrestrial and no aquatic data are available. The aquatic MPC is derived using QSARs (Van de Plassche et al., 1993). No safety factor was applied to these estimates. However, the MPCs for water, soil and sediment were adjusted downwards by a factor 10 after harmonisation with air.

These QSAR values used are shown in Table A6. 11. The log K_{ow} value used for the calculations was 1.52 (Van de Plassche et al., 1993; Otte et al., 2001). On the basis of

statistical extrapolation an HC50(aquatic species) of 8.0 mg/l and an HC5(aquatic species) of 0.84 mg/l are derived from these QSARs, after application of a safety factor of 10 for the use of QSAR estimates or for harmonisation. The log K_p for soil and sediment is 0.33, resulting in an HC50 for soil and sediment of **17 mg/kg** and an MPC of **1.8 mg/kg**. These values should be regarded as unreliable because vinylchloride probably is a reactive chemical and the QSAR estimates are solely derived for narcotic chemicals.

3.5.6 SRC_{eco} for trichloroethene (trichloroethylene)

For trichloroethene the same motivation can be used to derive the HC50 for aquatic species as for 1,2-dichloromethane and trichloromethane. Chronic toxicity data are available for 6 taxonomic groups of aqueous species (bacteria, cyanophyta, algae, protozoa and crustaceans; Table A6. 13 and annelids; Table A6. 14). The only study with a marine species fits well in the overall log-normal distribution ($P = 33\%$) and therefore both sets are combined. The HC50 from this distribution is 50 mg/l (90% CI: 13 – 193 mg/l).

Again, compared to the acute toxicity data these taxonomic groups are rather insensitive (Figure 3.33). The geometric mean of the extensive set of acute toxicity data is almost equal: 51 mg/l. Further, the data for *Jordonella floridae* and *Ophryotrocha labronica* show that there are differences between acute and chronic toxicity, with ACRs of 5 and 10, respectively. The acute toxicity data are represented by 9 taxonomic groups.

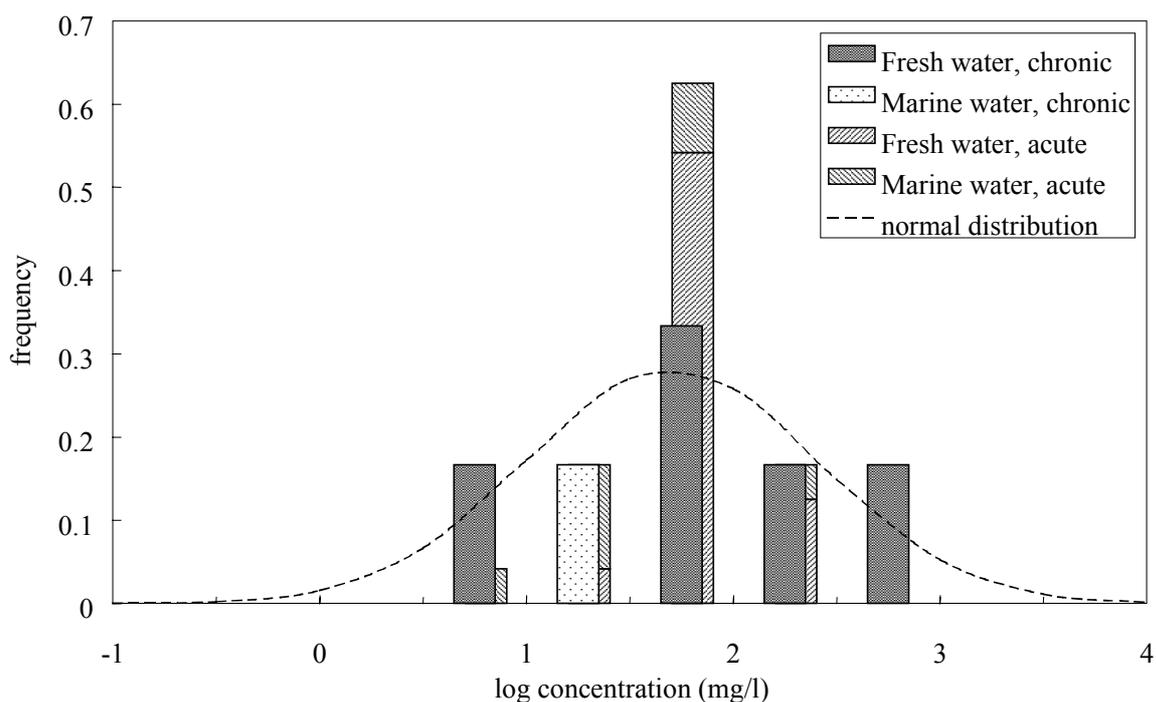


Figure 3.33: Trichloroethene: Distribution of chronic and acute toxicity data for aquatic species. The estimated curve is based on the chronic toxicity data ($n = 6$, $\bar{x} = 1.70$, $s = 1.71$).

Also in this case a comparison with QSAR estimates is made. The QSAR data are tabulated in Table A6. 15. For the calculation of the QSAR data a log K_{ow} value of 2.61 was used (Otte et al., 2001). The HC50 derived from these QSARs is **20 mg/l** (90% CI: 11 – 36 mg/l). This value is proposed as SRC_{eco} for surface water.

The MPC of 2.4 mg/l for trichloroethene was derived from chronic QSARs for narcosis to which statistical extrapolation was applied (Van de Plassche et al., 1993). With the same set of QSARs but a different log K_{ow} value, an HC5 of **1.6 mg/l** (90% CI: 0.5 – 3.4 mg/l) was

derived. The HC5 from the log-normal distribution of the chronic toxicity data is 2.9 mg/l (90% CI: 0.1 – 12.1 mg/l).

For trichloroethene data for processes are available too (Table A6. 12), which were not included in the derivation of the MPC. Although 5 NOECs for different processes are available, it is impossible to apply statistical extrapolation, because 4 processes are from one study and have the same value. These data for terrestrial processes are suitable to base the HC50 for soil upon. The proposed SRC_{eco} for soil is **2.5** mg/kg. The log K_p for soil and sediment is 0.83 resulting in an HC50 for sediment of **1.3·10²** mg/kg. Applying equilibrium partitioning to the MPC value of 1.6 mg/l for surface water gives an MPC for sediment and soil of **11** mg/kg. From these data it is obvious that the MPC derived by equilibrium partitioning is too high for soil, because all NOECs for the reported enzymatic activities are exceeded.

3.5.7 SRC_{eco} for tetrachloroethene (tetrachloroethylene)

The geometric mean of the chronic toxicity data for tetrachloroethene is 1.0 mg/l (Table A6. 17). Acute toxicity data for aquatic species are available for fresh water as well as marine species (Table A6. 17 and Table A6. 18). The acute toxicity data for fresh water and marine species are not significantly different ($P = 0.49$). The geometric mean of the combined sets is 15 mg/l. Therefore, the HC50(aquatic species) is based on the chronic data: **1.0** mg/l. The MPC of 0.33 mg/l for water was derived from QSARs and application of the statistical extrapolation method (Van de Plassche et al., 1993). The modified EPA method results in a value of 3.5 µg/l by applying a factor of 1000 to the lowest L(E)C50. No MPC can be derived according to the EU/TGD method, because the base set is not complete (no data for algae). The log K_p for soil and sediment is 1.19 resulting in an HC50(EqP) for soil and sediment of 16 mg/kg. The only study with terrestrial species (Table A6. 16) presents an L(E)C50 of 160 mg/kg, resulting in the same value for the HC50. Consequently, the HC50s for soil and sediment are **16** mg/kg. The terrestrial processes given by Van de Plassche et al. (1993) are in the same range as this HC50 (3.9 - >39). If equilibrium partitioning is applied to the MPC derived with the modified EPA method, an MPC for soil and sediment of **0.050** mg/kg is obtained. This value is lower than the MPC derived from the terrestrial toxicity study. According to the modified EPA method as well as the EU/TGD method an assessment factor of 1000 is applied resulting in an MPC(direct) of 0.16 mg/kg.

3.5.8 Summary and comparison with old values and MPCs

In Table 3.9 the SRC_{eco} for halogenated aliphatic hydrocarbons are summarised. Also included in this table are the old values derived in Denneman and Van Gestel (1990), the MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (Van de Plassche and Bockting, 1993) and the MPCs based on the same experimental data that were used for the SRC_{eco}.

The ERLs for water are presented in Table 3.10. For 3 compounds chronic aquatic toxicity data were available for 4 or more taxonomic groups. However, just as in the case of the non-halogenated monocyclic aromatic hydrocarbons the groups bacteria, cyanophyta, protozoa and algae were predominant in the distribution. Again, these groups appeared rather insensitive, compared with the acute toxicity data. Also for these compounds a comparison with QSAR estimates was made.

It should be noted that some of the MPCs that were derived from QSARs are close to the SRC_{eco} that were derived from experimental data. The MPCs derived with preliminary risk

assessment from the experimental data are generally much lower. The equilibrium concentrations in air of these MPCs for surface water are also closer to the tentative MPC for the air compartment.

The values as proposed by Denneman and van Gestel (1990) concern tetrachloroethene and the sum of chlorinated aliphatic hydrocarbons. No sum value is proposed here, because of possible differences in BSAF values and in mode of toxic action. For the derivation of the MPCs, Van de Plassche et al. (1993) assumed that these compounds mainly act by narcosis and therefore a QSAR approach was used.

Assuming the same mode of toxic action and similar BSAF values for these compounds, an SRC_{eco} for the sum of chlorinated aliphatic hydrocarbons could be derived. By taking the geometric mean of the HC50 values derived from experimental data, the proposed SRC_{eco} for the sum of chlorinated aliphatic hydrocarbons would be 25 mg/kg in standard soil. This value is very close to old value proposed by Denneman and van Gestel (1990). For sediment this value would be 85 mg/kg. Because different chlorinated aliphatic hydrocarbons have not the same molecular weight, these values are preferably expressed on a molar basis. The SRC_{eco} for the sum of these compounds would be $2.1 \cdot 10^2 \mu\text{mol/kg}$ for soil and $7.0 \cdot 10^2 \mu\text{mol/kg}$ for sediment.

Table 3.9: Summary of new SRC_{eco} values for halogenated aliphatic hydrocarbons in soil or sediment, values as derived by Denneman and van Gestel (1990), MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report. Values are given as concentrations in mg/kg standard soil/sediment (soil containing 10% organic matter and 25% clay, sediment containing 10% organic matter and 25% clay).

Compound	Compartment	SRC _{eco} [mg/kg]	Method* / reliability score	Denneman and van Gestel (1990) [mg/kg]	MPC this report [mg/kg]	Method*	MPC ^a INS [mg/kg]
sum chlorinated aliphatic hydrocarbons	soil	-		30	-		-
1,2-dichloroethane	sediment	240	EqP / medium	-	20	EqP	1.5^c
dichloromethane	soil	240	EqP / medium	-	20	EqP	1.5^c
	sediment	3.9	1 c pr. / medium	-	0.018	EqP<h pr.	36
trichloromethane ^e	soil	40	EqP / low	-	0.018	EqP	36
	sediment	170	EqP / medium	-	28	EqP	1.9^c
tetrachloromethane	soil	170	EqP / medium	-	28	EqP	1.9^c
	sediment	29	EqP / low	-	0.17	EqP	37
vinyl chloride ^d	soil	29	EqP / low	-	0.17	EqP	37
	sediment	17	EqP / -	-	1.8	EqP	1.4^c
trichloroethene ^e	soil	17	EqP / -	-	1.8	EqP	1.4^c
	sediment	2.5	1 c pr. / medium	-	0.0078	50 h pr.	13
tetrachloroethene ^e	soil	130	EqP / medium	-	11	EqP	13
	sediment	16	EqP=10 a sp. / medium	15	0.054	EqP<a sp.	0.16 ^b
	sediment	16	EqP / low	-	0.054	EqP	4.0

* For the SRC_{eco} and the MPC, EqP (equilibrium partitioning) or the assessment factor together with the designation according to Table 2.1 and Table 2.6 is given. Whether the SRC_{eco} or the MPC is based on species or processes is indicated by the abbreviation sp. and pr.

- MPCs for water are derived from QSARs for narcosis, whereupon statistical extrapolation on these data is performed (Van de Plassche et al., 1993). The MPCs for soil are derived from these values with equilibrium partitioning and comparison with soil toxicity data and harmonisation with the air compartment (Van de Plassche and Bocking, 1993).
- From experimental terrestrial data
- Adjusted downwards after harmonisation with the air compartment; bold value indicates that no update of the MPC is proposed.
- Derived from QSARs for aquatic species with equilibrium partitioning and a safety factor of 10.
- For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

Table 3.10: Summary of new SRC_{eco} values for halogenated aliphatic hydrocarbons in surface water, MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report.

Compound	Compartment	SRC _{eco} [µg/l]	Method* / reliability score	MPC this report [µg/l]	Method*	MPC ^a INS [µg/l]
1,2-dichloroethane	surface water	130000	ref. / high	11000	ref.	700^b
dichloromethane	surface water	40000	10 a / low	18	1000 a	20000
trichloromethane ^d	surface water	63000	QSAR / high	6000	QSAR / ref.	590^b
tetrachloromethane	surface water	8700	10 a / low	50	1000 incompl.	1100
vinyl chloride ^c	surface water	8000	QSAR/10 / -	840	QSAR/10 / ref.	840 ^b
trichloroethene ^d	surface water	20000	QSAR / high	1600	QSAR / ref.	2400
tetrachloroethene ^d	surface water	1000	1 c / medium	3.5	1000 incompl.	330

* For the SRC_{eco} and the MPC the abbreviation ref. is used in case of refined risk assessment. The assessment factor together with the designation according to Table 2.1 and Table 2.5 is given in case of preliminary risk assessment. An incomplete base set is indicated by the abbreviation incompl.

- a MPCs for water are derived from QSARs for narcosis, whereupon statistical extrapolation on these data is performed (Van de Plassche et al., 1993). The MPCs for soil are derived from these values with equilibrium partitioning and comparison with soil toxicity data and harmonisation with the air compartment (Van de Plassche and Bocking, 1993).
- b Adjusted downwards after harmonisation with the air compartment; bold value indicates that no update of the MPC is proposed.
- c Derived from QSARs with a safety factor of 10.
- d For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

3.6 SRC_{eco} for halogenated aromatic hydrocarbons

The following chlorinated aromatic hydrocarbons were considered and discussed below: chlorobenzenes (each isomer separately), chlorophenols (each isomer separately), polychlorinated biphenyl (limited data on some of the isomers) and monochloronaphthalene (2 isomers). The selected data used for extrapolation are included in Appendix 7.

3.6.1 SRC_{eco} for chlorobenzenes

All data for chlorobenzenes were collected in the framework of the project 'Setting Integrated Environmental Quality Standards' (Hesse et al., 1991). For 1,4-dichlorobenzene and 1,2,4-trichlorobenzene an European evaluation (EU commission regulation 1488/94) will be available on a short term.

3.6.1.1 SRC_{eco} for monochlorobenzene

For monochlorobenzene toxicity data are available for fresh water and marine species (Table A7. 1 and Table A7. 2). The chronic toxicity data for fresh water and marine species are not significantly different ($P = 0.12$). The geometric mean of the combined sets is 6.2 mg/l. The only acute toxicity study for a marine species is at the end of the 90% confidence interval of the overall log-normal distribution ($P = 94\%$). The geometric mean of the combined acute toxicity data is 11 mg/l. Applying an ACR of 10 to this geometric mean gives an HC50(aquatic species) of 1.1 mg/l.

The MPC of monochlorobenzene for surface water was derived from QSARs and statistical extrapolation (Van de Plassche et al., 1993). This MPC is 0.69 mg/l. Because chronic and acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish, a safety factor of 10 can be applied to lowest NOEC according to the modified EPA method as well as the EU/TGD method. The MPC derived in this way is 32 µg/l.

No terrestrial data are available for monochlorobenzene. Therefore, the HC50 has to be derived by equilibrium partitioning. The log K_p for standard soil and sediment is 1.11, resulting in an HC50 for soil and sediment of 15 mg/kg and an MPC of 0.41 mg/kg.

3.6.1.2 SRC_{eco} for 1,2-dichlorobenzene

Toxicity data of 1,2-dichlorobenzene are available for fresh water and marine species (Table A7. 3 and Table A7. 4). The only NOEC for fresh water species deviates from the rest of the aquatic data and has a low probability density ($P = 1.2\%$). However, this study is performed with crustaceans while the rest of the data are mainly for algae. Therefore, the data are combined and the geometric mean of the chronic toxicity data is 4.5 mg/l. The acute toxicity data are not significantly different ($P = 0.28$, Welch-corrected). The geometric mean of the acute toxicity data is almost equal to that of the chronic toxicity data: 7.4 mg/l. Applying an ACR of 10 to the geometric mean of the acute toxicity data gives an HC50(aquatic species) of 0.74 mg/l.

The MPC of 1,2-dichlorobenzene for surface water was derived from QSARs and statistical extrapolation (Van de Plassche et al., 1993). This MPC is 0.27 mg/l. The final MPC of 0.25 mg/l is an average for the three dichlorobenzene isomers. Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. According to the modified EPA method a safety factor of 100 can be applied to lowest L(E)C50 resulting in an MPC of 12 µg/l. Because more than 3 NOECs are available and the lowest NOEC as well as L(E)C50 are for *Daphnia magna*, a safety factor of 10 is applied to the lowest NOEC, according to the EU/TGD method. The MPC derived in this way is 31 µg/l.

No terrestrial data are available for 1,2-dichlorobenzene. Therefore, the HC50 has to be derived by equilibrium partitioning. The log K_p for standard soil and sediment is 1.37, resulting in an HC50 for soil and sediment of **17 mg/kg** and an MPC of **0.73 mg/kg**.

3.6.1.3 SRC_{eco} for 1,3-dichlorobenzene

For 1,3-dichlorobenzene 2 chronic NOECs are available for fresh water species (Table A7. 5). The geometric mean of these data is $8.2 \cdot 10^2$ µg/l. The only acute toxicity study with a marine species (Table A7. 6) fits well in the overall log-normal distribution (P = 41%). The geometric mean of the acute toxicity data is 9.5 mg/l. The HC50(aquatic species) is thus determined by the chronic toxicity data.

The MPC of 1,3-dichlorobenzene for surface water was derived from QSARs and statistical extrapolation (Van de Plassche et al., 1993). The MPC is 0.21 mg/l. The final MPC of 0.25 mg/l is an average for the three dichlorobenzene isomers. According to the modified EPA method a safety factor of 100 can be applied to lowest L(E)C50, because acute toxicity data are available for algae, crustaceans and fish. The MPC derived in this way would be 33 µg/l. With the EU/TGD method an assessment factor of 50 is applied to the lowest of two NOECs, because both the lowest NOEC and the lowest L(E)C50 are for *Daphnia magna*. The resulting MPC is **14 µg/l**.

No terrestrial data are available for 1,3-dichlorobenzene. Therefore, the HC50 has to be derived by equilibrium partitioning. The log K_p for standard soil and sediment is 1.46, resulting in an HC50 for soil and sediment of **24 mg/kg** and an MPC of **0.39 mg/kg**.

3.6.1.4 SRC_{eco} for 1,4-dichlorobenzene

For 1,4-dichlorobenzene 3 chronic NOECs are available for fresh water species (Table A7. 8). The geometric mean of these data is $4.6 \cdot 10^2$ µg/l. Fresh water and marine species (Table A7. 9) do not differ significantly in sensitivity in acute toxicity studies (P = 0.11). The geometric mean of the acute toxicity data is 7.1 mg/l. The HC50(aquatic species) is determined by the chronic toxicity data.

The MPC of 1,4-dichlorobenzene for surface water was derived from QSARs and statistical extrapolation (Van de Plassche et al., 1993). The MPC is 0.26 mg/l. The final MPC of 0.25 mg/l is an average for the three dichlorobenzene isomers. Because chronic and acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish, a safety factor of 10 can be applied to lowest NOEC according to both the modified EPA method and the EU/TGD method. The MPC derived in this way is **30 µg/l**.

Some terrestrial toxicity data are available for 1,4-dichlorobenzene (Table A7. 7). Additional data in the original report (Hesse et al., 1991) show LC50 values of 390 for two species of earthworms in a soil with approximately 10% organic matter. However, the geometric mean of the acute toxicity data still remains higher than 500 mg/kg. Therefore, the HC50(terrestrial species) is determined by the chronic NOEC of 50 mg/kg. According to the modified EPA method and the EU/TGD method, a factor of 1000 is applied to the lowest L(E)C50 resulting in an MPC(terrestrial species) of 0.39 mg/kg.

Because of the limited amount of terrestrial species a comparison with equilibrium partitioning is made. The log K_p for standard soil and sediment is 1.59, resulting in an HC50 for soil and sediment of 18 mg/kg and an MPC of 1.2 mg/kg. The MPC derived directly from terrestrial toxicity data is lower than the value derived by equilibrium partitioning. Thus the proposed SRC_{eco} for soil and sediment is **18 mg/kg**. The MPC for soil is **0.39 mg/kg** and for sediment **1.2 mg/kg**.

3.6.1.5 SRC_{eco} for 1,2,3-trichlorobenzene

For 1,2,3-trichlorobenzene chronic and acute toxicity data are available for fresh water species (Table A7. 11), and for marine species one acute toxicity study (Table A7. 12), which fits well in the overall log-normal distribution (P = 58%). The geometric mean of the chronic toxicity data is $1.0 \cdot 10^2$ µg/l and that of the acute toxicity data is 2.1 mg/l. The HC50(aquatic species) is consequently determined by the chronic toxicity data.

The MPC of 1,2,3-trichlorobenzene for surface water was derived from QSARs and statistical extrapolation (Van de Plassche et al., 1993). The MPC is 64 µg/l. The final MPC of 67 µg/l is an average for the three trichlorobenzene isomers. The lowest of three NOECs is 40 µg/l.

According to the modified EPA method as well as the EU/TGD method an assessment factor of 10 can be applied to lowest NOEC, because chronic and acute toxicity data are available for algae, crustaceans (*Daphnia*) and fish. The MPC derived in this way is **4.0** µg/l.

Acute and chronic toxicity data are available for terrestrial species (Table A7. 10). The geometric mean of the acute toxicity data is 98 mg/kg. The HC50(terrestrial species) is determined by the chronic NOEC of 5 mg/kg. According to the modified EPA method and the EU/TGD method, a factor of 1000 is applied to the lowest L(E)C50 after comparison with the chronic NOEC. This MPC derived directly from the acute terrestrial toxicity data is 0.010 mg/kg.

This value is compared with equilibrium partitioning. The log K_p for standard soil and sediment is 2.00, resulting in an HC50(EqP) of 10 mg/kg. The HC50(soil) is therefore **5.0** mg/kg, which is directly derived from the terrestrial toxicity data and the HC50(sediment) is **10** mg/kg. The MPC(EqP) is 0.40 mg/kg. The value from the terrestrial data is lower than the value derived by equilibrium partitioning due to the application of safety factor of 1000.

Therefore, the MPC for soil is **0.010** mg/kg and the MPC for sediment **0.40** mg/kg.

3.6.1.6 SRC_{eco} for 1,2,4-trichlorobenzene

Acute toxicity data of 1,2,4-trichlorobenzene are available for fresh water and marine species and chronic toxicity data for fresh water species only (Table A7. 14 and Table A7. 15). The acute toxicity data for both sets are very similar (P = 0.91, Welch-corrected). The geometric mean of the chronic toxicity data is **46** µg/l and that of the acute toxicity data is 3.4 mg/l. The HC50(aquatic species) is also determined by the chronic toxicity data.

The MPC of 1,2,4-trichlorobenzene for surface water was derived from QSARs and statistical extrapolation (Van de Plassche et al., 1993). The MPC is 79 µg/l. The final MPC of 67 µg/l is an average for the three trichlorobenzene isomers. According to the modified EPA method and the EU/TGD method an assessment factor of 10 can be applied to lowest NOEC of 1 µg/l, because chronic and acute toxicity data are available for algae, crustaceans (*Daphnia*) and fish. The MPC derived in this way is **0.10** µg/l.

Acute and chronic toxicity data are available for terrestrial species (Table A7. 13). The geometric mean of the acute toxicity data is 190 mg/kg. The only chronic NOEC has a value of 50 mg/kg. Application of an ACR of 10 to the mean of the acute toxicity data gives the HC50(terrestrial species) of 19 mg/kg. This value is compared with equilibrium partitioning. According to the modified EPA method and the EU/TGD method, a factor of 1000 is applied to the lowest L(E)C50 after comparison with the chronic NOEC. The resulting MPC derived directly from the acute terrestrial toxicity data is 0.13 mg/kg

The log K_p for standard soil and sediment is 2.05, resulting in an HC50(EqP) for of 5.1 mg/kg. The SRC_{eco} for soil and sediment is therefore **5.1** mg/kg. Also the MPC for soil and sediment derived by equilibrium partitioning of **0.011** mg/kg is lower than the value derived directly from the acute terrestrial toxicity data.

3.6.1.7 SRC_{eco} for 1,3,5-trichlorobenzene

For 1,3,5-trichlorobenzene two L(E)C50s for fresh water species (Table A7. 17) and one chronic study for a marine species (Table A7. 18) are available. The HC50(aquatic species) of **31** µg/l is equal to the geometric mean of these data of $3.1 \cdot 10^2$ µg/l with an ACR of 10. The MPC of 1,3,5-trichlorobenzene for surface water was derived from QSARs and statistical extrapolation (Van de Plassche et al., 1993). The MPC is 57 µg/l. The final MPC of 67 µg/l is an average for the three trichlorobenzene isomers. According to the modified EPA method an MPC of 3.3 µg/l is derived by applying a factor of 1000 to the lowest L(E)C50. Although the base set is incomplete, an MPC can be derived according to the EU/TGD method too, because 1,3,5-trichlorobenzene has a log K_{ow} value higher than 3. The resulting MPC is also **3.3** µg/l. Terrestrial data are available for a macrophyt (Table A7. 16). The NOEC of 50 mg/kg is more than 10 times as low as the L(E)C50 value of 620 mg/kg and is consequently chosen as the HC50(terrestrial species). This value is compared with equilibrium partitioning. The log K_p for standard soil and sediment is 2.75, resulting in an HC50(EqP) of $1.7 \cdot 10^2$ mg/kg. The HC50 for sediment is therefore **$1.7 \cdot 10^2$** mg/kg and for soil **50** mg/kg. The MPC for soil and sediment derived by equilibrium partitioning and is 1.9 mg/kg. With the modified EPA method, an assessment factor of 1000 is applied to the lowest L(E)C50, after comparison with the chronic toxicity data, resulting in an MPC of 0.62 mg/kg. With the EU/TGD method, a factor of 100 is applied to the lowest NOEC after comparison with the acute toxicity data. This MPC is 0.50 mg/kg. Therefore, the MPC for soil is **0.50** mg/kg and the MPC for sediment **1.9** mg/kg.

3.6.1.8 SRC_{eco} for 1,2,3,4-tetrachlorobenzene

For 1,2,3,4-tetrachlorobenzene 2 NOECs and 3 L(E)C50s are available for fresh water species (Table A7. 20). The geometric mean of the chronic toxicity data is **83** µg/l and that of the acute toxicity data 2.1 mg/l. Therefore, HC50(aquatic species) is based on the chronic toxicity data. The MPC of 1,2,3,4-tetrachlorobenzene for surface water was derived from QSARs and statistical extrapolation (Van de Plassche et al., 1993). This MPC is 23 µg/l. The final MPC of 24 µg/l is an average for the three tetrachlorobenzene isomers. According to the modified EPA method an MPC of 1.1 µg/l is derived by applying a factor of 1000 to the lowest L(E)C50. Because 1,2,3,4-tetrachlorobenzene has a log K_{ow} value higher than 3, an MPC can be derived according to the EU/TGD method too. With 3 NOECs available, also for the same taxonomic group as the minimum LC50, an assessment factor of 10 is applied to the lowest NOEC. The resulting MPC is **2.3** µg/l.

Terrestrial data are available for a macrophyt (Table A7. 16), with a NOEC of 50 mg/kg and an L(E)C50 of 160 mg/kg. The HC50(terrestrial species) is derived by application of an ACR of 10 to the L(E)C50 and is 16 mg/kg. This value is compared with equilibrium partitioning. The log K_p for standard soil and sediment is 2.68, resulting in an HC50(EqP) for of 40 mg/kg. Consequently, the HC50 for soil is **16** mg/kg and for sediment **40** mg/kg. The MPC for soil derived directly from the terrestrial data is **0.16** mg/kg, both with the assessment factors of the EU/TGD and of the modified EPA method. The MPC for sediment is derived by equilibrium partitioning and is **1.1** mg/kg.

3.6.1.9 SRC_{eco} for 1,2,3,5-tetrachlorobenzene

Some acute toxicity data are available for 1,2,3,5-tetrachlorobenzene for fresh water species (Table A7. 22) and one for marine species (Table A7. 23). This value fits well into the overall log-normal distribution (P = 78%). The geometric mean of the combined data is 2.1 mg/l. Application of an ACR of 10 leads to the HC50(aquatic species) of **$2.1 \cdot 10^2$** µg/l. The MPC of 1,2,3,5-tetrachlorobenzene for surface water was derived from QSARs and statistical

extrapolation (Van de Plassche et al., 1993). This MPC is 22 µg/l. The final MPC of 24 µg/l is an average for the three tetrachlorobenzene isomers. According to the modified EPA method a safety factor of 100 can be applied because acute toxicity data are available for algae, crustaceans and fish. The resulting MPC is 8.0 µg/l. According to the EU/TGD method a factor of 1000 is applied to the lowest L(E)C50, resulting in an MPC of **0.80** µg/l. One terrestrial L(E)C50 of 6.5 mg/kg is available for a macrophyt (Table A7. 21). With an ACR of 10 the HC50(terrestrial species) is 0.65 mg/kg. This value is compared with equilibrium partitioning. The log K_p for standard soil and sediment is 2.34, resulting in an HC50(EqP) for of 47 mg/kg. The HC50 for soil is therefore **0.65** mg/kg and for sediment **47** mg/kg. The MPC for soil derived directly from the terrestrial data of **0.0065** mg/kg is very low due to the high assessment factor of 1000 with the modified EPA method as well as the EU/TGD method. The MPC for sediment derived by equilibrium partitioning is **0.17** mg/kg.

3.6.1.10 SRC_{eco} for 1,2,4,5-tetrachlorobenzene

Acute toxicity data and one chronic study are available for 1,2,4,5-tetrachlorobenzene (Table A7. 25 and Table A7. 26). The acute study for a marine fish species fits well into the overall log-normal distribution ($P = 44\%$). The geometric mean of the combined acute toxicity data is $9.4 \cdot 10^2$ µg/l. The only NOEC has a value of **90** µg/l, which value is taken as the HC50(aquatic species). The MPC of 1,2,4,5-tetrachlorobenzene for surface water was derived from QSARs and statistical extrapolation (Van de Plassche et al., 1993). The MPC is 26 µg/l. The final MPC of 24 µg/l is an average for the three tetrachlorobenzene isomers. According to the modified EPA method a safety factor of 1000 is applied to the lowest L(E)C50. The resulting MPC is 0.3 µg/l. Although the base set is not complete, an MPC is also derived with the EU/TGD method, because 1,2,4,5-tetrachlorobenzene has a log K_{ow} value higher than 3. One NOEC is available for the same taxonomic group as the minimum L(E)C50. Therefore, an assessment factor of 100 is applied to this NOEC, leading to an MPC of **0.90** µg/l. One acute terrestrial study is available (Table A7. 24) with an EC50 of 10 mg/kg. Application of an ACR of 10 yields the HC50(terrestrial species) of 1.0 mg/kg. This value is compared with equilibrium partitioning. The log K_p for standard soil and sediment is 2.54, resulting in an HC50(EqP) for of 31 mg/kg. The HC50 for soil is therefore **1.0** mg/kg and for sediment **31** mg/kg. The MPC for soil derived directly from the terrestrial data of **0.010** mg/kg is very low due to the high assessment factor of 1000. The MPC for sediment derived by equilibrium partitioning is **0.31** mg/kg.

3.6.1.11 SRC_{eco} for pentachlorobenzene

For pentachlorobenzene chronic and acute toxicity data are available for fresh water species (Table A7. 28) and one acute study for a marine species (Table A7. 29). The geometric mean of the NOECs is **32** µg/l. The only marine study fits well in the overall log-normal distribution ($P = 42\%$). The geometric mean of the combined sets of acute data is $7.1 \cdot 10^2$ µg/l. The geometric mean of the chronic toxicity data is thus taken as the HC50(aquatic species). The MPC of pentachlorobenzene for surface water is based on secondary poisoning for birds and mammals (Van de Plassche, 1994). This MPC is 0.030 µg/l, which is almost 100 times lower than the MPC according to the modified EPA method (2.5 µg/l) and 20 times lower than the MPC according to the EU/TGD method (0.62 µg/l). One terrestrial acute toxicity study with a macrophyt is available (Table A7. 27). An HC50(terrestrial species) of 28 mg/kg is obtained after application of an ACR of 10. This value is compared with equilibrium partitioning. The log K_p for standard soil and sediment is 2.69, resulting in an HC50(EqP) for of 16 mg/kg. The HC50 for soil and sediment is therefore **16** mg/kg. The MPC for soil derived directly from the terrestrial data is 0.28 mg/kg. The MPC

for soil is based on secondary poisoning and is equal to **0.12** mg/kg. The MPC for sediment of 0.012 mg/kg was derived by equilibrium partitioning from the MPC for surface water (Van de Plassche, 1994). With the log K_p used here, this value is **0.015** mg/kg.

3.6.1.12 SRC_{eco} for hexachlorobenzene

For hexachlorobenzene toxicity data are available for fresh water species (Table A7. 31). The geometric mean of the chronic toxicity data is 5.0 µg/l. The only suitable acute toxicity study provides an L(E)C50 of 30 µg/l. Application of an ACR of 10 leads to the HC50(aquatic species) of **3.0** µg/l. The MPC of hexachlorobenzene for surface water is based on secondary poisoning for birds and mammals (Van de Plassche, 1994). The MPC is **2.1·10⁻⁵** µg/l, which is more than 1000 times lower than the MPC according to the modified EPA method (0.30 µg/l; factor of 1000 to L(E)C50) or the EU/TGD method (0.36 µg/l; factor of 50 to lowest NOEC).

One terrestrial chronic toxicity study with a macrophyt is available (Table A7. 30), which leads to an HC50(terrestrial species) of 500 mg/kg. This value is compared with equilibrium partitioning. The log K_p for standard soil and sediment is 2.83, resulting in an HC50(EqP) of 2.0 mg/kg. The HC50 for soil and sediment is therefore **2.0** mg/kg. The MPC for soil based on secondary poisoning is 0.028 mg/kg. With the MPC for surface water derived by the EU/TGD method an MPC of **0.024** mg/kg is derived for soil by equilibrium partitioning. This value is lower than the MPC for secondary poisoning. The MPC for sediment of 0.0012 mg/kg was derived by equilibrium partitioning from the MPC for surface water (Van de Plassche, 1994). With the log K_p used here, this value is **1.4·10⁻³** mg/kg.

3.6.1.13 SRC_{eco} for the sum of chlorobenzenes

Probably, all chlorobenzenes mainly act by narcosis (Van de Plassche et al., 1993). Therefore, a geometric mean of the data can be selected for the sum of chlorobenzenes, provided that the different compounds concentrate into the organisms to the same extent. For the water compartment this assumption will only be valid for the isomers with the same degree of chlorination. Consequently, an HC50 value for water cannot be derived for the sum of all chlorobenzenes. Values for mono-, di-, tri-, tetra-, penta- and hexachlorobenzene are 1.1·10³, 6.5·10², 1.4·10², 1.2·10², 32 and 3.0 µg/l, respectively.

For the soil compartment average values for different compounds can be taken if the compounds are taken up by the organisms from the soil to the same extent (see section 2.5). Considering the uncertainty due to the limited number of toxicity studies, the differences in available data and the application of the equilibrium partitioning theory, it can be concluded that differences in the derived HC50s for soil and sediment are not very large.

The HC50-values for mono-, di-, tri-, tetra-, penta- and hexachlorobenzene are respectively 15, 19, 11, 2.2, 16 and 2.0 mg/kg for soil and 15, 19, 25, 39, 16 and 2.0 mg/kg for sediment. If equal BSAF values are assumed, the value for the sum of all chlorobenzenes might be derived by taking the geometric mean of the HC50s derived directly from terrestrial toxicity studies and indirectly by the equilibrium partitioning theory. The resulting values for the SRC_{eco} would be 15 mg/kg for soil and 20 mg/kg for sediment. Because the molecular weight is not the same for all chlorobenzenes, these values are preferably expressed on a molar basis. The SRC_{eco} would then be 73 and 1.1·10² µmol/kg.

The MPCs of single isomers are highly influenced by the safety factor that is applied and thus, by the available data. If however, a geometric mean is taken for the sum of all chlorobenzenes, derived in the same way as the HC50, the resulting MPCs would be 0.12 mg/kg for soil and 0.30 mg/kg for sediment, or on a molar basis 0.56 µmol/kg and 1.6 µmol/kg for soil and sediment, respectively.

Because the mode of toxic action is the same but no detailed information is available for the BSAF, the toxic unit approach is proposed for the sum of all chlorobenzenes in water, sediment and soil.

3.6.2 SRC_{eco} for chlorophenols

Most of the data for chlorophenols were collected in the framework of the project 'Setting Integrated Environmental Quality Standards'. Additional new data were collected and are included in the annex to this report. Data were used as they are reported. No correction was made for dissociation of the compounds at neutral pH. In doing so, it is assumed that the average pH in the laboratory tests is close to that in most of the natural soils, sediments or water. There are several reasons why the data are not corrected. First, in most of the cases the pH is not properly reported, and this would cause a great loss of data. Second, it is not clear to what extent the dissociated compounds do still contribute to the toxicity. Correcting the concentrations for the ionised part of the compound may result in an underestimation of the effect concentrations. For compounds such as chlorophenols the uptake of the ionised form is less than for the neutral form but not negligible (Van Wezel, 1998). Third, the shift of the values due to correction for the dissociated part are in most cases small compared to the large differences in sensitivity between different species. As can be seen from effect studies with fish (*P. reticulata*) the shift in toxicity between pH 5 and 8 is at most a factor of 25 for almost completely dissociated compounds but usually much less (Könemann and Musch, 1981; Saarikoski and Viluksela, 1981). Moreover, the median pH used in the toxicity experiments can be regarded as representative for the environmental situation. Therefore, the ERLs that are derived here apply to the total amount (i.e. neutral and ionised) of the compound in soil, sediment or water.

3.6.2.1 SRC_{eco} for 2-chlorophenol

For 2-chlorophenol acute as well as chronic aquatic toxicity data are available (Table A7. 33 and Table A7. 34). The geometric mean of the 2 chronic NOECs is **1.4** mg/l. The acute toxicity data for fresh water and marine species are not significantly different ($P = 0.20$). The geometric mean of the combined sets is 37 mg/l. Hence, the HC50(aquatic species) is determined by the geometric mean of the chronic toxicity data.

Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. With the modified EPA method an MPC of 50 µg/l is derived by applying a safety factor of 10 to the lowest NOEC. This value is slightly lower than the lowest L(E)C50 divided by 100. With the assessment factors of the EU/TGD a factor of 50 is applied to the lowest of 2 NOECs, because a NOEC is available for the taxonomic group of the lowest L(E)C50. The resulting MPC is **10** µg/l. The old MPC of 25 µg/l was a mean value for the sum of the three monochlorophenol isomers (Janus et al., 1991).

One terrestrial L(E)C50 is available for 2-chlorophenol (Table A7. 32). Applying an ACR of 10 to this value results in an HC50(terrestrial species) of 22 mg/kg. This value is compared with a value derived by equilibrium partitioning. The log K_p for standard soil and sediment is 0.74, resulting in an HC50(EqP) of 7.8 mg/kg. The SRC_{eco} for soil and sediment is therefore **7.8** mg/kg. Applying a factor of 1000 to the terrestrial L(E)C50 gives an MPC(terrestrial species) of 0.22 mg/kg. The old MPC for the sum of the three monochlorophenol in soil of 0.20 mg/kg was deduced from this value. With the equilibrium partitioning theory, the MPC for soil and sediment is **0.055** mg/kg. The old MPC in sediment for the sum of the three monochlorophenol isomers was also derived by equilibrium partitioning from the MPC in water. This MPC was 0.22 mg/kg.

3.6.2.2 SRC_{eco} for 3-chlorophenol

Only acute toxicity data are available for 3-chlorophenol (Table A7. 36 and Table A7. 37). The only value for a marine species fits well in the overall log-normal distribution ($P = 29\%$). The geometric mean of all acute toxicity data is 25 mg/l. With an ACR of 10 the resulting HC50(aquatic species) is 2.5 mg/l. According to the modified EPA method an assessment factor of 100 can be applied to the lowest L(E)C50, because data are available for algae, crustaceans and fish. The resulting MPC for surface water is 55 µg/l. According to the EU/TGD method, this factor is 1000 in this case. This leads to an MPC of 5.5 µg/l. The old MPC of 25 µg/l was a mean value for the sum of the three monochlorophenol isomers (Janus et al., 1991).

There are some acute terrestrial toxicity studies (Table A7. 35). After application of an ACR of 10 to the geometric mean of these data the HC50(terrestrial species) becomes 14 mg/kg. This value is compared with a value derived by equilibrium partitioning. The log K_p for standard soil and sediment is 1.33, resulting in an HC50(EqP) of 54 mg/kg. The SRC_{eco} for soil is therefore 14 mg/kg and for sediment 54 mg/kg. Applying a factor of 1000 to the lowest terrestrial L(E)C50 gives an MPC for soil of 0.035 mg/kg. With the equilibrium partitioning theory, the MPC for sediment is 0.12 mg/kg. The old MPCs for the sum of the three monochlorophenols were 0.20 and 0.22 mg/kg in soil and sediment, respectively (Janus et al., 1991).

3.6.2.3 SRC_{eco} for 4-chlorophenol

For 4-chlorophenol acute as well as chronic aquatic toxicity data are available (Table A7. 38 and Table A7. 39). The marine study fits in the overall log-normal distribution with the fresh water studies ($P = 82\%$). The geometric mean of the 3 chronic NOECs is 2.9·10² µg/l. The acute toxicity data for fresh water and marine species are not significantly different ($P = 0.45$). The geometric mean of the combined sets is 14 mg/l. Hence, the HC50(aquatic species) is determined by the geometric mean of the chronic toxicity data.

Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. With the modified EPA method an MPC of 19 µg/l is derived by applying a safety factor of 100 to the lowest L(E)C50, which is slightly lower than the lowest NOEC divided by 10. With 3 NOECs but not from the same taxonomic group as the lowest L(E)C50 an assessment factor of 50 is applied to the lowest NOEC according to the EU/TGD method. The resulting MPC is 4.0 µg/l. The old MPC of 25 µg/l was a mean value for the sum of the three monochlorophenol isomers (Janus et al., 1991).

No terrestrial data are available for 4-chlorophenol. The log K_p for standard soil and sediment is 0.70, resulting in an HC50 for soil and sediment of 1.4 mg/kg and an MPC of 0.020 mg/kg. The old MPCs for the sum of the three monochlorophenols were 0.20 and 0.22 mg/kg in soil and sediment, respectively (Janus et al., 1991).

3.6.2.4 SRC_{eco} for 2,3-dichlorophenol

Only acute toxicity data are available for aquatic species (Table A7. 40 and Table A7. 41). One marine study fits in the overall log-normal distribution ($P = 22\%$). Applying an ACR of 10 to the geometric mean of the data results in an HC50(aquatic species) of 1.4 mg/l. Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. The MPC for 2,3-dichlorophenol according to the modified EPA method is 35 µg/l, derived by applying a safety factor of 100 to the lowest L(E)C50. With the assessment factor of the EU/TGD of 1000 for a complete base set the MPC is 3.5 µg/l. The old MPC of 15 µg/l was a value for the sum of the six dichlorophenol isomers (Janus et al., 1991).

No terrestrial data are available for 2,3-dichlorophenol. The $\log K_p$ for standard soil and sediment is 1.33, resulting in an HC50 for soil and sediment of **31 mg/kg** and an MPC of **0.075 mg/kg**. The old MPCs for the sum of the dichlorophenols in soil was 0.20 mg/kg. This value was a mean of the MPCs derived for three isomers. The old MPCs for the sum of the dichlorophenols in sediment was 0.33 mg/kg, which was derived from the MPC in water by means of equilibrium partitioning (Janus et al., 1991).

3.6.2.5 SRC_{eco} for 2,4-dichlorophenol

For dichlorophenol chronic toxicity studies are available for 6 taxonomic groups (Table A7. 43 and Table A7. 44). The fresh water and marine species are from different taxonomic groups and taking into account this variability, the data sets are not significantly different ($P = 0.29$, Welch-corrected). Therefore, statistical extrapolation is performed (Figure 3.34). The HC50(aquatic species from this distribution is $4.1 \cdot 10^2 \mu\text{g/l}$ (90% CI: $0.6 \cdot 10^2 - 27.7 \cdot 10^2 \mu\text{g/l}$). The MPC for 2,4-dichlorophenol is determined from the HC5 of this distribution and is $1.5 \mu\text{g/l}$ (90% CI: $0.03 - 14.6 \mu\text{g/l}$). The old MPC of $15 \mu\text{g/l}$ was a value for the sum of the six dichlorophenol isomers (Janus et al., 1991).

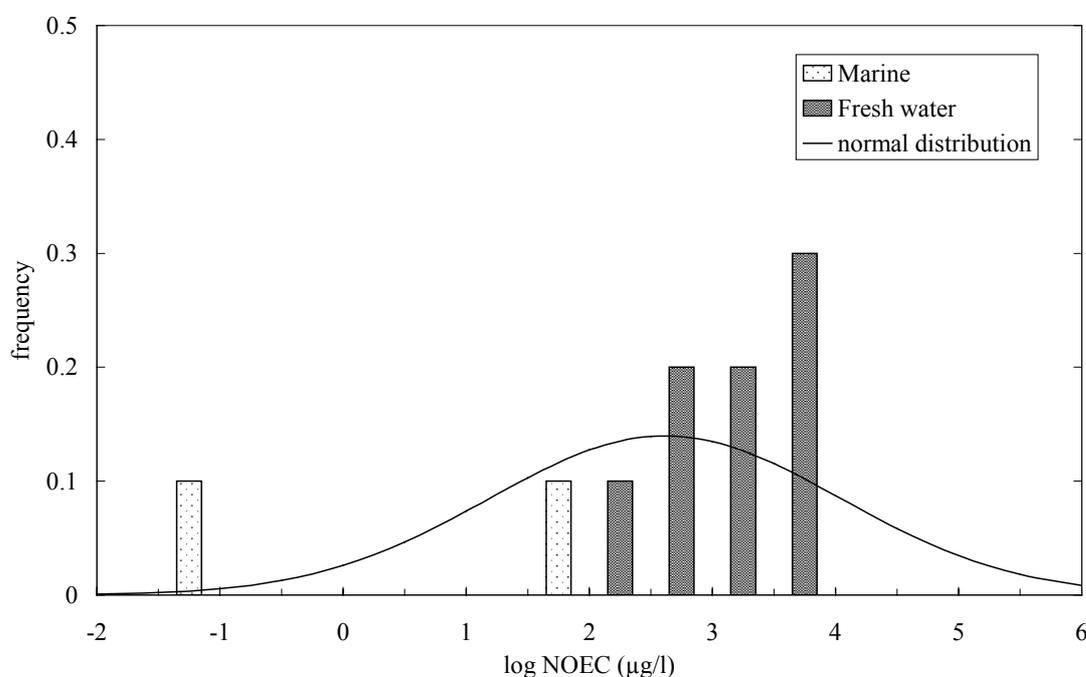


Figure 3.34: 2,4-Dichlorophenol: Distribution of chronic toxicity data for aquatic species and estimated sensitivity distribution ($n = 10$, $\bar{x} = 2.62$, $s = 1.43$).

One acute toxicity study is available for terrestrial species. With an ACR of 10 the resulting HC50(terrestrial species) is 27 mg/kg. A value for the MPC of 0.27 mg/kg is obtained after application of a safety factor of 1000, according to the modified EPA method as well as the EU/TGD method. The $\log K_p$ for standard soil and sediment is 1.31, resulting in a lower value for the HC50(soil). The HC50 for soil and sediment is **8.4 mg/kg** and the MPC is **0.031 mg/kg**. The old MPCs for the sum of the dichlorophenols were 0.20 and 0.33 mg/kg in soil and sediment, respectively (Janus et al., 1991).

3.6.2.6 SRC_{eco} for 2,5-dichlorophenol

The only available toxicity data for 2,5-dichlorophenol are acute studies for aquatic species (Table A7. 45). The only study for a marine species fits well in the overall log-normal

distribution ($P = 40\%$). The geometric mean of all acute toxicity data is 13 mg/l. With an ACR of 10 the HC50(aquatic species) is 1.3 mg/l. The MPC according to the modified EPA method is 2.8 $\mu\text{g/l}$ derived by application of a factor of 1000 to the lowest L(E)C50. Although the base set is not complete, the same MPC can be derived by the EU/TGD method because the $\log K_{ow}$ of 2,5-dichlorophenol is little higher than 3 (Otte et al., 2001). The old MPC of 15 $\mu\text{g/l}$ was a value for the sum of the six dichlorophenol isomers (Janus et al., 1991). No terrestrial data are available. Therefore, the SRC_{eco} and MPC for soil and sediment are derived by equilibrium partitioning. The $\log K_p$ for standard soil and sediment is 1.60. The HC50 for soil and sediment is 53 mg/kg and the MPC is 0.11 mg/kg. The old MPCs for the sum of the dichlorophenols were 0.20 and 0.33 mg/kg in soil and sediment, respectively (Janus et al., 1991).

3.6.2.7 SRC_{eco} for 2,6-dichlorophenol

Acute toxicity data and one chronic study with aquatic species are available for 2,6-dichlorophenol (Table A7. 46 and Table A7. 47). The data for fresh water and marine species are not significantly different ($P = 0.72$). The geometric mean of all acute toxicity is almost equal to the chronic NOEC. Therefore, the HC50(aquatic species) of 2.3 mg/l is derived from the acute toxicity data with application of an ACR of 10. Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. According to the modified EPA method the MPC for 2,6-dichlorophenol is 37 $\mu\text{g/l}$, derived by applying a safety factor of 100 to the lowest L(E)C50. Following the EU/TGD protocol an assessment factor of 1000 is applied to lowest L(E)C50. The resulting MPC is 3.7 $\mu\text{g/l}$. The old MPC of 15 $\mu\text{g/l}$ was a value for the sum of the six dichlorophenol isomers (Janus et al., 1991).

No terrestrial data are available. Therefore, the SRC_{eco} and MPC for soil and sediment are derived by equilibrium partitioning. The $\log K_p$ for standard soil and sediment is 1.60. The HC50 for soil and sediment is 57 mg/kg and the MPC is 0.093 mg/kg. The old MPCs for the sum of the dichlorophenols were 0.20 and 0.33 mg/kg in soil and sediment, respectively (Janus et al., 1991).

3.6.2.8 SRC_{eco} for 3,4-dichlorophenol

For 3,4-dichlorophenol acute toxicity data are available for fresh water and marine species (Table A7. 49 and Table A7. 50). There are no significant differences in sensitivity ($P = 0.79$). The HC50 derived from the geometric mean of the acute toxicity data with an ACR of 10 is $5.9 \cdot 10^2$ $\mu\text{g/l}$. Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. According to the modified EPA method the MPC for 3,4-dichlorophenol is 11 $\mu\text{g/l}$, derived by applying a safety factor of 100 to the lowest L(E)C50. Following the EU/TGD protocol an assessment factor of 1000 is applied to lowest L(E)C50. The resulting MPC is 1.1 $\mu\text{g/l}$. The old MPC of 15 $\mu\text{g/l}$ was a value for the sum of the six dichlorophenol isomers (Janus et al., 1991).

Also some acute data for earthworms are available for 3,4-dichlorophenol (Table A7. 48). The geometric mean of these data is 420 mg/kg and as a result the HC50(terrestrial species) is 42 mg/kg. The MPC derived directly from the terrestrial data is equal to 0.30 mg/kg. The $\log K_p$ for standard soil and sediment is 1.67. The HC50(EqP) is 27 mg/kg and the MPC(EqP) is 0.051 mg/kg. Therefore, the SRC_{eco} for soil and sediment is 27 mg/kg and the MPC for soil and sediment is 0.051 mg/kg. The old MPCs for the sum of the dichlorophenols were 0.20 and 0.33 mg/kg in soil and sediment, respectively (Janus et al., 1991).

3.6.2.9 SRC_{eco} for 3,5-dichlorophenol

For 3,5-dichlorophenol acute toxicity data are available for fresh water and marine species (Table A7. 52 and Table A7. 53). There are no significant differences in sensitivity ($P = 0.40$). The HC50 derived from the geometric mean of the acute toxicity data with an ACR of 10 is $4.2 \cdot 10^2 \mu\text{g/l}$. Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. According to the modified EPA method the MPC for 3,5-dichlorophenol is $15 \mu\text{g/l}$, derived by applying a safety factor of 100 to the lowest L(E)C50. Following the EU/TGD protocol an assessment factor of 1000 is applied to lowest L(E)C50. The resulting MPC is **1.5** $\mu\text{g/l}$. The old MPC, which was also $15 \mu\text{g/l}$, was a value for the sum of the six dichlorophenol isomers (Janus et al., 1991).

One acute study with a macrophyt is available for 3,5-dichlorophenol (Table A7. 48) with an EC50 of 160 mg/kg . As a result the HC50(terrestrial species) is 16 mg/kg and the MPC derived directly from the terrestrial data is equal to 0.16 mg/kg . The $\log K_p$ for standard soil and sediment is 1.11. The HC50(EqP) is 5.4 mg/kg and the MPC(EqP) is 0.019 mg/kg . Therefore, the SRC_{eco} for soil and sediment is **5.4** mg/kg . The MPC for soil and sediment is **0.019** mg/kg . The old MPCs for the sum of the dichlorophenols were 0.20 and 0.33 mg/kg in soil and sediment, respectively (Janus et al., 1991).

3.6.2.10 SRC_{eco} for 2,3,4-trichlorophenol

For 2,3,4-trichlorophenol acute toxicity data are available for fresh water and marine species (Table A7. 54 and Table A7. 55), which are not significantly different ($P = 0.33$). The HC50 derived from the geometric mean of the acute toxicity data with an ACR of 10 is $4.2 \cdot 10^2 \mu\text{g/l}$. Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. According to the modified EPA method the MPC for 2,3,4-trichlorophenol is $12 \mu\text{g/l}$, derived by applying a safety factor of 100 to the lowest L(E)C50. Following the EU/TGD protocol an assessment factor of 1000 is applied to lowest L(E)C50. The resulting MPC is **1.2** $\mu\text{g/l}$. The old MPC of $2.5 \mu\text{g/l}$ was a value for the sum of the six trichlorophenol isomers (Janus et al., 1991).

There are no terrestrial toxicity data for 2,3,4-trichlorophenol. The $\log K_p$ for standard soil and sediment is 1.85. The resulting SRC_{eco} for soil and sediment is equal to **30** mg/kg and the MPC is equal to **0.085** mg/kg . The old MPC of 0.04 mg/kg for the sum of the six trichlorophenol isomers was based on the lowest terrestrial LC50 value for one of the trichlorophenols (Janus et al., 1991). For sediment, The old MPC for the sum of trichlorophenols was 0.10 mg/kg (Janus et al., 1991).

3.6.2.11 SRC_{eco} for 2,3,5-trichlorophenol

For 2,3,5-trichlorophenol acute toxicity data are available for fresh water and marine species (Table A7. 57 and Table A7. 58), which are not significantly different ($P = 0.73$). The HC50, derived from the geometric mean of the acute toxicity data with an ACR of 10, is **$2.6 \cdot 10^2$** $\mu\text{g/l}$. No data for algae are available. The MPC for 2,3,5-trichlorophenol is **0.60** $\mu\text{g/l}$, derived by applying a safety factor of 1000 to the lowest L(E)C50, both with the modified EPA method and the EU/TGD method ($\log K_{ow} > 3$). The old MPC of $2.5 \mu\text{g/l}$ was a value for the sum of the six trichlorophenol isomers (Janus et al., 1991).

One chronic and one acute value for a macrophyt are available. The L(E)C50 is 45 mg/kg and the NOEC is 16 mg/kg . The HC50(terrestrial species) of 4.5 mg/kg is derived by application of an ACR of 10 to the EC50 value. The MPC derived directly from the terrestrial data is **0.045** mg/kg according to both the modified EPA and EU/TGD method. The $\log K_p$ for standard soil and sediment is 1.93. The HC50(EqP) is 22 mg/kg and the MPC(EqP) is 0.051 mg/kg . Therefore, the SRC_{eco} for soil **4.5** mg/kg and for sediment **22** mg/kg . The MPC for soil is **0.045** mg/kg and the MPC for sediment is **0.051** mg/kg . The old MPCs for the sum of

the six trichlorophenols were 0.04 and 0.10 mg/kg in soil and sediment, respectively (Janus et al., 1991).

3.6.2.12 SRC_{eco} for 2,3,6-trichlorophenol

For 2,3,6-trichlorophenol acute toxicity data are available for fresh water and marine species (Table A7. 59 and Table A7. 60), which are not significantly different ($P = 0.57$). The HC50 is $9.9 \cdot 10^2$ µg/l, derived from the geometric mean of the acute toxicity data with an ACR of 10. No data are available for algae. The MPC for 2,3,6-trichlorophenol is 2.7 µg/l, derived by applying a safety factor of 1000 to the lowest L(E)C50, both with the modified EPA method and the EU/TGD method ($\log K_{ow} > 3$). The old MPC of 2.5 µg/l was a value for the sum of the six trichlorophenol isomers (Janus et al., 1991).

There are no terrestrial toxicity data for 2,3,6-trichlorophenol. The $\log K_p$ for standard soil and sediment is 2.05. The resulting SRC_{eco} for soil and sediment is equal to $1.1 \cdot 10^2$ mg/kg and the MPC is equal to 0.30 mg/kg. The old MPCs for the sum of the six trichlorophenols were 0.04 and 0.10 mg/kg in soil and sediment, respectively (Janus et al., 1991).

3.6.2.13 SRC_{eco} for 2,4,5-trichlorophenol

A number of acute toxicity data of 2,4,5-trichlorophenol are available for fresh water as well as marine species (Table A7. 62 and Table A7. 63). The fresh water and marine species do not differ in sensitivity ($P = 0.63$). The geometric mean of the acute toxicity data is 2.3 mg/l. Further, there is one chronic study for a fresh water species. This NOEC is $1.6 \cdot 10^2$ µg/l. The HC50(aquatic species) is determined by this value. Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. According to the modified EPA method the MPC for 2,4,5-trichlorophenol is 4.5 µg/l, derived by applying a safety factor of 100 to the lowest L(E)C50. Following the EU/TGD protocol an assessment factor of 100 is applied to the NOEC, which is for the same taxonomic group as the lowest L(E)C50. The resulting MPC is 1.6 µg/l. The old MPC of 2.5 µg/l was a value for the sum of the six trichlorophenol isomers (Janus et al., 1991).

Two L(E)C50 values are available for earthworms (Table A7. 61). The geometric mean of these data is $2.4 \cdot 10^2$ mg/kg. An ACR of 10 leads to an HC50(terrestrial species) of 24 mg/kg. The MPC derived from these data is 0.11 mg/kg. These values are compared with values derived by equilibrium partitioning. The $\log K_p$ for standard soil and sediment is 2.13. The resulting HC50 for soil and sediment is equal to 22 mg/kg. The MPC(EqP) is equal to 0.22 mg/kg. Accordingly, the MPC for soil is 0.11 mg/kg and for sediment 0.22 mg/kg. The old MPCs for the sum of the six trichlorophenols were 0.04 and 0.10 mg/kg in soil and sediment, respectively (Janus et al., 1991).

3.6.2.14 SRC_{eco} for 2,4,6-trichlorophenol

For 2,4,6-trichlorophenol both chronic and acute toxicity data are available for aquatic species (Table A7. 65 and Table A7. 66). The geometric mean of the chronic toxicity data is $4.8 \cdot 10^2$ µg/l. The only acute toxicity study for marine species fits well in the overall log-normal distribution ($P = 53\%$). The geometric mean of the combined sets is 7.4 mg/l. Consequently, the geometric mean of the chronic toxicity data is taken as the HC50(aquatic species). Acute toxicity data are available for algae, crustaceans (*Daphnia*) and fish. According to the modified EPA method the MPC for 2,4,6-trichlorophenol is derived by applying a safety factor of 100 to the lowest L(E)C50. This MPC is 3.6 µg/l. Because 3 chronic NOECs are available, also for the taxonomic group of the lowest L(E)C50, an assessment factor of 10 is applied to lowest NOEC according to the EU/TGD method. The resulting MPC is 18 µg/l.

The old MPC of 2.5 µg/l was a value for the sum of the six trichlorophenol isomers (Janus et al., 1991).

Several data for terrestrial toxicity are available for 2,4,6-trichlorophenol (Table A7. 64). Chronic NOECs are available for 3 plant species with a geometric mean of $2.5 \cdot 10^2$ mg/kg. Further, some acute toxicity data are available for 4 species of earthworms and a plant. With an ACR of 10 the resulting HC50(terrestrial species) is **8.1** mg/kg. According to the modified EPA method the MPC for soil is derived by applying a factor of 1000 to the lowest L(E)C50 after comparison with the chronic toxicity data. The resulting MPC is 0.058 mg/kg. According to the EU/TGD method a factor of 50 is applied to the lowest NOEC, because 3 NOECs are available, although not for the same taxonomic group as the lowest L(E)C50. The MPC derived in this way is 2.4 mg/kg. These values are compared with values derived by equilibrium partitioning. The log K_p for standard soil and sediment is 2.22. The resulting HC50(EqP) is 80 mg/kg and the MPC(EqP) is 3.0 mg/kg. Thus, the SRC_{eco} are **8.1** and **80** mg/kg and the MPCs **2.4** and **3.0** mg/kg for soil and sediment respectively. The old MPCs for the sum of the six trichlorophenols were 0.04 and 0.10 mg/kg in soil and sediment, respectively (Janus et al., 1991).

3.6.2.15 SRC_{eco} for 3,4,5-trichlorophenol

For 3,4,5-trichlorophenol only acute toxicity data are available (Table A7. 67 and Table A7. 68). The marine study fits in the overall log-normal distribution (P = 13%). The geometric mean of all acute toxicity data is 1.9 mg/l, which leads to an HC50(aquatic species) of **1.9·10²** µg/l. No data are available for algae. According to the modified EPA method an MPC of **0.38** µg/l is derived. Because 3,4,5-trichlorophenol has a log $K_{ow} > 3$, also an MPC according to the EU/TGD can be derived. This MPC is also derived by application of an assessment factor of 1000 to the lowest L(E)C50. The old MPC of 2.5 µg/l was a value for the sum of the six trichlorophenol isomers (Janus et al., 1991).

No terrestrial data are available for 3,4,5-trichlorophenol. The log K_p for standard soil and sediment is 2.31. The resulting HC50 for soil and sediment is **39** mg/kg and the MPC is **0.078** mg/kg. The old MPCs for the sum of the six trichlorophenols were 0.04 and 0.10 mg/kg in soil and sediment, respectively (Janus et al., 1991).

3.6.2.16 SRC_{eco} for 2,3,4,5-tetrachlorophenol

For 2,3,4,5-tetrachlorophenol acute toxicity data are available for fresh water species and one marine species (Table A7. 70 and Table A7. 71). The marine study fits in the overall log-normal distribution (P = 11%). The geometric mean of the combined toxicity data is 1.5 mg/l. Application of an ACR of 10 leads to an HC50(aquatic species) of **1.5·10²** µg/l. No data are available for algae. The MPC according to the modified EPA method is **0.21** µg/l. Because 2,3,4,5-tetrachlorophenol has a log $K_{ow} > 3$, also an MPC according to the EU/TGD can be derived. This MPC is also derived by application of an assessment factor of 1000 to the lowest L(E)C50. The old MPC of 1.0 µg/l was a value for the sum of the three tetrachlorophenol isomers (Janus et al., 1991).

Two L(E)C50 values are available for earthworms (Table A7. 69). The geometric mean of these data is $6.4 \cdot 10^2$ mg/kg. The HC50(terrestrial species) derived from these data with an ACR of 10 is 64 mg/kg. The log K_p for standard soil and sediment is 2.64. The resulting HC50(EqP) is 67. Therefore, the SRC_{eco} for soil is **64** mg/kg and for sediment **67** mg/kg. The MPC derived directly from the terrestrial data is 0.29 mg/kg, derived by applying a factor 1000 to the lowest value. The old MPC(soil) for the sum of the three tetrachlorophenol isomers was set equal to this value of 0.3 mg/kg. The MPC derived by equilibrium partitioning is lower than this value. This MPC of **0.092** mg/kg is taken as the MPC for soil

and sediment for 2,3,4,5-tetrachlorophenol. The old MPC(sediment) for the sum of the three tetrachlorophenol isomers was 0.086 mg/kg.

3.6.2.17 SRC_{eco} for 2,3,4,6-tetrachlorophenol

Acute toxicity data of 2,3,4,6-tetrachlorophenol are available for fresh water as well as marine species (Table A7. 74 and Table A7. 75). The fresh water and marine species do not differ in sensitivity ($P = 0.28$). The geometric mean of the acute toxicity data is 1.6 mg/l. Further, there is one chronic study for a fresh water species. This NOEC is $6.5 \cdot 10^2 \mu\text{g/l}$. The HC50(aquatic species) of $1.6 \cdot 10^2 \mu\text{g/l}$ is derived by applying an ACR of 10 to the geometric mean of the acute toxicity data. Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. With the modified EPA method the MPC for 2,3,4,6-tetrachlorophenol is derived by applying an assessment factor of 100 to the lowest L(E)C50 after comparison with the chronic toxicity data. This MPC is 1.4 $\mu\text{g/l}$. With the EU/TGD method the same approach is followed except that the assessment factors for both the chronic and acute toxicity data are a factor of 10 lower in this case. The resulting MPC is **0.14** $\mu\text{g/l}$. The old MPC of 1.0 $\mu\text{g/l}$ was a value for the sum of the three tetrachlorophenol isomers (Janus et al., 1991).

No terrestrial data are available for 2,3,4,6-tetrachlorophenol. Therefore, both the SRC_{eco} and the MPC for soil and sediment are derived by equilibrium partitioning. The log K_p for standard soil and sediment is 1.90. The SRC_{eco} for soil and sediment is **13** mg/kg. The MPC for soil and sediment derived by equilibrium partitioning is **0.011** mg/kg. The old MPCs for the sum of the three tetrachlorophenol isomers were 0.3 and 0.086 mg/kg in soil and sediment, respectively.

3.6.2.18 SRC_{eco} for 2,3,5,6-tetrachlorophenol

Acute toxicity data of 2,3,5,6-tetrachlorophenol are available for fresh water as well as marine species (Table A7. 74 and Table A7. 75). The fresh water and marine species do not differ in sensitivity ($P = 0.89$). The geometric mean of the acute toxicity data is 2.6 mg/l. Further, there is one chronic study for a fresh water species. This NOEC is **95** $\mu\text{g/l}$. The HC50(aquatic species) is determined by this value. No data are available for algae but the log K_{ow} of 2,3,5,6-tetrachlorophenol is higher than 3. According to the modified EPA method the MPC for 2,3,5,6-tetrachlorophenol is derived by applying an assessment factor of 1000 to the lowest L(E)C50 after comparison with the chronic NOEC. This MPC is 0.17 $\mu\text{g/l}$. The chronic NOEC is for a species from the same taxonomic group as the lowest L(E)C50. Therefore, the MPC according to the EU/TGD method is derived by application of an assessment factor of 100 to the lowest NOEC. The resulting MPC is The old MPC of 1.0 $\mu\text{g/l}$ was a value for the sum of the three tetrachlorophenol isomers (Janus et al., 1991).

No terrestrial data are available for 2,3,4,6-tetrachlorophenol. Therefore, both the HC50 and the MPC for soil and sediment are derived by equilibrium partitioning. The log K_p for standard soil and sediment is 2.11. The HC50 for soil and sediment is **12** mg/kg. The MPC for soil and sediment derived by equilibrium partitioning is **0.12** mg/kg. The old MPCs for the sum of the three tetrachlorophenol isomers were 0.3 and 0.086 mg/kg in soil and sediment, respectively.

3.6.2.19 SRC_{eco} for pentachlorophenol

For pentachlorophenol, enough chronic toxicity data are available for aquatic species to perform statistical extrapolation (Table A7. 78 and Table A7. 79). Fresh water and marine species do not differ in sensitivity ($P = 0.80$) and therefore, both sets are combined (Figure 3.35).

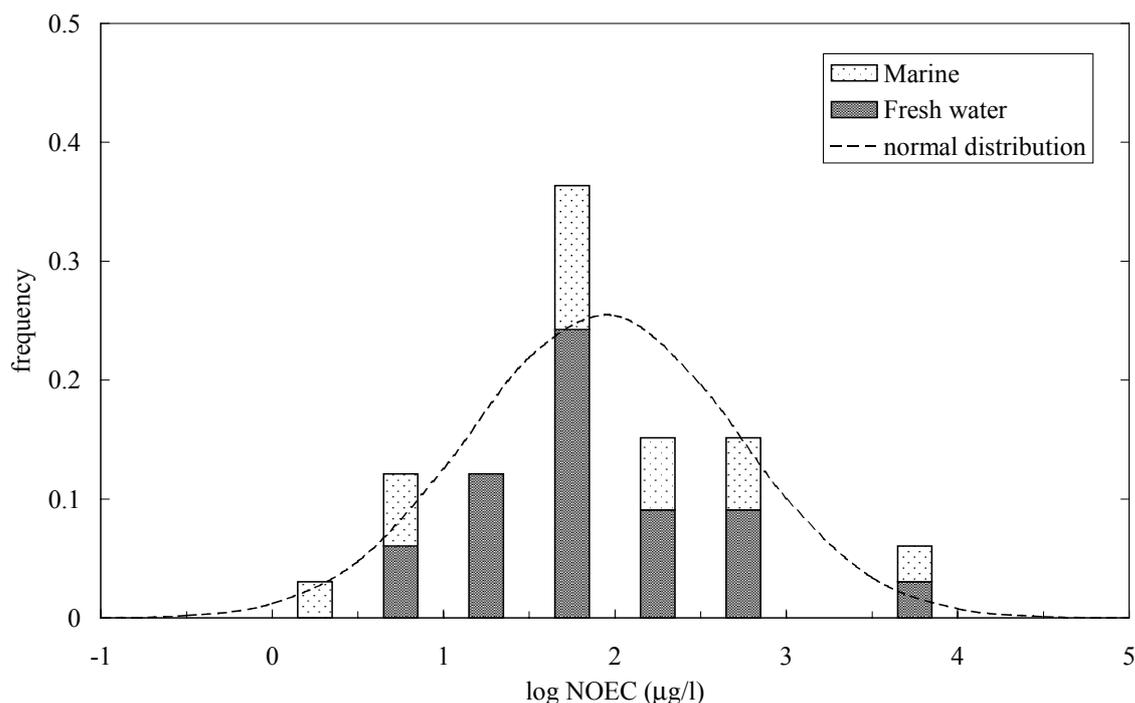


Figure 3.35: Pentachlorophenol: Distribution of chronic toxicity data for aquatic species and estimated sensitivity distribution ($n = 33$, $\bar{x} = 1.93$, $s = 0.78$).

The HC50 of this distribution is 85 µg/l (90% CI: 50 - 145 µg/l). The HC5 is 4.3 µg/l (90% CI: 1.7 - 8.8 µg/l). The MPC for pentachlorophenol based on data for secondary poisoning is higher than this HC5: 13 µg/l (Van de Plassche, 1994). Therefore, the new MPC for pentachlorophenol is **4.3** µg/l.

For pentachlorophenol terrestrial data are available for both species and processes (Table A7.76 and Table A7.77). The distribution of these data is shown in Figure 3.36. For processes, the HC50 is 72 mg/kg (90% CI: 30-175 mg/kg). The HC5 of this distribution is 1.1 mg/kg (90% CI: 0.2 - 3.6 mg/kg). However, species appear to be more sensitive. The geometric mean of the chronic toxicity data is 16 mg/kg, while that of the acute toxicity data is $1.2 \cdot 10^2$ mg/kg. After application of an ACR of 10, the resulting value for the HC50 is 12 mg/kg. The log K_p for standard soil and sediment is 1.97. The resulting HC50 is 8.0 mg/kg, slightly lower than the values derived directly from the terrestrial toxicity data. Therefore, the proposed SRC_{s_{eco}} are **12** mg/kg for soil and **8.0** mg/kg for sediment.

According to the modified EPA method an assessment factor of 10 can be applied to the lowest NOEC, because data are available for bacteria, macrophytes and annelids. This value directly calculated from the terrestrial toxicity data is 0.16 mg/kg. Three NOECs are available for terrestrial species, including the same taxonomic as for the minimum L(E)C50. Therefore, the same MPC is derived according to the EU/TGD method. The MPC for soil calculated for secondary poisoning is 1.3 mg/kg and thus the MPC for soil is **0.16** mg/kg (Van de Plassche, 1994). The MPC for sediment is calculated from the MPC for surface water with equilibrium partitioning and is **0.40** mg/kg. Although the MPC for surface water is lower, this MPC for sediment is higher than the old MPC value of 0.17 mg/kg. This is caused by the use of a new value for the K_{oc} , which is slightly higher.

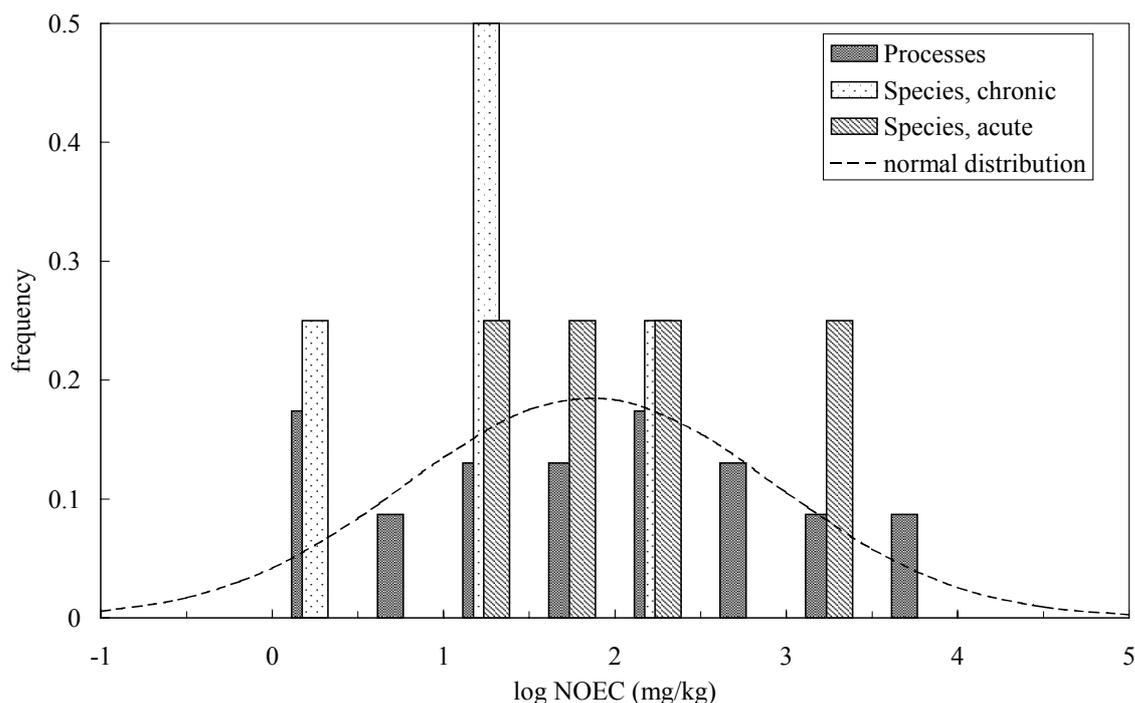


Figure 3.36: Pentachlorophenol: Distribution of toxicity data for terrestrial processes and species. The estimated distribution is based on processes ($n = 23$, $\bar{x} = 1.86$, $s = 1.08$).

3.6.2.20 SRC_{eco} for the sum of chlorophenols

Chlorophenols mainly act by polar narcosis, a mode of action that is probably the same as narcosis of nonpolar chemicals (Verhaar et al., 1996; Urrestarazu-Ramos et al., 1998; Vaes et al., 1998). In the same manner, as was done for chlorobenzenes, risk limits can be derived for the sum of chlorophenol isomers. HC50-values for water for mono-, di-, tri-, tetra- and pentachlorophenol are $1.0 \cdot 10^3$, $8.7 \cdot 10^2$, $3.4 \cdot 10^2$, $1.3 \cdot 10^2$, and $85 \mu\text{g/l}$, respectively. These values are very similar to the values for chlorobenzenes with the same degree of chlorination. The HC50-values for mono-, di-, tri-, tetra- and pentachlorophenol are respectively 5.4, 22, 22, 21, and 12 mg/kg for soil and 8.5, 22, 41, 22, and 8.0 mg/kg for sediment. Again these values are very similar to the values for chlorobenzenes.

A value for the sum of all chlorophenols is not proposed in this report, because some of the chlorophenols may exhibit a more specific mode of toxic action than polar narcosis, such as uncoupling activity (see e.g. Escher et al., 1999). However, by taking the geometric mean of the HC50s derived directly from terrestrial toxicity studies and indirectly by the equilibrium partitioning theory, the resulting proposed values for the SRC_{eco} would be 18 mg/kg for soil and 22 mg/kg for sediment, or on a molar basis $1.0 \cdot 10^2$ and $1.2 \cdot 10^2 \mu\text{mol/kg}$. For comparison, these values were 15 and 20 mg/kg (73 and $1.1 \cdot 10^2 \mu\text{mol/kg}$) for chlorobenzenes. By taking the geometric mean of the MPCs of all chlorophenols in the same way as for the HC50, the resulting MPCs for the sum of all chlorophenols would be 0.13 mg/kg for soil and 0.22 mg/kg for sediment or, on a molar basis, 1.0 and $0.49 \mu\text{mol/kg}$. For comparison, these values were 0.15 and 0.34 mg/kg (0.56 and $1.6 \mu\text{mol/kg}$) for chlorobenzenes.

It can be concluded that for compounds that act by the same mode of action (narcosis or polar narcosis for most chlorophenols) the effect concentrations in water are mainly influenced by the physicochemical properties of the compounds and that in soil and sediment the effect concentrations are approximately at the same level for all compounds. These levels are

100 $\mu\text{mol/kg}$ (~ 20 mg/kg) for the HC50 and 1 $\mu\text{mol/kg}$ (~ 0.20 mg/kg) for the MPC for narcotic chemicals.

3.6.3 SRC_{eco} for monochloronaphthalenes

For monochloronaphthalenes new data have been collected. These data are reported in the annex to this report. Data for 1-, and 2-chloronaphthalene are first considered separately. For 1-chloronaphthalene aquatic toxicity data are available for fresh water and marine species (Table A7. 80 and Table A7. 81). One chronic NOEC of $3.9 \cdot 10^2$ $\mu\text{g/l}$ is available. The acute toxicity data for fresh water and marine species are not significantly different ($P = 0.30$). The geometric mean of the combined sets of acute toxicity data is 1.2 mg/l. After application of an ACR of 10, the HC50(aquatic species) becomes $1.2 \cdot 10^2$ $\mu\text{g/l}$. Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. According to the modified EPA method an assessment factor of 100 can be applied to the lowest L(E)C50 value resulting in an MPC of 3.7 $\mu\text{g/l}$. With the EU/TGD method an assessment factor of 1000 is applied to the lowest L(E)C50. This MPC is 0.37 $\mu\text{g/l}$. In both cases a comparison with the chronic NOEC is made. For 2-chloronaphthalene two acute toxicity data are available (Table A7. 82 and Table A7. 83). The geometric mean of these data 1.9 mg/l, which results in an HC50(aquatic species) of $1.9 \cdot 10^2$ $\mu\text{g/l}$. With a safety factor of 1000 to the lowest L(E)C50, an MPC of 1.6 $\mu\text{g/l}$ is derived according to the modified EPA method and the EU/TGD method ($\log K_{ow} > 3$). For both 1- and 2-chloronaphthalene the $\log K_p$ for standard soil and sediment is 2.19. The resulting SRC_{eco} for soil and sediment are 18 and 30 mg/kg for 1- and 2-chloronaphthalene respectively. The corresponding MPCs are 0.057 and 0.25 mg/kg.

Because no obvious differences are observed between the two isomers, one value can be derived for the sum of the two. The values of the SRC_{eco} and MPC for surface water are $1.5 \cdot 10^2$ $\mu\text{g/l}$ and 0.77 $\mu\text{g/l}$. For soil and sediment the HC50 and MPC are 23 and 0.12 mg/kg.

3.6.4 SRC_{eco} for polychlorinated biphenyls (PCBs)

For PCBs only a few aquatic toxicity data are available (Van Wezel et al., 1999a). For the derivation of the HC50 for water the data from fish egg injection experiments were not considered suitable, because the data have to be recalculated from dose per egg to aqueous concentrations and the results deviate far from the NOECs for other studies. Only for the congeners #77, #105 and #126 aquatic toxicity data are available (Table A7. 84). For PCB77 one NOEC of 0.1 $\mu\text{g/l}$ for a crustacean is available. For PCB105 there is an EC50 for fish of 1.3 $\mu\text{g/l}$. Also for PCB126 a NOEC of 0.018 for a crustacean is available. Based on these three studies, the HC50s(aquatic species) would be 0.1, 0.13 and 0.018 $\mu\text{g/l}$ for PCB77, PCB105 and PCB126, respectively.

The $\log K_p$ for standard soil and sediment is 4.62 for PCB77, 4.90 for PCB105 and 4.71 for PCB126 (Otte et al., 2001). With equilibrium partitioning the resulting HC50s in soil are 4.2, 10, and 0.92 mg/kg for PCB77, PCB105, and PCB126, respectively.

The MPC for PCB77 was derived by probabilistic modelling with the data recalculated to organic carbon and performing statistical extrapolation on these data. For PCB77 all toxicity data were used for this purpose, including aquatic toxicity and secondary poisoning, for PCB105 only the most sensitive probability distribution was used and for PCB 126 only the mammal and bird data (secondary poisoning). The resulting MPCs, recalculated to standard soil and sediment were $4.2 \cdot 10^{-4}$, $1.5 \cdot 10^{-3}$ and $2.5 \cdot 10^{-6}$ mg/kg for PCB77, PCB105 and PCB126, respectively (Van Wezel et al., 1999a).

These three congeners are all mono- or non-*ortho* PCBs and are therefore planar. A mixture-MPC has been derived for six of these PCBs using scaling factors for the MPC of each single congener based on intrinsic potency and occurrence in congener patterns. This MPC is expressed as a concentration of PCB118 and is $5 \cdot 10^{-3}$ mg/kg_{o.c.} or for standard soil and sediment $3 \cdot 10^{-4}$ mg/kg. Aquatic toxicity data are not available for all these congeners and thus, no HC50 can be derived for a mixture of planar PCBs, unless a geometric mean of the three congeners is taken. This geometric mean is 3.4 mg/kg or 11 μ mol/kg.

It was decided not to include secondary poisoning in the derivation of the SRC_{s_{eco}} (see chapter 2) and therefore the SRC_{eco} for PCBs is based on relatively simple aquatic toxicity studies. However, secondary poisoning was of major importance in the derivation of the MPC for these three PCB congeners. Hence, the SRC_{eco} does not reflect the toxic potential of these planar PCBs. For this reason the SRC_{eco} for PCBs can be considered as preliminary value. On the other hand, it is clear that the SRC_{s_{eco}} for the three congeners follow the same order as the MPCs that were derived with secondary poisoning included. Further, the SRC_{eco} should be based on the HC50, which means that only 50% of the species is protected. For specific acting chemicals, such as planar PCBs by means of the Ah-receptor, it can be expected that the majority of the species (e.g. most invertebrates) are not particularly sensitive to these chemicals. Therefore, the derived values might serve as HC50 for the purpose of the SRC_{eco}, although it can be considered as undesirable if all species with Ah receptor (e.g. mammals and birds) would be endangered.

3.6.5 Summary and comparison with old values and MPCs

In Table 3.11 the SRC_{s_{eco}} for chlorobenzenes are summarised. Also included in this table are the old values derived in Denneman and Van Gestel (1990) and the MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards'. Probably, these compounds mainly act by narcosis (Van de Plassche et al., 1993) and all proposed SRC_{s_{eco}} for soil and sediment are very close to each other. For water the derived ERLs are given in Table 3.12. For the sum of all chlorobenzenes the toxic unit approach is proposed for the water, soil, and sediment compartment.

The same ERLs for chlorophenols are presented in Table 3.13 and Table 3.14 and for the other chlorinated aromatic hydrocarbons in Table 3.15 and Table 3.16. The ERLs for the chlorophenols and monochloronaphthalenes in soil and sediment are very similar as those for chlorobenzenes. The few data for PCBs lead to SRC_{eco} values that are almost an order of magnitude lower. However, the specific toxicity of planar PCBs is probably not very pronounced in the aquatic toxicity tests that underlie the SRC_{eco} for PCBs, because secondary poisoning is not included. Still the value of the SRC_{eco} for the sum of PCBs changes from 70 mg/kg (Denneman and van Gestel, 1990) to 3.4 mg/kg.

Table 3.11: Summary of new SRC_{eco} values for chlorobenzenes in soil or sediment, values as derived by Denneman and van Gestel (1990), MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report. Values are given as concentrations in mg/kg standard soil/sediment (soil containing 10% organic matter and 25% clay, sediment containing 10% organic matter and 25% clay).

Compound	Compartment	SRC _{eco} [mg/kg]	Method* / reliability score	Denneman and van Gestel (1990) [mg/kg]	MPC this report [mg/kg]	Method*	MPC ^a INS [mg/kg]
sum chlorobenzenes	soil / sediment	T.U. approach		-	T.U. approach		-
	soil	15	EqP / low	-	0.41	EqP	7.6
chlorobenzene	sediment	15	EqP / low	-	0.41	EqP	7.6
	soil	19		-	0.48		0.40 ^b
dichlorobenzenes	sediment	19		-	0.69		5.5
	soil	17	EqP / low	-	0.73	EqP	5.9
1,2-dichlorobenzene	sediment	17	EqP / low	-	0.73	EqP	5.9
1,3-dichlorobenzene	soil	24	EqP / low	-	0.39	EqP	4.6
	sediment	24	EqP / low	-	0.39	EqP	4.6
1,4-dichlorobenzene ^d	soil	18	EqP<1 c sp. / medium	50	0.39	1000 c sp.	0.4 ^b
	sediment	18	EqP / low	-	1.2	EqP	5.7
trichlorobenzenes	soil	11		30	0.038		0.24 ^b
	sediment	25		-	0.20		6.7
1,2,3-trichlorobenzene	soil	5.0	1 c sp. / medium	25	0.010	1000 c sp.	0.005 ^b
1,2,4-trichlorobenzene ^d	sediment	10	EqP / low	-	0.40	EqP	6.4
	soil	5.1	EqP<10 b sp. / medium	20	0.011	EqP<c sp.	0.10 ^b
1,3,5-trichlorobenzene	sediment	5.1	EqP / low	-	0.011	EqP	7.9
	soil	50	1 c sp. / medium	50	0.50	100 d sp.	0.6 ^b
tetrachlorobenzenes	sediment	310	EqP / low	-	1.9	EqP	5.7
	soil	2.2		10	0.022		0.072 ^b
1,2,3,4-tetrachlorobenzene	sediment	39		-	0.39		7.2
	soil	16	10 b sp. / medium	50	0.16	1000 c sp.	0.20 ^b
1,2,3,5-tetrachlorobenzene	sediment	40	EqP / low	-	1.1	EqP	6.9
	soil	0.65	10 a sp. / medium	2.5	0.0065	1000 a sp.	0.0070 ^b
1,2,4,5-tetrachlorobenzene	sediment	47	EqP / low	-	0.17	EqP	6.6
	soil	1.0	10 a sp. / medium	-	0.010	1000 a sp.	0.010 ^b
pentachlorobenzene	sediment	31	EqP / low	-	0.31	EqP	7.8
	soil	16	EqP<10 b sp. / medium	50	0.28	1000 c sp.	0.12 ^c
hexachlorobenzene	sediment	16	EqP / low	-	0.015 ^e	EqP	0.012 ^c
	soil	2.0	EqP / medium	500	0.024	EqP<b sp.	0.028 ^c
	sediment	2.0	EqP<1 c sp. / low	-	0.0014 ^e	EqP	0.0012 ^c

- * For the SRC_{eco} and the MPC, EqP (equilibrium partitioning) or the assessment factor together with the designation according to Table 2.1 and Table 2.6 is given. Whether the SRC_{eco} or the MPC is based on species or processes is indicated by the abbreviation sp. and pr.
- a Unless stated otherwise, MPCs for water are derived from QSARs for narcosis, whereupon statistical extrapolation on these data is performed (Van de Plassche et al., 1993). The MPCs for soil are derived from these values with equilibrium partitioning and comparison with soil toxicity data and harmonisation with the air compartment (Van de Plassche and Bocking, 1993).
- b From experimental terrestrial data
- c Based on secondary poisoning for the terrestrial food chain or the aquatic food chain for sediment. The MPC in sediment are calculated by equilibrium partitioning; bold value indicates that no update of the MPC is proposed.
- d For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.
- e Calculated by equilibrium partitioning from the MPC for secondary poisoning effects for the aquatic food chain (Van de Plassche, 1994) with the log K_p values used in this report (Otte et al., 2001).

Table 3.12: Summary of new SRC_{eco} values for chlorobenzenes in surface water, MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report.

Compound	Compartment	SRC _{eco} [µg/l]	Method* / reliability score	MPC this report [µg/l]	Method*	MPC ^d INS [µg/l]
sum chlorobenzenes	surface water	T.U. approach			T.U. approach	-
chlorobenzene	surface water	1100	10 b / medium	32	10 g	690
dichlorobenzenes	surface water	650		23		250
1,2-dichlorobenzene	surface water	740	10 b / medium	31	10 h	(270)
1,3-dichlorobenzene	surface water	820	1 c / medium	14	50 e	(210)
1,4-dichlorobenzene ^c	surface water	460	1 c / medium	30	10 g	(260)
trichlorobenzenes	surface water	140		1.1		67
1,2,3-trichlorobenzene	surface water	100	1 c / medium	4.0	10 g	(64)
1,2,4-trichlorobenzene ^c	surface water	46	1 c / medium	0.10	10 g	(79)
1,3,5-trichlorobenzene	surface water	550	10 a / low	3.3	1000 c	(57)
tetrachlorobenzenes	surface water	120		1.2		24
1,2,3,4-tetrachlorobenzene	surface water	83	1 c / medium	2.3	10 h	(23)
1,2,3,5-tetrachlorobenzene	surface water	210	10 a / low	0.80	1000 a	(22)
1,2,4,5-tetrachlorobenzene	surface water	90	1 c / medium	0.90	100 b	(26)
pentachlorobenzene	surface water	32	1 c / medium	0.62	50 e	0.030 ^b
hexachlorobenzene	surface water	3.0	10 b / medium	0.036	50 e	2.1·10⁻⁵ ^b

* For the SRC_{eco} and the MPC, the assessment factor together with the designation according to Table 2.1 and Table 2.5 is given.

- a MPCs for water are derived from QSARs for narcosis, whereupon statistical extrapolation on these data is performed (Van de Plassche et al., 1993). The MPCs for soil are derived from these values with equilibrium partitioning and comparison with soil toxicity data and harmonisation with the air compartment (Van de Plassche and Bocking, 1993).

- b Based on secondary poisoning for the aquatic food chain; bold value indicates that no update of the MPC is proposed.
 c For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

Table 3.13: Summary of new SRC_{eco} values for chlorophenols in soil or sediment, values as derived by Denneman and van Gestel (1990), MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report. Values are given as concentrations in mg/kg standard soil/sediment (soil containing 10% organic matter and 25% clay, sediment containing 10% organic matter and 25% clay).

Compound	Compartment	SRC _{eco} [mg/kg]	Method* / reliability score	Denneman and van Gestel (1990) [mg/kg]	MPC this report [mg/kg]	Method*	MPC INS [mg/kg]
monochlorophenols	soil	5.4		35	0.034		0.20
	sediment	8.5		-	0.051		0.22
2-chlorophenol	soil	7.8	EqP<10 a sp. / medium	45	0.055	EqP<a sp.	-
	sediment	7.8	EqP / low	-	0.055	EqP	-
3-chlorophenol	soil	14	10 a sp. / medium	30	0.035	1000 a sp.	-
	sediment	54	EqP / low	-	0.12	EqP	-
4-chlorophenol	soil	1.4	EqP / low	-	0.020	EqP	-
	sediment	1.4	EqP / low	-	0.020	EqP	-
dichlorophenols	soil	22		40	0.054		0.20
	sediment	22		-	0.054		0.33
2,3-dichlorophenol	soil	31	EqP / low	-	0.075	EqP	-
	sediment	31	EqP / low	-	0.075	EqP	-
2,4-dichlorophenol	soil	8.4	EqP<10 a sp. / medium	50	0.031	EqP<a sp.	-
	sediment	8.4	EqP / medium	-	0.031	EqP	-
2,5-dichlorophenol	soil	53	EqP / low	-	0.11	EqP	-
	sediment	53	EqP / low	-	0.11	EqP	-
2,6-dichlorophenol	soil	57	EqP / low	-	0.093	EqP	-
	sediment	57	EqP / low	-	0.093	EqP	-
3,4-dichlorophenol	soil	27	EqP<10 a sp. / medium	45	0.051	EqP<a sp.	-
	sediment	27	EqP / low	-	0.051	EqP	-
3,5-dichlorophenol	soil	5.4	EqP<10 a sp. / medium	30	0.019	EqP<a sp.	-
	sediment	5.4	EqP / low	-	0.019	EqP	-
trichlorophenols	soil	22		15	0.17		0.04
	sediment	41		-	0.20		0.10
2,3,4-trichlorophenol	soil	30	EqP / low	-	0.085	EqP	-
	sediment	30	EqP / low	-	0.085	EqP	-
2,3,5-trichlorophenol	soil	4.5	10 b sp. / medium	15	0.045	1000 c sp.	-

Compound	Compartment	SRC _{eco} [mg/kg]	Method* / reliability score	Denneman and van Gestel (1990) [mg/kg]	MPC this report [mg/kg]	Method*	MPC INS [mg/kg]
2,3,6-trichlorophenol	sediment	22	EqP / low	-	0.051	EqP	-
	soil	110	EqP / low	-	0.30	EqP	-
2,4,5-trichlorophenol	sediment	110	EqP / low	-	0.30	EqP	-
	soil	22	EqP < 10 a sp. / medium	25	0.11	1000 a sp.	-
2,4,6-trichlorophenol	sediment	22	EqP / low	-	0.22	EqP	-
	soil	8.1	10 b sp. / medium	10	2.4	50 h sp.	-
3,4,5-trichlorophenol	sediment	80	EqP / low	-	3.0	EqP	-
	soil	39	EqP / low	-	0.078	EqP	-
tetrachlorophenols	sediment	39	EqP / low	-	0.078	EqP	-
	soil	21	-	-	0.050	-	0.3
2,3,4,5-tetrachlorophenol	sediment	22	-	-	0.050	-	0.086
	soil	64	10 a sp. / medium	65	0.092	EqP < a sp.	-
2,3,4,6-tetrachlorophenol	sediment	67	EqP / low	-	0.092	EqP	-
	soil	13	EqP / low	-	0.011	EqP	-
2,3,5,6-tetrachlorophenol	sediment	13	EqP / low	-	0.011	EqP	-
	soil	12	EqP / low	-	0.12	EqP	-
pentachlorophenol	sediment	12	EqP / low	-	0.12	EqP	-
	soil	12	10 b sp. < ref. pr. / high.	5	0.16	10 g sp. < ref pr.	0.20 ^a
	sediment	8.0	EqP / medium	-	0.40	EqP	0.17

* For the SRC_{eco} and the MPC the abbreviation ref. is used in case of refined risk assessment. EqP (equilibrium partitioning) or the assessment factor together with the designation according to Table 2.1 and Table 2.6 is given in case of preliminary risk assessment. Whether the SRC_{eco} or the MPC is based on species or processes is indicated by the abbreviation sp. and pr.

- a MPC by Van de Plassche (1994) were based on secondary poisoning for the terrestrial food chain for soil or the aquatic food chain for sediment. The MPC in sediment was calculated by equilibrium partitioning. The new MPCs for pentachlorophenol should therefore be 0.16 mg/kg for soil and 0.40 mg/kg for sediment.

Table 3.14: Summary of new SRC_{eco} values for chlorophenols in surface water, MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report.

Compound	Compartment	SRC _{eco} [µg/l]	Method* / reliability score	MPC this report [µg/l]	Method*	MPC INS [µg/l]
monochlorophenols	surface water	1000		6.0		25
2-chlorophenol	surface water	1400	1 c / medium	10	50 e	-
3-chlorophenol	surface water	2500	10 a / low	5.5	1000 a	-
4-chlorophenol	surface water	290	1 c / medium	4.0	50 i	-
dichlorophenols	surface water	870		2.1		15
2,3-dichlorophenol	surface water	1400	10 a / low	3.5	1000 a	-
2,4-dichlorophenol	surface water	410	ref. / high	1.5	ref.	-
2,5-dichlorophenol	surface water	1300	10 a / low	2.8	1000 a	-
2,6-dichlorophenol	surface water	2300	10 b / medium	3.7	1000 c	-
3,4-dichlorophenol	surface water	590	10 a / low	1.1	1000 a	-
3,5-dichlorophenol	surface water	420	10 a / low	1.5	1000 a	-
trichlorophenols	surface water	340		1.7		2.5
2,3,4-trichlorophenol	surface water	420	10 a / low	1.2	1000 a	-
2,3,5-trichlorophenol	surface water	260	10 a / low	0.60	1000 a	-
2,3,6-trichlorophenol	surface water	990	10 a / low	2.7	1000 a	-
2,4,5-trichlorophenol	surface water	160	1 c / medium	1.6	100 b	-
2,4,6-trichlorophenol	surface water	480	1 c / medium	18	10 h	-
3,4,5-trichlorophenol	surface water	190	10 a / low	0.38	1000 a	-
tetrachlorophenols	surface water	130		0.30		1.0
2,3,4,5-tetrachlorophenol	surface water	150	10 a / low	0.21	1000 a	-
2,3,4,6-tetrachlorophenol	surface water	160	10 b / medium	0.14	1000 c	-
2,3,5,6-tetrachlorophenol	surface water	95	1 c / medium	0.95	100 b	-
pentachlorophenol	surface water	85	ref. / high	4.3	ref.	2.0

* For the SRC_{eco} and the MPC the abbreviation ref. is used in case of refined risk assessment. The assessment factor together with the designation according to Table 2.1 and Table 2.5 is given in case of preliminary risk assessment.

Table 3.15: Summary of new SRC_{eco} values for other chlorinated aromatic hydrocarbons in soil or sediment, values as derived by Denneman and van Gestel (1990), MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report. Values are given as concentrations in mg/kg standard soil/sediment (soil containing 10% organic matter and 25% clay, sediment containing 10% organic matter and 25% clay).

Compound	Compartment	SRC _{eco} [mg/kg]	Method* / reliability score	Denneman and van Gestel (1990) [mg/kg]	MPC this report [mg/kg]	Method*	MPC INS [mg/kg]
sum monochloronaphthalenes	soil	23		-	0.12		-
	sediment	23		-	0.12		-
1-chloronaphthalene	soil	18	EqP / low	-	0.057	EqP	-
	sediment	18	EqP / low	-	0.057	EqP	-
2-chloronaphthalene	soil	30	EqP / low	-	0.25	EqP	-
	sediment	30	EqP / low	-	0.25	EqP	-
sum PCBs (planar) (#77, #105, and #126)	soil	3.4 (11 µmol/kg)		70 ^a	(0.034)		3·10⁻⁴b
	sediment	3.4		-	(0.034)		3·10⁻⁴b
PCB77	soil	4.2	EqP / low	-	(0.042)	EqP	4.2·10⁻⁴c
	sediment	4.2	EqP / low	-	(0.042)	EqP	4.2·10⁻⁴c
PCB105	soil	10	EqP / low	-	(0.10)	EqP	1.5·10⁻³c
	sediment	10	EqP / low	-	(0.10)	EqP	1.5·10⁻³c
PCB126	soil	0.92	EqP / low	-	(0.0092)	EqP	2.5·10⁻⁶c
	sediment	0.92	EqP / low	-	(0.0092)	EqP	2.5·10⁻⁶c

* For the SRC_{eco} and the MPC EqP (equilibrium partitioning) is used.

a Refers to the technical PCB mixture Aroclor 1254

b Refers to a concentration of PCB 118 representative for the sum of planar PCBs; bold value indicates that no update of the MPC is proposed.

c Data for secondary poisoning through the aquatic food chain for sediment were included in the derivation of these MPCs; bold value indicates that no update of the MPC is proposed.

Table 3.16: Summary of new SRC_{eco} values for other chlorinated aromatic hydrocarbons in surface water, MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report.

Compound	Compartment	SRC _{eco} [µg/l]	Method* / reliability score	MPC this report [µg/l]	Method*
sum monochloronaphthalenes	surface water	150		0.77	
1-chloronaphthalene	surface water	120	10 b / medium	0.37	1000 c
2-chloronaphthalene	surface water	190	10 a / low	1.6	1000 a
PCB77	surface water	(0.10)	10 a / low	(0.0010) ^a	100 b
PCB105	surface water	(0.13)	1 c / low	(0.0013) ^a	1000 a
PCB126	surface water	(0.018)	10 a / low	(1.8·10 ⁻⁴) ^a	100 b

* For the SRC_{eco} and the MPC the assessment factor together with the designation according to Table 2.1 and Table 2.5 is given.

a Values are not relevant because no data for secondary poisoning through the aquatic food chain sediment were included in the derivation of these MPCs.

3.7 SRC_{eco} for pesticides

For the DDT related compounds (DDT/DDD/DDE), the drins (aldrin, dieldrin and endrin), the hexachlorocyclohexanes (α -, β - en γ -HCH) and carbofuran the data presented by van de Plassche et al. (1994) are used to derive the SRC_{eco} values. For carbaryl, maneb and atrazine the data from Crommentuijn et al. (1997c) have been used. The proposed SRC_{eco} are summarised in 3.7.8. together with old values as proposed by Denneman and van Gestel (1990) and MPCs/NCs as proposed in the framework of the project 'Setting Integrated Environmental Quality Standards'. The selected data used for extrapolation are included in Appendix 8.

3.7.1 SRC_{eco} for DDT related compounds

For DDT and its derivatives DDE and DDD separate limits are derived. Afterwards it is considered whether values can be derived for the sum of the three compounds.

3.7.1.1 SRC_{eco} for DDT

For DDT one acute toxicity study is available for a terrestrial insect (Table A8. 1). With an ACR of 10 the HC50(terrestrial species) is 1.0 mg/kg. The MPC derived from this study with either the modified EPA method or the EU/TGD method is 0.010 mg/kg. Because of the limited data for terrestrial species a comparison with equilibrium partitioning is made. The few chronic data for fresh water organisms are significantly ($P = 0.046$) lower than for marine species (Table A8. 2 and Table A8. 3). However, regarding acute toxicity the marine species are more sensitive than the fresh water species ($P = 0.046$). For crustaceans this effect is not observed ($P = 0.59$) but marine fish are more sensitive ($P = 0.0052$). The chronic toxicity data that are available for fish show the opposite effect. The differences in sensitivity are rather inconclusive and therefore, fresh and marine water studies are combined. The geometric mean of the chronic toxicity data is 1.7 $\mu\text{g/l}$ and of the acute toxicity data 4.3 $\mu\text{g/l}$. With an ACR of 10 the HC50(aquatic species) becomes **0.43** $\mu\text{g/l}$. The MPC of **$4.4 \cdot 10^{-4}$** $\mu\text{g/l}$ for surface water is based on secondary poisoning (Van de Plassche, 1994). This is about a factor of 10 lower than the MPC derived directly from the aquatic toxicity data using the modified EPA method or the EU/TGD method (0.005 $\mu\text{g/l}$).

The log K_p for standard soil and sediment is 4.35 (Otte et al., 2001). This results in an HC50(EqP) of 10 mg/kg. This value is higher than the value based on the study for the terrestrial species. Consequently, the SRC_{eco} for soil is **1.0** mg/kg and for sediment **10** mg/kg. The MPC for sediment is calculated by equilibrium partitioning from the MPC for surface water. This current MPC is $9.4 \cdot 10^{-3}$ mg/kg (Van de Plassche, 1994). With the log K_p used here, this MPC is **$9.8 \cdot 10^{-3}$** mg/kg. The MPC for soil is derived from the terrestrial toxicity study, which is lower than the MPC based on secondary poisoning for the terrestrial food chain. This MPC is **0.010** mg/kg and is almost the same as the MPC(sediment) (Van de Plassche, 1994).

3.7.1.2 SRC_{eco} for DDE

For DDE no terrestrial data are available. Therefore, the HC50 for both soil and sediment are based on equilibrium partitioning. Only one chronic NOEC is available for a marine crustacean (Table A8. 5). The acute toxicity data for fresh and marine water are significantly different ($P = 0.046$), but this can be attributed to the different taxonomic groups in both sets. Fresh water fish and marine crustaceans are comparable in sensitivity. Therefore, the data of fresh water and marine species are combined. The geometric mean of these acute toxicity data

is 50 µg/l. The HC50(aquatic species) is equal to the only chronic NOEC of **0.10** µg/l. The MPC for DDE was set equal to that of DDT, **$4.4 \cdot 10^{-4}$** µg/l (Van de Plassche, 1994). With the modified EPA method an MPC of 0.0025 µg/l is derived after application of an assessment factor of 1000 to the lowest L(E)C50. The log K_{ow} of DDE is higher than 3 (Otte et al., 2001). Therefore, also, an MPC according to the EU/TGD method can be derived. The chronic NOEC is for the same taxonomic group as the lowest L(E)C50. Therefore, a factor of 100 is applied to this NOEC value, resulting in an MPC of 0.0010 µg/l. Both values are higher than that based on secondary poisoning.

The log K_p for standard soil and sediment is 4.12. This results in an SRC_{eco} for soil and sediment of **1.3** mg/kg. The current MPC for soil is based on that for DDT and is 0.010 mg/kg (Van de Plassche, 1994). The value derived by equilibrium partitioning from the MPC(aquatic species) by the EU/TGD method is only slightly higher: **0.013** mg/kg. The MPC of 0.0015 mg/kg for sediment was derived by equilibrium partitioning from the MPC for water from secondary poisoning (Van de Plassche, 1994). With the log K_p used here, this value is **$5.8 \cdot 10^{-3}$** mg/kg.

3.7.1.3 SRC_{eco} for DDD

Also for DDD no terrestrial data are available. For surface water only acute toxicity data are available (Table A8. 6 and Table A8. 7). The data for fresh and marine water are not significantly different ($P = 0.48$) and are combined. The geometric mean is 38 µg/l. With an ACR of 10 this leads to an HC50(aquatic species) of **3.8** µg/l. Also for DDD the MPC was set equal to that of DDT, **$4.4 \cdot 10^{-4}$** µg/l (Van de Plassche, 1994). With the modified EPA method an MPC of 0.024 µg/l is derived by applying an assessment factor of 100 to the lowest L(E)C50, because data are available for algae, crustaceans (a.o. *Daphnia*) and fish. According to the EU/TGD method an assessment factor of 1000 is applied in this case resulting in an MPC of 0.0024 µg/l. Both values are higher than that based on secondary poisoning.

The log K_p for standard soil and sediment is 3.95. This results in an SRC_{eco} for soil and sediment of **34** mg/kg. The current MPC for soil is based on that for DDT and is 0.010 mg/kg (Van de Plassche, 1994). The value derived by equilibrium partitioning from the MPC(aquatic organisms) by the EU/TGD method is only slightly higher: **0.021** mg/kg. The MPC of 0.0018 mg/kg for sediment was derived by equilibrium partitioning from the MPC for water from secondary poisoning (Van de Plassche, 1994). With the log K_p used here, this value is **$3.9 \cdot 10^{-3}$** mg/kg.

3.7.1.4 Combined values for the DDT related compounds

DDT, DDE and especially DDD differ markedly in their properties, both regarding physico-chemical properties and toxicity. The acute toxicity data (L(E)C50s) of both DDE and DDD are significantly higher than those of DDT. Further, the difference in log K_{ow} is more than half a unit. Therefore, no combined SRC_{eco} value is derived for the DDT related compounds. Due to differences in the available information other assessment factors are used for the derivation of the MPC. For this reason, the MPCs for DDT, DDE and DDD derived from aquatic toxicity data are in the same order of magnitude. However, the MPC for water for DDT is based on secondary poisoning and the MPCs for DDE and DDD were set equal to this value (Van de Plassche, 1994). For soil the MPC for DDT based on direct effects was lower than that from secondary poisoning. Although these compounds show different toxicity, the MPCs for DDE and DDD derived by equilibrium partitioning are almost the same as this MPC for DDT.

3.7.2 SRC_{eco} for drins

In the derivation of the MPC in the framework of the project 'Setting Integrated Environmental Quality Standards' aldrin and dieldrin are treated as one, because aldrin is rapidly converted to dieldrin in surface water and soil (Van de Plassche, 1994). Also for the derivation of the SRC_{eco}, the data for dieldrin and aldrin are combined. For this goal the data for aldrin are recalculated as dieldrin, which contains one more oxygen atom.

3.7.2.1 SRC_{eco} for aldrin and dieldrin

Acute as well as chronic studies with terrestrial species are available for aldrin (Table A8. 8) and dieldrin (Table A8. 12). For dieldrin also a few data for terrestrial processes are available (Table A8. 11), but these are less sensitive than the species. The insect species tested with dieldrin in a chronic toxicity study is less sensitive than the taxonomic groups tested with aldrin, but still fits well in the overall distribution ($P = 7.1\%$). The acute toxicity data for aldrin and dieldrin compare very well to each other ($P = 0.41$). Because aldrin is rapidly converted to dieldrin, the data for aldrin and dieldrin are combined.

The geometric mean of the chronic toxicity data is 19 mg/kg and that of the acute toxicity data 2.2 mg/kg (expressed as dieldrin). With an ACR of 10 the HC50(terrestrial species) is equal to 0.22 mg/kg. This value for the sum of the two compounds is expressed as a concentration of dieldrin. Because aldrin and dieldrin do not have the same molecular weight it is better to express this value on a molar basis: 0.57 $\mu\text{mol/kg}$.

The MPC of 0.050 mg/kg in soil was based on direct effects by means of the modified EPA method (Van de Plassche, 1994). With the EU/TGD method an assessment factor of 50 is applied to the 3 NOECs of 34 mg/kg for terrestrial processes. The MPC(terrestrial processes) is thus 0.68 mg/kg. The lowest L(E)C50 for terrestrial species is for an insect species tested with aldrin. The insect species tested with dieldrin show comparable L(E)C50s. The lowest of 4 NOECs is for an insect species too, tested with dieldrin. Therefore, an assessment factor of 10 can be applied to this value according to the EU/TGD method, resulting in the same MPC of 0.050 mg/kg. On a molar basis this value for the sum of the two compounds is 0.13 $\mu\text{mol/kg}$.

Because of the limited number of data, both SRC_{eco} and MPC are compared with equilibrium partitioning. The acute toxicity data with fresh water and marine species (Table A8. 9 and Table A8. 10) are significantly different for aldrin ($P = 0.021$). This effect is only observed for fish species and not for crustaceans. For dieldrin no significant differences ($P = 0.19$) were found between fresh water and marine species (Table A8. 13 and Table A8. 14). The chronic data from aldrin are similar to those of dieldrin ($P = 0.27$) and therefore the data of both compounds are combined. Data are available for 5 taxonomic groups and statistical extrapolation is performed (Figure 3.37). The HC50(aquatic species) is 3.4 $\mu\text{g/l}$ (90% CI: 1.1 – 10.4 $\mu\text{g/l}$, expressed as dieldrin) or 0.0089 $\mu\text{mol/l}$.

The HC5 of this distribution is 0.075 $\mu\text{g/l}$ (90% CI: 0.008 – 0.293 $\mu\text{g/l}$). For dieldrin alone the HC5 would be 0.057 $\mu\text{g/l}$. With only one value for fresh water cyanophyta (Van de Plassche, 1994) the HC5 with the log-normal distribution is 0.032 $\mu\text{g/l}$, similar to the old value with the log-logistic distribution of 0.029 $\mu\text{g/l}$. The MPC of **0.018** $\mu\text{g/l}$ for dieldrin and aldrin is based on secondary poisoning (Van de Plassche, 1994).

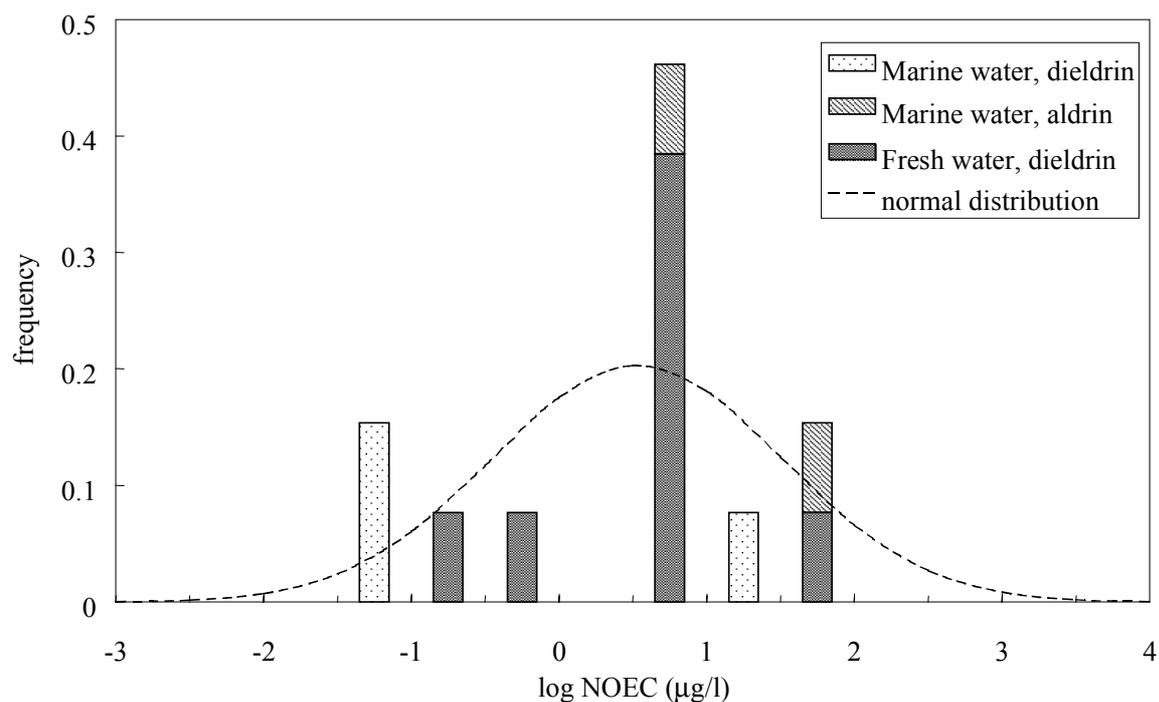


Figure 3.37: Dieldrin and aldrin: Chronic toxicity for fresh water and marine species. The estimated distribution is based on the combined sets ($n = 13$, $\bar{x} = 0.53$, $s = 0.98$).

The log K_p for standard soil and sediment is 2.76 for dieldrin and 2.71 for aldrin. With the HC50 of 3.4 µg/l, an HC50(EqP) of 1.9 mg/kg for dieldrin and 1.7 for aldrin is obtained. The HC50 for soil is directly obtained from the terrestrial data and is **0.22** mg/kg. For sediment the HC50s of **1.9** and **1.7** mg/kg, obtained by equilibrium partitioning, are used for dieldrin and aldrin, respectively. The MPCs for dieldrin and aldrin in soil and sediment were derived in the same way (Van de Plassche, 1994). The MPC for soil derived by the modified EPA method was 0.050 mg/kg and the MPCs for sediment were 0.12 mg/kg for aldrin and 0.67 mg/kg for dieldrin (Van de Plassche, 1994). However, with the lower values for the log K_p for standard soil and sediment used here, these values are much lower too. For soil, the MPC can be derived by equilibrium partitioning from the MPC of 0.075 µg/l derived for aquatic species. The resulting MPCs in soil for dieldrin and aldrin are **0.043** and **0.038** mg/kg. For sediment, the MPC can be derived from the MPC for water based on secondary poisoning. The resulting MPCs in sediment for dieldrin and aldrin are **0.010** and **0.0092** mg/kg.

3.7.2.2 SRC_{eco} for endrin

One acute toxicity study with terrestrial species is available for endrin (Table A8. 15). The value of 0.95 mg/kg from this study is compared with equilibrium partitioning. Both for acute and chronic toxicity there are no significant differences between fresh water and marine species (Table A8. 16 and Table A8. 17, $P = 0.41$ and 0.76 respectively). Chronic toxicity data are available for five different taxonomic groups and the data follow the log-normal distribution. Consequently, statistical extrapolation can be performed (Figure 3.38). The HC50(aquatic species) is **0.92** µg/l (90% CI: 0.17 – 4.96 µg/l).

The HC5 determined with the log-normal distribution is **0.0049** µg/l (90% CI: 0.0002 – 0.0369 µg/l). The slightly lower MPC of 0.0030 µg/l for endrin was derived using the modified EPA method (Van de Plassche, 1994). The value for indirect effects (secondary poisoning) was slightly higher than this HC50: 0.0063 µg/l.

The log K_p for standard soil and sediment is 2.72. The resulting HC50(EqP) is 0.48 mg/kg. However, with an ACR of 10 the HC50(terrestrial species) is lower and therefore, the HC50 for soil is equal to **0.095** mg/kg. For sediment the HC50 is **0.48** mg/kg.

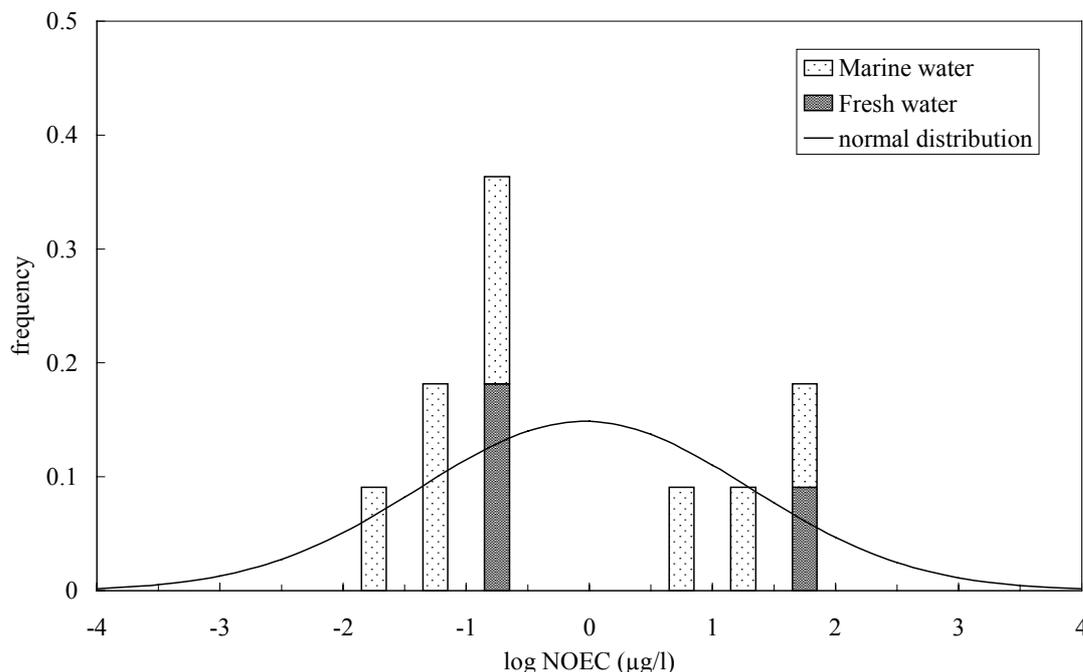


Figure 3.38: Endrin: Chronic toxicity for fresh water and marine species. The estimated log-normal distribution is based on the combined sets of data ($n = 11$, $\bar{x} = -0.04$, $s = 1.34$).

The old MPC of 0.0029 mg/kg for soil was based on equilibrium partitioning with the MPC for surface water, because there is only one acute terrestrial toxicity study (Van de Plassche, 1994). With one L(E)C50 an assessment factor of 1000 is applied according to both the modified EPA method and the EU/TGD method, resulting in a new MPC of $9.5 \cdot 10^{-4}$ mg/kg. The MPC for sediment derived by equilibrium partitioning is **0.0026** mg/kg.

3.7.2.3 Combined values for drins

For aldrin and dieldrin one value for both compounds has already been derived. Both the physico-chemical properties and the toxicity of endrin are similar to that of dieldrin and aldrin. If combined risk limits are desired, a value for drins can be established. For surface water SRC_{eco} is derived from the geometric mean of the 2 HC50s for aldrin/dieldrin and endrin and is **1.8** µg/l. The SRC_{eco} for soil is **0.14** mg/kg (geometric mean of dieldrin/aldrin and endrin) and for sediment **1.2** mg/kg (geometric mean of aldrin, dieldrin and endrin). For the MPCs, the geometric mean for surface water for secondary poisoning of **0.011** µg/l (geometric mean of dieldrin/aldrin and endrin) is lower than for direct aquatic toxicity studies (0.019 µg/l). With equilibrium partitioning the MPC for the sum of drins in sediment is **0.0068** mg/kg (geometric mean of aldrin, dieldrin and endrin), which is based on secondary poisoning throughout the aquatic food chain. For drins in soil the MPC is **0.012** (geometric mean of aldrin, dieldrin and endrin). All ERLs for the sum of drins are based on the molecular weight of dieldrin and endrin. Concentrations of aldrin should be recalculated to dieldrin.

3.7.3 SRC_{eco} for hexachlorocyclohexanes (HCHs)

For HCHs the data from the project ‘Setting Integrated Environmental Quality Standards’ have been used. Studies for three HCH isomers (α -, β - and γ -HCH or lindane) reported. These isomers are treated separately.

3.7.3.1 SRC_{eco} for α -HCH

No terrestrial data are available for α -HCH. Therefore, the SRC_{eco} for soil has to be derived by equilibrium partitioning. Chronic toxicity data are available for six fresh water and one marine species (Table A8. 18 and Table A8. 19). The marine species fits well in the overall log-normal distribution ($P = 0.43$) and both sets are combined. Because chronic toxicity data are available for 5 taxonomic groups, statistical extrapolation is applied to the data (Figure 3.39). The HC50(aquatic species) is $1.4 \cdot 10^2 \mu\text{g/l}$ (90% CI: $0.3 \cdot 10^2 - 6.1 \cdot 10^2 \mu\text{g/l}$).

The HC5 based on the log-normal distribution is $3.9 \mu\text{g/l}$ (90% CI: $0.1 - 20.6 \mu\text{g/l}$). The HC5 derived by the log-logistic distribution was $3.5 \mu\text{g/l}$. The MPC of $2.5 \mu\text{g/l}$ for α -HCH is based on secondary poisoning (Van de Plassche, 1994).

The log K_p for standard soil and sediment is 2.10. With equilibrium partitioning, the resulting HC50 for soil and sediment is 17 mg/kg . Equilibrium partitioning was also used to derive the MPC of 0.22 mg/kg for soil and sediment from the MPC for secondary poisoning through the aquatic food chain (Van de Plassche, 1994). For the terrestrial compartment, a comparison was also made with an estimate for secondary poisoning through the terrestrial food chain. With the log K_p used here, this value is 0.31 mg/kg .

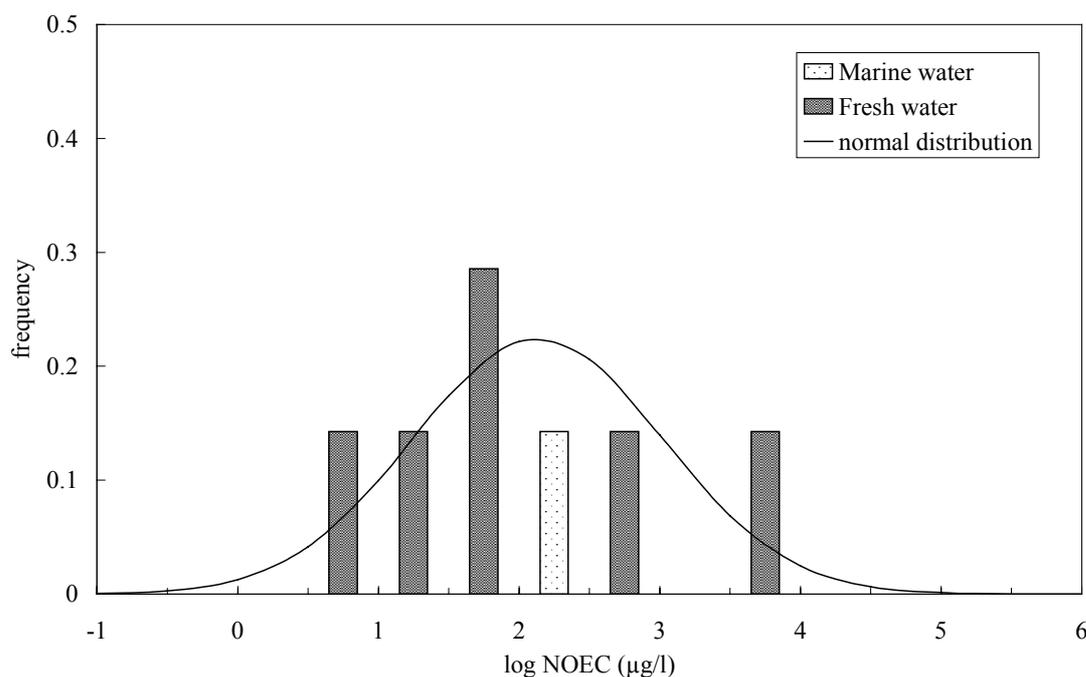


Figure 3.39: α -HCH: Chronic toxicity for fresh water and marine species. The estimated log-normal distribution is based on the combined sets of data ($n = 7$, $\bar{x} = 2.13$, $s = 0.89$).

3.7.3.2 SRC_{eco} for β -HCH

Also for β -HCH, no terrestrial data are available. Chronic toxicity data are available for five fresh water and one marine species (Table A8. 20 and Table A8. 21). The marine species fits in the overall log-normal distribution ($P = 0.20$) and both sets are combined. Because chronic

toxicity data are available for 4 taxonomic groups, statistical extrapolation is performed (Figure 3.40). The HC50(aquatic species) is **93** $\mu\text{g/l}$ (90% CI: 27 – 320 $\mu\text{g/l}$). The HC5 based on the log-normal distribution is 6.7 $\mu\text{g/l}$ (90% CI: 0.4 – 24.9 $\mu\text{g/l}$). The MPC of **0.080** $\mu\text{g/l}$ for β -HCH is based on secondary poisoning (Van de Plassche, 1994). The log K_p for standard soil and sediment is 2.14. With equilibrium partitioning, the resulting SRC_{eco} for soil and sediment is **13** mg/kg. Equilibrium partitioning was also used to derive the MPC of 0.092 mg/kg for soil and sediment from the MPC for secondary poisoning through the aquatic food chain (Van de Plassche, 1994). For the terrestrial compartment, a comparison was also made with an estimate for secondary poisoning through the terrestrial food chain. With the log K_p used here, this MPC becomes is **0.011** mg/kg.

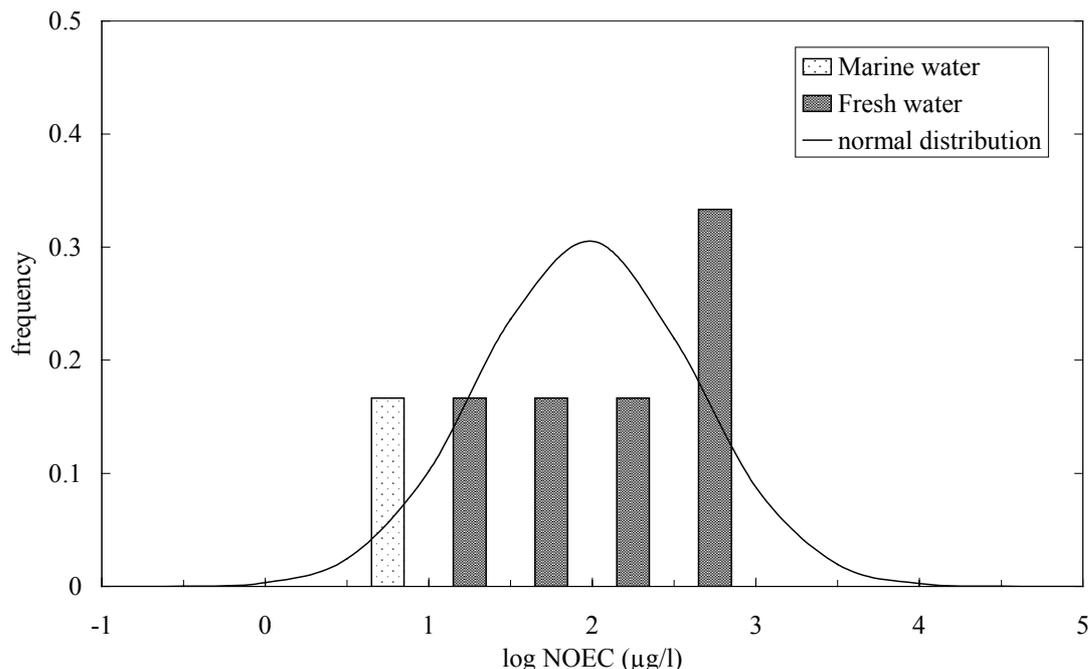


Figure 3.40: β -HCH: Chronic toxicity for fresh water and marine species. The estimated log-normal distribution is based on the combined sets of data ($n = 6$, $\bar{x} = 1.97$, $s = 0.65$).

3.7.3.3 SRC_{eco} for γ -HCH (lindane)

A few acute as well as chronic toxicity data for terrestrial species are available for lindane (Table A8. 22). The geometric mean of the chronic toxicity data is 1.2 mg/kg. Applying an ACR of 10 to the geometric mean of the acute toxicity data gives a slightly higher value of 1.7 mg/kg. Consequently, the HC50(terrestrial species) is 1.2 mg/kg. This value is compared with a value derived by equilibrium partitioning.

Enough aquatic toxicity data for fresh water and marine species (Table A8. 23 and Table A8. 24) are available to perform statistical extrapolation. The data for the marine species are significantly different from the data for fresh water species. However, these data are from one study for two marine molluscs, and from the fresh water species, it seems that molluscs are a relatively insensitive species to lindane. Therefore, both sets are combined in the statistical extrapolation (Figure 3.41). The HC50(aquatic species) is **87** $\mu\text{g/l}$ (90% CI: 26 – 287 $\mu\text{g/l}$). The HC5 based on the log-normal distribution is 1.2 $\mu\text{g/l}$ (90% CI: 0.1 – 5.5 $\mu\text{g/l}$). The MPC of **0.77** $\mu\text{g/l}$ for lindane is based on secondary poisoning (Van de Plassche, 1994).

The log K_p for standard soil and sediment is 1.76. With equilibrium partitioning, the resulting HC50(EqP) is 5.0 mg/kg. Therefore, the SRC_{eco} for sediment is **5.0** mg/kg and the SRC_{eco} for

soil is **1.2 mg/kg**, based on the terrestrial HC50. The MPC of 0.0050 mg/kg in soil was derived with the modified EPA method, by applying a factor of 10 on the lowest NOEC (Van de Plassche, 1994). Both values are for the same insect species, which can be considered to belong to a sensitive taxonomic group for lindane. However, if the modified EPA method is strictly followed, a comparison with the acute toxicity data is made. Applying an assessment factor of 1000 to the lowest L(E)C50 gives a value that is much lower: $8.4 \cdot 10^{-4}$ mg/kg. Because chronic NOECs are available for the same taxonomic groups as for the acute toxicity data, an assessment factor of 50 is applied to the lowest of 2 NOECs according to the EU/TGD method. This results in a similar MPC of **0.0010 mg/kg**. The MPC of 0.19 mg/kg for sediment was derived by equilibrium partitioning from the MPC for surface water. With the log K_p value used here this MPC is **0.044 mg/kg**.

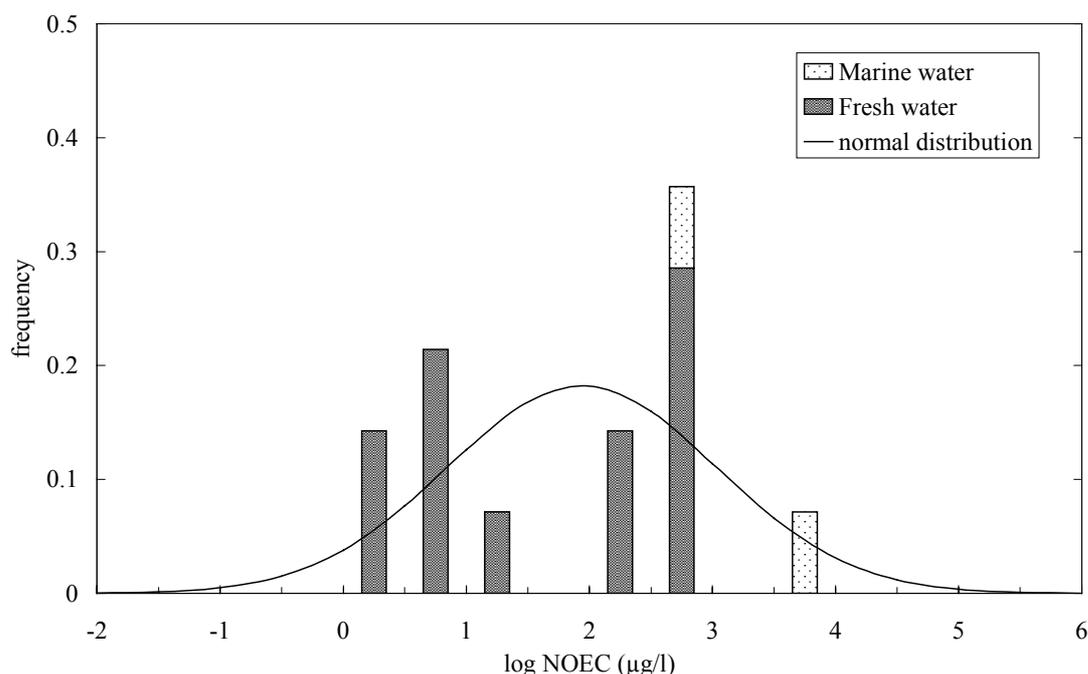


Figure 3.41: Lindane: Chronic toxicity for fresh water and marine species. The estimated log-normal distribution is based on the combined sets of data ($n = 14$, $\bar{x} = 1.94$, $s = 1.10$).

3.7.3.4 Combined values for HCHs

For the three considered HCH isomers, the toxicity and physico-chemical properties seem to be very similar to each other. The differences in the HC50 values for soil are mainly caused by the absence of terrestrial toxicity data for α - and β -HCH. Therefore, values can be presented for the sum of the three isomers, if desired. For surface water the geometric mean of the HC50 is $1.0 \cdot 10^2$ µg/l. The geometric mean of the HC50s(soil) of **6.4 mg/kg** can be taken as the SRC_{eco} for the sum of HCHs in soil. For sediment the SRC_{eco} for the sum of HCHs is **10 mg/kg**.

The geometric means of the MPCs are 3.2 µg/l for surface water, 0.077 mg/kg for soil, and 0.32 mg/kg for sediment if derived from direct toxicity data and equilibrium partitioning. If however, the data for secondary poisoning are considered, the resulting MPCs for the sum of HCHs are **0.54 µg/l** for water and **0.054 mg/kg** for soil and sediment.

3.7.4 SRC_{eco} for carbaryl

For carbaryl toxicity data are available for terrestrial organisms. However, most of these data are of deviating tests. These studies are often rejected because of the low purity of the pesticides (commercial products). To calculate a geometric mean for the derivation of the HC50 values these studies are nevertheless taken into account (Table A8. 25). The geometric mean of the chronic toxicity data is 97 mg/kg. The geometric mean of the acute toxicity data is 73 mg/kg. With an ACR of 10 the HC50(terrestrial species) becomes 7.3 mg/kg. Also one NOEC of $1.2 \cdot 10^2$ mg/kg for terrestrial processes is available (Table A8. 26). The minimum value of these two, the HC50(soil, direct), is compared with a value derived by equilibrium partitioning.

The chronic toxicity data for fresh water and marine species (Table A8. 27 and Table A8. 28) compare well to each other ($P = 0.70$) and consequently both sets of data are combined. Enough aquatic toxicity data are available to perform statistical extrapolation (Figure 3.42). The HC50(aquatic species) is **41** $\mu\text{g/l}$ (90% CI: 11 – 153 $\mu\text{g/l}$). The HC5 based on the log-normal distribution is **0.23** $\mu\text{g/l}$ (90% CI: 0.02 – 1.21 $\mu\text{g/l}$). The MPC derived by the log-logistic distribution was 0.23 $\mu\text{g/l}$ too (Crommentuijn et al., 1997b).

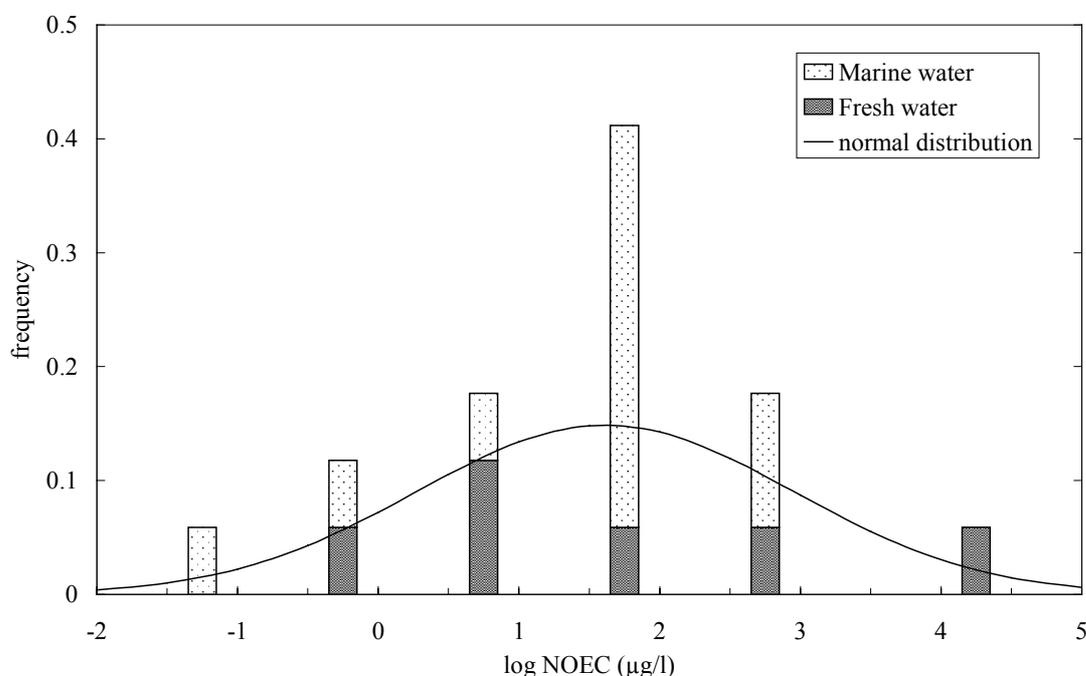


Figure 3.42: Carbaryl: Chronic toxicity for fresh water and marine species. The estimated log-normal distribution is based on the combined sets of data ($n = 17$, $\bar{x} = 1.61$, $s = 1.34$).

The log K_p for standard soil and sediment is 1.04. With equilibrium partitioning, the resulting HC50(EqP) is 0.45 mg/kg. Therefore, the SRC_{eco} for soil and sediment is equal to **0.45** mg/kg. The MPC of 0.12 mg/kg for soil is based on the lowest L(E)C50 with a safety factor of 100 (Crommentuijn et al., 1997b). A factor of 100 instead of 1000 was applied, because insects are expected to be a sensitive taxonomic group for carbaryl. If the deviating test are also considered, a similar value is derived with the EU/TGD method. Three NOECs are available including one for insects. Applying an assessment factor of 10 to this value results in an MPC of 0.16 mg/kg. With equilibrium partitioning the MPC is 0.0025 mg/kg. For soil no comparison with equilibrium was made with equilibrium partitioning in the case that an MPC could be derived from terrestrial data (Crommentuijn et al., 1997b). The MPC for

sediment of **0.0025** mg/kg was derived by equilibrium partitioning (Crommentuijn et al., 1997b).

3.7.5 SRC_{eco} for carbofuran

For carbofuran chronic and acute toxicity data are available for terrestrial species (Table A8. 29). The geometric mean of the chronic toxicity data is 2.4 mg/kg. The geometric mean of the acute toxicity data is 4.1 mg/kg. With an ACR of 10 the HC50(terrestrial species) of 0.41 mg/kg is obtained. Also three NOECs for terrestrial processes are available (Table A8. 30). From these data an HC50(terrestrial processes) of 8.0 mg/kg is derived. The minimum value of these two, the HC50(soil, direct), is compared with a value derived by equilibrium partitioning.

Chronic toxicity data are available for crustaceans and fish for both fresh and marine water (Table A8. 31 and Table A8. 32). These data are not significantly different ($P = 0.43$). The geometric mean of these data is 6.5 $\mu\text{g/l}$. Also the acute toxicity data are not significantly different ($P = 0.11$). The geometric mean of these data is 99 $\mu\text{g/l}$. Therefore, the HC50(aquatic species) is **6.5** $\mu\text{g/l}$. The MPC of carbofuran of 0.015 $\mu\text{g/l}$ is based on the lowest L(E)C50 with a safety factor of 100 (Van de Plassche, 1994). Although no data are available for algae, a factor of 100 was used because many other data for 4 taxonomic groups are available for carbofuran. Strictly no MPC can be derived according to the EU/TGD method because the base set is not complete and carbofuran has a $\log K_{ow}$ lower than 3 (Otte et al., 2001). If the same reasoning is followed as was done by Van de Plassche et al. (1994), the base set can be considered as complete. Then the lowest NOEC is for the same taxonomic group as the lowest L(E)C50 and an assessment factor of 10 can be applied to the lowest of 4 NOECs. This results in an MPC of **0.050** $\mu\text{g/l}$.

The $\log K_p$ for standard soil and sediment is 0.41. With equilibrium partitioning, the resulting HC50(EqP) is 0.017 mg/kg. Therefore, the HC50 for soil and sediment is equal to **0.017** mg/kg. The MPC for soil of 0.0047 mg/kg was obtained by the modified EPA method, after applying a factor of 100 to the lowest L(E)C50 (Van de Plassche, 1994). The MPC according to the EU/TGD method is 0.010 mg/kg in this case by applying a factor of 50 to the lowest of 3 NOECs. The MPC for sediment of $3.2 \cdot 10^{-5}$ mg/kg was derived by equilibrium partitioning (Van de Plassche, 1994). With the value for $\log K_p$ used here and the MPC of 0.050 $\mu\text{g/l}$, an MPC of **$1.3 \cdot 10^{-4}$** mg/kg is derived.

3.7.6 SRC_{eco} for maneb

For maneb terrestrial toxicity data are available for species (Table A8. 33) and processes (Table A8. 34). There is only one acute study for terrestrial species. Applying an ACR of 10 to this value of 220 mg/kg, gives an HC50(terrestrial species) of 22 mg/kg. The geometric mean of the NOECs for the terrestrial processes is 87 mg/kg. Because maneb is a polymeric pesticide, soil-water partitioning is not well defined and therefore, the SRC_{eco} for soil is directly derived from terrestrial data and not compared to equilibrium partitioning. The SRC_{eco} for soil is also **22** mg/kg. The same motivation was used for the derivation of the MPC for soil of **0.22** mg/kg, derived by the modified EPA method (Crommentuijn et al., 1997b). With the EU/TGD method the same value is derived. No separate value for sediment can be derived by equilibrium partitioning.

For water only the chronic toxicity data are taken into account (Table A8. 35), because the geometric mean of the acute toxicity data is obviously much higher than that of the chronic toxicity data and the solubility of this compound is not well defined. The geometric mean of

these data is **32** µg/l. The MPC for water of 0.012 µg/l was derived by the modified EPA method with a factor of 100 applied to the lowest L(E)C50 for *Vibrio fischeri*, because acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish (Crommentuijn et al., 1997b). With the EU/TGD method an assessment factor of 100 is applied to the lowest NOEC in this case. The resulting MPC is **0.18** µg/l.

3.7.7 SRC_{eco} for atrazine

Also for atrazine the studies from a deviating test with a compound purity of less than 80% have been used to derive the HC50 for terrestrial species (Table A8. 36). The geometric mean of the chronic toxicity data is 36 mg/kg. Chronic toxicity data are available for 4 taxonomic groups (Figure 3.43). However, one of these NOECs comes from a deviating test and the taxonomic groups are relatively insensitive compared to the acute toxicity data. Therefore, the acute toxicity data are used to base the HC50(terrestrial species) upon. The geometric mean of the acute toxicity data is 22 mg/kg. Applying an ACR of 10 to this value yields an HC50(terrestrial species) of 2.2 mg/kg. The geometric mean of 3.1 mg/kg of the NOECs for terrestrial processes is slightly higher (Table A8. 37). Because of the limited amount of studies from non-deviating tests, the HC50 of 2.2 mg/kg directly determined from terrestrial data is compared with equilibrium partitioning.

For the derivation of the MPC of 0.024 mg/kg a factor of 10 was applied to lowest NOEC for terrestrial processes according to the modified EPA method (Crommentuijn et al., 1997b).

The MPC for terrestrial species was derived by applying a safety factor of 100 to the lowest L(E)C50, although this was a value from a deviating test. The factor of 100 was used because acute data are available for earthworms and plants and chronic data for arthropods, which are not more sensitive (Crommentuijn et al., 1997b). For both terrestrial processes and species 3 or more NOECs are available. According to the EU/TGD method an assessment factor of 50 is applied to the lowest NOEC in both cases. The minimum MPC for soil is that for processes of 0.0048 mg/kg.

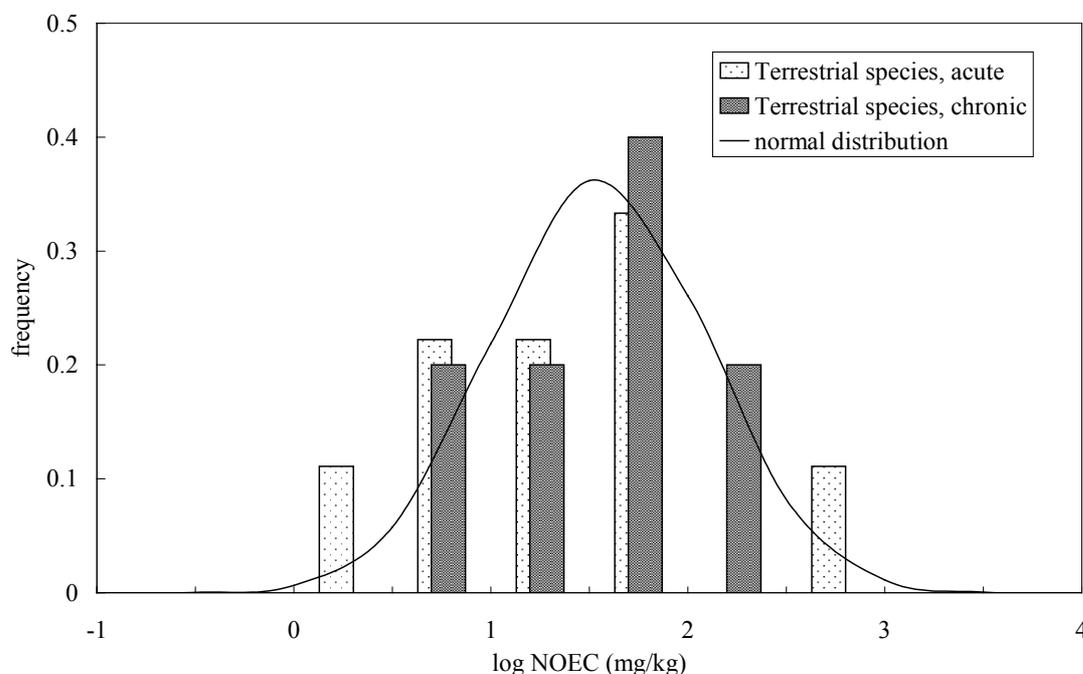


Figure 3.43: Atrazine: Chronic and acute toxicity for terrestrial species. The estimated log-normal distribution is based on the chronic data ($n = 5$, $\bar{x} = 1.55$, $s = 0.55$).

Chronic toxicity data are available for cyanophyta, algae, crustaceans, insects and fish for fresh water species (Table A8. 38) and for algae, crustaceans and fish for marine species (Table A8. 39). The fresh water and marine data are not significantly different ($P = 0.37$). Because sufficient taxonomic groups are available, statistical extrapolation can be performed (Figure 3.44). The HC50(aquatic species) is **76 $\mu\text{g/l}$** (90% CI: 38 – 153 $\mu\text{g/l}$). The HC5 based on the log-normal distribution is **2.9 $\mu\text{g/l}$** (90% CI: 0.8 – 7.3 $\mu\text{g/l}$) is the same as the MPC derived by the log-logistic distribution (Crommentuijn et al., 1997b).

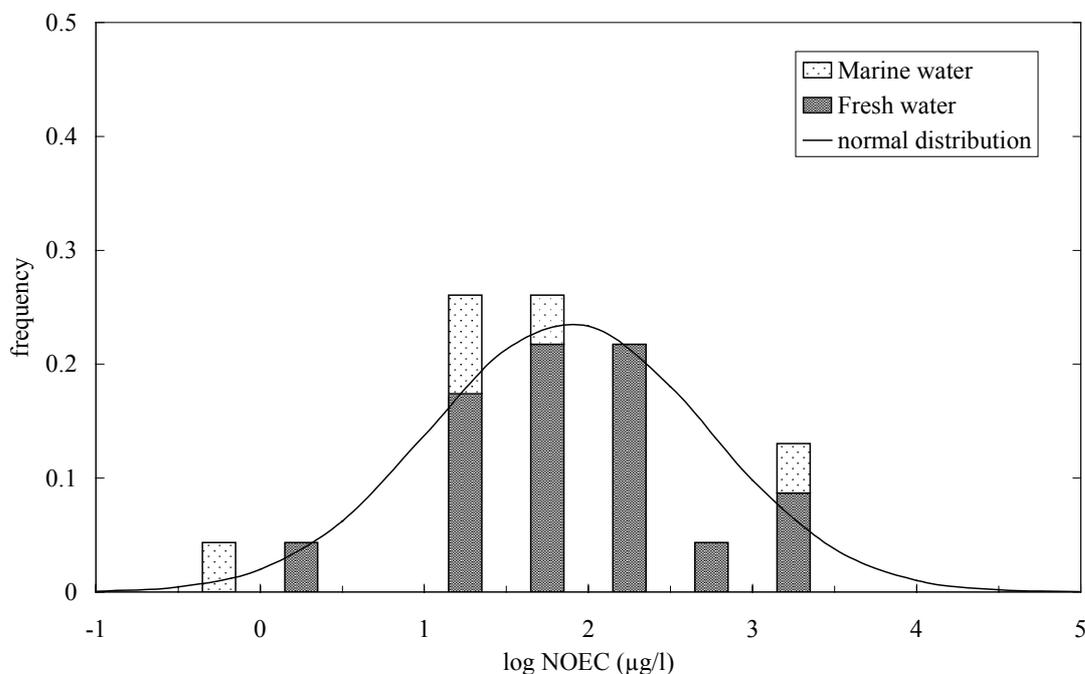


Figure 3.44: Atrazine: Chronic toxicity for fresh water and marine species. The estimated log-normal distribution is based on the combined sets of data ($n = 23$, $\bar{x} = 1.88$, $s = 0.85$).

The log K_p for standard soil and sediment is 0.97. With equilibrium partitioning, the resulting HC50(EqP) is 0.71 mg/kg. This value is a factor of 3 lower than the HC50 derived directly from terrestrial toxicity studies. Therefore, the SRC_{eco} for soil and sediment is equal to **0.71 mg/kg**. Applying equilibrium partitioning to the MPC for water results in an MPC of 0.027 mg/kg. The MPC for soil is thus **0.0048 mg/kg** and the MPC for sediment **0.027 mg/kg**.

3.7.8 Summary and comparison with old values and MPCs

In Table 3.17 the SRC_{eco} for pesticides are summarised. Besides the values derived in the present report also the old values derived in Denneman and Van Gestel (1990) and the MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards'. The ERLs for surface water are presented in Table 3.18. For drins and HCHs also values for the sum of these compounds have been derived.

Table 3.17: Summary of new SRC_{eco} values for pesticides in soil or sediment, values as derived by Denneman and van Gestel (1990) and MPC/NC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards'. Values are given as concentrations in mg/kg standard soil/sediment (soil containing 10% organic matter and 25% clay, sediment containing 10% organic matter and 25% clay).

Compound	Compartment	SRC _{eco} [mg/kg]	Method* / reliability score	Denneman and van Gestel (1990) [mg/kg]	MPC this report [mg/kg]	Method*	MPC/INS [mg/kg]
DDT	soil	1.0	10 a sp. / medium	1.3	0.010	1000 a	0.010 ^a
	sediment	10	EqP / low	-	0.0098 ^d	EqP	0.0094 ^c
DDE	soil	1.3	EqP / low	-	0.013	EqP	(0.010)
	sediment	1.3	EqP / low	-	0.0058 ^d	EqP	0.0015 ^c
DDD	soil	34	EqP / low	-	0.021	EqP	(0.010)
	sediment	34	EqP / low	-	0.0039 ^d	EqP	0.0018 ^c
sum drins	soil	0.14		-	0.012		-
	sediment	1.2		-	0.0068 ^e		-
aldrin/dieldrin	soil	0.22	10 b sp. / medium	-	-		-
	soil	-		0.35	0.038	EqP<g sp.<h pr.	0.050 ^a
aldrin	sediment	1.7	EqP / medium	-	0.0092 ^d	EqP	0.12 ^c
	soil	-		4.0	0.043	EqP<g sp.<h pr.	0.050 ^a
dieldrin	sediment	1.9	EqP / medium	-	0.010 ^d	EqP	0.67 ^c
	soil	0.095	10 a sp. / medium	0.05	9.5·10 ⁻⁴	1000 a sp.	9.5·10 ^{-4 a}
endrin	sediment	0.48	EqP / medium	-	0.0026	EqP	0.0029 ^b
	soil	6.4		-	0.054 ^f		-
sum HCHs	sediment	10		-	0.054 ^f		-
	soil	17	EqP / medium	-	0.31 ^d	EqP	0.22 ^c
<i>α</i> -HCH	sediment	17	EqP / medium	-	0.31 ^d	EqP	0.22 ^c
	soil	13	EqP / medium	-	0.011 ^d	EqP	0.092 ^c
<i>β</i> -HCH	sediment	13	EqP / medium	-	0.011 ^d	EqP	0.092 ^c
	soil	1.2	1 c sp. / medium	2	0.0010	50 e sp.	0.0050 ^a
<i>γ</i> -HCH	sediment	5.0	EqP / medium	-	0.044 ^d	EqP	0.19 ^c
	soil	0.45	EqP<10 b sp.<1 c pr. / medium	5	0.0025	EqP<g sp.<b pr.	0.12 ^a
carbaryl	sediment	0.45	EqP / medium	-	0.0025	EqP	0.0025 ^b
	soil	0.017	EqP<10 b sp.<1 c pr. / medium	1.5	1.3·10 ⁻⁴	EqP<h sp.<h pr.	0.0047 ^a
carbofuran	sediment	0.017	EqP / low	-	1.3·10 ⁻⁴	EqP	3.2·10 ^{-5 b}
	soil	22	10 a / sp. / medium	30	0.22	1000 a sp.<h pr.	0.22 ^a
maneb	sediment	-	-	-	-	-	-
	soil	0.71	EqP<10 b sp.<1 c pr. / medium	90	0.0048	50 h pr.<h sp.	0.024 ^a
atrazine	sediment	0.71	EqP / medium	-	0.027	EqP	0.026 ^b

- * For the SRC_{eco} and the MPC the abbreviation ref. is used in case of refined risk assessment. EqP (equilibrium partitioning) or the assessment factor together with the designation according to Table 2.1 and Table 2.6 is given in case of preliminary risk assessment. Whether the SRC_{eco} or the MPC is based on species or processes is indicated by the abbreviation sp. and pr.
- a Derived from direct effects to terrestrial organisms or processes.
 - b Derived by equilibrium partitioning from direct effects to aquatic organisms.
 - c Derived by equilibrium partitioning from secondary poisoning effects for the aquatic food chain.
 - d Calculated by equilibrium partitioning from the MPC for secondary poisoning effects for the aquatic food chain (Van de Plassche, 1994) with the log K_p values used in this report (Otte et al., 2001).
 - e Calculated from the data for secondary poisoning through the aquatic food chain (Van de Plassche, 1994). Direct aquatic toxicity data would result in an MPC of 0.016 mg/kg.
 - f Calculated from the data for secondary poisoning through the aquatic food chain (Van de Plassche, 1994). Direct aquatic and terrestrial toxicity data would result in an MPC of 0.077 mg/kg for soil and 0.32 mg/kg for sediment.

Table 3.18: Summary of new SRC_{eco} values for pesticides in surface water, MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report.

Compound	Compartment	SRC_{eco} [$\mu\text{g/l}$]	Method / reliability score	MPC this report [$\mu\text{g/l}$]	Method	MPC INS [$\mu\text{g/l}$]
DDT	surface water	0.43	10 b / medium	0.0050	10 g	$4.4 \cdot 10^{-4}$ ^a
DDE	surface water	0.10	1 c / medium	0.0010	100 b	$(4.4 \cdot 10^{-4})$
DDD	surface water	3.8	10 a / low	0.0024	1000 a	$(4.4 \cdot 10^{-4})$
sum drins	surface water	1.8		0.011 ^c		-
aldrin/dieldrin	surface water	3.4	ref. / high	0.075	ref.	0.018 ^a
endrin	surface water	0.92	ref. / high	0.0049	ref.	0.0030 ^b
sum HCHs	surface water	100		0.54		-
α -HCH	surface water	140	ref. / high	3.9	ref.	2.5 ^a
β -HCH	surface water	93	ref. / high	6.7	ref.	0.080 ^a
γ -HCH	surface water	87	ref. / high	1.2	ref.	0.77 ^a
carbaryl	surface water	41	ref. / high	0.23	ref.	0.23 ^b
carbofuran	surface water	6.5	1 c / medium	0.050	10 h	0.015 ^b
maneb	surface water	32	1 c / low	0.18	100 f	0.012 ^b
atrazine	surface water	76	ref. / high	2.9	ref.	2.9 ^b

* For the SRC_{eco} and the MPC the abbreviation ref. is used in case of refined risk assessment. The assessment factor together with the designation according to Table 2.1 and Table 2.5 is given in case of preliminary risk assessment.

a Derived from secondary poisoning effects for the aquatic food chain; bold value indicates that no update of the MPC is proposed.

b Derived from direct effects to aquatic organisms.

c Calculated from the data for secondary poisoning through the aquatic food chain (Van de Plassche, 1994). Direct aquatic toxicity data would result in an MPC of 0.019 $\mu\text{g/l}$.

d Calculated from the data for secondary poisoning through the aquatic food chain (Van de Plassche, 1994). Direct aquatic toxicity data would result in an MPC of 3.2 $\mu\text{g/l}$.

3.8 SRC_{eco} for other compounds

3.8.1 SRC_{eco} for phthalates

For phthalates new data have been collected for all phthalates. These data are reported in the annex to this report. Further, the data that have been collected in the framework of the project 'Setting Integrated Environmental Quality Standards' for *n*-dibutyl phthalate and diethylhexyl phthalate have been used (Van Wezel et al., 1999b). The selected data used for extrapolation are included in Appendix 9. For dibutyl phthalate, benzyl butyl phthalate, bis(2-ethylhexyl) phthalate (diethylhexyl phthalate), dioctyl phthalate, di-'isodecyl' phthalate, and di-'isononyl' phthalate an European evaluation (EU commission regulation 1488/94) will be available on a short term.

3.8.1.1 SRC_{eco} for dimethyl phthalate (DMP)

For dimethyl phthalate (DMP) aquatic toxicity data are available for both fresh water and marine species (Table A9. 2 and Table A9. 3). The acute toxicity data from both sets are not significantly different ($P = 0.10$). The geometric mean of these acute toxicity data is 81 mg/l, while that of the two chronic toxicity data is 9.8 mg/l. With an ACR of 10 the resulting HC50(aquatic species) is **8.1** mg/l.

Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. According to the modified EPA method, the MPC is derived by applying a safety factor of 100 to the lowest L(E)C50. This MPC is $1.7 \cdot 10^2$ µg/l. With the EU/TGD method an assessment factor of 50 is applied to the lowest of 2 NOECs, resulting in an MPC of **96** µg/l.

One acute terrestrial study for earthworms is available (Table A9. 1). With an ACR of 10 the resulting HC50(terrestrial species) is $3.2 \cdot 10^2$ mg/kg. The MPC derived directly from the terrestrial toxicity data is 3.2 mg/kg according to both the modified EPA method and the EU/TGD method. These values are compared with equilibrium partitioning. The log K_p for standard soil and sediment is 1.02. The resulting SRC_{eco} and MPC for soil and sediment are **84** and **1.0** mg/kg.

3.8.1.2 SRC_{eco} for diethyl phthalate (DEP)

For diethyl phthalate (DEP) aquatic toxicity data are available for both fresh water and marine species (Table A9. 5 and Table A9. 6). The acute toxicity data from both sets are significantly different ($P = 0.040$). However, when only algae, crustaceans and fish are considered this significance disappears ($P = 0.08$), although the difference is still markedly. However, for none of the other phthalates differences between fresh and salt water were observed.

Therefore, also for DEP both sets are combined. The geometric mean of these acute toxicity data is 30 mg/l. Chronic toxicity data are available for 4 taxonomic groups (cyanophyta, protozoa, algae and crustaceans). Therefore, statistical extrapolation is performed (see Figure 3.45). The HC50 from this distribution is 23 mg/l (90% CI: 13 – 39 mg/l). The HC5 is 7.0 mg/l (90% CI: 1.9 – 12.6 mg/l). As can be seen from the figure the difference between acute and chronic toxicity data is very small. A small difference is also observed for single species or taxonomic groups, e.g. *Daphnia magna* or *Scenedesmus* species. However, also the variance in the chronic toxicity data is very small in this case. Therefore, also a comparison with QSAR estimates is made. The used value for log K_{ow} is 2.47 (Otte et al., 2001). The QSAR estimates are shown in Table A9. 7. The HC50 from these QSAR estimates is 44 mg/l (90% CI: 24 – 80 mg/l). The HC5 is 3.7 mg/l (90% CI: 1.2 – 7.8 mg/l). The HC50 from the QSAR estimates is thus higher than that of the experimental data. However, the HC5 is lower.

Therefore, the SRC_{eco} for water is derived from the experimental data and is **23 mg/l**. The MPC is derived from the QSAR estimates and is **3.7 mg/l**.

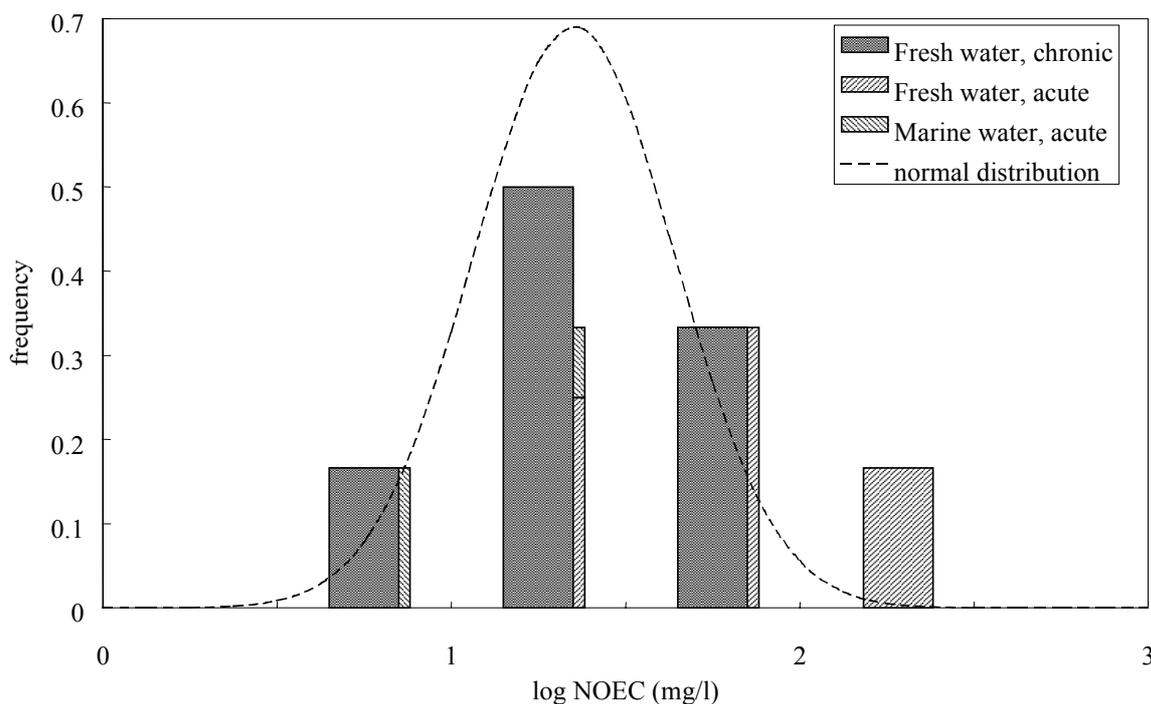


Figure 3.45: DEP: Chronic and acute toxicity for fresh water and marine species. The estimated log-normal distribution is based on the chronic data ($n = 6$, $\bar{x} = 1.35$, $s = 0.26$).

One acute terrestrial study for plants is available (Table A9. 4). With an ACR of 10 the resulting HC50(terrestrial species) is 53 mg/kg. The MPC derived directly from the terrestrial toxicity data is 0.53 mg/kg according to both the modified EPA method and the EU/TGD method.

These values are compared with equilibrium partitioning. The $\log K_p$ for standard soil and sediment is 1.41. The resulting HC50(EqP) is 78 mg/kg and the MPC(EqP) is 1.1 mg/kg. Therefore, the SRC_{eco} for soil is **53 mg/kg** and the SRC_{eco} for sediment **$5.8 \cdot 10^2$ mg/kg**. The MPC for soil is **0.53 mg/kg** and for sediment **94 mg/kg**.

3.8.1.3 SRC_{eco} for di-iso-butylphthalate (DIBP)

Two acute studies were collected for di-iso-butylphthalate (Table A9. 8 and Table A9. 9). The geometric mean of these data is 1.6 mg/l. Applying an ACR of 10 results in an HC50(aquatic species) of **$1.6 \cdot 10^2$ μ g/l**. According to the modified EPA method and the EU/TGD method ($\log K_{ow} > 3$) an assessment factor of 1000 is applied to the lowest L(E)C50, resulting in an MPC for surface water of **0.90 μ g/l**.

There are no terrestrial data for DIBP. The $\log K_p$ for standard soil and sediment is 2.01. The resulting SRC_{eco} for soil and sediment is **17 mg/kg** and the MPC is **0.092 mg/kg**.

3.8.1.4 SRC_{eco} for n-dibutyl phthalate (DBP)

Aquatic toxicity studies with n-dibutyl phthalate are available for both fresh water and marine species (Table A9. 11 and Table A9. 12). The only chronic study for marine species fits in the overall log-normal distribution ($P = 23\%$). The geometric mean of all chronic toxicity data is **$7.8 \cdot 10^2$ μ g/l**. Also the acute toxicity data for fresh and marine water are not significantly different ($P = 0.56$, Welch-corrected). Application of an ACR of 10 to the acute toxicity data

results in an HC50(aquatic species) of $1.7 \cdot 10^2$ µg/l. The MPC for surface water of **10** µg/l was derived from the same set of data using the modified EPA method (Van Wezel et al., 1999b). Because chronic and acute toxicity data are available for algae, *Daphnia* and fish, the same MPC is derived with the EU/TGD method.

One acute toxicity study with a terrestrial plant is available (Table A9. 10). With an ACR of 10, the HC50(terrestrial species) is $1.9 \cdot 10^2$ mg/kg. This value is compared with equilibrium partitioning. The log K_p for standard soil and sediment is 2.33. The resulting SRC_{eco} for soil and sediment is **36** mg/kg.

The MPC for soil and sediment was derived by equilibrium partitioning (Van Wezel et al., 1999b). For this goal the lowest K_{oc} value of $1.2 \cdot 10^3$ for suspended solids was used to prevent underestimation of the risk. The resulting MPC for soil and sediment is **0.7** mg/kg. With the log K_p for standard soil and sediment of 2.33 corresponding to a K_{oc} value of $3.6 \cdot 10^3$, a proportionally higher value of 2.1 mg/kg is obtained. By applying a safety factor of 1000 to the terrestrial L(E)C50 a value of 1.9 mg/kg is derived. The current MPC is thus a factor of 3 lower than these values.

3.8.1.5 SRC_{eco} for butyl benzyl phthalate (BBP)

Acute aquatic toxicity data of butyl benzyl phthalate (BBP) are available for fresh water and marine species (Table A9. 13 and Table A9. 14). No differences in sensitivity were observed ($P = 0.83$). The geometric mean of these data is 1.0 mg/l. One chronic toxicity study presents a NOEC of $2.9 \cdot 10^2$ µg/l. The HC50(aquatic species) is therefore **$1.0 \cdot 10^2$** µg/l, by applying an ACR of 10 to the acute toxicity data. Acute toxicity data are available for algae, crustaceans (a.o. *Daphnia*) and fish. According to the modified EPA method a safety factor of 100 can be applied to the lowest L(E)C50. This MPC is 2.9 µg/l. According to the EU/TGD method an assessment factor of 1000 is applied to the lowest L(E)C50 in this case, resulting in an MPC of **0.29** µg/l.

Terrestrial data were not found for BBP. The log K_p for standard soil and sediment is 2.68. The resulting HC50 for soil and sediment is **48** mg/kg and the MPC **0.14** mg/kg.

3.8.1.6 SRC_{eco} for dihexyl phthalate (DHP)

For dihexyl phthalate (DHP) one NOEC was found. On the basis of this NOEC the HC50 for surface water is **84** µg/l. It should be noted that this value might exceed the water solubility of DHP. According to the modified EPA method the MPC is 8.4 µg/l. The base set of the EU/TGD method is not complete, because no acute toxicity data are available. However, the log K_{ow} of DHP is much higher than 3 (Otte et al., 2001). Therefore, the maximum assessment factor of 100 is applied to the NOEC, leading to an MPC of **0.84** µg/l.

Terrestrial data were not found for DHP. The log K_p for standard soil and sediment is 3.42. The resulting HC50 for soil and sediment is **$2.2 \cdot 10^2$** mg/kg and the MPC **2.2** mg/kg.

3.8.1.7 SRC_{eco} for diethylhexyl phthalate (DEHP)

Almost all studies for diethylhexyl phthalate show effect concentration that are far above the aqueous solubility (Van Wezel et al., 1999b). There is only one NOEC that is close to the solubility (Table A9. 17). This value of **5** µg/l can be considered as the HC50 for surface water. The log K_p for standard soil and sediment is 4.14. The resulting SRC_{eco} for soil is **69** mg/kg. For DEHP there is also one study with a frog species, exposed via contaminated sediment (Table A9. 16). The NOEC for sediment is **10** mg/kg. This value can also be considered as the SRC_{eco} for sediment.

It should be noted that these values, that are meant to represent median hazardous concentrations, are based on the most sensitive species. Many studies had to be rejected,

because the water solubility was exceeded or no effects were observed in the study.

Consequently, the derived SRC_{eco} can be assumed to be at the safe end.

Chronic toxicity and acute studies were performed for algae, *Daphnia* and fish. Therefore, to derive an MPC from the aquatic toxicity data an assessment factor of 10 is sufficient with both the modified EPA method and the EU/TGD method. The resulting MPC for water would be 0.5 $\mu\text{g/l}$. The log K_p for standard soil and sediment is 3.42. Applying equilibrium partitioning would result in an MPC of 6.9 mg/kg.

The MPC of 1.0 mg/kg for soil and sediment was taken from the sediment study, with application of safety factor of 10. To prevent possible adverse estrogenic effects, the MPC for water was calculated from this study by applying equilibrium partitioning, with the lowest value for log K_{oc} of 4.94. This MPC is 0.19 $\mu\text{g/l}$ (Van Wezel et al., 1999b). With the current log K_{oc} of 5.37 the derived value would be 0.073 $\mu\text{g/l}$. Derived directly from the aquatic toxicity data the MPC is 0.5 $\mu\text{g/l}$. The MPC for water of 0.19 $\mu\text{g/l}$ is in between and relatively close to both of these values.

3.8.1.8 SRC_{eco} for the sum of phthalates

Also for phthalates it can be concluded that differences in the derived HC50s for soil and sediment are not very large, considering the uncertainty due to the limited number of toxicity studies, the differences in available data and the application of the equilibrium partitioning theory. However, a sum value for the sum of phthalates is not proposed here, because some of the phthalates merely act by narcosis, while others also exhibit an endocrine disruptive activity (Van Wezel et al., 2000). The geometric mean of the HC50s for soil and sediment of the individual phthalates is 57 mg/kg for soil and 61 mg/kg for sediment, similar to the value derived by Denneman and van Gestel (1990). The values for soil based on the terrestrial toxicity data alone are much higher ($1.5 \cdot 10^2$ mg/kg). Because also phthalates do not have the same molecular weight these values can be better expressed on a molar basis. Then, the geometric mean of the HC50s are $2.0 \cdot 10^2$ $\mu\text{mol/kg}$ for soil and $2.2 \cdot 10^2$ $\mu\text{mol/kg}$ for sediment. The geometric means of the MPCs for individual phthalates are 0.79 mg/kg (~ 2.8 $\mu\text{mol/kg}$) in soil and 1.7 mg/kg (~ 6.0 $\mu\text{mol/kg}$) in sediment.

3.8.2 SRC_{eco} for cyclohexanone

For cyclohexanone, new data were collected. These data are reported in the annex to this report. Only data for aquatic species are available. The selected data are presented in Table A9. 18 and Table A9. 19. The HC50 of the chronic toxicity data, which are for bacteria, cyanophyta, protozoa and algae, is $2.6 \cdot 10^2$ mg/l (90% CI: $1.2 \cdot 10^2 - 5.4 \cdot 10^2$ mg/l). The HC50 of this distribution is 54 mg/l (90% CI: 9 – 118 mg/l). The only acute toxicity study for marine species fits well in the overall log-normal distribution ($P = 27\%$). The acute toxicity data include studies for algae, crustaceans and fish. The geometric mean of the acute toxicity data is $2.5 \cdot 10^2$ mg/l, almost equal to that of the chronic toxicity data (Figure 3.46). Because of the relatively high chronic toxicity data a comparison with QSAR estimates is made. The log K_{ow} used for these estimates was 0.81 mg/l (Otte et al., 2001). However, both the HC5 and the HC50 from these QSAR estimates (data in Table A9. 20) were higher than those from the experimental data. The SRC_{eco} and the MPC for water are thus $2.6 \cdot 10^2$ and 54 mg/l. The log K_p for standard soil and sediment is -0.24 . The resulting HC50 for soil and sediment is $1.5 \cdot 10^2$ mg/kg and the MPC 31 mg/kg.

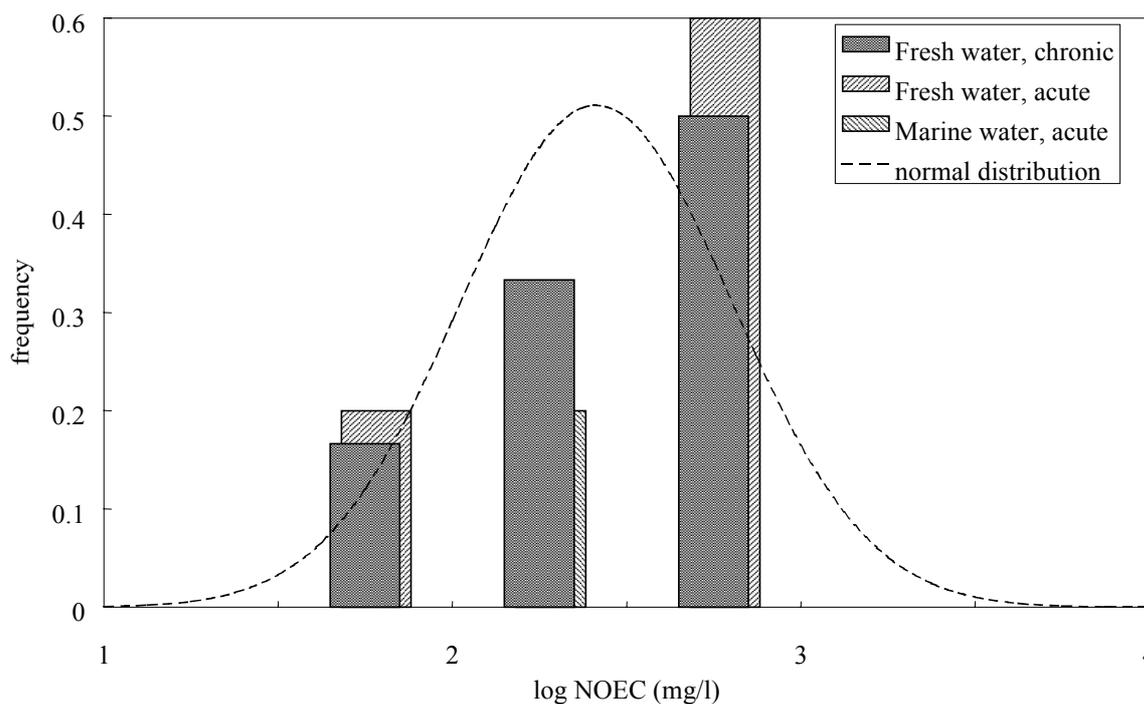


Figure 3.46: Cyclohexanone: Chronic and acute toxicity for aquatic species. The estimated log-normal distribution is based on the chronic toxicity data ($n = 6$, $\bar{x} = 2.41$, $s = 0.39$).

3.8.3 SRC_{eco} for pyridine

For pyridine new data were collected, which are reported in the annex to this report. The selected data for aquatic species are presented in Table A9. 22 and Table A9. 23. Chronic toxicity data are available for bacteria, cyanophyta, protozoa and algae. Therefore, a statistical extrapolation is performed (Figure 3.47). The HC50 from this extrapolation is **57 mg/l** (90% CI: 19 – 166 mg/l). The HC5 from this distribution is **2.9 mg/l** (90% CI: 0.3 – 10.2 mg/l). The acute toxicity data for fresh water and marine species are not significantly different ($P = 0.12$). The geometric mean of all acute toxicity data is $5.5 \cdot 10^2$ mg/l, which is about a factor of 10 higher than the chronic toxicity data. The acute toxicity data include studies for crustaceans and fish. Therefore, no further comparison is made with QSAR estimates.

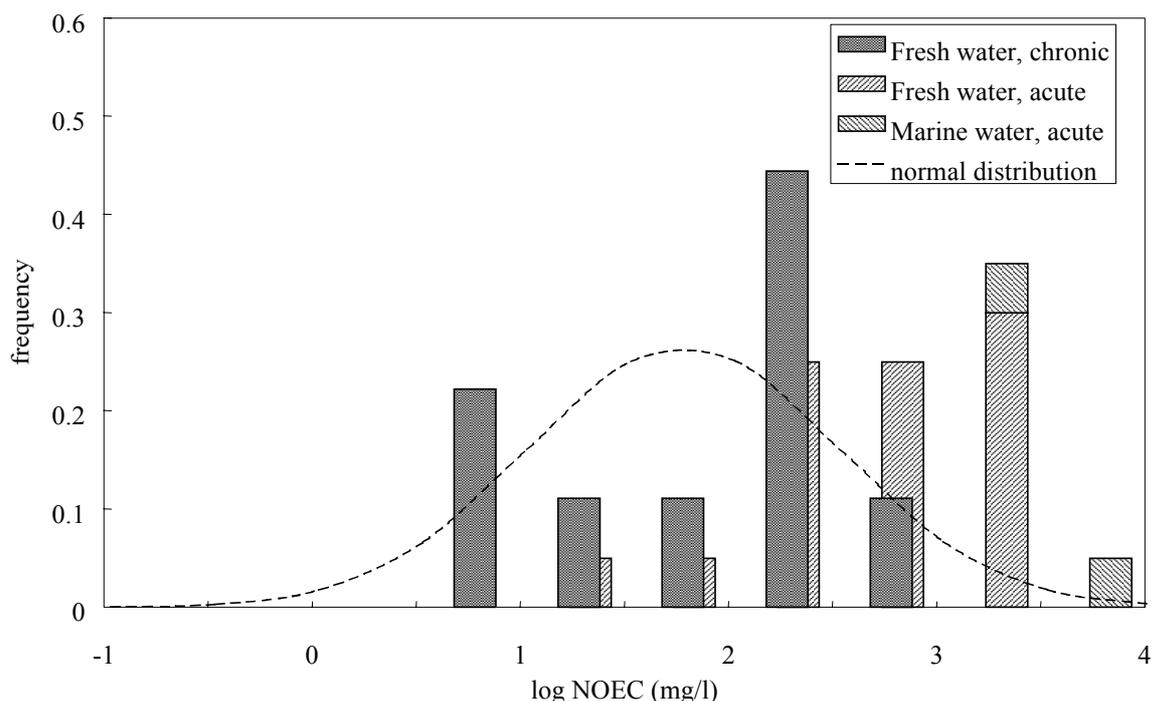


Figure 3.47: Pyridine: Chronic and acute toxicity for aquatic species. The estimated log-normal distribution is based on the chronic toxicity data ($n = 9$, $\bar{x} = 1.75$, $s = 0.75$).

The log K_p for standard soil and sediment is 0.70. The resulting HC50(EqP) is $2.8 \cdot 10^2$ mg/kg and the MPC(EqP) 15 mg/kg. For pyridine also some terrestrial toxicity data are available for plants (Table A9. 21). The HC50 derived from these values is equal to the NOEC of 50 mg/kg. According to the modified EPA method the MPC of 1.0 mg/kg is determined by applying a safety factor of 1000 to the L(E)C50 of 1000 mg/kg. With the EU/TGD method an assessment factor of 100 is applied to the NOEC, resulting in an MPC of 0.50 mg/kg. The SRC_{eco} for soil is thus 50 mg/kg and for sediment $2.8 \cdot 10^2$ mg/kg. The MPC for soil is 0.50 mg/kg and for sediment 15 mg/kg.

3.8.4 SRC_{eco} for tetrahydrofuran

For tetrahydrofuran chronic and acute aquatic toxicity data are available (Table A9. 24 and Table A9. 25). Chronic toxicity data are available for four taxonomic groups (Figure 3.48). Only one fish species is included and the rest of the data is for bacteria, protozoa and algae. The HC50 of this distribution is $8.0 \cdot 10^2$ mg/l (90% CI: $3.0 \cdot 10^2 - 21.8 \cdot 10^2$ mg/l). The HC5 is 97 mg/l (90% CI: 9 - 279 mg/l). For acute toxicity studies the only value for marine species fits in the overall log-normal distribution ($P = 10\%$). The geometric mean of the acute toxicity data is $2.4 \cdot 10^3$ mg/l. Because the difference between chronic and acute toxicity study is small and the diversity of the taxonomic groups for chronic toxicity studies is limited, a comparison with QSAR estimates is made. To calculate the QSAR estimates a log K_{ow} of 0.47 was used (Otte et al., 2001). The QSAR estimates are shown in Table A9. 26. The HC50 resulting from statistical extrapolation with these data is $7.2 \cdot 10^2$ mg/l (90% CI: $4.3 \cdot 10^2 - 11.9 \cdot 10^2$ mg/l). The HC5 is 87 mg/l (90% CI: 34 - 166 mg/l). The QSAR estimates for HC50 as well as HC5 are lower than those from the experimental data. Therefore, the SRC_{eco} and MPC for surface water are $7.2 \cdot 10^2$ mg/l and 87 mg/l.

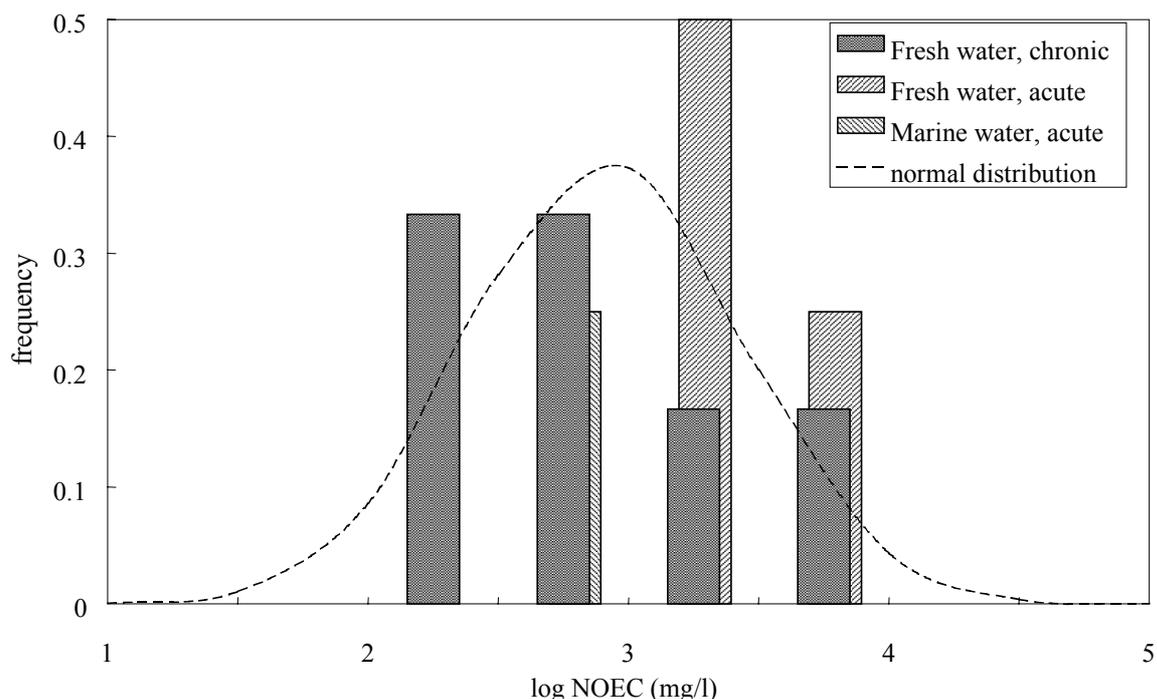


Figure 3.48: Tetrahydrofuran: Chronic and acute toxicity for aquatic species. The estimated log-normal distribution is based on the chronic toxicity data ($n = 6$, $\bar{x} = 2.91$, $s = 0.53$).

The $\log K_p$ for standard soil and sediment is -0.76 . The resulting SRC_{eco} for soil and sediment is $1.2 \cdot 10^2$ mg/kg and the MPC 15 mg/kg.

3.8.5 SRC_{eco} for tetrahydrothiophene

For tetrahydrothiophene no terrestrial and no aquatic data are available. The aquatic HC50 and MPC are therefore derived using QSARs, with the same set of QSARs as was used by Van de Plassche et al. (1993), assuming that the toxic mode of action of this chemical is narcosis. These QSAR values are shown in Table A9. 27. On the basis of statistical extrapolation an HC50(aquatic species) of 9.4 mg/l and an HC5(aquatic species) of 0.97 mg/l are derived from these QSARs, after application of a safety factor of 10 for the absence of experimental data and the use of QSAR estimates. The $\log K_p$ for soil and sediment is -0.03 , resulting in an HC50 for soil and sediment of 8.8 mg/kg and an MPC of 0.90 mg/kg.

3.8.6 Summary and comparison with old values and MPCs

In Table 3.19 the SRC_{eco} for the remaining compounds are summarised. Besides the values derived in the present report also the old values derived in Denneman and Van Gestel (1990) and the MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards'. For none of the compounds listed in this table an SRC_{eco} is determined that is substantially lower than that of the compounds that act mainly by narcosis, such as the chlorobenzenes.

Table 3.19: Summary of new SRC_{eco} values for phthalates and cyclic compounds in soil or sediment, values as derived by Denneman and van Gestel (1990), MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report. Values are given as concentrations in mg/kg standard soil/sediment (soil containing 10% organic matter and 25% clay, sediment containing 10% organic matter and 25% clay).

Compound	Compartment	SRC _{eco} [mg/kg]	Method / reliability score	Denneman and van Gestel (1990) [mg/kg]	MPC this report [mg/kg]	Method	MPC INS [mg/kg]
sum phthalates ^d	soil	61		50 (indicative)	1.3		-
	sediment	57		-	1.4		-
DMP	soil	84	EqP<10 a sp./ medium	20	1.0	EqP<1000 a sp.	-
	sediment	84	EqP / low	-	1.0	EqP	-
DEP	soil	53	10 a / medium	150	0.53	1000 a sp.	-
	sediment	580	EqP / medium	-	94 ^b	EqP	-
DIBP	soil	17	EqP / low	-	0.092	EqP	-
	sediment	17	EqP / low	-	0.092	EqP	-
DBP ^d	soil	36	EqP<10 a sp./ medium	150	1.9 ^c	1000 a sp.	0.7
	sediment	36	EqP / low	-	2.1 ^c	EqP	0.7
BBP ^d	soil	48	EqP / low	-	1.4	EqP	-
	sediment	48	EqP / low	-	1.4	EqP	-
DHP	soil	220	EqP / low	-	22	EqP	-
	sediment	220	EqP / low	-	22	EqP	-
DEHP ^d	soil	69	EqP / low	-	6.9 ^c	EqP	1.0
	sediment	10	1 c sp./ medium	-	- ^c	EqP	1.0
cyclohexanone	soil	150	EqP / medium	-	0.19	EqP	-
	sediment	150	EqP / medium	-	0.19	EqP	-
pyridine	soil	50	1 c sp./ medium	150	1.0	100 d sp.	-
	sediment	280	EqP / medium	-	1.5	EqP	-
tetrahydrofuran	soil	120	EqP / medium	-	1.6 ^b	EqP	-
	sediment	120	EqP / medium	-	1.6 ^b	EqP	-
tetrahydrothiophene ^a	soil	8.8	EqP / -	-	0.90	EqP	-
	sediment	8.8	EqP / -	-	0.90	EqP	-

* For the SRC_{eco} and the MPC EqP (equilibrium partitioning) or the assessment factor together with the designation according to Table 2.1 and Table 2.6 is given. Whether the SRC_{eco} or the MPC is based on species or processes is indicated by the abbreviation sp. and pr.

a Calculated by equilibrium partitioning from aquatic ERLs based on QSAR estimates only to which a safety factor of 10 is applied.

b Calculated from aquatic ERLs based on QSAR estimates after comparison with experimental data.

c No update of the MPCs is proposed for these compounds; bold value indicates that no update of the MPC is proposed.

d For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

Table 3.20: Summary of new SRC_{eco} values for phthalates and cyclic compounds in surface water, MPC values as derived in the context of the project 'Setting Integrated Environmental Quality Standards' (INS) and MPC values derived in this report.

Compound	Compartment	SRC _{eco} [µg/l]	Method / reliability score	MPC [µg/l]	Method	MPC INS [µg/l]
DMP	surface water	8100	10 b / medium	96	100 f	-
DEP	surface water	23000	ref. / high	3700 ^b	QSAR / ref.	-
DIBP	surface water	160	10 a / low	0.90	1000 a	-
DBP ^d	surface water	170	10 b / medium	10	10 g	10
BBP ^d	surface water	100	10 b / medium	0.29	1000 c	-
DHP	surface water	84	1 c / low	0.84	1000 incompl.	-
DEHP ^d	surface water	5.0	1 c / medium	0.50 ^c	10 g	0.19
cyclohexanone	surface water	260000	ref. / high	54000	ref.	-
pyridine	surface water	57000	ref. / high	2900	ref.	-
tetrahydrofuran	surface water	800000	QSAR / high	87000 ^b	QSAR / ref.	-
tetrahydrothiophene ^a	surface water	9400	QSAR/10 / -	970	QSAR/10 / ref.	-

* For the SRC_{eco} and the MPC the abbreviation ref. is used in case of refined risk assessment. The assessment factor together with the designation according to Table 2.1 and Table 2.5 is given in case of preliminary risk assessment. An incomplete base set is indicated by the abbreviation incompl.

- a Based on QSAR estimates only to which a safety factor of 10 is applied.
- b Based on QSAR estimates after comparison with experimental data.
- c No update of the MPCs is proposed for these compounds; bold value indicates that no update of the MPC is proposed.
- d For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

4 Discussion

4.1 Revised SRC_{eco}

In 1990 the first series of SRC_{eco} values were proposed by Denneman and van Gestel to serve as trigger values for the purpose of soil remediation, the Intervention Values. However, since then new toxicological data have become available, mostly collected in the framework of the project 'Setting Integrated Environmental Quality Standards' to derive the MPC/NC values. Further, new data were retrieved for compounds of the first series that have not yet been evaluated in the framework of the current report. Also the methodology to derive the SRC_{eco} has been changed since the first series of SRC_{eco} . The concentration that is hazardous to 50% of the species (HC50) is proposed as the SRC_{eco} . This HC50 is determined by refined risk assessment (log-normal extrapolation) or preliminary risk assessment, which is a comparison of chronic and acute toxicity data together with equilibrium partitioning (EqP). In this report this information has been evaluated and new values for the SRC_{eco} are proposed. In addition, if necessary the old MPC/NC values have been updated.

The SRC_{eco} , are reported in Table 4.1. In this table also the reliability of the SRC_{eco} is indicated. The QSAR estimates without any comparison with experimental toxicity data have been assigned no reliability score, but can be regarded as having a low reliability. The SRC_{eco} for all compounds presented in this table are based on standard soil and sediment. However, this soil is representative for only a few soil types. For a site-specific risk assessment a normalisation on organic matter can be performed in the case of organic compounds. The values for metals consist of an added part and a natural background in standard soil. Here, for a site-specific risk assessment the background concentration can be corrected based on organic matter and lutum of the specific soil. For the added part the use of this correction method is still subject to debate.

Most of the new SRC_{eco} values are in the same order of magnitude as the current values. Exceptions to this are dichloromethane, trichloroethene, hexachlorobenzene, drins, carbaryl, and carbofuran. For these organic chemicals the new SRC_{eco} is substantially lower (> factor of 10). For dichloromethane and trichloroethene this can be attributed to the inclusion of terrestrial processes in the derivation of the SRC_{eco} . The use of equilibrium partitioning is the cause of the difference for hexachlorobenzene, carbaryl, and carbofuran. For the rest of the organic chemicals the new SRC_{eco} values are on average not particularly higher or lower than the old values. The same conclusion can be drawn for the metals. The new values for arsenic, mercury, and lead are higher than the old values, while the new values for copper, nickel and zinc are lower than the old values. High partition coefficients for metals in sediment give rise to much higher SRC_{eco} values in sediment than in soil (see also 4.3.2).

The changes in SRC_{eco} can be attributed to changes in both data and methodology or a combination of these two aspects. Regarding the data used, both the toxicity data and the partitioning coefficients used for equilibrium partitioning have been evaluated. The methodology has been changed on several aspects too. In comparison with Denneman and van Gestel, species are now used as entries instead of taxonomic groups, all acute toxicity data are grouped instead of separate values for LC50s and EC50s, the number and type of data to apply statistical extrapolation upon is different, data on processes are also included to base the SRC_{eco} upon, and the way in which it is determined whether to use chronic, acute or equilibrium partitioning data to derive the SRC_{eco} in case of preliminary risk assessment has been changed.

The derived SRC_{eco} are still based on a limited amount of toxicity data. As a result, preliminary risk assessment is mostly used for both the water and the soil compartment. For only slightly more than half of the compounds terrestrial toxicity data were available. Finally, almost two out of three SRC_{eco} values for soil is derived by equilibrium partitioning (see also 4.3.1).

4.2 Revised MPCs

For all compounds considered in this report the MPCs are discussed (see Table 4.2). As far as preliminary risk assessment is concerned, new MPCs were derived according to the EU/TGD method instead of the modified EPA method that was used until now in the framework of the project 'Setting Integrated Environmental Quality Standards'. In addition to the preliminary risk assessment methods statistical extrapolation was used. Also the method for this refined risk assessment was changed, from log-logistic extrapolation to log-normal extrapolation, although the influence of this change on the numerical values is marginal. Data on secondary poisoning or harmonisation with the air compartment were not considered in this report and therefore, all MPCs derived by this EU/TGD method can only be regarded as a proposal for the MPC if they are lower than the MPCs that were formerly derived for secondary poisoning or after harmonisation with the air compartment. In general, the EU/TGD method gives MPC values that are rather comparable with those derived by the modified EPA method, but tending to be slightly lower, on average a factor of 2 (see also 4.3.5).

The MPCs that were derived in the framework of 'Setting Integrated Environmental Quality Standards' by means of QSARs are high compared to the SRC_{eco} . Using the experimental data as a starting point usually results in much lower MPCs, especially when preliminary risk assessment was used. It is open to discussion whether or not these QSARs in combination with statistical extrapolation can be used to derive MPCs. Statistical extrapolation uses the standard deviation of the data points for the range of extrapolation. For each QSAR however, the variability in sensitivity of a species for different compounds is averaged. In this way, the standard deviation of all QSAR estimates might be deviating from that of experimental data. The fact that many MPCs derived with statistical extrapolation from experimental data are still close to the QSAR estimates can also be explained by a limited diversity in taxonomic groups (see 4.3), which may also greatly diminish the standard deviation of the experimental data points.

Table 4.1: Summary of SRC_{eco} values for soil, sediment and surface and ground water.

Compound	Dennemman and van Gestel [mg/kg _{d.w.}]	current SRC _{eco} soil [mg/kg _{d.w.}]	new SRC _{eco} soil [mg/kg _{d.w.}]	reliability score	new SRC _{eco} sediment [mg/kg _{d.w.}]	reliability score	new SRC _{eco} groundwater [µg/l]	reliability score
arsenic	40	40	85	high	5900	low	890	high
barium	650	650	890	high	7200	low	7100	medium
cadmium ^a	12	12	13	high	820	low	9.7	high
chromium ^a	230	230	220	high	43000	low	220	high
cobalt	120	240	180	high	3200	low	810	high
copper	190	190	96	high	660	low	19	high
mercury	10	10	36	high	1500	low	14	high
methyl-mercury	-	-	4.0	medium	-	-	0.37	high
lead	290	290	580	high	63000	low	150	high
molybdenum	<480	<480	190	high	23000	low	27000	medium
nickel ^a	210	210	100	medium	2600	low	500	high
zinc ^a	720	720	350	high	6600	low	91	high
free cyanide (as CN ⁻)	-	-	-	-	-	-	31	high
thiocyanate (as SCN ⁻)	-	-	620	low	-	-	10000	medium
complex cyanide (CN ⁻)	-	-	-	-	-	-	29	medium
benzene ^a	25	25	130	medium	130	medium	30000	high
toluene ^a	150	130	47	medium	79	medium	11000	high
ethylbenzene ^a	-	-	110	medium	110	medium	5500	high
sum xylenes	-	-	17	-	17	-	1100	-
o-xylene	-	-	9.3	low	9.3	low	1000	medium
m-xylene	-	-	18	low	18	low	1200	medium
p-xylene	-	-	30	low	30	low	1100	medium
styrene ^a	-	-	86	low	86	low	3800	medium
phenol ^a	40	40	14	medium	14	medium	7000	high
sum cresols	50	50	13	-	27	-	10000	-
o-cresol	150	-	50	medium	66	medium	29000	high
m-cresol	15	-	16	medium	110	medium	36000	high
p-cresol	-	-	2.6	low	2.6	low	1000	medium
sum dihydroxybenzenes	-	-	8.0	-	8.0	-	3100	-
catechol	-	-	2.6	low	2.6	low	630	low
resorcinol	-	-	4.6	low	4.6	low	5700	medium

Compound	Denneman and van Gestel [mg/kg _{d.w.}]	current SRC _{eco} soil [mg/kg _{d.w.}]	new SRC _{eco} soil [mg/kg _{d.w.}]	reliability score	new SRC _{eco} sediment [mg/kg _{d.w.}]	reliability score	new SRC _{eco} groundwater [µg/l]	reliability score
hydroquinone	-	-	43	medium	43	medium	8200	high
sum PAHs	40	40	-	-	-	-	-	-
naphthalene ^a	30	-	17	low	17	low	290	medium
anthracene ^a	-	-	1.6	medium	1.6	low	1.4	medium
phenanthrene	100	-	31	low	31	low	30	medium
fluoranthene	-	-	260	low	260	low	30	medium
benzo[<i>a</i>]anthracene	-	-	2.5	medium	49	low	1.0	low
chrysene	-	-	35	QSAR	35	QSAR	1.2	QSAR
benzo[<i>k</i>]fluoranthene	-	-	38	low	38	low	0.36	low
benzo[<i>a</i>]pyrene	-	-	7.0	medium	28	low	0.72	medium
benzo[<i>ghi</i>]perylene	-	-	33	QSAR	33	QSAR	0.18	QSAR
indeno[1,2,3- <i>cd</i>]pyrene	-	-	1.9	QSAR	1.9	QSAR	0.036	QSAR
sum chlorinated aliphatic hydrocarbons	30	-	-	-	-	-	-	-
1,2-dichloroethane	-	60	240	medium	240	medium	130000	high
dichloromethane	-	60	3.9	medium	40	low	40000	low
trichloromethane ^a	-	60	170	medium	170	medium	63000	high
tetrachloromethane	-	60	29	low	29	low	8700	low
vinylchloride	-	60	17	QSAR	17	QSAR	8000	QSAR
trichloroethene ^a	-	60	2.5	medium	130	medium	20000	high
tetrachloroethene ^a	15	60	16	medium	16	low	1000	medium
sum chlorobenzenes	-	30	T.U. approach	T.U. approach	T.U. approach	T.U. approach	T.U. approach	T.U. approach
chlorobenzene	-	-	15	low	15	low	1100	medium
dichlorobenzenes	-	-	19	-	19	-	650	-
1,2-dichlorobenzene	-	-	17	low	17	low	740	medium
1,3-dichlorobenzene	-	-	24	low	24	low	820	medium
1,4-dichlorobenzene ^a	50	-	18	medium	18	low	460	medium
trichlorobenzenes	30	-	11	-	25	-	140	-
1,2,3-trichlorobenzene	25	-	5.0	medium	10	low	100	medium
1,2,4-trichlorobenzene ^a	20	-	5.1	medium	5.1	low	46	medium
1,3,5-trichlorobenzene	50	-	50	medium	310	low	550	low
tetrachlorobenzenes	10	-	2.2	-	39	-	120	-
1,2,3,4-tetrachlorobenzene	50	-	16	medium	40	low	83	medium

<i>Compound</i>	<i>Denneman and van Gestel</i> [mg/kg _{d.w.}]	<i>current SRC_{eco} soil</i> [mg/kg _{d.w.}]	<i>new SRC_{eco} soil</i> [mg/kg _{d.w.}]	<i>reliability score</i>	<i>new SRC_{eco} sediment</i> [mg/kg _{d.w.}]	<i>reliability score</i>	<i>new SRC_{eco} groundwater</i> [µg/l]	<i>reliability score</i>
1,2,3,5-tetrachlorobenzene	2.5	-	0.65	medium	47	low	210	low
1,2,4,5-tetrachlorobenzene	-	-	1.0	medium	31	low	90	medium
pentachlorobenzene	50	50	16	medium	16	low	32	medium
hexachlorobenzene	500	500	2.0	medium	2.0	low	3.0	medium
sum chlorophenols	-	10	-	-	-	-	-	-
monochlorophenols	35	10	5.4	-	8.5	-	1000	-
2-chlorophenol	45	-	7.8	medium	7.8	low	1400	medium
3-chlorophenol	30	-	14	medium	54	low	2500	low
4-chlorophenol	-	-	1.4	low	1.4	low	290	medium
dichlorophenols	40	10	22	-	22	-	870	-
2,3-dichlorophenol	-	-	31	low	31	low	1400	low
2,4-dichlorophenol	50	-	8.4	medium	8.4	medium	410	high
2,5-dichlorophenol	-	-	53	low	53	low	1300	low
2,6-dichlorophenol	-	-	57	low	57	low	2300	medium
3,4-dichlorophenol	45	-	27	medium	27	low	590	low
3,5-dichlorophenol	30	-	5.4	medium	5.4	low	420	low
trichlorophenols	15	10	22	-	41	-	340	-
2,3,4-trichlorophenol	-	-	30	low	30	low	420	low
2,3,5-trichlorophenol	15	-	4.5	medium	22	low	260	low
2,3,6-trichlorophenol	-	-	110	low	110	low	990	low
2,4,5-trichlorophenol	25	-	22	medium	22	low	160	medium
2,4,6-trichlorophenol	10	-	8.1	medium	80	low	480	medium
3,4,5-trichlorophenol	-	-	39	low	39	low	190	low
tetrachlorophenols	-	10	21	-	22	-	130	-
2,3,4,5-tetrachlorophenol	65	-	64	medium	67	low	150	low
2,3,4,6-tetrachlorophenol	-	-	13	low	13	low	160	medium
2,3,5,6-tetrachlorophenol	-	-	12	low	12	low	95	medium
pentachlorophenol	5	5	12	high	8	medium	85	high
sum monochloronaphthalenes	-	-	23	-	23	-	150	-
1-chloronaphthalene	-	-	18	low	18	low	120	medium
2-chloronaphthalene	-	-	30	low	30	low	190	low
sum PCBs	70	1	3.4	-	3.4	-	-	-
PCB 77	-	-	4.2	low	4.2	low	0.10	low

Compound	Denneman and van Gestel [mg/kg _{d.w.}]	current SRC _{eco} soil [mg/kg _{d.w.}]	new SRC _{eco} soil [mg/kg _{d.w.}]	reliability score	new SRC _{eco} sediment [mg/kg _{d.w.}]	reliability score	new SRC _{eco} groundwater [µg/l]	reliability score
PCB105	-	-	10	low	10	low	0.13	low
PCB 126	-	-	0.92	low	0.92	low	0.018	low
Sum DDT/DDE/DDD	-	4	-	-	-	-	-	-
DDT	1.3	-	1.0	medium	9.5	low	0.43	medium
DDE	-	-	1.3	low	1.3	low	0.10	medium
DDD	-	-	34	low	34	low	3.8	low
sum drins	-	4	0.14	-	1.2	-	1.8	-
aldrin / dieldrin	-	-	0.22	medium	-	-	3.4	high
aldrin	0.35	-	-	-	1.7	medium	-	-
dieldrin	4.0	-	-	-	1.9	medium	-	-
endrin	0.05	-	0.095	medium	0.48	medium	0.92	high
sum HCHs	-	2	6.4	-	10	-	100	-
α-HCH	-	-	17	medium	17	medium	140	high
β-HCH	-	-	13	medium	13	medium	93	high
γ-HCH	2	-	1.2	medium	5.0	medium	87	high
carbaryl	5	5	0.45	medium	0.45	medium	41	high
carbofuran	1.5	1.5	0.017	medium	0.017	low	6.5	medium
maneb	30	35	22	medium	-	-	32	low
atrazine	90	6	0.71	medium	0.71	medium	76	high
sum phthalates ^a	50	60	-	-	-	-	-	-
(indicative)								
dimethylphthalate	20	-	84	medium	84	low	8100	medium
diethylphthalate	150	-	53	medium	580	medium	23000	high
di-iso-butylphthalate	-	-	17	low	17	low	160	low
di-n-butylphthalate ^a	150	-	36	medium	36	low	170	medium
butylbenzylphthalate ^a	-	-	48	low	48	low	100	medium
dihexylphthalate	-	-	220	low	220	low	84	low
diethylhexylphthalate ^a	-	-	69	low	10	medium	5.0	medium
cyclohexanone	-	-	150	medium	150	medium	260000	high
pyridine	150	150	50	medium	280	medium	57000	high
tetrahydrofuran	-	-	120	medium	120	medium	800000	high
tetrahydrothiophene	-	-	8.8	QSAR	8.8	QSAR	9400	QSAR

a For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

Table 4.2: Summary of MPC or MPA (for metals) values for soil, sediment and surface water.

Compound	current MPC/MPA		new proposal		current MPC/MPA		new proposal	
	soil [mg/kg _{d.w.}]	soil [mg/kg _{d.w.}]	soil [mg/kg _{d.w.}]	soil [mg/kg _{d.w.}]	sediment [mg/kg _{d.w.}]	sediment [mg/kg _{d.w.}]	surface water [µg/l]	surface water [µg/l]
arsenic	4.5	0.90	160	160	-	160	24	24
barium	9.0	180	150	150	-	29	150	29
cadmium ^a	0.76	0.79	29	29	-	29	0.34	0.34
chromium ^a	3.8	0.38	1620	1620	-	1700	8.5	8.7
cobalt	24	2.4	10	10	-	12	2.6	3.0
copper	3.5	3.4	37	37	-	36	1.1	1.1
mercury	1.9	1.9	26	26	-	26	0.23	0.23
methyl-mercury	0.37	0.037	-	-	-	-	0.01	0.011
lead	55	55	4700	4700	-	4500	11	11
molybdenum	253	39	250	250	-	25	290	29
nickel ^a	2.6	0.26	9.4	9.4	-	10	1.8	1.9
zinc ^a	16	16	480	480	-	530	6.6	7.3
free cyanide (as CN ⁻)	-	-	-	-	-	-	-	0.23
thiocyanate (as SCN ⁻)	-	6.2	-	-	-	-	-	3.6
complex cyanide (CN ⁻)	-	-	-	-	-	-	-	0.13
benzene ^a	0.95	0.95	0.95	0.95	-	0.95	240	240
toluene ^a	1.4	0.14	4.2	4.2	-	5.6	730	770
ethylbenzene ^a	3.1	6.2	3.1	3.1	-	6.2	370	310
sum xylenes	14	0.13	14	14	-	0.13	380	8.6
<i>o</i> -xylene	-	0.089	-	-	-	0.089	-	10
<i>m</i> -xylene	-	0.11	-	-	-	0.11	-	7.0
<i>p</i> -xylene	-	0.24	-	-	-	0.24	-	9.0
styrene ^a	25	0.20	25	25	-	0.20	570	9.1
phenol ^a	-	0.20	-	-	-	0.20	-	100
sum cresols	-	0.16	-	-	-	1.0	-	400
<i>o</i> -cresol	-	0.50	-	-	-	13	-	5700
<i>m</i> -cresol	-	1.6	-	-	-	17	-	5500
<i>p</i> -cresol	-	0.0051	-	-	-	0.0051	-	2.0
sum dihydroxybenzenes	-	0.062	-	-	-	0.062	-	24
catechol	-	0.0032	-	-	-	0.0032	-	0.77
resorcinol	-	0.034	-	-	-	0.034	-	42
hydroquinone	-	2.2	-	-	-	2.2	-	410
naphthalene ^a	0.14	0.12	0.14	0.14	-	0.12	1.2	2.1

Compound	current MPC/MPA		new proposal		current MPC/MPA		new proposal	
	soil [mg/kg _{d.w.}]	soil [mg/kg _{d.w.}]	sediment [mg/kg _{d.w.}]	sediment [mg/kg _{d.w.}]	surface water [µg/l]	surface water [µg/l]	water [µg/l]	water [µg/l]
anthracene ^a	0.12	0.039	0.12	0.039	0.07	0.034	0.034	
phenanthrene	0.51	3.3	0.51	3.3	0.3	3.2	3.2	
fluoranthene	2.6	1.0	2.6	1.0	0.3	0.12	0.12	
benzo[<i>a</i>]anthracene	0.25	0.025	0.36	0.49	0.01	0.010	0.010	
chrysene	10.7	8.1	10.7	8.1	0.34	0.28	0.28	
benzo[<i>k</i>]fluoranthene	2.4	0.38	2.4	0.38	0.04	0.0036	0.0036	
benzo[<i>a</i>]pyrene	0.26	0.052	2.7	0.19	0.05	0.0050	0.0050	
benzo[<i>ghi</i>]perylene	7.5	0.57	7.5	0.57	0.03	0.0031	0.0031	
indeno[1,2,3- <i>cd</i>]pyrene	5.9	0.031	5.9	0.031	0.04	6.1·10 ⁻⁴	6.1·10 ⁻⁴	
1,2-dichloroethane	1.5	1.5	1.5	1.5	700	700	700	
dichloromethane	36	0.018	36	0.018	20000	18	18	
trichloromethane ^a	1.9	1.9	1.9	1.9	590	590	590	
tetrachloromethane	37	0.17	37	0.17	1100	50	50	
vinylchloride	1.4	1.4	1.4	1.4	840	840	840	
trichloroethene ^a	13	0.0078	13	11	2400	1600	1600	
tetrachloroethene ^a	0.16	0.054	4.0	0.054	330	3.5	3.5	
sum chlorobenzenes	-	T.U. approach	-	T.U. approach	-	T.U. approach	T.U. approach	
monochlorobenzene	7.6	0.41	7.6	0.41	690	32	32	
dichlorobenzenes	0.40	0.48	5.5	0.69	250	23	23	
1,2-dichlorobenzene	5.9	0.73	5.9	0.73	(270)	31	31	
1,3-dichlorobenzene	4.6	0.39	4.6	0.39	(210)	14	14	
1,4-dichlorobenzene ^a	0.4	0.39	5.7	1.2	(260)	30	30	
trichlorobenzenes	0.24	0.038	6.7	0.20	67	1.1	1.1	
1,2,3-trichlorobenzene	0.005	0.010	6.4	0.40	(64)	4.0	4.0	
1,2,4-trichlorobenzene ^a	0.10	0.011	7.9	0.011	(79)	0.10	0.10	
1,3,5-trichlorobenzene	0.6	0.50	5.7	1.9	(57)	3.3	3.3	
tetrachlorobenzenes	0.072	0.022	7.2	0.39	24	1.2	1.2	
1,2,3,4-tetrachlorobenzene	0.20	0.16	6.9	1.1	(23)	2.3	2.3	
1,2,3,5-tetrachlorobenzene	0.0070	0.0065	6.6	0.17	(22)	0.80	0.80	
1,2,4,5-tetrachlorobenzene	0.010	0.010	7.8	0.31	(26)	0.90	0.90	
pentachlorobenzene	0.12	0.12	0.012	0.015	0.030	0.030	0.030	
hexachlorobenzene	0.028	0.024	0.0012	0.0014	2.1·10 ⁻⁵	2.1·10 ⁻⁵	2.1·10 ⁻⁵	
monochlorophenols	0.20	0.034	0.22	0.051	25	6.0	6.0	
2-chlorophenol	-	0.055	-	0.055	-	10	10	
3-chlorophenol	-	0.035	-	0.12	-	5.5	5.5	

Compound	current MPC/MPA		new proposal		current MPC/MPA		new proposal	
	soil [mg/kg _{d.w.}]	soil [mg/kg _{d.w.}]	sediment [mg/kg _{d.w.}]	sediment [mg/kg _{d.w.}]	surface water [µg/l]	surface water [µg/l]	water [µg/l]	water [µg/l]
4-chlorophenol	-	0.020	-	0.020	-	-	-	4.0
dichlorophenols	0.20	0.054	0.33	0.054	15	15	2.1	2.1
2,3-dichlorophenol	-	0.075	-	0.075	-	-	3.5	3.5
2,4-dichlorophenol	-	0.031	-	0.031	-	-	1.5	1.5
2,5-dichlorophenol	-	0.11	-	0.11	-	-	2.8	2.8
2,6-dichlorophenol	-	0.093	-	0.093	-	-	3.7	3.7
3,4-dichlorophenol	-	0.051	-	0.051	-	-	1.1	1.1
3,5-dichlorophenol	-	0.019	-	0.019	-	-	1.5	1.5
trichlorophenols	0.04	0.17	0.10	0.20	2.5	2.5	1.7	1.7
2,3,4-trichlorophenol	-	0.085	-	0.085	-	-	1.2	1.2
2,3,5-trichlorophenol	-	0.045	-	0.051	-	-	0.60	0.60
2,3,6-trichlorophenol	-	0.30	-	0.30	-	-	2.7	2.7
2,4,5-trichlorophenol	-	0.11	-	0.22	-	-	1.6	1.6
2,4,6-trichlorophenol	-	2.4	-	3.0	-	-	18	18
3,4,5-trichlorophenol	-	0.078	-	0.078	-	-	0.38	0.38
tetrachlorophenols	0.3	0.050	0.086	0.050	1.0	1.0	0.30	0.30
2,3,4,5-tetrachlorophenol	-	0.092	-	0.092	-	-	0.21	0.21
2,3,4,6-tetrachlorophenol	-	0.011	-	0.011	-	-	0.14	0.14
2,3,5,6-tetrachlorophenol	-	0.12	-	0.12	-	-	0.95	0.95
pentachlorophenol	0.20	0.16	0.17	0.40	2.0	2.0	4.3	4.3
sum monochloronaphthalenes	-	0.12	-	0.12	-	-	0.77	0.77
1-chloronaphthalene	-	0.057	-	0.057	-	-	0.37	0.37
2-chloronaphthalene	-	0.25	-	0.25	-	-	1.6	1.6
sum PCBs ^b	3·10 ⁻⁴	3·10 ⁻⁴	3·10 ⁻⁴	3·10 ⁻⁴	-	-	-	-
PCB 77	4.2·10 ⁻⁴	4.2·10 ⁻⁴	4.2·10 ⁻⁴	4.2·10 ⁻⁴	-	-	-	-
PCB105	1.5·10 ⁻³	1.5·10 ⁻³	1.5·10 ⁻³	1.5·10 ⁻³	-	-	-	-
PCB 126	2.5·10 ⁻⁶	2.5·10 ⁻⁶	2.5·10 ⁻⁶	2.5·10 ⁻⁶	-	-	-	-
DDT	0.010	0.010	0.0094	0.0098	4.4·10 ⁻⁴	4.4·10 ⁻⁴	4.4·10 ⁻⁴	4.4·10 ⁻⁴
DDE	0.010	0.013	0.0015	0.0058	4.4·10 ⁻⁴	4.4·10 ⁻⁴	4.4·10 ⁻⁴	4.4·10 ⁻⁴
DDD	0.010	0.021	0.0018	0.0039	4.4·10 ⁻⁴	4.4·10 ⁻⁴	4.4·10 ⁻⁴	4.4·10 ⁻⁴
aldrin / dieldrin	-	-	-	-	0.018	0.018	0.018	0.018
aldrin	0.050	0.038	0.050	0.0092	-	-	-	-
dieldrin	0.12	0.043	0.67	0.010	-	-	-	-
endrin	9.5·10 ⁻⁴	9.5·10 ⁻⁴	0.0029	0.0026	0.0030	0.0030	0.0049	0.0049
α-HCH	0.22	0.31	0.22	0.31	2.5	2.5	2.5	2.5

Compound	current MPC/MPA soil [mg/kg _{d.w.}]	new proposal MPC/MPA soil [mg/kg _{d.w.}]	current MPC/MPA sediment [mg/kg _{d.w.}]	new proposal MPC/MPA sediment [mg/kg _{d.w.}]	current MPC/MPA surface water [µg/l]	new proposal MPC/MPA surface water [µg/l]
β-HCH	0.092	0.011	0.092	0.011	0.080	0.080
γ-HCH	0.0050	0.0010	0.19	0.044	0.77	0.77
carbaryl	0.12	0.0025	0.0025	0.0025	0.23	0.23
carbofuran	0.0047	1.3·10 ⁻⁴	3.2·10 ⁻⁵	1.3·10 ⁻⁴	0.015	0.050
maneb	0.22	0.22	-	-	0.012	0.18
atrazine	0.024	0.0048	0.026	0.027	2.9	2.9
dimethylphthalate	-	1.0	-	1.0	-	96
diethylphthalate	-	0.53	-	94	-	3700
di- <i>iso</i> -butylphthalate	-	0.092	-	0.092	-	0.90
di- <i>n</i> -butylphthalate ^a	0.7	0.7	0.7	0.7	10	10
butylbenzylphthalate ^a	-	1.4	-	1.4	-	0.29
dihexylphthalate	-	22	-	22	-	0.84
diethylhexylphthalate ^a	1.0	1.0	1.0	1.0	0.19	0.19
cyclohexanone	-	0.19	-	0.19	-	54000
pyridine	-	1.0	-	1.5	-	2900
tetrahydrofuran	-	1.6	-	1.6	-	87000
tetrahydrothiophene	-	0.90	-	0.90	-	970

a For these compounds an European evaluation (EU commission regulation 1488/94) will be available on a short term.

b Refers to a concentration of PCB 118 representative for the sum of planar PCBs

4.3 Uncertainty and reliability of the derived ERLs

4.3.1 Number of available toxicity data

In most cases enough data are available to do a refined risk assessment for the metals, both for water and soil. Therefore, most of the derived risk limits for metals have a high reliability score. For cyanides only data for water were available, except one terrestrial study with thiocyanate. A refined risk assessment was possible for free cyanide. For thiocyanate only a few aquatic toxicity data were available.

Only for a minority of the organic compounds a refined risk assessment was possible for the aquatic compartment and for almost a quarter of the compounds only acute aquatic toxicity data are available. The terrestrial toxicity data are even more limited. For organic compounds only one SRC_{eco} for soil has a high reliability score. Further, more than half of the organic compounds have the low reliability score on SRC_{eco} for soil, which means that no terrestrial data were found for these compounds.

In Figure 4.1 the methods used for derivation of the $SCRs_{eco}$ are presented by compartment. From this figure it is clear that most data are available for aquatic species. The number of $SRCs_{eco}$ for soil that is derived by equilibrium partitioning is substantial (more than 50%), which also reflects the limited data for terrestrial species and processes. The $SRCs_{eco}$ for sediment are almost solely derived by equilibrium partitioning, because no toxicity data are available for sediment.

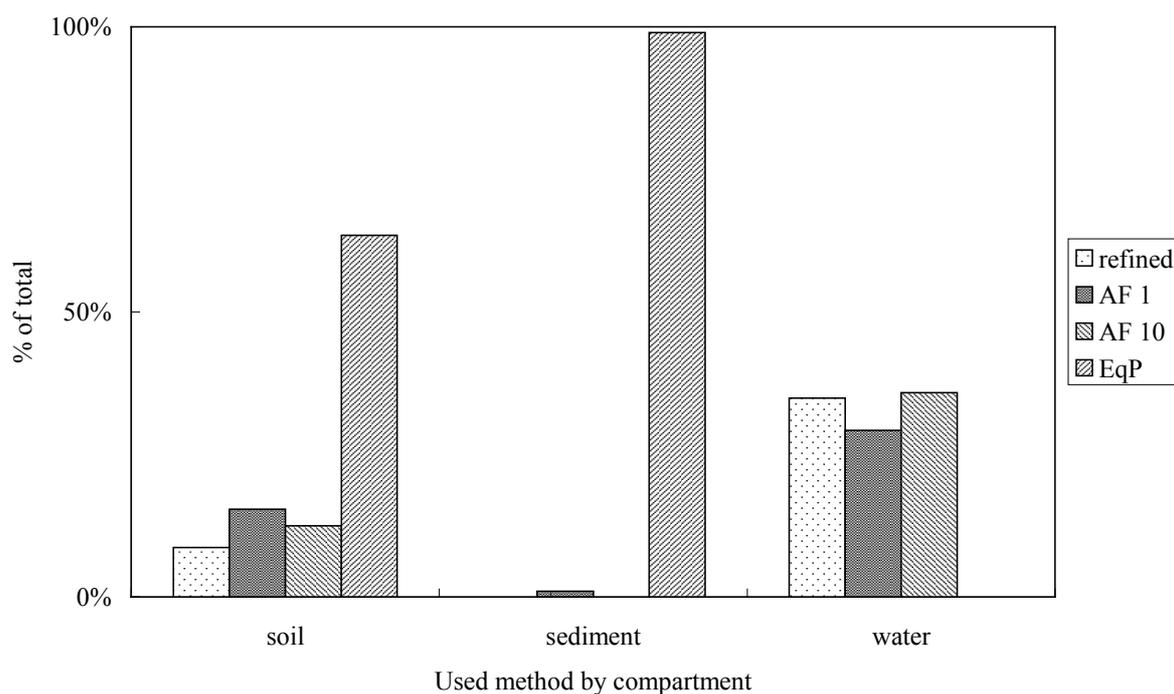


Figure 4.1: Overview of the methods used for the derivation of the $SCRs_{eco}$ for the compartments soil, sediment and water: refined risk assessment, preliminary risk assessment factors (AF) of 1 and 10, for NOECs and L(E)C50s respectively, or equilibrium partitioning (EqP).

4.3.2 Uncertainty in ERLs for metals

The high reliability score for metals is based on the number of taxonomic groups available for extrapolation, and this denotes that refined risk assessment is applied. However, in the case of essential metals the application of statistical extrapolation is subject to debate at this moment.

In a project guided by the workgroup VEM (Slijkerman et al., 2000) it is examined if it is better to do a separate risk assessment for individual ecological systems (environmental type with accompanying species). Differences in ERLs derived for all ecological systems together or for each individual system will probably be most pronounced in the MPCs, which depend on the standard deviation in the data, and are not expected to greatly influence the SRC_{eco} , which is solely determined by the geometric mean of the data. Therefore, the classification 'highly reliable' is still used if statistical extrapolation could be applied.

4.3.3 High ERLs for some organic compounds

The SRC_{eco} in surface water for some organic compounds can be erroneously for two reasons. First, it appears that refined risk assessment of these compounds results in generally much higher SRC_{eco} values, compared to preliminary risk assessment (see also Figure 4.2). For several compounds, the taxonomic groups bacteria, cyanophyta, algae and protozoa prevailed in the distributions of the chronic toxicity data. For other taxonomic groups, such as fish and crustaceans, the acute toxicity data, were often as low as these chronic toxicity data. The acute toxicity studies (e.g. LC50 studies) are mostly performed with higher organisms, while lower organisms tend to be more pronounced among the chronic toxicity studies. Statistical extrapolation requires a kind of random sampling of the data among the taxonomic groups. It can be concluded that this requirement is often not met. If still the criterion of four taxonomic groups is applied to perform statistical extrapolation, it might be better to use *monera* instead of *bacteria* and *cyanophyta*, and *protista* instead of *protozoa* and *algae* as taxonomic groups. This proposal is a more stringent guideline to apply statistical extrapolation only in those cases where more taxonomic groups (at least two) are available than the four mentioned above. In this report this rule would apply to the following compounds: toluene, ethylbenzene, hydroquinone, *o*- and *m*-cresol, trichloromethane, β -HCH, cyclohexanone, pyridine, tetrahydrofuran, and diethyl phthalate. Preliminary risk assessment would then be used instead of refined risk assessment for these eleven compounds. The guidelines to apply statistical extrapolation used by Denneman and van Gestel (1990) were also more rigid than those from the project 'Setting Integrated Environmental Quality Standards' used in this report (see 2.7).

A second possibility for the fact that some of the derived SRC_{eco} can be too high lies in the fact that some compounds, i.e. the non-chlorinated monoaromatic and chlorinated aliphatic hydrocarbons, are very volatile. As a consequence, actual exposure concentrations are generally much lower than nominal concentrations. Many of the underlying data for the compound groups above are subject to this effect, which can severely influence the ERLs (Van de Plassche et al., 1993). In this case the derived ERLs from these experiments are too high as well.

4.3.4 A generic value for the ERLs in soil and sediment of narcotic chemicals

For most organic compounds the BSAF values are very similar (Hendriks et al., 1998; Tracey and Hansen, 1996). If compounds have the same intrinsic toxicity this will also result in almost constant effect concentrations in soil or sediment. Many organic chemicals have no specific mode of toxic action and act mainly by narcosis (McCarthy and Mackay, 1993; Hermens and Leeuwangh, 1982). The presence of a more specific mode of toxic action will of course be more pronounced in the 5th percentile of the most sensitive species to a compound than in the geometric mean of all species. Therefore, a generic a-specific mode of toxic action

will be of more relevance for the SRC_{eco} than for the MPC: the SRC_{eco} is subject to the differences in the derivation of the toxicity data for each compound to a lesser extent than the MPC. A generic value for the ERLs, or at least the SRC_{eco} , can thus be considered for narcotic chemicals.

All SRC_{eco} that were derived in this report for organic chemicals in soil are shown in Figure 4.2, including SRC_{eco} derived directly from terrestrial toxicity studies as well as those derived by equilibrium partitioning from aquatic toxicity studies. In the upper part of the figure the compounds that are supposed to have no specific toxic mode of action (narcotic chemicals) are shown and in the lower part the other chemicals, which are the pesticides and PCBs. For soil and sediment the MPCs derived by either the modified EPA method or the EU/TGD method are shown in Figure 4.3 and Figure 4.4. As can be seen from these figures a clear difference exists between the chemicals that are assumed to act mainly by narcosis and those with a specific mode of action.

The differences for narcotic chemicals are likely caused by differences and uncertainty in the available data on toxicity and partition coefficients and differences in extrapolation methods, rather than differences in toxicity. This facilitates the use of one value for this type of chemicals. Further, if effect concentrations are additive, which is the case for narcotic chemicals, this generic value for narcotic chemicals (e.g. Broderius and Kahl, 1985) can also be considered as a sum value for the group of these compounds (see also 2.5).

A similar approach for deriving ERLs has also been suggested by DiToro and McGrath (2000). A general SRC_{eco} for soil and sediment would be in the order of $100 \mu\text{mol/kg}$, which is approximately the value derived for chlorobenzenes and chlorophenols. A general value for the MPC would be in the range of $1.0 \mu\text{mol/kg}$, a value that is approximately the geometric mean for chlorobenzenes and chlorophenols. Consequently, for these chemicals the difference between SRC_{eco} and MPC is approximately a factor of 100. This approach should be worked out in more detail before it can be used for the purpose of deriving SRC_{eco} in sediment or soil.

4.3.5 Preliminary risk assessment: the use of equilibrium partitioning and extrapolation factors

The SRC_{eco} derived by equilibrium partitioning are consistent with the SRC_{eco} derived from terrestrial toxicity data (Figure 4.2). Similar to the SRC_{eco} , no significant differences exist for the MPCs derived directly from terrestrial toxicity data or derived indirectly from aquatic toxicity data by equilibrium partitioning (Figure 4.3 and Figure 4.4). This is a strong indication that equilibrium partitioning is an effective method for calculating ERLs for organic compounds.

The MPCs cover a broader range of concentrations than the SRC_{eco} (see Figure 4.2 to Figure 4.4). This is expected because the MPC (which is based on the 5th percentile or derived from the lowest value with different assessment factors) is much more influenced by the composition of the available toxicity data than the SRC_{eco} (which is based on the geometric mean only). Further, the MPCs derived by the modified EPA method and the MPC derived by the EU/TGD method seem to cover almost the same range.

For MPCs of narcotic chemicals derived by equilibrium partitioning the difference between the values originating from preliminary and refined risk assessment is even more obvious than for the SRC_{eco} (see 4.3.3). The distribution of the MPCs seems to be bimodal and not uniform. A possible explanation is that the assessment factors for preliminary risk assessment are too high. It is also plausible that the limited diversity of the underlying data or volatilisation of many of the narcotic chemicals is causing this bimodality (4.3.3).

Considering this, it can be concluded that the extrapolation factors of the preliminary risk assessment are rather consistent with the statistical extrapolation.

4.4 Recommendations for further studies

Only one toxicity study for sediment has been used for the derivation of the ERLs. This means that almost all ERLs for sediment are based on equilibrium partitioning. Because environmental conditions, such as redox potential and pH, can be very different in sediment, data on benthic processes or single species would be very useful.

The available toxicity data that originate from older studies are in some cases rather limited. For these compounds, which are the monoaromatic hydrocarbons, the chlorinated aliphatic hydrocarbons and the chlorobenzenes, new toxicity data should be searched for.

Further, an update of the SRC_{eco} is advisable if the compound has been evaluated in a European framework (EU commission regulation 1488/94). The compounds of the first series of Intervention Values that are listed in the first priority list of the European Union are nickel, cadmium, several chromium salts, zinc, benzene, toluene, ethylbenzene, styrene, phenol, naphthalene, anthracene, chloroform, trichloroethylene, tetrachloroethylene, 1,4-dichlorobenzene, 1,2,4-trichlorobenzene, dibutyl phthalate, benzyl butyl phthalate, bis(2-ethylhexyl) phthalate and other phthalates. For these compounds an European evaluation will be available on a short term.

Until now for all acute toxicity data a general ACR of 10 has been used to compare ERLs derived from acute toxicity data with those derived from chronic toxicity data. Further, the specific sensitivity of a certain species towards a chemical is not included in the extrapolation from usually a limited number of toxicity studies from even less taxonomic groups. From knowledge about the toxic mode of action of a compound and from toxicity databases, more scientifically based assessment factors might be derived. The resulting assessment factors should be specific for a particular taxonomic group or group of compounds.

The use of a generic value for ERLs for sediment and soil for organic compounds without a specific mode of toxic action has been put forward in section 4.3. The applicability of such a concept for the purpose of ERLs should be further explored. It should be investigated if differences in ERLs can be completely attributed to uncertainties in toxicity data and partition coefficients or to differences in taxonomic groups among the available toxicity data.

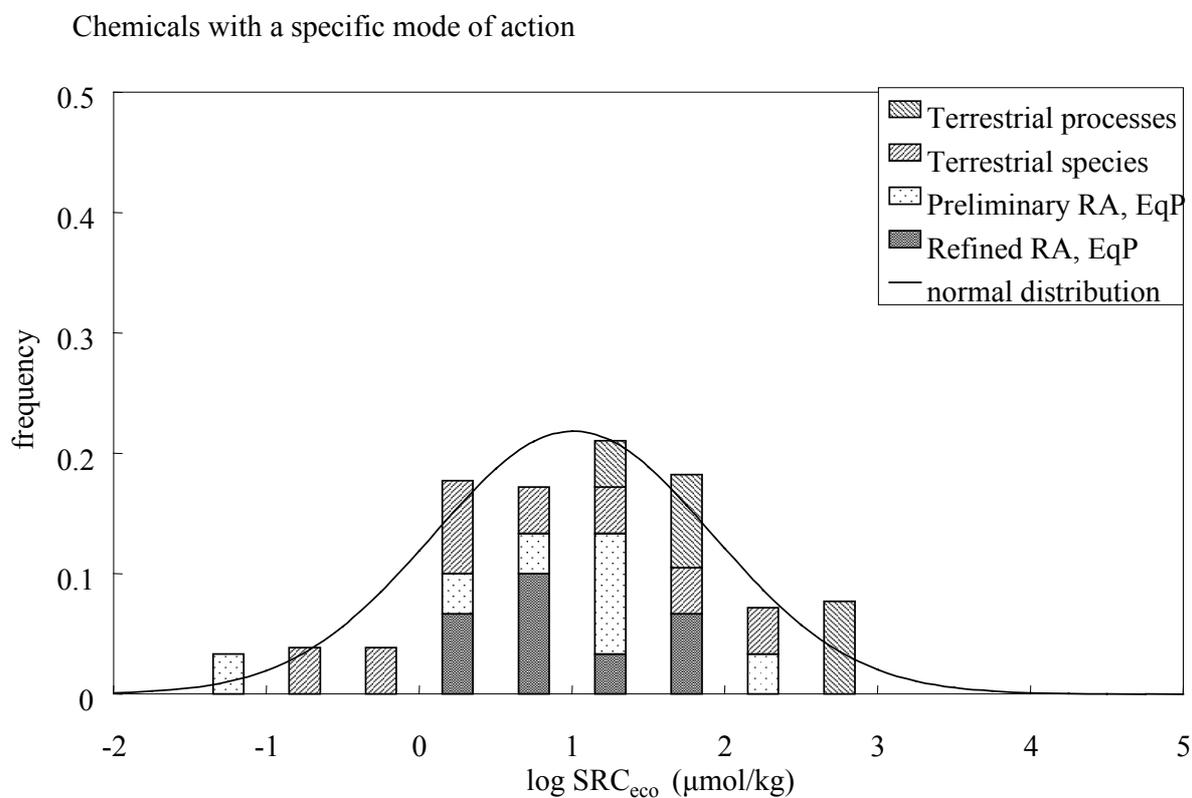
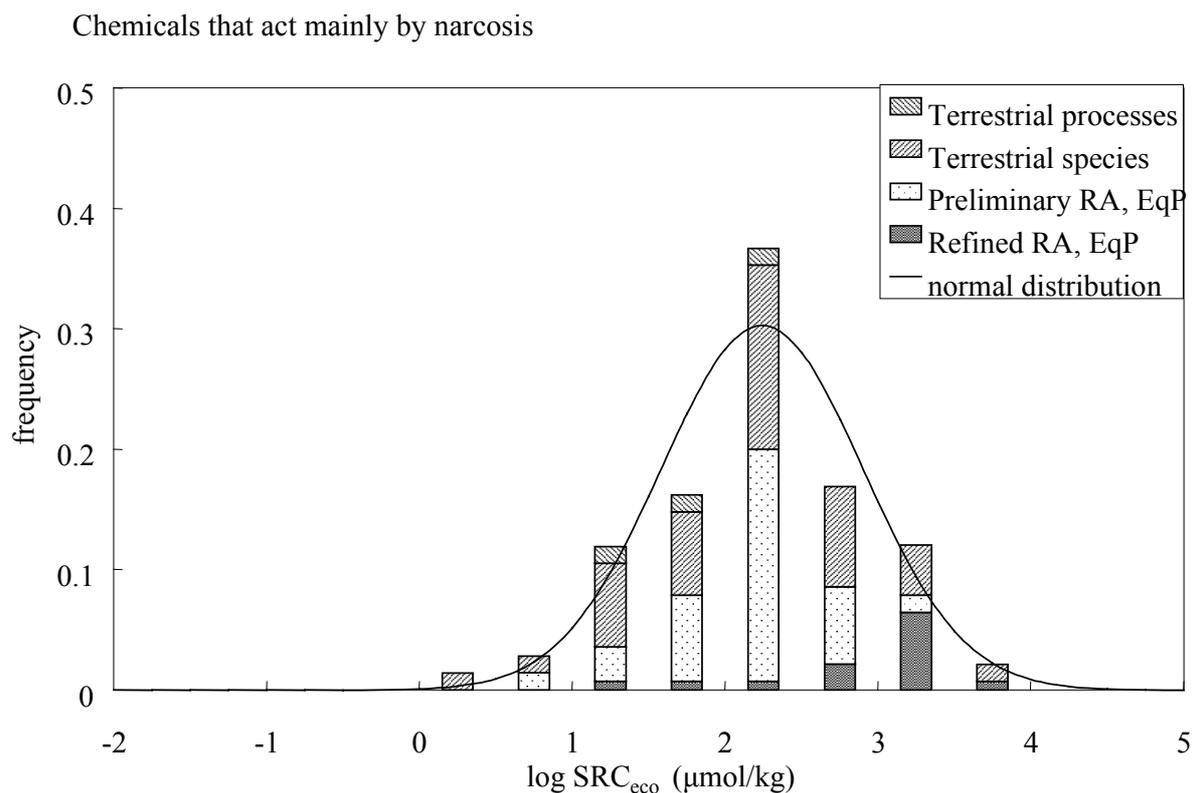


Figure 4.2: Distribution of the SRC_{eco} derived in this report for organic compounds. A separation is made between chemicals that are assumed to act mainly by narcosis (most of the organic compounds, $n = 106$, $\bar{x} = 2.24$, $s = 0.66$) and chemicals with a more specific mode of action (all pesticides and PCBs, $n = 28$, $\bar{x} = 1.01$, $s = 0.91$).

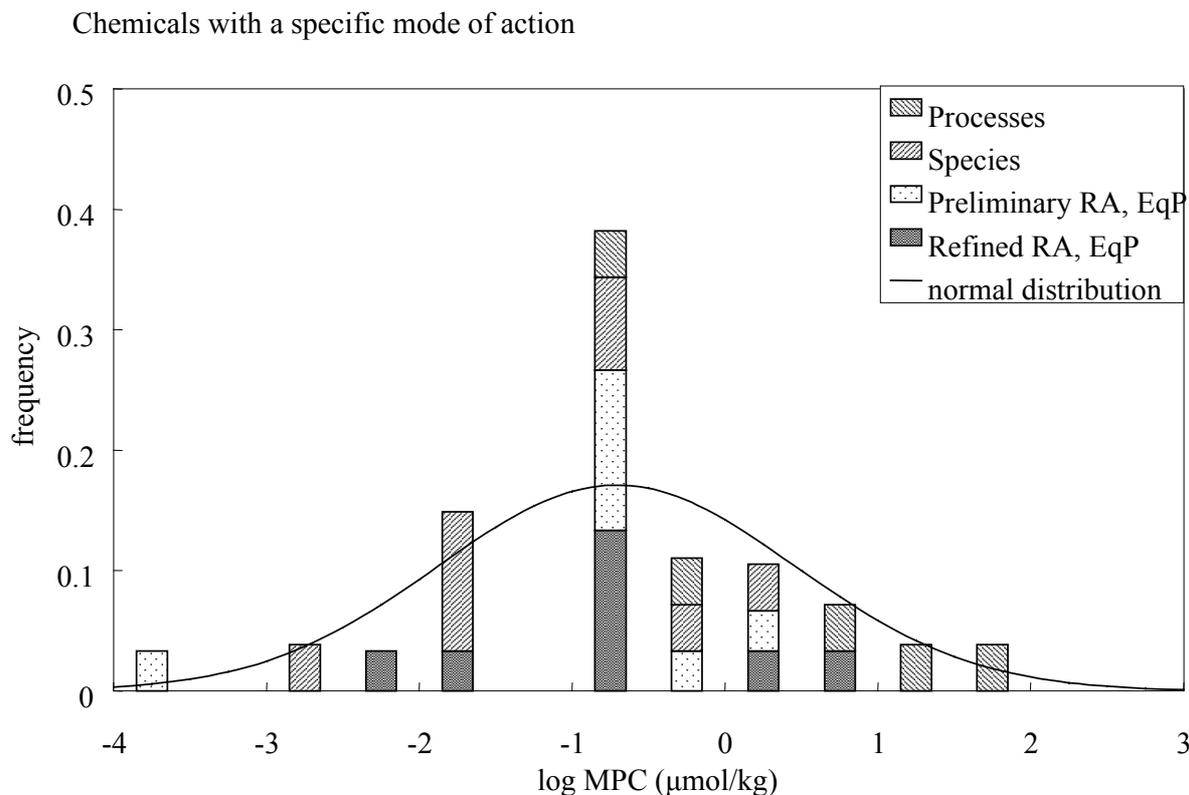
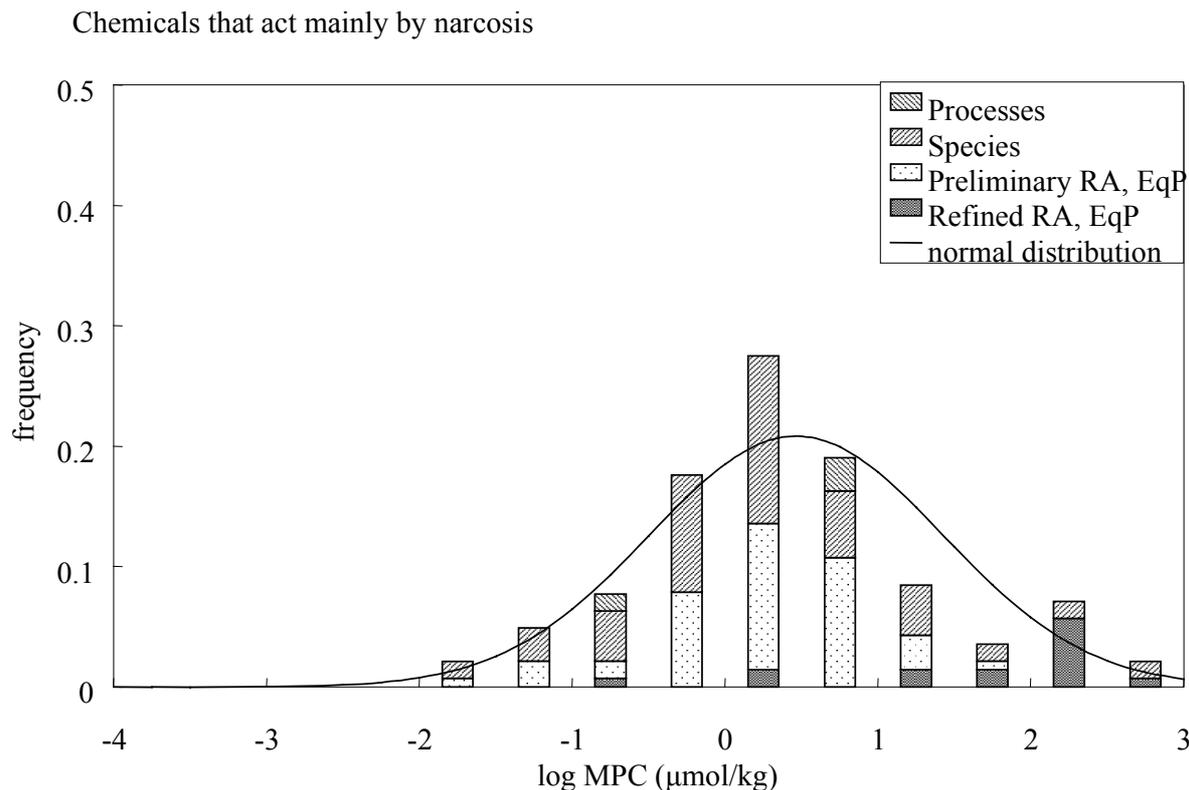


Figure 4.3: Distribution of the MPCs derived in this report for organic compounds by the modified EPA method or statistical extrapolation. A separation is made between chemicals that are assumed to act mainly by narcosis (most of the organic compounds, $n = 106$, $\bar{x} = 0.47$, $s = 0.96$) and chemicals with a more specific mode of action (all pesticides and PCBs, $n = 28$, $\bar{x} = -0.71$, $s = 1.17$).

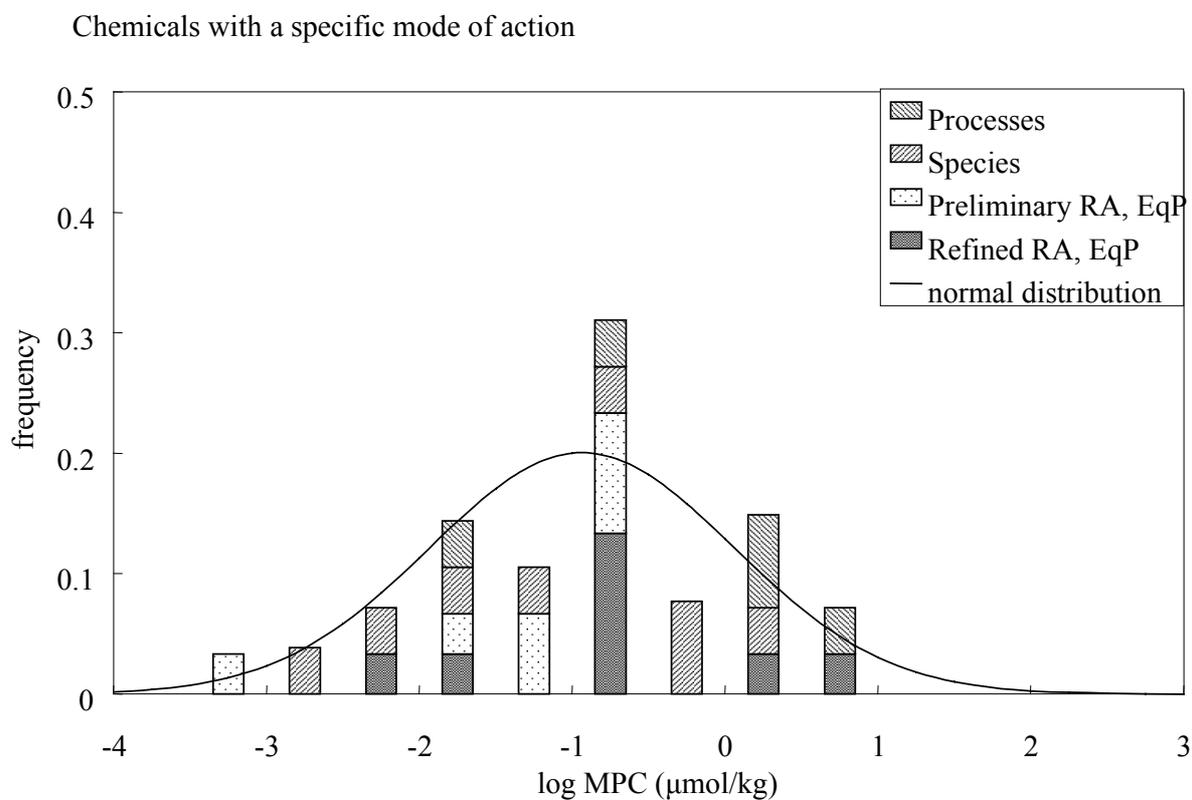
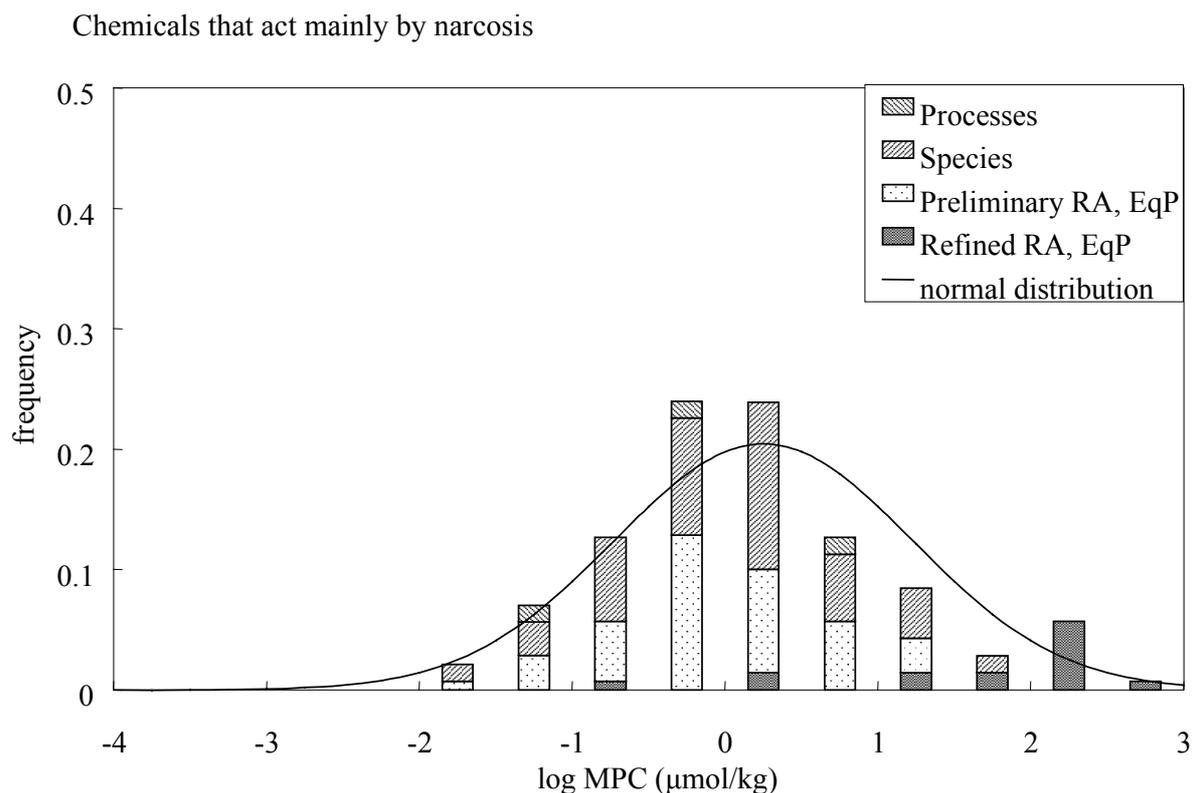


Figure 4.4: Distribution of the MPCs derived in this report for organic compounds by the EU/TGD method or statistical extrapolation. A separation is made between chemicals that are assumed to act mainly by narcosis (most of the organic compounds, $n = 106$, $\bar{x} = 0.25$, $s = 0.98$) and chemicals with a more specific mode of action (all pesticides and PCBs, $n = 106$, $\bar{x} = -0.94$, $s = 1.00$).

5 Conclusions

Generally, the SRC_{eco} derived in this report are in the same order of magnitude as the current Intervention Values and on average, the new SRC_{eco} values are equally high, with exception of a few organic chemicals. Differences with the old values derived by Denneman and van Gestel can be attributed to both a different methodology and different toxicity data. The number of ecotoxicological data on which most SRC_{eco} are based is limited, especially for the group of organic chemicals. This lack of sufficient data has considerable implications for the reliability of the values derived in this report. Most toxicity data be found for the water compartment. For soil much less toxicity data were reported and as good as no data are available for sediment. Consequently, a substantial part of the SRC_{eco} for soil and almost all values for sediment had to be derived by equilibrium partitioning. The equilibrium partitioning method seems to give results that are comparable with the ERLs derived from direct terrestrial toxicity data. Therefore, this method is suitable to derive ERLs for soil and sediment in the absence of sufficient terrestrial toxicity data. However, the reliability of this method also depends on the used partition coefficients. For this reason, this method seems to be less reliable to derive ERLs for metals in soil and sediment. The assessment factors for preliminary risk assessment seem to be linked with the statistical extrapolation of the refined risk assessment fairly well for the SRC_{eco} as well as the MPCs. However, the taxonomic diversity necessary to apply refined risk assessment is not very stringent at this moment.

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List of abbreviations

Terrestrial species

ann	annelida (oligochaeta)
ara	arachnida
bact	bacteria
crus	crustacea
fung	fungi
iso	isopoda
ins	insecta
mac	macrophyta
moll	mollusca
nema	nematoda

Microbial processes

N-min	N-mineralisation
nitr	nitrification
ac-min	acetate mineralisation
am	ammonification
arg-am	arginine ammonification
ATP	ATP content
bio C	biomass carbon
cel-resp	cellulose respiration
cel-min	cellulose mineralisation
Fe(III)-red	Fe(III) reduction
glu-resp	glucose respiration
H ₂ -oxy	H ₂ oxidising potential
N ₂ -fix	N ₂ fixation
resp	respiration
eth	ethylene production
glu-min	glucose mineralisation

Enzymatic activity

aryl	arylsulfatase
amy	amylase
β-gluc	β-glucosidase
β-acet	β-acetylglucoseaminidase
cellu	cellulase
dehy	dehydrogenase
glut	glutamase
inv	invertase
nit-red	nitrate reductase
nitro	nitrogenase
phos	phosphatase
phos diest	phosphodiesterase
prot	proteinase
ure	urease activity
xyl	xylanase

Aquatic species

bact	bacteria
coel	coelenterata
cyan	cyanophyta
echi	echinodermata
fung	fungi (mycophyta)
alg	algae
prot	protozoa
crus	crustacea
pisc	pisces
mac	macrophyta
nema	nematoda
plat	platyhelminthes
roti	rotifera
moll	mollusca
ann	annelida
ins	insecta
amph	amphibia

Risk limits

ACR	Acute to chronic ratio
BCF	Bioconcentration factor: the ratio of the substance concentration in (part of) an organism to the concentration in water at steady state
BSAF	Biota to soil/sediment accumulation factor: the ratio of the substance concentration in (part of) an organism to the concentration in soil or sediment at steady state
C_b	background concentration
ECOTOX-SCC	Ecotoxicological Serious Contamination Concentration (currently SRC_{eco})
EC50	Effect Concentration causing 50% effect
ERL	Ecotoxicological Risk Limit
EqP	Equilibrium Partitioning
HC5	Hazardous Concentration for which for 5% of the species or processes are not protected
HC50	Hazardous Concentration for which for half of the species or processes are not protected
HUMTOX SCC	Human-toxicological Serious Contamination Concentration (currently SRC_{human})
INS	Setting Integrated Environmental Quality Standards (Integrale Normstelling Stoffen)
IW	Technical evaluation of Intervention Values for soil/sediment and groundwater Intervention Values (Interventiewaarden)
K_{oc}	Organic carbon-water partition coefficient
K_{ow}	Octanol-water partition coefficient
K_p	Solid-water partition coefficient (between soil or sediment and water soil/w and sed/w)
LC50	Lethal concentration for 50% of the population
MPA	Maximal Permissible Addition (for metals)

MPC	Maximal Permissible Concentration
NA	Negligible Addition (for metals)
NC	Negligible Concentration
NOEC	No Observed Effect Concentration
QSAR	Quantitative structure activity relationship
SRA _{eco}	Serious Risk Addition for ecosystems (for metals)
SRC _{eco}	Serious Risk Concentration for ecosystems (formerly called ECOTOX-SCC)
SRC _{human}	Serious Risk Concentration for humans (formerly called HUMTOX SCC)
TGD	Technical guidance document
T.U.	Toxic Unit

Organisations

EPA	Environmental Protection Agency (U.S.)
EU	European Union
RIVM	National Institute of Public Health and the Environment (The Netherlands)
TCB	Technical Soil Protection Committee (The Netherlands)
VROM	Ministry of Housing Spatial Planning and the Environment (The Netherlands)

Appendix 1 Mailing list

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Table A2. 1: Arsenic: selected data on terrestrial species

taxonomic group	NOEC [mg/kg]	taxonomic group	NOEC [mg/kg]
mac	72	ann	45
mac	55a		

All data originate from Appendix 2II in Crommentuijn et al. (1997a).

a: geometric mean of 140 and 22 mg/kg, parameter growth for *G. hirsutum*

Table A2. 2: Arsenic: selected data on terrestrial processes

process	NOEC [mg/kg]	process	NOEC [mg/kg]
N-min	420 ^a	phos	980 ^k
N-min	310 ^b	ure	48
N-min	370 ^c	ure	370
N-min	340 ^d	ure	140
phos	120 ^e	ure	37
phos	1100 ^f	ure	100
phos	380 ^g	ure	17
phos	340 ^h	nitr	42 ^l
phos	98 ⁱ	nitr	67 ^m
phos	200 ^j	nitr	76 ⁿ

All data originate from Appendix 2V in Crommentuijn et al. (1997a).

a: geometric mean of 420 and 420 mg/kg, process N-mineralisation in soil with pH 5.8

b: geometric mean of 310 and 310 mg/kg, process N-mineralisation in soil with pH 6.6

c: geometric mean of 370 and 370 mg/kg, process N-mineralisation in soil with pH 7.8

d: geometric mean of 340 and 340 mg/kg, process N-mineralisation in soil with pH 7.4

e: geometric mean of 210 and 71 mg/kg, process phosphatase(acid) in Webster soil with pH 5.8

f: geometric mean of 1900 and 620 mg/kg, process phosphatase(acid) in Harps soil with pH 7.8

g: geometric mean of 850 and 170 mg/kg, process phosphatase(acid) in Okoboji soil with pH 7.4

h: geometric mean of 620 and 190 mg/kg, process phosphatase(alkaline) in Harps soil with pH 7.8

i: geometric mean of 170 and 57 mg/kg, process phosphatase(alkaline) in Okoboji soil with pH 7.4

j: geometric mean of 140 and 280 mg/kg, process phosphatase in spar-mor soil with pH 4.3

k: geometric mean of 680 and 1400 mg/kg, process phosphatase in mull soil with pH 6.3

l: geometric mean of 42 and 42 mg/kg, process nitrification in Webster soil with pH 5.8

m: geometric mean of 37 and 120 mg/kg, process nitrification in Harps soil with pH 7.8

n: geometric mean of 34 and 170 mg/kg, process nitrification in Okoboji soil with pH 7.4

Table A2. 3: Arsenic: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC in [$\mu\text{g/l}$]
bact	9700	crus	400 ^a
cyan	11000	crus	88
alg	10	pisc	2100
alg	86	pisc	2100
alg	4700	pisc	76
alg	10000	pisc	8400
prot	4800	pisc	1900 ^b
crus	570		

All data originate from Appendix 2 in Crommentuijn et al. (1997a).

a: most sensitive parameter (reproduction) for *Daphnia magna*, geometric mean of 630 and 260 $\mu\text{g/l}$

b: most sensitive parameter (mortality/reproduction) for *Pimephales promelas*, geometric mean of 1700 and 2100 $\mu\text{g/l}$

Table A2. 4: Arsenic: selected data for marine water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
alg	95a	crus	630

All data originate from Appendix 2I in Crommentuijn et al. (1997a).

a: most sensitive parameter (reproduction) for *Champia parvula*

Table A2. 5: Barium: selected data on terrestrial processes

process	NOEC [mg/kg]	process	NOEC [mg/kg]
phos (acid)	2800	aryl	1300
phos (acid)	2600	ure	930
phos (acid)	1100 ^a	ure	590
phos (alkaline)	1400	ure	370
phos (alkaline)	820 ^b	ure	190 ^e
aryl	930	ure	450
aryl	380 ^c	ure	170 ^f
aryl	750 ^d		

All data originate from Appendix 4 in Van de Plassche et al. (1992).

a: geometric mean of 3600 and 360 mg/kg, process acid phosphatase in loam with pH 5.8

b: geometric mean of 2600 and 260 mg/kg, process alkaline phosphatase in silty clay loam with pH 7.4

c: geometric mean of 970 and 150 mg/kg, process arylsulfatase in soil with pH 7.6

d: geometric mean of 1700 and 340 mg/kg, process arylsulfatase in soil with pH 6.5

e: geometric mean of 590 and 59 mg/kg, process urease in soil with pH 7.8

f: geometric mean of 540 and 54 mg/kg, process urease in soil with pH 7.4

Table A2. 6: Barium: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	17000	crus	55000 ^a
crus	2900	pisc	570000
		mac	26000

All data originate from Appendix 2 in van de Plassche et al. (1992).

a: geometric mean of 200 and 15 mg/l for *Daphnia* sp.

Table A2. 7: Cadmium: selected data on terrestrial species

taxonomic group	NOEC [mg/kg]	taxonomic group	NOEC [mg/kg]
mac	18 ^a	ann	14
mac	14	ann	250
mac	2.0 ^b	iso	2.8 ^e
moll	7.8	ins	57 ^f
ann	130	ins	2.9 ^g
ann	5.3 ^c	ara	1.2 ^h
ann	23 ^d		

All data originate from Appendix 2II in Crommentuijn et al. (1997a).

a: geometric mean of 20, 7.9, 55, 10, 71 and 6.1 mg/kg, parameter growth for grain species

b: geometric mean of 1.5, 2.2, 1.1, 2.5, 2.3 and 3.4 mg/kg, parameter growth for *S. oleracea*

c: lowest parameter (reproduction) for *Eisenia andrei*

d: lowest parameter (reproduction) for *Eisenia fetida*, geometric mean of 13 and 41 mg/kg

e: lowest parameter (growth) for *P. scaber*, geometric mean of 4.6 and 1.7 mg/kg

f: lowest parameter (reproduction) for *F. candida*, geometric mean of 36 and 89 mg/kg

g: lowest parameter (growth) for *O. cincta*

h: lowest parameter (reproduction) for *P. peltifer*

Table A2. 8: Cadmium: selected data on terrestrial processes

process	NOEC [mg/kg]	process	NOEC [mg/kg]
arg-am	110	dehy	170
ATP	80	dehy	31
cel-resp	200	dehy	110
Fe(III)-red	62	dehy	91
glu-resp	200	dehy	98
nitr	60	dehy	69
nitr	54	dehy	33
nitr	40	dehy	24
N-min	340	dehy	29
N-min	180	dehy	120
N-min	200	dehy	81
N-min	270	dehy	67
N-min	650	dehy	96
N-min	2100	dehy	81
N-min	480	phos	380
N-min	370	phos	1000
N-min	310	phos	170
resp	200 ^a	phos	300
resp	270 ^b	phos	270
resp	200 ^c	phos	300
resp	450 ^d	phos	90
resp	130	phos	29 ^h
resp	83	phos	11000
resp	65	phos	18 ⁱ
resp	63	phos	750 ^j
resp	160	ure	71 ^k
resp	120	ure	380 ^l
resp	310	ure	2.7 ^m
aryl	6.1 ^e	ure	2200
aryl	4.7	ure	77
aryl	9.2 ^f	ure	60
aryl	25 ^g	ure	67
aryl	3000	ure	30
dehy	54	ure	52
dehy	27	ure	26

All data originate from Appendix 2V in Crommentuijn et al. (1997a).

a: respiration, result from test with sandy loam with pH 5.1 with longest exposure

b: respiration, result from test with sand with pH 7.7 with longest exposure

c: respiration, result from test with silty loam with pH 7.4 with longest exposure

d: respiration, result from test with sandy peat with pH 4.3 with longest exposure

e: arylsulphatase, result from test with sand with pH 7.7 with longest exposure

f: arylsulphatase, result from test with silty loam with pH 7.4 with longest exposure

g: arylsulphatase, result from test with clay with pH 6.8 with longest exposure

h: phosphatase, result from test with sand with pH 7.7 with longest exposure

i: phosphatase, result from test with silty loam with pH 7.4 with longest exposure

j: phosphatase, result from test with clay with pH 6.8 with longest exposure

k: urease, result from test with sand with pH 7.7 with longest exposure

l: urease, result from test with silty loam with pH 7.4 with longest exposure
 m: urease, result from test with clay with pH 6.8 with longest exposure

Table A2. 9: Cadmium: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
bact	80	ann	30 ^g
bact	220	crus	0.41 ^h
cyan	50	crus	0.86 ⁱ
cyan	70	crus	1.6 ^j
alg	52 ^a	crus	1.2
alg	83	crus	0.29
alg	330 ^b	crus	1.0 ^k
alg	33 ^c	ins	2.0 ^l
alg	900	pisc	4.2 ^m
alg	31	pisc	4.2
alg	11	pisc	15 ⁿ
alg	15 ^d	pisc	3.0 ^o
alg	1.1	pisc	180 ^p
mac	33	pisc	4.3
mac	9.0	pisc	10
mac	20	pisc	1.3
mac	5.0	pisc	2.1 ^q
mac	2.2 ^e	pisc	3.8
mac	6.9 ^f	pisc	5.0 ^r
prot	11	pisc	2.5 ^s
prot	670	pisc	4.4
roti	40	pisc	9.0
moll	2.5	amph	3.0
moll	3.0		

All data originate from Appendix 2 in Crommentuijn et al. (1997a).

a: parameter growth for *C. reinhardtii*, geometric mean of 38 and 70 $\mu\text{g/l}$

b: parameter growth for *C. pyrenoidosa*, geometric mean of 36 and 3100 $\mu\text{g/l}$

c: lowest parameter (growth) for *C. vulgaris*

d: parameter growth for *S. capricornutum*, geometric mean of 2, 4, 10 and 700 $\mu\text{g/l}$

e: parameter growth for *S. minima*, geometric mean of 1, 3.3 and 3.3 $\mu\text{g/l}$

f: parameter growth for *S. punctata*, geometric mean of 10, 10 and 3.3 $\mu\text{g/l}$

g: parameter growth for *A. headleyi*, geometric mean of 54 and 17 $\mu\text{g/l}$

h: parameter(reproduction) for *C. dubia*, geometric mean of 1.0, 0.33, 0.33, 0.1 and 1.1 $\mu\text{g/l}$

i: lowest parameter (growth) for *Daphnia magna*, geometric mean of 0.5, 1, 0.5, 1, 1.2, 1.2, 4.1, 2, 0.11, 1, 0.16, and 3.2 $\mu\text{g/l}$

j: lowest parameter (reproduction) for *Daphnia pulex*, geometric mean of 0.03, 3.8, 7.5 and 7.5 $\mu\text{g/l}$

k: lowest parameter (reproduction) for *M. macrocopa*

l: lowest parameter (mortality/reproduction) for *C. riparius*

m: lowest parameter (mortality) for *C. commersoni*

n: parameter growth for *I. punctatus*, geometric mean of 20 and 12 $\mu\text{g/l}$

o: lowest parameter (mortality) for *J. floridae*

p: lowest parameter (growth) for *L. macrochirus*, geometric mean of 1100 and 31 $\mu\text{g/l}$

q: geometric mean of 1.3, 2.6 and 2.6 $\mu\text{g/l}$, parameter mortality for *Oncorhynchus mykiss*

r: lowest parameter (growth) for *Pimephales promelas*

s: lowest parameter (growth) for *S. fontinalis*, geometric mean of 1.7, 1.1, 3.0 and 7.0 $\mu\text{g/l}$

Table A2. 10: Cadmium: selected data for marine water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
cyan	39	alg	3.4
alg	1.1	nema	500
alg	11	nema	5000
alg	11	nema	25000
alg	3.4	moll	5.0
alg	39	moll	110
alg	110	ann	320
alg	34	ann	1000 ^a
alg	1100	ann	560
alg	1.1	ann	500 ^b
alg	11	ann	200
alg	3.4	crus	2.1 ^c
alg	1.1	crus	1.1
alg	3.4	crus	320
alg	0.56	crus	5.0 ^d
alg	1.1	crus	3.7 ^e
alg	11	crus	5.1
alg	34	pisc	100
alg	3.4	pisc	45 ^f
alg	11	pisc	1000

All data originate from Appendix 2I in Crommentuijn et al. (1997a).

a: geometric mean of 1000 and 1000 $\mu\text{g/l}$, parameter reproduction for *Ctenodrilus serratus*

b: geometric mean of 500 and 500 $\mu\text{g/l}$, parameter reproduction for *O. diadema*

c: lowest parameter (growth) for *A. compressa*

d: lowest parameter (mortality) for *C. anthonyi*

e: lowest parameter (mortality) for *M. bahia*, geometric mean of 2.5, 0.6, 0.6, 4, 5, 25, 15 and 5.1 $\mu\text{g/l}$

f: geometric mean of 20 and 100 $\mu\text{g/l}$, parameter mortality for *M. cephalus*

Table A2. 11: Chromium(III): selected data on terrestrial species

taxonomic group	NOEC [mg/kg]	taxonomic group	NOEC [mg/kg]
mac	380 ^a	ann	38 ^b

All data originate from Appendix 2II in Crommentuijn et al. (1997a).

a: geometric mean of 960, 200, 160, 720 and 350 mg/kg for grain species

b: lowest parameter (reproduction) for *Eisenia andrei*

Table A2. 12: Chromium(III): selected data on terrestrial processes

process	NOEC [mg/kg]	process	NOEC [mg/kg]
aryl	3.9	phos	1,300 ^c
aryl	1.5 ^a	phos	320 ^f
aryl	94	phos	1300 ^g
aryl	160 ^b	phos	630
aryl	4,600 ^c	resp	220 ^h
nitr	120	resp	140 ⁱ
nitr	27	resp	120
nitr	24	resp	240
nitr	22	ure	720 ^j
N-min	90	ure	1000 ^k
N-min	93	ure	210 ^l
N-min	120	ure	600
N-min	73	ure	31
phos	140	ure	79
phos	390	ure	90
phos	370	ure	24
phos	55	ure	120
phos	390	ure	11
phos	1300 ^d		

All data originate from Appendix 2V in Crommentuijn et al. (1997a).

a: arylsulphatase, result from test with sandy loam with pH 5.1 with longest exposure

b: arylsulphatase, result from test with clay with pH 6.8 with longest exposure

c: arylsulphatase, result from test with sandy peat with pH 3.0 with longest exposure

d: phosphatase, result from test with sand with pH 7.7 with longest exposure

e: phosphatase, result from test with sandy loam with pH 5.1 with longest exposure

f: phosphatase, result from test with silty loam with pH 7.4 with longest exposure

g: phosphatase, result from test with clay with pH 7.5 with longest exposure

h: respiration, result from test with sandy loam with pH 5.1 with longest exposure

i: respiration, geometric mean of 100 and 210 mg/kg

j: urease, result from test with sand, with pH 7.7 with longest exposure

k: urease, result from test with silty loam, with pH 7.4 with longest exposure

l: urease, result from test with clay, with pH 7.5 with longest exposure

Table A2. 13: Chromium(VI): selected data on terrestrial processes

process	NOEC [mg/kg]	process	NOEC [mg/kg]
phos	1400 ^a	phos	680 ^b

All data originate from Appendix 2V in Crommentuijn et al. (1997a).

a: geometric mean of 1000 and 2000 mg/kg

b: geometric mean of 480 and 960 mg/kg

Table A2. 14: Chromium(III): selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
bact	1300	crus	700
alg	100	pisc	200
alg	100	pisc	88 ^a
alg	170		

All data originate from Appendix 2 in Crommentuijn et al. (1997a).

a: geometric mean of 48 and 160 $\mu\text{g/l}$, parameter mortality/growth/reproduction for *Oncorhynchus mykiss*

Table A2. 15: Chromium(VI): selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
bact	570 ^a	coel	1100
bact	380	roti	2000
cyan	83 ^b	moll	110 ^h
cyan	3300	crus	44 ⁱ
alg	33 ^c	crus	44 ^j
alg	35	crus	20
alg	35	ins	1100
alg	110 ^d	pisc	4700 ^k
alg	580	pisc	290
alg	86 ^e	pisc	6700 ^l
alg	130 ^f	pisc	305 ^m
mac	100	pisc	520
mac	35 ^g	pisc	1100 ⁿ
mac	100	pisc	100 ^o
mac	100	pisc	10
prot	0.058	pisc	3500 ^p
prot	3200	pisc	1000 ^q
prot	9600	pisc	3500 ^r
prot	6400	pisc	100 ^s
prot	1000	pisc	190 ^t
prot	100	pisc	110 ^u
		amph	350 ^v

All data originate from Appendix 2 in Crommentuijn et al. (1997a).

- a: geometric mean of 130 and 2500 $\mu\text{g/l}$, parameter mortality for *E. coli*
b: geometric mean of 1.9, 200, 200, 350, 110 and 110 $\mu\text{g/l}$, parameter growth for *M. aeruginosa*
c: lowest parameter (photosynthesis) for *C. pyrenoidosa*
d: geometric mean of 110 and 110 $\mu\text{g/l}$, parameter growth for *S. pannonicus*
e: geometric mean of 230 and 32 $\mu\text{g/l}$, parameter growth for *S. subspicatus*
f: geometric mean of 180, 110, 200 and 70 $\mu\text{g/l}$, parameter growth for *S. capricornutum*
g: geometric mean of 11 and 110 $\mu\text{g/l}$, parameter growth for *L. minor*
h: lowest parameter (reproduction) for *L. stagnalis*
i: lowest parameter (reproduction) for *C. dubia*, geometric mean of 32, 5.7, 65, 110 and 120 $\mu\text{g/l}$
j: lowest parameter (reproduction) for *Daphnia magna*, geometric mean of 18, 270, 350, 35 and 2.9 $\mu\text{g/l}$
k: lowest parameter (growth) of the most sensitive life-stage(eggs) for *Brachydanio rerio*
l: lowest parameter (growth) for *G. aculeatus*
m: most sensitive life-stage (eggs)/parameter (growth) for *I. punctatus*
n: lowest parameter (growth) for *J. floridae*
o: lowest parameter (growth) of most sensitive life-stage (eggs) for *Oncorhynchus mykiss*, geometric mean of 200 and 51 $\mu\text{g/l}$
p: lowest parameter (mortality/growth) for *O. latipes*
q: lowest parameter (mortality) for *Pimephales promelas*, geometric mean of 1000, 900 and 1100 $\mu\text{g/l}$
r: lowest parameter (growth) for *P. reticulata*, geometric mean of 3500 and 3500 $\mu\text{g/l}$
s: lowest parameter (growth) for *S. gairdneri*, geometric mean of 190 and 51 $\mu\text{g/l}$
t: lowest parameter (mortality/growth) for *S. fontinalis*, geometric mean of 100 and 350 $\mu\text{g/l}$
u: lowest parameter (growth) for *S. namaycush*
v: lowest parameter (mortality) for *X. laevis*

Table A2. 16: Chromium(VI): selected data for marine water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
alg	400 ^a	crus	88 ^d
ann	50	crus	520 ^e
ann	57 ^b	crus	5200 ^f
ann	25 ^c	crus	1000
ann	500	crus	360
crus	770	crus	320

All data originate from Appendix 2I in Crommentuijn et al. (1997a).

a: geometric mean of 300, 600, 800, 1400, 350 and 60 $\mu\text{g/l}$, parameter growth for *S. costatum*

b: lowest parameter (reproduction) for *D. gyrociliatus*, geometric mean of 100 and 33 $\mu\text{g/l}$

c: lowest parameter (reproduction) for *N. arenaceodantata*

d: most sensitive life-stage for *M. bahia*, parameter(reproduction)

e: most sensitive parameter (reproduction) for *P. elegans*

f: geometric mean of 5200, 5200 and 5200 $\mu\text{g/l}$, parameter mortality for *P. varians*

Table A2. 17: Cobalt: selected data on terrestrial species

taxonomic group	NOEC [mg/kg]		
ann	240		

All data originate from Appendix 4 in van de Plassche et al. (1992).

Table A2. 18: Cobalt: selected data on terrestrial processes

process	NOEC [mg/kg]	process	NOEC [mg/kg]
resp	30 ^a	phos (acid)	510 ^e
resp	31 ^b	phos (alkaline)	650
resp	62 ^c	phos (alkaline)	380 ^f
resp	97 ^d	aryl	1300
N-min	160	aryl	210 ^g
N-min	180	aryl	470 ^h
N-min	250	aryl	1200
N-min	230	ure	130
nitr	32	ure	130
nitr	87	ure	110
nitr	77	ure	34 ⁱ
phos (acid)	1300	ure	67
phos (acid)	1200	ure	24 ^j

All data originate from Appendix 4 in Van de Plassche et al. (1992).

a: geometric mean of 0.93 and 930 mg/kg, process respiration in silt loam with pH 6.7.

b: geometric mean of 1.7 and 570 mg/kg, process respiration in clay with pH 5.8.

c: geometric mean of 3.4 and 1100 mg/kg, process respiration in silt loam with pH 7.2.

d: geometric mean of 5.3 and 1800 mg/kg, process respiration in sandy loam with pH 8.2.

e: geometric mean of 1600 and 160 mg/kg, process acid phosphatase in loam with pH 5.8.

f: geometric mean of 1200 and 120 mg/kg, process alkaline phosphatase in silty clay loam with pH 7.4

g: geometric mean of 650 and 65 mg/kg, process arylsulphatase in soil with pH 7.6.

h: geometric mean of 1500 and 150 mg/kg, process arylsulphatase in soil with pH 6.5.

i: geometric mean of 87 and 13 mg/kg, process urease in soil with pH 7.8.

j: geometric mean of 77 and 7.7 mg/kg, process urease in soil with pH 7.4.

Table A2. 19: Cobalt: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
cyan	500	crus	5.0
alg	58 ^a	pisc	1100
alg	500		

All data originate from Appendix 2 in van de Plassche et al. (1992).

a: geometric mean of 49 and 69 $\mu\text{g/l}$ for *Chlorella pyrenoidosa*.

Table A2. 20: Cobalt: selected marine data

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
crus	110000	pisc	45000
crus	450		

All data originate from Appendix 3 in van de Plassche et al. (1992).

Table A2. 21: Copper: selected data on terrestrial species

taxonomic group	NOEC [mg/kg]	taxonomic group	NOEC [mg/kg]
mac	1500	ann	180
mac	1500	ann	61 ^d
mac	1500	ann	110 ^e
mac	290 ^a	ann	26 ^f
nema	430 ^b	ins	2800
ann	94 ^c	ara	180

All data originate from Appendix 2II in Crommentuijn et al. (1997a).

a: geometric mean of 350, 220, 180, 390 and 340 mg/kg, parameter growth for grain species

b: geometric mean of 300, 290, 1100, 810 and 190 mg/kg, parameter mortality for *C. elegans*

c: lowest parameter (reproduction) for *A. caliginosa*

d: lowest parameter (growth/reproduction) for *Eisenia andrei*

e: lowest parameter (reproduction) for *Eisenia fetida*, geometric mean of 35 and 380 mg/kg

f: lowest parameter (reproduction) for *L. rubellus*, geometric mean of 40 and 17 mg/kg

Table A2. 22: Copper: selected data on terrestrial processes

process	NOEC [mg/kg]	process	NOEC [mg/kg]
am	360	resp	310 ^c
eth	6.7	resp	520
eth	7.8	aryl	13 ^d
eth	11	aryl	520 ^e
eth	12	aryl	370 ^f
eth	11	aryl	1800 ^g
eth	7.3	aryl	4700 ^h
eth	12	phos	91 ⁱ
eth	8.2	phos	520 ^j
eth	13	phos	470 ^k
eth	11	phos	520 ^l
eth	11	phos	140 ^m
eth	11	phos	17 ⁿ
eth	12	phos	660
eth	14	phos	220 ^o
eth	14	phos	650 ^p
eth	11	phos	81 ^q
eth	6.7	ure	42 ^r
eth	10	ure	180
eth	14	ure	440
nitr	310	ure	350 ^s
nitr	36	ure	290 ^t
nitr	100	ure	25 ^u
nitr	90	ure	26 ^v
N-min	250	ure	78 ^w
N-min	310	ure	60 ^x
resp	21	ure	37 ^y
resp	9.8 ^a	ure	10 ^z
resp	560 ^b	ure	26 ^{aa}
		ure	14 ^{ab}

All data originate from Appendix 2V in Crommentuijn et al. (1997a).

- a: respiration, result from test with longest exposure
- b: respiration, result from test with longest exposure
- c: respiration, result from test with longest exposure
- d: arylsulphatase, result from test with longest exposure
- e: arylsulphatase, result from test with longest exposure
- f: arylsulphatase, result from test with longest exposure
- g: arylsulphatase, result from test with longest exposure
- h: arylsulphatase, result from test with longest exposure
- i: geometric mean of 91 and 91 mg/kg
- j: geometric mean of 520 and 520 mg/kg
- k: geometric mean of 470 and 470 mg/kg
- l: geometric mean of 520 and 520 mg/kg
- m: geometric mean of 140 and 140 mg/kg
- n: phosphatase, result from test with longest exposure
- o: phosphatase, result from test with longest exposure
- p: phosphatase, result from test with longest exposure
- q: phosphatase, result from test with longest exposure
- r: urease, result from test with longest exposure
- s: urease, result from test with longest exposure
- t: urease, result from test with longest exposure

- u: geometric mean of 25 and 25 mg/kg
v: geometric mean of 26 and 26 mg/kg
w: geometric mean of 43 and 140 mg/kg
x: geometric mean of 32 and 110 mg/kg
y: geometric mean of 37 and 37 mg/kg
z: geometric mean of 10 and 10 mg/kg
aa: geometric mean of 26 and 26 mg/kg
ab: geometric mean of 14 and 14 mg/kg

Table A2. 23: Copper: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
bact	10	crus	5.0
alg	11 ^a	crus	3.3 ⁱ
alg	40 ^b	ins	20
alg	5.3	ins	34
alg	50	ins	10 ^j
alg	330	pisc	0.06 ^k
alg	10	pisc	13
alg	10	pisc	43
alg	33 ^c	pisc	50
alg	64	pisc	35
alg	28 ^d	pisc	9.5 ^l
prot	3800	pisc	29 ^m
roti	20	pisc	37
moll	8.0	pisc	120
moll	17	pisc	16 ⁿ
moll	8.0	pisc	22 ^o
crus	15 ^e	pisc	13 ^p
crus	20 ^f	pisc	3.4 ^q
crus	8.2 ^g	pisc	22
crus	1.7 ^h	pisc	10 ^r

All data originate from Appendix 2 in Crommentuijn et al. (1997a).

- a: lowest parameter (mortality/immobility, deflagellation, encysted cells) for *C. reinhardtii*, geometric mean of 5, 19, 12 and 14 $\mu\text{g/l}$
b: lowest parameter (photosynthesis) for *C. pyrenoidosa*, geometric mean of 33 and 50 $\mu\text{g/l}$
c: lowest parameter (photosynthesis) for *S. gaudricauda*
d: geometric mean of 64, 15, 19, 24, 21 and 57 $\mu\text{g/l}$, parameter growth for *S. capricornutum*
e: geometric mean of 0.25 and 20 $\mu\text{g/l}$, parameter reproduction
e: lowest parameter (reproduction) for *C. dubia*, geometric mean of 12, 6.3, 6.4, 23, 27 and 40 $\mu\text{g/l}$
f: lowest parameter (growth) for *Daphnia ambigua*
g: lowest parameter (reproduction) for *Daphnia magna*, geometric mean of 10, 11 and 5 $\mu\text{g/l}$
h: lowest parameter (reproduction) for *Daphnia pulex*, geometric mean of 0.3 and 10 $\mu\text{g/l}$
i: lowest parameter (mortality) for *G. pulex*
j: reproduction for *C. magnifica* geometric mean of 8 and 13 $\mu\text{g/l}$
k: lowest parameter (reproduction) for *Brachydanio rerio*
l: lowest parameter (growth) for *I. punctatus*, geometric mean of 9 and 10 $\mu\text{g/l}$
m: lowest parameter (mortality) for *L. macrochirus*, geometric mean of 40 and 21 $\mu\text{g/l}$
n: lowest parameter (growth) for *Oncorhynchus mykiss*
o: most sensitive life-stage for *O. trutta*
p: most sensitive parameter (growth) for *Pimephales promelas*, geometric mean of 11, 11, 33, 3.1, 9.9, 31 and 20 $\mu\text{g/l}$,

q: most sensitive parameter (growth) for *S. fontinalis*, geometric mean of 9, 9, 22, 1, 0.67, 2 and 2 µg/l

r: most sensitive parameter (mortality/growth) for *S. vitreum*

Table A2. 24: Copper: selected data for marine water

taxonomic group	NOEC [µg/l]	taxonomic group	NOEC [µg/l]
cyan	5.0	alg	6.4 ^h
alg	64	alg	6.4
alg	130	alg	130
alg	6.4	coel	10
alg	250	coel	2.5
alg	2.5	coel	10
alg	17	moll	100
alg	0.64	moll	10
alg	250	moll	5.0
alg	66 ^a	moll	0.5 ⁱ
alg	64	moll	6.7
alg	190	moll	10
alg	130	ann	50
alg	110 ^b	ann	5.6 ^j
alg	10	ann	100
alg	250	ann	100
alg	1.0	crus	4.4 ^k
alg	6.4 ^c	crus	0.2
alg	14 ^d	crus	60
alg	64	crus	3.3 ^l
alg	130	crus	38 ^m
alg	170 ^e	crus	10
alg	64 ^f	pisc	76 ⁿ
alg	8.5 ^g		

All data originate from Appendix 2I in Crommentuijn et al. (1997a).

a: geometric mean of 6.4, 64, 190 and 250 µg/l, parameter reproduction for *E. huxleyi*

b: geometric mean of 64 and 190 µg/l, parameter reproduction for *H. carterae*

c: geometric mean of 6.4 and 6.4 µg/l, parameter reproduction for *Peridinium* spec.

d: geometric mean of 0.64, 64 and 64 µg/l, parameter reproduction for *Prorocentrum* spec.

e: lowest parameter (growth) for *S. costatum*

f: geometric mean of 64 and 64 µg/l, parameter reproduction for *S. tamesis*

g: geometric mean of 0.64, 0.64, 6.4, 6.4, 6.4, 64, 64 and 64 µg/l, parameter reproduction for *Synechococcus* spec.

h: geometric mean of 0.64, 6.4, 6.4 and 64 µg/l parameter reproduction for *Thoracosphaera* spec.

i: lowest parameter (mortality) for most sensitive life-stage (larva) for *M. edulis*

j: geometric mean of 3.9 and 8 µg/l, parameter mortality for *N. arenaceodentata*

k: lowest parameter (growth) for *A. compressa*, geometric mean of 5.2 and 3.7 µg/l

l: most sensitive parameter (reproduction) for *C. anthonyi*

m: most sensitive parameter (reproduction) for *M. bahia*

n: lowest parameter (abnormalities) for *A. affinis*, geometric mean of 120, 63, 120, 68, 55 and 55 µg/l

Table A2. 25: Lead: selected data on terrestrial species

taxonomic group	NOEC [mg/kg]	taxonomic group	NOEC [mg/kg]
mac	750 ^a	ann	1400 ^c
mac	1500	ann	240 ^d
mac	1500	moll	1000
mac	120	crus	40
mac	1500	ins	1100
mac	120	ara	400
ann	450 ^b		

All data originate from Janus et al. (2000).

a: geometric mean of 1100, 760, 700, 1200, 1100, 960 and 180 mg/kg, parameter yield for *Avena sativa*

b: geometric mean of 740, 740 and 170 mg/kg, parameter reproduction for *Dendrobaena rubida*

c: most sensitive parameter (reproduction) for *Eisenia fetida*, geometric mean of 2000 and 1000 mg/kg

d: most sensitive parameter (reproduction) for *Lumbricus rubellus*

Table A2. 26: Lead: selected data on terrestrial processes

process	NOEC [mg/kg]	process	NOEC [mg/kg]
resp	240	nitr	1500
resp	200	glu-min	1400
resp	1200	cel-min	330 ^a
resp	2300	amy	1000
resp	190	cellu	1000
resp	15	dehy	490
resp	24	dehy	6200
resp	5200	dehy	7700
resp	1500	phos	570 ^b
resp	1000	phos	470 ^c
resp	500	ure	50 ^d
N-min	180	ure	49 ^e
N-min	570	ure	900 ^f
N-min	440	ure	580 ^g
N-min	340	ure	250 ^h
N-min	950	ure	320 ⁱ
am	1500	ure	890 ^j
nitr	380	ure	94 ^k
nitr	1000	xyl	1000
nitr	950		

All data originate from Janus et al. (2000).

a: geometric mean of 160, 180 and 1200 mg/kg

b: geometric mean of 570 and 570 mg/kg

c: geometric mean of 470 and 470 mg/kg

d: geometric mean of 50 and 50 mg/kg

e: geometric mean of 49 and 49 mg/kg

f: geometric mean of 630 and 1,300 mg/kg

g: geometric mean of 1,000 and 340 mg/kg

h: geometric mean of 570 and 110 mg/kg

i: geometric mean of 1000 and 100 mg/kg

j: geometric mean of 890 and 890 mg/kg

k: geometric mean of 94 and 94 mg/kg

Table A2. 27: Lead: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
bact	1300	prot	70
bact	1800	moll	12 ^b
cyan	450	crus	26
alg	500	crus	40 ^c
alg	500	pisc	120
alg	1000	pisc	120
alg	500	pisc	250
alg	500	pisc	75
alg	1300 ^a	pisc	70
alg	10	pisc	120
alg	2100	pisc	41 ^d
alg	300	pisc	20
prot	220	pisc	39 ^e
prot	20	pisc	48 ^f
prot	1300	pisc	240 ^g

All data originate from Janus et al. (2000).

a: geometric mean of 1300, 1900, 3000, 500 and 1000 $\mu\text{g/l}$, parameter growth for *Scenedesmus quadricauda*

b: lowest parameter (survival) for *L. palustris*

c: lowest parameter (reproduction) for *Daphnia magna*, geometric mean of 1.0, 15, 250 and 670 $\mu\text{g/l}$

d: lowest parameter (abnormalities) for *Oncorhynchus mykiss*, geometric mean of 190, 7.0, 8.0, 28, 250 and 60 $\mu\text{g/l}$

e: lowest parameter (hatching/abnormalities/growth) for *Salvelinus fontinalis*

f: lowest parameter (survival) for *Salvelinus namaycush*

g: lowest parameter (survival/abnormalities) for *Stizostedion vitreum*

Table A2. 28: Lead: selected data for marine water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
alg	60	moll	200
alg	9.0	moll	200
prot	150	crus	1000
coel	300	crus	10
ann	500	crus	17
ann	1000	crus	50

All data originate from Janus et al. (2000).

Table A2. 29: Mercury, inorganic: selected data on terrestrial processes

process	NOEC [mg/kg]	process	NOEC [mg/kg]
resp	79	resp	40
resp	9.0	resp	250
resp	99	am	6.0
resp	120	am	10
resp	12	nitr	6.0
resp	31	nitr	10
resp	35	amy	79
resp	40	phos	2400
resp	210	ATP	1.4

All data originate from Slooff et al. (1995).

Table A2. 30: Methyl-mercury: selected data on terrestrial species

taxonomic group	NOEC [mg/kg]	
ann	3.7	

All data originate from Slooff et al. (1995).

Table A2. 31: Mercury, inorganic: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
bact	11 ^a	prot	500
bact	1.0	prot	780 ^b
cyan	2.5	prot	34
alg	100	moll	45 ^c
alg	100	crus	18 ^d
alg	20	crus	8.5
alg	35	crus	0.7 ^e
mac	20	crus	10 ^f
prot	8.0	pisc	1.0 ^g
prot	9.0	pisc	0.3 ^h

All data originate from Slooff et al. (1995).

a: geometric mean of 5 and 25 $\mu\text{g/l}$, parameter growth for *Pseudomonas putida*

b: most sensitive parameter (growth) for *Tetrahymena pyriformis*

c: geometric mean of 20, 40, 100, 20, 60 and 90 $\mu\text{g/l}$, parameter survival for *Viviparus bengalensis*

d: most sensitive parameter (reproduction) for *Cyclops spec.*

e: most sensitive parameter (reproduction) for *Daphnia magna*, geometric mean of 0.07, 1.7 and 3 $\mu\text{g/l}$

f: most sensitive parameter (mortality) for *Daphnia similis*

g: most sensitive parameter (mortality) for *Brachydanio rerio*

h: most sensitive parameter (growth) for *Pimephales promelas*, geometric mean of 0.63, 0.31, 0.26 and 0.09 $\mu\text{g/l}$

Table A2. 32: Mercury, inorganic: selected data for marine water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
alg	5.0	moll	1.0 ^c
alg	9.0	moll	0.25 ^d
alg	9.0	moll	2.0
alg	0.9	moll	4.0
alg	0.9	crus	2.0
prot	2.5	crus	4.9
coel	0.1	crus	0.8 ^e
ann	10 ^a	crus	6.0
ann	71 ^b	pisc	10 ^f

All data originate from Slooff et al. (1995).

a: geometric mean of 10 and 10 $\mu\text{g/l}$, parameter reproduction for *Ctenodrilus serratus*

b: geometric mean of 50 and 100 $\mu\text{g/l}$, parameter reproduction for *Ophryotrocha diadema*

c: most sensitive parameter (hatching) for *Crassostrea virginica*

d: most sensitive parameter (reproduction) for *Crepidula fornatica*

e: geometric mean of 0.8 and 0.8 $\mu\text{g/l}$, parameter reproduction/mortality for *Mysidopsis bahia*

f: most sensitive parameter (hatching) for *Fundulus heteroclitus*

Table A2. 33: Methyl-mercury: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
bact	0.2	pisc	0.17
prot	0.2	pisc	19 ^b
prot	14	pisc	0.07 ^c
plat	0.03 ^a	pisc	0.8
crus	0.09	pisc	0.15 ^d

All data originate from Slooff et al. (1995).

a: most sensitive parameter for *Dugesia dorotocephala*

b: geometric mean of 13 and 29 $\mu\text{g/l}$, parameter mortality for *Oncorhynchus kisutch*

c: most sensitive parameter (mortality) for *Pimephalis promelas*

d: most sensitive parameter (growth) for *Salvelinus fontinalis*, geometric mean of 0.29 and 0.08 $\mu\text{g/l}$

Table A2. 34: Methyl-mercury: selected data for marine water

taxonomic group	NOEC [$\mu\text{g/l}$]	
moll	0.3	

All data originate from Slooff et al. (1995).

Table A2. 35: Molybdenum: selected data on terrestrial processes

process	NOEC [mg/kg]	process	NOEC [mg/kg]
N-min	480	phos	96
N-min	160	phos	96
N-min	160	aryl	240
N-min	48	aryl	140 ^b
nitr	48	aryl	140 ^c
nitr	160	aryl	1200
nitr	160	ure	480
phos (acid)	800	ure	240
phos (acid)	240	ure	240
phos (acid)	24	ure	77 ^d
phos (alkaline)	800	ure	480
phos (alkaline)	310 ^a	ure	110 ^c

All data originate from Appendix 4 in Van de Plassche et al. (1992).

a: geometric mean of 800 and 120 mg/kg, process alkaline phosphatase in silty clay loam with pH 7.4.

b: geometric mean of 240 and 80 mg/kg, process arylsulphatase in soil with pH 7.6.

c: geometric mean of 240 and 80 mg/kg, process arylsulphatase in soil with pH 6.5

d: geometric mean of 240 and 25 mg/kg, process urease in soil with pH 7.8.

e: geometric mean of 240 and 50 mg/kg, process urease in soil with pH 7.4.

Table A2. 36: Molybdenum: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	27000	ann	29000
		crus	2700000
		pisc	1000000 ^a

All data originate from Appendix 2 in van de Plassche et al. (1992).

a: geometric mean of 1300 and 800 mg/l for *Oncorhynchus mykiss*

Table A2. 37: Molybdenum: selected data for marine water

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
moll	150000	crus	1100000
moll	1900000	crus	1900000
crus	250000	pisc	2600000

All data originate from Appendix 3 in van de Plassche et al. (1992).

Table A2. 38: Nickel: selected data on terrestrial species

taxonomic group	NOEC [mg/kg]	
ann	65	

All data originate from Van de Meent et al. (1990).

Table A2. 39: Nickel: selected data on terrestrial processes

process	NOEC [mg/kg]	process	NOEC [mg/kg]
resp	520	ure	26

All data originate from Van de Meent et al. (1990).

Table A2. 40: Nickel: selected fresh water data

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
bact	100000	alg	10000
bact	6000	alg	1300
bact	5000	prot	820
bact	130000	prot	42
bact	2.5	prot	140
cyan	25	crus	90
cyan	5	pisc	380 ^a
		pisc	104 ^b

All data originate from Van de Meent et al. (1990).

a: geometric mean of 380 and 380 $\mu\text{g/l}$ for *Pimephales promelas*, parameter growth/survival

b: geometric mean of 62, 134 and 134 $\mu\text{g/l}$ for *Oncorhynchus mykiss*, parameter growth/survival

Table A2. 41: Zinc: selected data on terrestrial species

taxonomic group	NOEC [mg/kg]	taxonomic group	NOEC [mg/kg]
mac	280 ^a	ann	1200 ^e
mac	220 ^b	moll	380
mac	210 ^c	crus	510
mac	420 ^d		

All data originate from Janus (1993) and adapted Janus et al. (1996).

a: geometric mean of 340, 340, 320, 320, 280, 360, 340, 68, 340 and 340 mg/kg, parameter yield for *Medicago sativa*

b: geometric mean of 340, 340, 320, 320, 280, 360, 340, 68, 340, 340, 340 and 14 mg/kg, parameter yield for *Zea mays*

c: geometric mean of 340, 340, 320, 320, 280, 360, 340, 14, 68, 340 and 340 mg/kg, parameter yield for *Latuca sativa*

d: geometric mean of 160, 160, 550, 420, 740, and 1200 mg/kg, parameter yield for *Avena sativa*

e: geometric mean of 1300, 1300, 1300, 320, and 3200 mg/kg, parameter survival/growth/reproduction for *Eisenia fetida*

Table A2. 42: Zinc: selected data on terrestrial processes

process	NOEC [mg/kg]	process	NOEC [mg/kg]
resp	89	glut	1600
resp	130	glut	500
resp	9.0	glut	270
resp	310	glut	1700
resp	240	amy	1300
resp	3800	cellu	1300
resp	270	phos	180
resp	250	phos	140
N-min	75	ure	30
am	1300	ure	27
nitr	130	ure	48
nitr	100	ure	47
nitr	180	xyl	1300
nitr	21		

All data originate from Janus (1993) and adapted Janus et al. (1996).

Table A2. 43: Zinc: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
alg	470 ^a	moll	25
alg	200	crus	25 ^e
alg	95	crus	37 ^f
alg	190	ins	12 ^g
alg	1000	pisc	1300
alg	250 ^b	pisc	44 ^h
alg	15 ^c	pisc	50
alg	390	pisc	120 ⁱ
alg	60	pisc	100 ^j
alg	1000	pisc	540
prot	3.3 ^d		

All data originate from Janus (1993) and adapted Janus et al. (1996), corrected for background in this report.

- a: geometric mean of 400 and 560 $\mu\text{g/l}$, parameter growth for *Chlorella vulgaris*
- b: geometric mean of 100, 230 and 700 $\mu\text{g/l}$, parameter growth for *Scenedesmus quadricauda*
- c: geometric mean of 5, 15 and 50 $\mu\text{g/l}$, parameter growth for *Selenastrum capricornutum*
- d: value corrected for background concentration (0.65 $\mu\text{g/l}$)
- e: geometric mean of 25, 8, 25, 25, 50, 25, 25, 50 and 17 $\mu\text{g/l}$, parameter reproduction for *Ceriodaphnia dubia*
- f: most sensitive parameter (growth) for *Daphnia magna*
- g: value corrected for background concentration (9.0 $\mu\text{g/l}$)
- h: geometric mean of 26 and 75 $\mu\text{g/l}$, parameter growth for *Jordanella floridae*
- i: most sensitive parameter(deformities) for *Pimephalis promelas*
- j: most sensitive parameter(survival) for *Oncorhynchus mykiss*, geometric mean of for background corrected values (320-30), (140-11) and (36-11) $\mu\text{g/l}$

Table A2. 44: Zinc: selected data for marine water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
alg	100	alg	100
alg	15 ^a	coel	300
alg	24 ^b	ann	320
alg	500	ann	100 ^g
alg	35 ^c	ann	100
alg	2700 ^d	ann	100 ^h
alg	100	moll	50
alg	15	moll	19
alg	10	moll	50
alg	100	moll	1000
alg	34 ^e	crus	440
alg	140 ^f	crus	18
alg	10	crus	120
alg	200	echi	10

All data originate from Janus (1993) and adapted Janus et al. (1996).

a: geometric mean of 30, 7, 20, 7, 7, 20 and 40 $\mu\text{g/l}$, parameter growth for *Asterionella japonica*

b: geometric mean of 10 and 60 $\mu\text{g/l}$, parameter growth for *Chaetoceros compressum*

c: geometric mean of 40, 60, 10 and 60 $\mu\text{g/l}$, parameter growth for *Nitzschia closterium*

d: geometric mean of 10000, 4000 and 500 $\mu\text{g/l}$, parameter growth for *Phaeodactylum tricornutum*

e: geometric mean of 25, 50, 100, 20, 60, 7, 7, 30, 200 and 50 $\mu\text{g/l}$, parameter growth for *Skeletonema costatum*

f: geometric mean of 100 and 200 $\mu\text{g/l}$, parameter growth for *Thalassiosira pseudonana*

g: geometric mean of 100 and 100 $\mu\text{g/l}$, parameter reproduction for *Ctenodrilus serratus*

h: geometric mean of 100 and 100 $\mu\text{g/l}$, parameter reproduction for *Nereis arenaceodentata*

Appendix 3 Data for cyanides used for extrapolation

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Table A3. 1: Free cyanide: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
bact	1.0	prot	270
cyan	70	crus	28
alg	270	pisc	8.8 ^b
alg	95 ^a	pisc	12 ^c
prot	1200	pisc	5.5 ^d
prot	1800	pisc	0.040

All data are taken from the annex to this report

a: geometric mean of 30 and 300 $\mu\text{g/l}$ for *Scenedesmus quadricauda*

b: most sensitive life stage (eggs) for *Lepomis macrochirus*

c: most sensitive parameter (egg production) for *Pimephales promelas*

d: most sensitive parameter (egg production) for *Salvelinus fontinalis*

Table A3. 2: Free cyanide: selected data for marine water

taxonomic group	NOEC [$\mu\text{g/l}$]		
crus	43		

All data are taken from the annex to this report

Table A3. 3: Thiocyanates: selected data for terrestrial species

taxonomic group	L(E)C50 [mg/kg]		
ins	6200 ^a		

All data are taken from the annex to this report

a: in soil with 2.9% organic matter. No correction applicable for organic matter.

Table A3. 4: Thiocyanates: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
mac	770 ^a	crus	5.9 ^f
crus	0.36 ^b	mac	3700
pisc	5.1 ^c	ins	250
pisc	77 ^d	ann	1200
pisc	1.1 ^e	pisc	400
		pisc	140
		pisc	300
		pisc	220
		pisc	490
		pisc	140 ^g
		pisc	270
		pisc	7.8
		pisc	75
		amph	280
		amph	230

All data are taken from the annex to this report

a: most sensitive parameter (growth) for *Lemna minor*

b: most sensitive parameter (reproduction) for *Daphnia magna*

c: most sensitive parameter (weight) for *Carassius auratus gibelio*

d: most sensitive life stage (juvenile) for *Oncorhynchus mykiss*

e: most sensitive parameter (time to first spawn, egg production) for *Pimephales promelas*

- f: geometric mean of 3.52, 1.9, 0.63, 14.57, 10.1, 1.42, 32.09, 19.32, 3.21, 57.4, and 3.02 mg/l for *Daphnia magna*
- g: geometric mean of 250, 177, 218, 264, 244, 191, 233, 250, 141, 83, 20.8, and 25 mg/l for *Oncorhynchus mykiss*

Table A3. 5: Cyanide complexes: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	0.026	pisc	0.19
		pisc	0.90

All data are taken from the annex to this report
 $\text{Na}_3[\text{Cu}(\text{CN})_4]$ was tested.

Table A3. 6: Cyanide complexes: selected data for marine water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	0.031	alg	0.13
alg	0.031	alg	0.28
		moll	0.13
		moll	0.69
		crus	5.0
		crus	12

All data are taken from the annex to this report
 $\text{K}_3\text{Fe}(\text{CN})_6$ and $\text{K}_4\text{Fe}(\text{CN})_6$ were tested.

Appendix 4 Data for monocyclic non-halogenated aromatic hydrocarbons used for extrapolation

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Table A4. 1: Benzene: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	92	alg	310 ^a
alg	600	alg	460
prot	490	coel	34
prot	490	crus	250 ^b
prot	390	crus	68 ^c
nema	78	crus	370
		crus	120
		crus	42
		ins	110 ^d
		ins	71
		ins	100
		ins	48
		ins	10
		ins	130
		ins	34
		moll	230
		moll	74
		pisc	40 ^e
		pisc	14
		pisc	390
		pisc	22
		pisc	21 ^f
		pisc	65 ^g
		pisc	8.7 ^h
		pisc	9.0 ⁱ
		pisc	10
		pisc	10
		pisc	250
		pisc	52 ^j
		pisc	100 ^k
		pisc	17 ^l
		pisc	12
		pisc	11
		pisc	13
		amph	190
		amph	370

All data originate from Knaap et al. (1988).

a: most sensitive parameter (growth) for *Chlorella vulgaris*

b: geometric mean of 400, 203, 200, and 250 mg/l for *Daphnia magna*

c: geometric mean of 305 and 15 mg/l for *Daphnia pulex*

d: geometric mean of 59 and 200 mg/l for 3rd and 4th instar larvae of *Aedes aegypti*

e: geometric mean of 46 and 34 mg/l for *Carassius auratus*

f: geometric mean of 20 and 23 mg/l for *Lepomis macrochirus*

g: geometric mean of 33, 62, and 132 mg/l for *Leuciscus idus melanotus*

h: geometric mean of 5 and 15 mg/l for fry (most sensitive life stage) *Oncorhynchus gorbuscha*

i: most sensitive life stage (fry) of *Oncorhynchus kisutch*

j: geometric mean of 32 and 84 mg/l for *Pimephales promelas*

k: geometric mean of 37, 420, and 64 mg/l for *Poecilia reticulata*

l: geometric mean of 5 and 56 mg/l for *Oncorhynchus mykiss*

Table A4. 2: Benzene: selected data for marine water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
alg	19 ^a	alg	180
alg	1.0 ^b	crus	92 ^d
alg	10	crus	110
crus	0.18 ^c	crus	18
		crus	44 ^e
		crus	380
		crus	96 ^f
		moll	920
		moll	170
		pisc	22 ^g
		pisc	22 ^h
		pisc	7.5 ⁱ
		pisc	40

Data originate from van de Plassche et al. (1993) and Knaap et al. (1988).

a: geometric mean of 10, 35, and 20 mg/l for *Skeletonema costatum*

b: geometric mean of 0.1 and 10 mg/l for *Dunaliella tertiolecta*

c: parameter mortality for larvae of *Cancer magister*

d: geometric mean of 66 and 127 mg/l for *Artemia* species

e: geometric mean of 27.0, 90.8, 74.4, 38.0, 33.5, and 33 mg/l for larvae/adult *Palaemonetes pugio*

f: geometric mean of 82 and 112 mg/l for *Nitrocra spinipes*

g: geometric mean of 20 and 25 mg/l for the most sensitive life stage (larvae) of *Clupea harengus pallasii*

h: geometric mean of 20 and 25 mg/l for larvae of *Engraulis mordax*

i: geometric mean of 5.8 and 9.6 mg/l for *Morone saxatilis*

Table A4. 3: Benzene: selected QSAR data.

taxonomic group	NOEC [mg/l]	taxonomic group	NOEC [mg/l]
bact	720	moll	9.6
bact	32	crus	12
bact	85	crus	9.5
bact	84	ins	16
alg	87	ins	12
alg	45	pisc	4.9
alg	11	amph	13
fung	760	amph	13
prot	81	amph	15
coel	10		

Table A4. 4: Toluene: selected data for terrestrial species

taxonomic group	NOEC [mg/kg]	taxonomic group	NOEC [mg/kg]
mac	14	ann	160

All data originate from Appendix 4 in van de Plassche et al. (1993).

Table A4. 5: Toluene: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	20	crus	35 ^b
bact	29	ins	22
cyan	110	pisc	170 ^c
alg	250	pisc	43 ^d
alg	10	pisc	36 ^e
prot	140	pisc	18 ^f
crus	0.53 ^a	pisc	63 ^g
pisc	16	pisc	25
pisc	4.0	pisc	32 ^h
pisc	1.4	pisc	5.5

All data originate from van der Heijden et al. (1988).

a: lowest parameter (reproduction) for *Daphnia magna*

b: geometric mean of 3.8, 1.4, 60, 310, 470, 270, 11.5, and 14.9 mg/l for *Daphnia magna*

c: geometric mean of 70 and 422 mg/l for *Leuciscus idus*

d: geometric mean of 58, 58, and 23 mg/l for *Carassius auratus*

e: geometric mean of 55, 72, 28, 36, 18, 30, 34, and 42 mg/l for different life stages of *Pimephales promelas*

f: geometric mean of 24 and 13 mg/l for *Lepomis macrochirus*

g: geometric mean of 59 and 68 mg/l for *Poecilia reticulata*

h: most sensitive life stage (fry) of *Oyzias latipes*

Table A4. 6: Toluene: selected data for marine water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
alg	10	alg	56
alg	10	crus	19 ^a
alg	10	crus	28
alg	10	crus	13
pisc	3.2	crus	4.3
		crus	19 ^b
		crus	30
		crus	9.5
		crus	150
		pisc	48 ^c
		pisc	7.3
		pisc	6.8 ^d
		pisc	90

All data originate from van der Heijden et al. (1988) and Appendix 3 van de Plassche et al. (1993).

a: geometric mean of 59 and 33 mg/l for nauplii of *Artemia* species

b: geometric mean of 21.4, 20.2, and 14.7 mg/l for *Eualus* species

c: geometric mean of 13 and 180 mg/l for *Cyprinodon variegatus*

d: geometric mean of 6.41, 7.63, 8.09, and 5.38 mg/l for fry of *Oncorhynchus gorbuscha*

Table A4. 7: Toluene: selected QSAR data.

taxonomic group	NOEC [mg/l]	taxonomic group	NOEC [mg/l]
bact	270	moll	3.4
bact	15	crus	5.0
bact	41	crus	2.7
bact	39	ins	4.3
alg	38	ins	4.3
alg	16	pisc	1.7
alg	3.3	amph	4.7
fung	310	amph	3.3
prot	32	amph	5.2
coel	3.7		

Table A4. 8: Ethylbenzene: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	6.0	alg	51
cyan	17	alg	63
alg	1.0	alg	4.6
prot	470	crus	16 ^a
prot	70	pisc	94
		pisc	97
		pisc	69 ^b
		pisc	22 ^c
		pisc	9.6
		pisc	4.2

All data originate from Appendix 2 in van de Plassche et al. (1993).

a: geometric mean of 2.2, 75, 180, and 2.1 mg/l for *Daphnia magna*

b: geometric mean of 32 and 150 mg/l for *Lepomis macrochirus*

c: geometric mean of 42 and 12 mg/l for *Pimephales promelas*

Table A4. 9: Ethylbenzene: selected data for marine water

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
crus	15	pisc	280
crus	13	pisc	4.3
crus	0.49	pisc	30

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A4. 10: Ethylbenzene: selected QSAR data.

taxonomic group	NOEC [mg/l]	taxonomic group	NOEC [mg/l]
bact	140	moll	1.7
bact	9.5	crus	2.7
bact	26	crus	1.1
bact	23	ins	1.7
alg	22	ins	2.2
alg	8.1	pisc	0.86
alg	1.5	amph	2.3
fung	170	amph	1.3
prot	17	amph	2.5
coel	1.8		

Table A4. 11: *o*-Xylene: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
alg	1.0	bact	9.2
prot	9.0	alg	4.7
		crus	6.7 ^a
		ins	1.6
		pisc	20
		pisc	19 ^b
		pisc	16
		pisc	35
		pisc	18 ^c
		pisc	21 ^d
		pisc	12
		pisc	7.8 ^e
		amph	73

All data originate from Appendix 2 in van de Plassche et al. (1993).

a: geometric mean of 1, 3.8, 170, and 3.2 mg/l for *Daphnia magna*

b: geometric mean of 13, 16, 17, 37 mg/l for *Carassius auratus*

c: geometric mean of 16 and 21 mg/l for *Lepomis macrochirus*

d: geometric mean of 16 and 27 mg/l for *Pimephales promelas*

e: geometric mean of 7.6 and 8.1 mg/l for *Oncorhynchus mykiss*

Table A4. 12: *o*-Xylene: selected data for marine water

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
crus	24	echi	4.1
crus	6.0	pisc	11
crus	1.3		

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A4. 13: *m*-Xylene: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
alg	0.70	alg	4.9
prot	28	crus	18 ^a
		ins	1.6
		pisc	20
		pisc	22 ^b
		pisc	35
		pisc	21
		pisc	27
		pisc	13
		pisc	8.4

All data originate from Appendix 2 in van de Plassche et al. (1993).

a: geometric mean of 4.7, 9.6, 14, and 170 mg/l for *Daphnia magna*

b: geometric mean of 16, 17, and 37 mg/l for *Carassius auratus*

Table A4. 14: *m*-Xylene: selected data for marine water

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
crus	19	crus	3.7
crus	12	pisc	9.2

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A4. 15: *p*-Xylene: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
alg	0.90	alg	46
prot	9.0	alg	110
		alg	3.2
		crus	17 ^a
		ins	1.6
		pisc	20
		pisc	22 ^b
		pisc	35
		pisc	21
		pisc	16 ^c
		pisc	8.8
		pisc	2.6

All data originate from Appendix 2 in van de Plassche et al. (1993).

a: geometric mean of 3.6, 8.5, and 170 mg/l for *Daphnia magna*

b: geometric mean of 18, 17, and 37 mg/l for *Carassius auratus*

c: geometric mean of 27 and 8.9 mg/l for *Pimephales promelas*

Table A4. 16: *p*-Xylene: selected data for marine water

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
crus	25	pisc	2.0
crus	2.0		

All data originate from Appendix 2 in van de Plassche et al. (1993).

Table A4. 17: Styrene: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	36	crus	64 ^a
cyan	34	pisc	41 ^b
prot	93	pisc	75
		pisc	25
		pisc	33 ^c
		pisc	46

All data originate from Appendix 2 in van de Plassche et al. (1993).

a: geometric mean of 23 and 180 mg/l for *Daphnia magna* (immobility/mortality)

b: geometric mean of 26 and 65 mg/l for *Carassius auratus*

c: geometric mean of 17 and 66 mg/l for *Leuciscus idus melanotus*

Table A4. 18: Styrene: selected data for marine water

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
crus	68	pisc	9.1

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A4. 19: Phenol: selected data for terrestrial species

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	160	mac	400

All data are taken from the annex to this report.

Table A4. 20: Phenol: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	NOEC [mg/l]
prot	65	alg	7.5
prot	33	crus	0.84 ^a
prot	140	crus	0.28 ^b
bact	64	pisc	2.2 ^c
bact	280	pisc	0.1
cyan	4.6	pisc	0.75 ^d

All data are taken from the annex to this report.

a: most sensitive parameter (survival) for *Ceriodaphnia dubia*

b: geometric mean of 0.16 and 0.5 mg/l for the most sensitive parameter (growth) for *Daphnia magna*

c: most sensitive parameter (growth) for *Brachydanio rerio*

d: most sensitive parameter (growth) for eggs of *Pimephales promelas*

Table A4. 21: Phenol: selected data for marine water

taxonomic group	NOEC [mg/l]		
alg	13		

All data are taken from the annex to this report.

Table A4. 22: o-Cresol: selected data for terrestrial species

taxonomic group	NOEC [mg/kg]		
mac	50		

All data are taken from the annex to this report.

Table A4. 23: *o*-Cresol: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
prot	130	prot	210
prot	17	ins	34
prot	31	ins	50
bact	33	ins	80
cyan	6.8	ins	46
alg	34	ins	10
alg	36	coel	75
alg	11	ann	24
alg	65	ann	140
		ann	170
		moll	160
		crus	23
		crus	16
		crus	13 ^a
		crus	9.6
		crus	21
		pisc	24
		pisc	23
		pisc	21
		pisc	8.4
		pisc	14 ^b
		pisc	19
		amph	40
		amph	38

All data are taken from the annex to this report.

a: geometric mean of 9.2, 23.5, 14.5, 19, 17.9, and 5 mg/l for *Daphnia magna*

b: geometric mean of 18.2, 12.6, 13.4, and 14 mg/l for *Pimephales promelas*

Table A4. 24: *o*-Cresol: selected data for marine water

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	18 ^a	echi	30
crus	10	pisc	12

All data are taken from the annex to this report.

a: geometric mean of 19, 11, and 25.9 mg/l for *Vibrio fisheri*

Table A4. 25: *o*-Cresol: selected QSAR data.

taxonomic group	NOEC [mg/l]	taxonomic group	NOEC [mg/l]
bact	1400	moll	19
bact	57	crus	24
bact	150	crus	20
bact	150	ins	35
alg	160	ins	24
alg	89	pisc	9.7
alg	24	amph	27
fung	1500	amph	27
prot	160	amph	31
coel	20		

Table A4. 26: *m-Cresol*: selected data for terrestrial species

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	16	mac	480

All data are taken from the annex to this report.

Table A4. 27: *m-Cresol*: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
prot	110	prot	130
prot	31	crus	17 ^a
prot	62	pisc	16
bact	53	pisc	18
cyan	13	pisc	8.9
alg	15	pisc	56

All data are taken from the annex to this report.

a: geometric mean of 25, 8.9, 19.2, and 18.8 mg/l for *Daphnia magna*

Table A4. 28: *m-Cresol*: selected data for marine water

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	7.5	echi	30

All data are taken from the annex to this report.

Table A4. 29: *m-Cresol*: selected QSAR data.

taxonomic group	NOEC [mg/l]	taxonomic group	NOEC [mg/l]
bact	1400	moll	19
bact	56	crus	23
bact	150	crus	20
bact	150	ins	34
alg	160	ins	23
alg	87	pisc	9.5
alg	23	amph	26
fung	1400	amph	27
prot	150	amph	30
coel	20		

Table A4. 30: *p-Cresol*: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
crus	1.0	prot	110 ^a
		bact	410
		alg	7.8
		crus	6.2 ^b
		crus	23
		pisc	7.7 ^c
		pisc	21 ^d

All data are taken from the annex to this report.

a: geometric mean of 69 and 165 mg/l for *Tetrahymena pyriformis*

b: geometric mean of 4.9, 14, 7.7, 12.5, and 1.4 mg/l for *Daphnia magna*

c: geometric mean of 7.5 and 7.9 mg/l for *Oncorhynchus mykiss*

d: geometric mean of 16 and 28.6 mg/l for *Pimephales promelas*

Table A4. 31: *p-Cresol*: selected data for marine water

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	2.0 ^a	echi	5.0
bact	74	pisc	5.0

All data are taken from the annex to this report.

a: geometric mean of 1.5, 2.3, and 2.3 mg/l for *Vibrio fisheri*

Table A4. 32: *Catechol*: selected data for fresh water

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	0.77	pisc	8.9
bact	4.0	pisc	3.5
prot	20		

All data are taken from the annex to this report.

Table A4. 33: *Catechol*: selected data for marine water

taxonomic group	L(E)C50 [mg/l]		
bact	32		

All data are taken from the annex to this report.

Table A4. 34: *Resorcinol*: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
pisc	32	crus	110
pisc	1.0	pisc	77
		mac	140
		mac	170

All data are taken from the annex to this report.

Table A4. 35: *Resorcinol*: selected data for marine water

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	110	crus	42

All data are taken from the annex to this report.

Table A4. 36: *Hydroquinone*: selected data for terrestrial species

taxonomic group	NOEC [mg/kg]	taxonomic group	NOEC [mg/kg]
mac	760 ^a	mac	890

All data are taken from the annex to this report.

a: geometric mean of 1087, 893, and 446 mg/kg for *Triticum aestivum*

Table A4. 37: Hydroquinone: selected data for fresh water

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
prot	22	prot	73
prot	11	prot	37
prot	21	roti	0.24
bact	58	bact	83 ^a
cyan	1.1	bact	34 ^b
alg	0.93	fung	3800
		fung	2800
		fung	1000
		alg	50
		alg	0.30
		alg	0.34
		crus	0.16 ^c
		crus	0.16
		crus	0.070
		crus	0.10
		pisc	0.17
		pisc	0.15
		pisc	0.25 ^d
		pisc	0.044
		mac	43
		mac	7.7

All data are taken from the annex to this report.

a: most sensitive parameter (luminescence) for *Beneckeia harveyi*

b: two studies of 34 mg/l for *Escherichia coli*

c: geometric mean of 0.32, 0.29, 0.09, 0.12, 0.14, and 0.13 mg/l for *Daphnia magna*

d: geometric mean of 0.097 and 0.64 mg/l for *Oncorhynchus mykiss*

Table A4. 38: Hydroquinone: selected data for marine water

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	0.095 ^a	crus	21 ^b

All data are taken from the annex to this report.

a: geometric mean of 0.31, 0.038, and 0.072 mg/l for *Vibrio fisheri*

b: most sensitive life stage of *Artemia salina*

Appendix 5 Data for PAHs used for extrapolation

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Table A5. 1: Naphthalene: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
pisc	450 ^a	alg	33000
pisc	2300	moll	5000
		crus	5700 ^b
		crus	2700 ^c
		ins	13000
		ins	2800
		ins	12600
		pisc	680
		pisc	120
		pisc	3500 ^d

All data originate from Appendix 2 in Kalf et al. (1995)

a: most sensitive parameter (hatchability, growth) for *Pimephales promelas*

b: geometric mean of 3400, 16600, 2200, 22600 and 2200 $\mu\text{g/l}$, parameter survival/immobility for *Daphnia magna*

c: geometric mean of 4700, 1000, 3400 and 3400 $\mu\text{g/l}$, parameter survival/immobility for *Daphnia pulex*

d: geometric mean of 6100 and 2000 $\mu\text{g/l}$, parameter survival for *Pimephales promelas*

Table A5. 2: Naphthalene: selected marine data.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	21	moll	2300 ^b
pisc	260 ^a	ann	3800
pisc	370	crus	3200
		crus	1400
		crus	2700
		crus	3800
		crus	1900 ^c
		crus	1100 ^d
		pisc	5300
		pisc	750
		pisc	5100 ^e

All data originate from Appendix 3 in Kalf et al. (1995)

a: geometric mean of 120 and 560 $\mu\text{g/l}$, parameter growth for *Oncorhynchus gorboscha*

b: geometric mean of 2900, 2200 and 2000 $\mu\text{g/l}$, parameter survival for *Callinectes sapidus*

c: geometric mean of 1100, 2100 and 2800 $\mu\text{g/l}$, parameter survival for *Hemigrapsus nudus*

d: geometric mean of 1300 and 850 $\mu\text{g/l}$, parameter survival for *Neomysis americanus*

e: geometric mean of 4200, 5700 and 5500 $\mu\text{g/l}$, parameter survival for *Metapenaeus monocerus*

Table A5. 3: Anthracene: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	150 ^a	mac	3600

All data originate from Appendix 4 in Kalf et al. (1995)

a: most sensitive parameter (growth) for *Avena sativa*

Table A5. 4: Anthracene: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
mac	300	pisc	6.9 ^c
alg	2.5 ^a	ins	27
crus	1.7 ^b		

All data originate from Appendix 2 in Kalf et al. (1995)

- a: geometric mean of 1.5, 2.5, 2.3, 8.7 and 7.8 $\mu\text{g/l}$, parameter growth for *Selenastrum capricornutum*.
 b: geometric mean of 4.5, 2.2, 1.9, 1.1 and 0.63 $\mu\text{g/l}$, most sensitive parameter (reproduction) for *Daphnia magna*.
 c: geometric mean of 1.3, 8.0, 3.8, 8.3, 2.8, 12, 18 and 26 $\mu\text{g/l}$, parameter survival for *Lepomis spec.*

Table A5. 5: Phenanthrene: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
mac	600	crus	720 ^d
crus	32 ^a	crus	410 ^e
crus	60 ^b	pisc	250
pisc	42 ^c	pisc	30

All data originate from Appendix 2 in Kalf et al. (1995)

- a: most sensitive parameter (growth) for *Daphnia magna*
 b: most sensitive parameter (growth) for *Daphnia pulex*
 c: most sensitive parameter (growth) for *Brachydanio rerio*, geometric mean of 32 and 56 $\mu\text{g/l}$
 d: geometric mean of 1200, 380, 840 and 700 $\mu\text{g/l}$, parameter survival/immobility for *Daphnia magna*
 e: geometric mean of 350, 730, 100 and 1140 $\mu\text{g/l}$, parameter survival/immobility for *Daphnia pulex*

Table A5. 6: Phenanthrene: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	150	ann	600
		crus	590 ^a

All data originate from Appendix 3 in Kalf et al. (1995)

- a: geometric mean of 680 and 520 $\mu\text{g/l}$, parameter survival/immobility for *Artemia salina*

Table A5. 7: Fluoranthene: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
mac	200	pisc	12 ^a

All data originate from Appendix 2 in Kalf et al. (1995)

- a: most sensitive parameter (growth) for *Brachydanio rerio*, geometric mean of 6.9 and 22 $\mu\text{g/l}$.

Table A5. 8: Fluoranthene: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
ann	300		

All data originate from Appendix 3 in Kalf et al. (1995)

Table A5. 9: Benzo[a]anthracene: selected data on terrestrial species

taxonomic group	NOEC [mg/kg]		
crus	2.5		

All data originate from Appendix 4 in Kalf et al. (1995)

Table A5. 10: Benzo[a]anthracene: selected data for fresh water

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
crus	10		

All data originate from Appendix 2 in Kalf et al. (1995)

Table A5. 11: Chrysene: selected QSAR data

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
alg	6.9	ins	24
coel	21	pisc	9.0
moll	19	amph	23
crus	49	amph	3.6
crus	4.1	amph	22
ins	4.6		

Table A5. 12: Benzo[k]fluoranthene: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]		
pisc	0.36 ^a		

All data originate from Appendix 2 in Kalf et al. (1995)

a: most sensitive parameter (growth) for *Brachydanio rerio*, geometric mean of 0.27 and 0.48 $\mu\text{g/l}$

Table A5. 13: Benzo[a]pyrene: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	NOEC [mg/kg]
ann	8.7	crus	11
ann	2.6	crus	9.6 ^a

All data originate from Appendix 4 in Kalf et al. (1995)

a: geometric mean of 11 and 8.3 mg/kg, parameter growth for *Porcellio scaber*

Table A5. 14: Benzo[a]pyrene: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
pisc	6.3	alg	5
		alg	15
		crus	5

All data originate from Appendix 2 in Kalf et al. (1995)

Table A5. 15: Benzo[ghi]perylene: selected QSAR data

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
crus	1.9	amph	1.6
ins	2.0		

Table A5. 16: Indeno[1,2,3-cd]pyrene: selected QSAR data

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
crus	0.40	amph	0.30
ins	0.39		

Appendix 6 Data for halogenated aliphatic hydrocarbons used for extrapolation

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Table A6. 1: 1,2-Dichloroethane: selected data for fresh water.

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	68	bact	1100
cyan	53	bact	840
alg	360	alg	130
prot	470	crus	330 ^b
prot	560	pisc	1.8
prot	530	pisc	490 ^c
crus	11 ^a	pisc	130 ^d
pisc	29		

All data originate from Appendix 2 in van de Plassche et al. (1993).

- a: most sensitive parameter (reproduction) for *Daphnia magna*
b: geometric mean of 160, 220, 540, and 600 mg/l for *Daphnia magna*
c: geometric mean of 550 and 430 mg/l for *Lepomis macrochirus*
d: geometric mean of 140 and 120 mg/l for *Pimephales promelas*

Table A6. 2: 1,2-Dichloroethane: selected data for marine water.

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
ann	200 ^a	crus	170 ^b
		crus	170
		moll	190
		ann	400
		pisc	180
		pisc	120

All data originate from Appendix 3 in van de Plassche et al. (1993).

- a: most sensitive parameters (mortality, % hatching) for *Ophiotrocha labronica*
b: geometric mean of 320 and 93.6 mg/l for nauplii of *Artemia salina*

Table A6. 3: 1,2-Dichloroethane: selected QSAR data

taxonomic group	NOEC [μ g/l]	taxonomic group	NOEC [μ g/l]
bact	3200	moll	45
bact	110	crus	51
bact	280	crus	58
bact	300	ins	110
alg	330	ins	56
alg	210	pisc	23
alg	65	amph	65
fung	3200	amph	84
prot	350	amph	76
coel	48		

Table A6. 4: Dichloromethane: selected data for terrestrial processes.

process	NOEC [mg/kg]	process	NOEC [mg/kg]
β -gluc	3.9	phos	3.9
β -acet	3.9	phos diest	3.9
prot	3.9		

All data originate from van Appendix 4 in van de Plassche et al. (1993).

Table A6. 5: Dichloromethane: selected data for fresh water.

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	2900	pisc	190 ^a
alg	2300	pisc	290
alg	1500	amph	18
crus	220		

All data originate from van Apeldoorn et al. (1988).

a: geometric mean of 310, 193, 99, and 220 mg/l for *Pimephales promelas*

Table A6. 6: Dichloromethane: selected data for marine water.

taxonomic group	L(E)C50 [mg/l]		
pisc	330		

All data originate from van Apeldoorn et al. (1988).

Table A6. 7: Trichloromethane: selected data for fresh water.

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	63	alg	380
cyan	93	alg	410
alg	550	alg	440
alg	110	crus	87 ^b
crus	12 ^a	pisc	100
		pisc	97
		pisc	75
		pisc	18
		pisc	92
		pisc	51
		pisc	130 ^c
		pisc	18

All data originate from Appendix 2 in van de Plassche et al. (1993).

a: geometric mean of 15 and 9.7 mg/l for *Daphnia magna*

b: geometric mean of 29, 79, and 290 mg/l for *Daphnia magna*

c: geometric mean of 130, 170, and 100 mg/l for *Pimephales promelas*

Table A6. 8: Trichloromethane: selected data for marine water.

taxonomic group	NOEC [mg/l]		
alg	220		

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A6. 9: Trichloromethane: selected QSAR data

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
bact	1500	moll	20
bact	61	crus	25
bact	160	crus	21
bact	160	ins	37
alg	170	ins	25
alg	94	pisc	10
alg	25	amph	28
fung	1500	amph	29
prot	170	amph	33
coel	22		

Table A6. 10: Tetrachloromethane: selected data for marine water.

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
pisc	50	pisc	150

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A6. 11: Vinylchloride: selected QSAR data.

taxonomic group	NOEC [mg/l]	taxonomic group	NOEC [mg/l]
bact	1800	moll	26
bact	62	crus	30
bact	170	crus	33
bact	170	ins	60
alg	190	ins	32
alg	120	pisc	13
alg	37	amph	37
fung	1800	amph	47
prot	200	amph	43
coel	27		

Table A6. 12: Trichloroethene: selected data for terrestrial processes.

process	NOEC [mg/kg]	process	NOEC [mg/kg]
β -gluc	3.9	phos	3.9
β -acet	0.39	phos. diest.	3.9
prot	3.9		

All data originate from van Appendix 4 in van de Plassche et al. (1993).

Table A6. 13: Trichloroethene: selected data for fresh water.

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
bact	33	bact	190
cyan	32	crus	57
alg	180	crus	48 ^b
prot	600	crus	45
pisc	5.8 ^a	crus	200
		ins	48
		ins	55
		coel	75
		moll	56
		pisc	60
		pisc	28
		pisc	45
		pisc	146 ^c
		pisc	44 ^d
		pisc	42
		amph	48
		amph	45

All data originate from Appendix 2 in van de Plassche et al. (1993).

a: most sensitive life stage (eggs) for *Jordanella floridae*

b: geometric mean of 7.8, 1300, 65, 21, and 18 mg/l for *Daphnia magna*

c: geometric mean of 79 and 270 mg/l for *Oryzias latipes*

d: geometric mean of 41, 44, 45, and 47 mg/l for *Pimephales promelas*

Table A6. 14: Trichloroethene: selected data for marine water.

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
ann	25 ^a	alg	8
		alg	95
		ann	250
		crus	14
		moll	20
		pisc	52
		pisc	16

All data originate from Appendix 3 in van de Plassche et al. (1993).

a: most sensitive life stage (eggs) for *Ophryotrocha labronica*

Table A6. 15: Trichloroethene: selected QSAR data.

taxonomic group	NOEC [mg/l]	taxonomic group	NOEC [mg/l]
bact	490	moll	6.2
bact	26	crus	8.8
bact	70	crus	5.1
bact	67	ins	8.2
alg	66	ins	7.8
alg	29	pisc	3.1
alg	6.3	amph	8.5
fung	540	amph	6.4
prot	56	amph	9.5
coel	6.7		

Table A6. 16: Tetrachloroethene: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]		
ann	160		

All data originate from Appendix 4 in van de Plassche et al. (1993).

Table A6. 17: Tetrachloroethene: selected data for fresh water.

taxonomic group	NOEC [mg/l]	taxonomic group	L(E)C50 [mg/l]
crus	0.51	crus	28 ^b
pisc	2.0 ^a	crus	63
		pisc	8.4
		pisc	13
		pisc	40
		pisc	17 ^c
		pisc	4.9

All data originate from Appendix 2 in van de Plassche et al. (1993).

a: most sensitive life stage (eggs) for *Jordanella floridae*

b: geometric mean of 8.5, 18 and 150 mg/l for *Daphnia magna*

c: geometric mean of 17 and 18 mg/l for *Pimephales promelas*

Table A6. 18: Tetrachloroethene: selected data for marine water.

taxonomic group	L(E)C50 [mg/l]	taxonomic group	L(E)C50 [mg/l]
moll	3.5	pisc	41
pisc	5.0		

All data originate from Appendix 3 in van de Plassche et al. (1993).

Appendix 7 Data for halogenated aromatic hydrocarbons used for extrapolation

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Table A7. 1: Monochlorobenzene: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	320 ^a	alg	33000
pisc	2900	alg	50000
pisc	4800 ^b	crus	6900 ^c
		crus	7900
		pisc	11000
		pisc	4100
		pisc	16000
		pisc	22000
		pisc	4100
		pisc	660

All data originate from Hesse et al. (1991).

a: most sensitive parameter (growth) for *Daphnia magna*

b: most sensitive life stage (adult) for *Branchydanio rerio*

c: geometric mean of 4300, 13000, and 5810 $\mu\text{g/l}$ for *Daphnia magna*

Table A7. 2: Monochlorobenzene: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	100000	alg	200000
		pisc	10000

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A7. 3: 1,2-Dichlorobenzene: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	310 ^a	alg	2200
		alg	17000
		alg	20000
		crus	1200 ^b
		pisc	10000
		pisc	6800
		pisc	5600

All data originate from Hesse et al. (1991).

a: geometric mean of 505 and 185 $\mu\text{g/l}$ for *Daphnia magna*

b: geometric mean of 780, 2350, 740, and 1700 $\mu\text{g/l}$ for *Daphnia magna* (immobility)

Table A7. 4: 1,2-Dichlorobenzene: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	7600	crus	15000
alg	7600	crus	9700 ^a
alg	7600	pisc	9700
alg	7600	pisc	7300
alg	7600		
moll	5000		

All data originate from Appendix 3 in van de Plassche et al. (1993).

a: geometric mean of 9400 and 10000 $\mu\text{g/l}$ for *Palaemonetes pugio*

Table A7. 5: 1,3-Dichlorobenzene: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	680 ^a	alg	31000
pisc	1000 ^b	alg	23000
		crus	3300 ^c
		pisc	7800 ^d
		pisc	5000

All data originate from Hesse et al. (1991).

a: geometric mean of 690, 650, and 690 $\mu\text{g/l}$ for *Daphnia magna* (reproduction)

b: most sensitive life stage (adult) for *Pimephales promelas*

c: geometric mean of 4200, 1200, and 7000 $\mu\text{g/l}$ for *Daphnia magna* (immobility)

d: two studies of 7800 $\mu\text{g/l}$ for *Pimephales promelas*

Table A7. 6: 1,3-Dichlorobenzene: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
pisc	7800		

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A7. 7: 1,4-Dichlorobenzene: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	50	mac	1300

All data originate from Hesse et al. (1991).

Table A7. 8: 1,4-Dichlorobenzene: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	570	alg	5200
crus	300 ^a	alg	31000
pisc	570	alg	20000
		crus	1500 ^b
		pisc	1180
		pisc	4300
		pisc	3500 ^c
		pisc	4300

All data originate from Hesse et al. (1991).

a: geometric mean of 690, 650, and 690 $\mu\text{g/l}$ for *Daphnia magna* (reproduction)

b: geometric mean of 1600, 700, and 3200 $\mu\text{g/l}$ for *Daphnia magna* (immobility)

c: geometric mean of 4200, 2400, 4000, and 3600 $\mu\text{g/l}$ for *Pimephales promelas* (adults and fry)

Table A7. 9: 1,4-Dichlorobenzene: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	14000	pisc	7400
crus	64000 ^a		

All data originate from Appendix 3 in van de Plassche et al. (1993).

a: geometric mean of 69000 and 60000 $\mu\text{g/l}$ for *Paleomonetes pugio*

Table A7. 10: 1,2,3-Trichlorobenzene: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	5.0	mac	10 ^a
		ann	300 ^b
		ann	310 ^c

All data originate from Hesse et al. (1991).

a: geometric mean of 5 and 20 mg/kg for *Lactuca sativa*

b: geometric mean of 362, 393, 83, and 675 mg/kg for *Eisenia andrei*

c: geometric mean of 310, 340, 122, and 695 mg/kg for *Lumbricus rubellus*

Table A7. 11: 1,2,3-Trichlorobenzene: selected data for fresh water.

taxonomic group	NOEC [μ g/l]	taxonomic group	L(E)C50 [μ g/l]
alg	110	alg	2200
crus	40	alg	6000
pisc	250	crus	1100 ^a
		pisc	710
		pisc	3100

All data originate from Hesse et al. (1991).

a: geometric mean of 350, 2720, and 1450 μ g/l for *Daphnia magna*

Table A7. 12: 1,2,3-Trichlorobenzene: selected data for marine water.

taxonomic group	L(E)C50 [μ g/l]		
crus	2400		

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A7. 13: 1,2,4-Trichlorobenzene: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	50	ann	200
		ann	250
		ann	130
		ann	180
		mac	240

All data originate from Hesse et al. (1991).

Table A7. 14: 1,2,4-Trichlorobenzene: selected data for fresh water.

taxonomic group	NOEC [μ g/l]	taxonomic group	L(E)C50 [μ g/l]
alg	1	alg	3900
crus	190 ^a	alg	6000
pisc	500	crus	1600 ^b
		pisc	2800 ^c
		pisc	2000
		pisc	6300
		pisc	3400

All data originate from Hesse et al. (1991).

a: geometric mean of 360 and 100 μ g/l for the most sensitive parameter (growth) for *Daphnia magna*

b: geometric mean of 1200 and 2100 μ g/l for *Daphnia magna*

c: geometric mean of 2800 and 2900 μ g/l for *Pimephales promelas*

Table A7. 15: 1,2,4-Trichlorobenzene: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	2600	pisc	6000
crus	540	pisc	21000

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A7. 16: 1,3,5-Trichlorobenzene: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	50	mac	620

All data originate from Hesse et al. (1991).

Table A7. 17: 1,3,5-Trichlorobenzene: selected data for fresh water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	9100	pisc	3300

All data originate from Hesse et al. (1991).

Table A7. 18: 1,3,5-Trichlorobenzene: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]		
moll	1000		

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A7. 19: 1,2,3,4-Tetrachlorobenzene: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	50	mac	160

All data originate from Hesse et al. (1991).

Table A7. 20: 1,2,3,4-Tetrachlorobenzene: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	23 ^a	alg	4100
pisc	250	pisc	1100 ^b
pisc	100		

All data originate from Hesse et al. (1991).

a: geometric mean of 10 and 55 $\mu\text{g/l}$ for the most sensitive parameter (reproduction) for *Daphnia magna*

b: two studies of 1100 $\mu\text{g/l}$ for *Pimephales promelas*

Table A7. 21: 1,2,3,5-Tetrachlorobenzene: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]		
mac	6.5		

All data originate from Hesse et al. (1991).

Table A7. 22: 1,2,3,5-Tetrachlorobenzene: selected data for fresh water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	1600	pisc	6400
alg	2500	pisc	800
alg	3000	pisc	800
crus	2400 ^a		

All data originate from Hesse et al. (1991).

a: geometric mean of 9700, 1730, and 860 $\mu\text{g/l}$ for *Daphnia magna*

Table A7. 23: 1,2,3,5-Tetrachlorobenzene: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
pisc	3700		

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A7. 24: 1,2,4,5-Tetrachlorobenzene: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]		
mac	10		

All data originate from Hesse et al. (1991).

Table A7. 25: 1,2,4,5-Tetrachlorobenzene: selected data for fresh water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	5000	pisc	300
pisc	1200	pisc	300
pisc	1600		

All data originate from Hesse et al. (1991).

Table A7. 26: 1,2,4,5-Tetrachlorobenzene: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
pisc	90	pisc	800

All data originate from Appendix 3 in van de Plassche et al. (1993).

Table A7. 27: Pentachlorobenzene: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	50	mac	280

All data originate from Hesse et al. (1991).

Table A7. 28: Pentachlorobenzene: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	31 ^a	alg	1300
pisc	34	crus	1300 ^b
		pisc	250

All data originate from Hesse et al. (1991).

a: geometric mean of 100, 31, and 10 $\mu\text{g/l}$ for the *Daphnia magna* (reproduction)

b: geometric mean of 5300, 1250, and 300 $\mu\text{g/l}$ for *Daphnia magna*

Table A7. 29: Pentachlorobenzene: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
pisc	610 ^a		

All data originate from Appendix 3 in van de Plassche et al. (1993).

a: geometric mean of 800 and 460 $\mu\text{g/l}$ for the *Cyprinodon variegatus*

Table A7. 30: Hexachlorobenzene: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]		
mac	500		

All data originate from Hesse et al. (1991).

Table A7. 31: Hexachlorobenzene: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	14	alg	30
crus	1.8		

All data originate from Hesse et al. (1991).

Table A7. 32: 2-Chlorophenol: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]		
mac	220		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 33: 2-Chlorophenol: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	500	prot	76000 ^a
pisc	4000	bact	200000 ^b
		bact	700000
		bact	410000
		bact	170000
		bact	120000
		alg	170000
		alg	70000
		alg	50000
		alg	150000
		crus	7000 ^c
		crus	21000
		crus	5200
		crus	25000
		pisc	15000
		pisc	14000 ^d
		pisc	8100 ^e
		pisc	11000 ^f
		pisc	12000 ^g
		pisc	10000

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 68000 and 48000 $\mu\text{g/l}$ for *Tetrahymena pyriformis*

b: geometric mean of 372000 and 104000 $\mu\text{g/l}$ for activated sludge bacteria

- c: geometric mean of 6300, 17900, 23000, 2600, 3900, 6200, 7400, 9000, and 3700 µg/l for *Daphnia magna* (immobility/mortality)
- d: geometric mean of 12400 and 16000 µg/l for *Carassius auratus*
- e: geometric mean of 6600 and 10000 µg/l for *Lepomis macrochirus*
- f: geometric mean of 12000, 14000, 11600, 14500, 9400, and 6300 µg/l for *Pimephales promelas*
- g: geometric mean of 13500, 11200, 7100, 20000, and 13800 µg/l for *Poecilia reticulata*

Table A7. 34: 2-Chlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [µg/l]	taxonomic group	L(E)C50 [µg/l]
bact	19000 ^a	crus	5300

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

- a: geometric mean of 9300 and 39700 µg/l for *Vibrio fisheri*

Table A7. 35: 3-Chlorophenol: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
ann	210 ^a	mac	35
ann	410 ^b		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

- a: geometric mean of 271, 160, 220, and 203 mg/kg for *Eisenia andrei*

- b: geometric mean of 406, 305, 561, and 405 mg/kg for *Lumbricus rubellus*

Table A7. 36: 3-Chlorophenol: selected data for fresh water.

taxonomic group	L(E)C50 [µg/l]	taxonomic group	L(E)C50 [µg/l]
prot	16000 ^a	alg	50000
bact	67000	crus	16000
bact	450000	pisc	15000
bact	30000	pisc	8200
alg	29000	pisc	5500

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

- a: geometric mean of 14200 and 17300 µg/l for *Tetrahymena pyriformis*

Table A7. 37: 3-Chlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [µg/l]		
bact	13000		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 38: 4-Chlorophenol: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	200 ^a	prot	37000
crus	300 ^b	bact	100000 ^c
		bact	400000
		bact	130000
		bact	20000
		alg	29000
		alg	14000 ^d
		alg	8000
		alg	75000
		crus	9000
		crus	4900 ^e
		crus	12000
		crus	10000
		crus	4600
		mac	55000 ^f
		mac	32000 ^g
		pisc	8700
		pisc	3800
		pisc	1900
		pisc	5100 ^h
		pisc	7800 ⁱ
		pisc	3800
		pisc	9000

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: most sensitive parameter (mortality) for *Ceriodaphnia dubia*

b: most sensitive parameter (mean brood size) for *Daphnia magna*

c: geometric mean of 155000 and 71000 $\mu\text{g/l}$ for activated sludge bacteria

d: geometric mean of 38000 and 5000 $\mu\text{g/l}$ for *Pseudokirchneriella subcapitata*

e: geometric mean of 6000, 2500, 8600, 8100, 4100, 4800, 7400, and 2300 $\mu\text{g/l}$ for *Daphnia magna* (immobility/mortality)

f: geometric mean of 54000 and 56000 $\mu\text{g/l}$ for *Lemna gibba*

g: geometric mean of 25000 and 41000 $\mu\text{g/l}$ for *Lemna minor*

h: geometric mean of 4200 and 6200 $\mu\text{g/l}$ for *Pimephales promelas*

i: geometric mean of 6300, 7800, 8500, and 9000 $\mu\text{g/l}$ for *Poecilia reticulata*

Table A7. 39: 4-Chlorophenol: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	390 ^a	bact	6300 ^b
		alg	6500 ^c
		ann	13000 ^d
		crus	4600
		crus	34000 ^e
		crus	30000
		pisc	5400

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: most sensitive parameter (total cell volume) for *Skeletonema costatum*

b: geometric mean of 4300 and 9100 $\mu\text{g/l}$ for *Vibrio fisheri*

c: geometric mean of 3300 and 13000 $\mu\text{g/l}$ for *Skeletonema costatum*

d: most sensitive life stage (7-d larvae) of *Platynereis dumerilii*

e: geometric mean of 28000 and 42000 $\mu\text{g/l}$ for *Mesidotea entomon*

Table A7. 40: 2,3-Dichlorophenol: selected data for fresh water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
prot	8600	alg	5000
bact	55000	crus	4000 ^a
bact	130000	pisc	4700
bact	46000	pisc	3500
bact	80000		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 3100 and 5200 $\mu\text{g/l}$ for *Daphnia magna* (immobility/mortality)

Table A7. 41: 2,3-Dichlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
bact	4800		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 42: 2,4-Dichlorophenol: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]		
mac	270		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 43: 2,4-Dichlorophenol: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
prot	5800	prot	15000
prot	500	bact	50000 ^b
prot	1600	bact	75000
bact	6000	bact	54000
alg	2000	bact	78000
alg	3600	bact	20000
crus	490 ^a	bact	70000
pisc	290	fung	43000
		fung	17000
		mac	58000
		alg	9200
		alg	12000
		alg	14000
		crus	3400 ^c
		crus	7000
		crus	6600
		pisc	4300 ^d
		pisc	13000 ^e
		pisc	2800 ^f
		pisc	4700 ^g
		pisc	1700 ^h
		pisc	1300 ⁱ
		pisc	4800 ^j
		pisc	1700

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 320 and 740 $\mu\text{g/l}$ for *Daphnia magna* (reproduction/mortality)

b: geometric mean of 53000 and 47000 $\mu\text{g/l}$ for activated sludge bacteria

- c: geometric mean of 1400, 3900, 11000, 2700, 2600, 2600, 6000, and 2600 µg/l for *Daphnia magna* (immobility/mortality)
 d: geometric mean of 3900 and 4800 µg/l for *Brachydanio rerio*
 e: geometric mean of 7800 and 23000 µg/l for *Carassius auratus*
 f: geometric mean of 4000 and 2000 µg/l for *Lepomis macrochirus*
 g: geometric mean of 5000 and 4500 µg/l for *Leuciscus idus melanotus*
 h: geometric mean of 2600 and 1160 µg/l for *Oncorhynchus mykiss*
 i: geometric mean of 8.39, 7700, 7800, and 6500 µg/l for *Pimephales promelas*
 j: geometric mean of 5900, 4200, 3300, 3500, 5500, and 7600 µg/l for *Poecilia reticulata*

Table A7. 44: 2,4-Dichlorophenol: selected data for marine water.

taxonomic group	NOEC [µg/l]	taxonomic group	L(E)C50 [µg/l]
mac	0.1 ^a	bact	5400 ^c
crus	50 ^b		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

- a: 7 d-old embryos of *Phyllospora comosa*, no NOEC could be established for zygotes
 b: most sensitive life stage (10 mm) for *Allorchestes compressa*
 c: geometric mean of 5800 and 5000 µg/l for *Vibrio fisheri*

Table A7. 45: 2,5-Dichlorophenol: selected data for fresh water.

taxonomic group	L(E)C50 [µg/l]	taxonomic group	L(E)C50 [µg/l]
prot	12000	crus	4900
bact	50000	pisc	3100
bact	85000	pisc	2800
bact	50000		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 46: 2,6-Dichlorophenol: selected data for fresh water.

taxonomic group	NOEC [µg/l]	taxonomic group	L(E)C50 [µg/l]
prot	20000	prot	26000
		prot	30000
		bact	65000
		bact	550000
		bact	120000
		bact	130000
		alg	9700
		alg	29000
		crus	9400 ^a
		crus	26000
		crus	17000
		pisc	7300
		pisc	8200 ^b
		pisc	3700 ^c
		pisc	4000

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

- a: geometric mean of 3400, 9400, 20000, and 12200 µg/l for *Daphnia magna* (immobility/mortality)
 b: geometric mean of 3900, 7800, and 17900 µg/l for *Poecilia reticulata*
 c: geometric mean of 3500 and 4000 µg/l for *Leuciscus idus melanotus*

Table A7. 47: 2,6-Dichlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	14000	crus	19000

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 48: 3,4-Dichlorophenol: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
ann	300 ^a	ann	600 ^b

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 271, 212, 393, and 362 mg/kg for *Eisenia andrei*

b: geometric mean of 436, 398, 797, and 951 mg/kg for *Lumbricus rubellus*

Table A7. 49: 3,4-Dichlorophenol: selected data for fresh water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
prot	3000	alg	3200
bact	43000	crus	2800
bact	52000	pisc	1700
bact	20000	pisc	1100

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 50: 3,4-Dichlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	4000 ^a	crus	5300

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 9300 and 1700 $\mu\text{g/l}$ for *Vibrio fisheri*

Table A7. 51: 3,5-Dichlorophenol: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]		
mac	160		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 52: 3,5-Dichlorophenol: selected data for fresh water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
prot	4500	crus	4100
bact	26000 ^a	crus	4200
bact	25000	crus	4200
bact	10000	pisc	1700
alg	2300	pisc	3200 ^c
crus	2400 ^b	pisc	1800

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: Geometric mean of 12000 and 58000 $\mu\text{g/l}$ for activated sludge bacteria

b: Geometric mean of 2800 and 2100 $\mu\text{g/l}$ for *Daphnia magna*

c: Geometric mean of 4700, 2700 and 2600 for *Poecilia reticulata*

Table A7. 53: 3,5-Dichlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	3200	crus	1500
crus	8900	ann	1900 ^a

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: most sensitive life stage(7-d-old larvae) for *Platynereis dumerilii*

Table A7. 54: 2,3,4-Trichlorophenol: selected data for fresh water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	27000	crus	2200
bact	13000	pisc	1900
bact	40000	pisc	1200
alg	2000		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 55: 2,3,4-Trichlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	1600	crus	2000

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 56: 2,3,5-Trichlorophenol: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	16	mac	45

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 57: 2,3,5-Trichlorophenol: selected data for fresh water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
prot	840	pisc	1400
bact	22000	pisc	1900 ^a
bact	10000	pisc	600
bact	20000	pisc	800
crus	2300		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean 4700, 1600, and 880 $\mu\text{g/l}$ for *Poecilia reticulata*

Table A7. 58: 2,3,5-Trichlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	1400	crus	2700

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 59: 2,3,6-Trichlorophenol: selected data for fresh water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	39000	pisc	4000 ^a
bact	190000	pisc	2900
crus	7400	pisc	5400
pisc	7500		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean 13300, 5100, and 950 $\mu\text{g/l}$ for *Poecilia reticulata*

Table A7. 60: 2,3,6-Trichlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	13000	crus	2700

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 61: 2,4,5-Trichlorophenol: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
ann	110 ^a	ann	540 ^b

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 105, 78, 125, and 124 mg/kg for *Eisenia andrei*

b: geometric mean of 561, 447, 518, and 635 mg/kg for *Lumbricus rubellus*

Table A7. 62: 2,4,5-Trichlorophenol: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
pisc	160	prot	1600
		bact	24000
		bact	12000
		bact	8300
		bact	20000
		crus	1700 ^a
		pisc	1300
		pisc	450
		pisc	740 ^b
		pisc	950 ^c
		pisc	1500 ^d
		pisc	1700
		pisc	900

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 900, 1300, 2100, 1200, 2700, and 3500 $\mu\text{g/l}$ for *Daphnia magna* (immobility/mortality)

b: geometric mean of 1000, 400, and 1000 for *Leuciscus idus*

c: geometric mean of 1270, 900, and 740 for *Pimephales promelas*

d: geometric mean of 990, 1200, and 3100 for *Poecilia reticulata*

Table A7. 63: 2,4,5-Trichlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	1200	crus	3800
alg	990	pisc	1700
ann	2600 ^a		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: most sensitive life stage (embryos) of *Platynereis dumerilii*

Table A7. 64: 2,4,6-Trichlorophenol: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	370 ^a	ann	58
mac	120 ^b	ann	110
mac	370 ^c	ann	85
		ann	78
		mac	80

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 270 and 500 mg/kg for *Avena sativa*

b: geometric mean of 86 and 160 mg/kg for *Lactuca sativa*

c: geometric mean of 270 and 500 mg/kg for *Lycopersicum esculentum*

Table A7. 65: 2,4,6-Trichlorophenol: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	650	prot	6200 ^b
pisc	180 ^a	bact	42000
pisc	970	bact	240000
		bact	38000
		bact	43000
		bact	170000
		alg	10000
		alg	5600
		alg	3500
		crus	2400 ^c
		crus	7500
		crus	3900
		pisc	2500
		pisc	2200
		pisc	360 ^d
		pisc	730
		pisc	5900 ^e
		pisc	1800 ^f

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: most sensitive parameter (growth) for fry of *Jordanella floridae*

b: geometric mean of 4000, 7700, and 7800 $\mu\text{g/l}$ for *Tetrahymena pyriformis*

c: geometric mean of 2200, 5500, 6000, 690, and 1700 $\mu\text{g/l}$ for *Daphnia magna* (immobility/mortality)

d: geometric mean of 410 and 320 $\mu\text{g/l}$ for *Lepomis macrochirus*

e: geometric mean of 9200, 2740, 9200, 4900, and 6100 for *Pimephales promelas*

f: geometric mean of 610, 890, 2300, and 7900 for *Poecilia reticulata*

Table A7. 66: 2,4,6-Trichlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
bact	8200		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 67: 3,4,5-Trichlorophenol: selected data for fresh water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	20000	pisc	1000
bact	5000	pisc	1400 ^a
crus	900		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 2400, 1100, and 1100 for *Poecilia reticulata*

Table A7. 68: 3,4,5-Trichlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
bact	380		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 69: 2,3,4,5-Tetrachlorophenol: selected data for fresh water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
prot	450	crus	1800
bact	20000	pisc	880
bact	4000	pisc	420 ^a
bact	10000	pisc	920 ^b
bact	12000	pisc	210

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 440, 400, 410, and 440 $\mu\text{g/l}$ for *Pimephales promelas*

b: geometric mean of 2300, 770, and 440 $\mu\text{g/l}$ for *Poecilia reticulata*

Table A7. 70: 2,3,4,5-Tetrachlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
bact	210		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 71: 2,3,4,5-Tetrachlorophenol: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
ann	290 ^a	ann	1400 ^b

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 272 and 316 mg/kg for *Eisenia andrei*

b: geometric mean of 1434 and 1392 mg/kg for *Lumbricus rubellus*

Table A7. 72: 2,3,4,6-Tetrachlorophenol: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	650	bact	40000
		prot	1400
		roti	5200
		roti	960
		alg	10000
		alg	1300
		crus	690 ^a
		crus	580
		crus	2300
		crus	1400
		pisc	140
		pisc	1000
		pisc	1100 ^b
		pisc	750
pisc	1000		
pisc	500		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 2660, 290, 180, and 1600 $\mu\text{g/l}$ for *Daphnia magna*

b: geometric mean of 340, 1100, and 3700 $\mu\text{g/l}$ for *Poecilia reticulata*

Table A7. 73: 2,3,4,6-Tetrachlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	1500	crus	12000 ^a

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 11800 and 11900 $\mu\text{g/l}$ for *Crangon septemspinosa*

Table A7. 74: 2,3,5,6-Tetrachlorophenol: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	Taxonomic group	L(E)C50 [$\mu\text{g/l}$]
pisc	95 ^a	prot	1200 ^b
		bact	44000
		bact	54000
		crus	1100 ^c
		pisc	3600
		pisc	1200
		pisc	170
		pisc	1200 ^d

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: most sensitive life stage (fry) for *Jordonella floridae*

b: geometric mean of 1400 and 1100 $\mu\text{g/l}$ for *Tetrahymena pyriformis*

c: geometric mean of 2300 and 570 $\mu\text{g/l}$ for *Daphnia magna*

d: geometric mean of 3900, 1400, 390, 3700, 1100, and 340 $\mu\text{g/l}$ for *Poecilia reticulata*

Table A7. 75: 2,3,5,6-Tetrachlorophenol: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	2500	pisc	1900

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

Table A7. 76: Pentachlorophenol: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	1.6 ^a	mac	13 ^c
mac	18	ann	78 ^d
bact	190	ann	150 ^e
ann	11 ^b	ann	1400 ^f

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: geometric mean of 1.6 and 1.7 mg/kg for *Lactuca sativa*

b: geometric mean of 10, 12.5, 25, 11.2, 7, and 5.6 mg/kg for reproduction or cocoon hatchability of *Eisenia fetida/andrei*

c: geometric mean of 16, 40, and 3.7 mg/kg for growth of *Lactuca sativa*

d: geometric mean of 322, 102, 233, 227, 87, 37, 80, 260, 28, 72, 19, and 12 mg/kg for *Eisenia fetida/andrei*

e: two values of 136 mg/kg for *Enchytraeus albidus*

f: geometric mean of 1473, 447, 1661, and 3259 mg/kg for *Lumbricus rubellus*

Table A7. 77: Pentachlorophenol: selected data for terrestrial processes.

process	NOEC [mg/kg]	process	NOEC [mg/kg]
H ₂ -oxy	59 ^a	ac-min	570
ATP	6.5	bio C	2.0 ^a
ATP	6.5	dehy	2.0 ^a
ac-min	840	ure	2.0 ^a
ac-min	170	nit-red	2.0 ^a
ac-min	4000	nitr	18
ac-min	24	nitr	40
ac-min	3800 ^b	nitr	17
ac-min	240 ^b	resp	420
ac-min	210	resp	170
ac-min	1500	N ₂ -fix	50
ac-min	1300		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: calculated from EC_x value (50-80%) divided by a factor of 10

b: lowest NOEC for same soil but different exposure times for acetate mineralisation

Table A7. 78: Pentachlorophenol: selected data for fresh water.

taxonomic group	NOEC [µg/l]	taxonomic group	NOEC [µg/l]
bact	1000	ins	3200
prot	80 ^a	coel	32
roti	200	moll	3.2 ^d
cyan	1000	moll	50
alg	30 ^a	pisc	55 ^e
alg	100	pisc	32 ^f
alg	135 ^b	pisc	100 ^g
mac	1000	pisc	28 ^h
crus	130 ^c	pisc	8.9
crus	23	amph	32
crus	23		

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

a: for protozoa and algae the lower NOEC values determined after 48 and 72 h are preferred above NOECs from longer exposure periods, which might be affected by growth of the organisms

b: most sensitive parameter (growth) for *Scenedesmus subspicatus*

- c: geometric mean 180 and 100 µg/l for most sensitive parameter (mortality) for *Daphnia magna*
 d: lowest NOEC for *Lymnea stagnalis* after 7 d of exposure instead of 40 d
 e: most sensitive life stage (eggs) for *Jordanella floridae*
 f: most sensitive parameter (mortality) for eggs of *Jordanella floridae*
 g: most sensitive parameter (growth) for *Poecilia reticulata*
 h: geometric mean 36, 6, 45, and 66 µg/l for *Pimephales promelas*

Table A7. 79: Pentachlorophenol: selected data for marine water.

taxonomic group	NOEC [µg/l]	taxonomic group	NOEC [µg/l]
alg	500	crus	100
alg	125	ann	3 ^a
alg	500	ann	84 ^b
alg	250	pisc	10
crus	5800	pisc	10
crus	100	pisc	47

Data originate from Janus et al. (1991); additional data are taken from the annex to this report.

- a: most sensitive parameter/life stage (mortality in egg mass, reproduction potential) for *Ophryotrocha diadema*
 b: geometric mean of 156 and 45 µg/l for *Arenicola cristata*

Table A7. 80: 1-Chloronaphthalene: selected data for fresh water.

taxonomic group	NOEC [µg/l]	taxonomic group	L(E)C50 [µg/l]
pisc	390	alg	1000
		crus	1600
		pisc	2300

All data are taken from the annex to this report.

Table A7. 81: 1-Chloronaphthalene: selected data for marine water.

taxonomic group	L(E)C50 [µg/l]	taxonomic group	L(E)C50 [µg/l]
bact	1700	crus	370
alg	1100	pisc	1300 ^b
crus	1100 ^a		

All data are taken from the annex to this report.

- a: geometric mean of 780, 1800, and 910 µg/l for different life stages of *Artemia salina*
 b: geometric mean of 690 and 2400 µg/l for *Cyprinodon variegatus*

Table A7. 82: 2-Chloronaphthalene: selected data for fresh water.

taxonomic group	L(E)C50 [µg/l]		
crus	1600		

All data are taken from the annex to this report.

Table A7. 83: 2-Chloronaphthalene: selected data for marine water.

taxonomic group	L(E)C50 [µg/l]		
crus	2300		

All data are taken from the annex to this report.

Table A7. 84: Polychlorinated (PCB) congeners: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
PCB 77 crus	0.10	pisc	1.3
PCB 105			
PCB 126 crus	0.018		

All data originate from Appendix 2 in Van Wezel et al. (1999a).

Appendix 8 Data for pesticides used for extrapolation

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Table A8. 1: DDT: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]		
ins	10 ^a		

All data originate from Van de Plassche et al. (1994).

a: geometric mean of 22, 7.4, 12, 0.8, 35, 29.4, 17.3, 4.7, 7.4, 10.9, 11.4, and 12 mg/kg, parameter mortality for *Gryllus pennsylvanicus*

Table A8. 2: DDT: selected data for fresh water

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	0.050 ^a	crus	4.0
pisc	0.35	crus	15
		crus	1.2 ^b
		crus	0.63 ^c
		crus	1.7 ^d
		crus	3.0 ^e
		crus	28
		crus	2.6 ^f
		ins	17
		ins	7.4
		ins	4.7
		ins	3.5
		ins	1.2
		ins	1.2
		ins	20
		ins	32
		ins	1.5
		ins	1.9
		ins	7.0
		ins	1.6
		pisc	17 ^g
		pisc	9.7
		pisc	2.7
		pisc	27
		pisc	4.9 ^h
		pisc	14 ⁱ
		pisc	8.9 ^j
		pisc	7.4 ^k
		pisc	8.7 ^l
		pisc	1.7 ^m
		pisc	5.8
		pisc	9.0
		pisc	12 ⁿ
		pisc	5.6
		pisc	3.9 ^o
		pisc	6.4 ^p
		pisc	8.8 ^q
		pisc	1.8
		pisc	1.8
		pisc	12
		pisc	3.7 ^r
		pisc	11 ^s
		pisc	16
		amph	30

All data originate from Van de Plassche et al. (1994).

a: most sensitive parameter (reproduction) for *Daphnia magna*

b: geometric mean of 4.7, 1.1, 1.1, 1.3, 0.5, 0.68 and 1.2 $\mu\text{g/l}$, parameter mortality/immobility for *Daphnia magna*

c: geometric mean of 1.1 and 0.36 $\mu\text{g/l}$, parameter immobility for *Daphnia pulex*

d: geometric mean of 0.8, 1.8 and 3.2 $\mu\text{g/l}$, parameter mortality for *Gammarus fasciatus*

- e: geometric mean of 1 and 9 µg/l, parameter mortality for *Gammarus lacustris*
 f: geometric mean of 2.5 and 2.8 µg/l, parameter immobility for *Simocephalus serrulatus*
 g: geometric mean of 15.5, 14.7 and 21 µg/l, parameter mortality for *Carassius auratus*
 h: geometric mean of 5.1 and 4.8 µg/l, parameter mortality for *Ictalurus melas*
 i: geometric mean of 21.5, 17.3, 6.9, 22, 16, 7 and 16 µg/l, parameter mortality for *Ictalurus punctatus*
 j: geometric mean of 6.5, 10.9 and 9.9 µg/l, parameter mortality for *Lepomis cyanellus*
 k: geometric mean of 7, 8.6, 6.3, 4.3, 5.8, 8 and 16 µg/l, parameter mortality for *Lepomis macrochirus*
 l: geometric mean of 5 and 15 µg/l, parameter mortality for *Lepomis microlophus*
 m: geometric mean of 1.5 and 2.0 µg/l, parameter mortality for *Micropterus salmoides*
 n: geometric mean of 12.4, 13.2, 19, 21, 8.6 and 5.3 µg/l, parameter mortality for *Pimephales promelas*
 o: geometric mean of 5.5, 7.9 and 1.4 µg/l, parameter mortality for *Oncorhynchus clarki*
 p: geometric mean of 7, 9.6, 2.4, 18, 1.7, 8.7, 7.6, 4.7 and 11.4 µg/l, parameter mortality for *Oncorhynchus mykiss*
 q: geometric mean of 4 and 19.3 µg/l, parameter mortality for *Salmo kisutch*
 r: geometric mean of 2.9 and 4.6 µg/l, parameter mortality for *Stizostedion vitreum*
 s: geometric mean of 5.1, 14 and 17 µg/l, parameter mortality for *Tilapia mossambica*

Table A8. 3: DDT: selected data for marine water.

taxonomic group	NOEC [µg/l]	taxonomic group	L(E)C50 [µg/l]
alg	2.0 ^a	alg	10
alg	1.0 ^b	alg	10
alg	0.50	alg	30
alg	8.0	alg	20
alg	1.0 ^c	crus	14
alg	25	crus	10
pisc	33	crus	1.1
		crus	0.40
		crus	3.8
		crus	0.45
		crus	30
		crus	0.80
		crus	10
		crus	0.60
		crus	0.70
		moll	9.0
		pisc	1.8 ^d
		pisc	3.7 ^e
		pisc	3.0
		pisc	3.9 ^f
		pisc	15 ^g
		pisc	0.30
		pisc	2.0
		pisc	0.41
		pisc	0.40
		pisc	0.40

All data originate from Van de Plassche et al. (1994).

a: most sensitive parameter (photosynthesis) for *Coccolithus huxleyi*

b: most sensitive parameter (growth) for *Cyclotella nana*

- c: most sensitive parameter (growth) for *Skeletonema costatum*
 d: geometric mean of 7.6 and 0.45 µg/l, parameter mortality for *Cymatogaster aggregata*
 e: geometric mean of 5.0, 5.0, and 2.0 µg/l, parameter mortality for *Cyprinodon variegatus*
 f: geometric mean of 2.8 and 5.5 µg/l, parameter mortality for *Fundulus similis*
 g: geometric mean of 18 and 12 µg/l, parameter mortality for *Gasterosteus aculeatus*

Table A8. 4: DDE: selected data for fresh water.

taxonomic group	L(E)C50 [µg/l]	taxonomic group	L(E)C50 [µg/l]
plat	1100	pisc	32
pisc	240	pisc	96

All data originate from Van de Plassche et al. (1994).

Table A8. 5: DDE: selected data for marine water.

taxonomic group	NOEC [µg/l]	taxonomic group	L(E)C50 [µg/l]
crus	0.10	crus	2.5
		crus	28 ^a
		moll	14

All data originate from Van de Plassche et al. (1994).

a: from two studies

Table A8. 6: DDD: selected data for fresh water.

taxonomic group	L(E)C50 [µg/l]	taxonomic group	L(E)C50 [µg/l]
crus	6.4 ^a	pisc	42
crus	3.2	pisc	70
crus	4.5	pisc	14
ins	380	amph	140
pisc	1500	amph	400
pisc	42		

All data originate from Van de Plassche et al. (1994).

a: geometric mean of 4.6 and 8.9 µg/l, parameter immobility for *Daphnia magna*

Table A8. 7: DDD: selected data for marine water.

taxonomic group	L(E)C50 [µg/l]	taxonomic group	L(E)C50 [µg/l]
alg	790	pisc	42
crus	60	pisc	20
crus	2.4	pisc	2.5
moll	25		

All data originate from Van de Plassche et al. (1994).

Table A8. 8: Aldrin: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
bact	59 ^a	ann	11
bact	130 ^b	nema	3.5 ^d
fung	32 ^c	ins	2.8 ^e
		ins	0.55

All data originate from Van de Plassche et al. (1994).

- a: geometric mean of 42 and 83 mg/kg derived from two ECx values (EC20 of 125 mg/kg and EC20 of 125 mg/kg standard soil divided by a factor of 3 in both cases) for *Actinomyces* in the same soil
- b: geometric mean of 125 and 125 mg/kg derived from two ECx values (EC7 of 125 mg/kg and EC13 divided by a factor of 2 of 250 mg/kg standard soil) for bacteria species in the same soil
- c: geometric mean of 42 and 25 mg/kg derived from two ECx values (EC33 of 125 mg/kg and EC65 250 mg/kg standard soil divided by a factor of 3 and 10 respectively) for fungi species in the same soil
- d: calculated from 8 LCx data for larvae of *Melanotus communis* in 3 different soils ($r^2=0.93$)
- e: geometric mean of 3.8 and 2.1 µg/l, parameter mortality for *Folsomia candida*

Table A8. 9: Aldrin: selected data for fresh water.

taxonomic group	L(E)C50 [µg/l]	taxonomic group	L(E)C50 [µg/l]
crus	8.0	pisc	4.0
crus	18	pisc	19
crus	29 ^a	pisc	53
crus	28	pisc	27 ^c
crus	9.8	pisc	20
crus	23	pisc	8.4 ^d
ins	143	pisc	5.0
ins	3.0	pisc	100
ins	1.0	pisc	19 ^e
ins	9.0	pisc	42
ins	42	pisc	6.8 ^f
ins	18	pisc	46
ins	22 ^b	pisc	10 ^g
pisc	32	amph	68

All data originate from Van de Plassche et al. (1994).

- a: geometric mean of 28 and 30 µg/l, parameter mortality for *Daphnia magna*
- b: geometric mean of 43, 180 and 1.3 µg/l, parameter mortality for *Pteronarcys* species, different life stages
- c: geometric mean of 37 and 20 µg/l, parameter mortality for *Lebistis reticulatis*
- d: geometric mean of 5.6, 10, 13, 6.2, 12, 9.7, 7.7, 6.2, 15 and 4.6 µg/l, parameter mortality for *Lepomis macrochirus*
- e: geometric mean of 28, 8.2 and 32 µg/l, parameter mortality for *Pimephales promelas*
- f: geometric mean of 18, 2.6, 8.2, 9.3, 3.2, 3.4, 2.2, 10 and 36 µg/l, parameter mortality for *Oncorhynchus mykiss*
- g: geometric mean of 7.5 and 14 µg/l, parameter mortality for *Salmo tshawytscha*

Table A8. 10: Aldrin: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
moll	83	crus	33 ^a
pisc	3.3	crus	8.0
		crus	33
		crus	9.0
		crus	0.44 ^b
		moll	15
		pisc	4.0
		pisc	33 ^c
		pisc	3.2
		pisc	7.2
		pisc	2.0
		pisc	2.8

All data originate from Van de Plassche et al. (1994).

a: geometric mean of 23 and 42 $\mu\text{g/l}$, parameter loss of equilibrium/immobility/mortality for *Callinectes sapidus*

b: geometric mean of 0.6 and 0.32 $\mu\text{g/l}$, parameter loss of equilibrium/immobility/mortality for *Penaeus duorarum*

c: geometric mean of 40 and 27 $\mu\text{g/l}$, parameter mortality for *Gasterosteus aculeatus*

Table A8. 11: Dieldrin: selected data on terrestrial processes.

process	NOEC [mg/kg]	process	NOEC [mg/kg]
resp	34	inv	34
amy	34		

All data originate from Van de Meent et al. (1990).

Table A8. 12: Dieldrin: selected data on terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
ins	0.50	ins	1.1
		ins	1.4

All data originate from Van de Meent et al. (1990).

Table A8. 13: Dieldrin: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
cyan	10	crus	32
cyan	10	pisc	5.0
cyan	10	pisc	0.75
moll	10	pisc	0.12

All data originate from Van de Meent et al. (1990).

Table A8. 14: Dieldrin: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
alg	0.10	pisc	0.10
crus	18		

All data originate from Van de Meent et al. (1990).

Table A8. 15: Endrin: selected data on terrestrial species.

taxonomic group	L(E)C50 [mg/kg]		
ins	0.95		

All data originate from Van de Plassche et al. (1994).

Table A8. 16: Endrin: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
cyan	95	crus	1.5
pisc	0.21 ^a	crus	41 ^c
pisc	0.17 ^b	crus	20
		crus	1.8
		crus	3.1 ^d
		crus	3.0
		crus	3.2 ^e
		crus	20
		ins	0.35 ^f
		ins	0.90
		ins	0.76
		ins	62
		ins	2.2 ^g
		ins	0.54
		ins	0.77 ^h
		ins	0.83
		pisc	0.65 ⁱ
		pisc	0.32
		pisc	0.87 ^j
		pisc	0.89 ^k
		pisc	0.85
		pisc	0.28 ^l

All data originate from Van de Plassche et al. (1994).

- a: most sensitive parameter (reproduction) for *Jordonella floridae*
b: lowest NOEC for *Pimephales promelas*
c: geometric mean of 230, 4.2, 74, and 41 $\mu\text{g/l}$ for *Daphnia magna*
d: geometric mean of 1.3, 4.3, and 5.5 $\mu\text{g/l}$ for *Gammarus fasciatus*
e: most sensitive life stage (3-5 w) for *Orconectes nais*
f: geometric mean of 0.32 and 0.39 $\mu\text{g/l}$ for *Acroneuria pacifica*
g: geometric mean of 2.4 and 2.1 $\mu\text{g/l}$ for *Ischnuria verticalis*
h: geometric mean of 0.25 and 2.4 $\mu\text{g/l}$ for *Pteronarcis californica*
i: geometric mean of 0.44 and 0.95 $\mu\text{g/l}$ for *Carassius auratus*
j: geometric mean of 1.1 and 0.69 $\mu\text{g/l}$ for *Gambusia affinis*
k: geometric mean of 0.42 and 1.9 $\mu\text{g/l}$ for *Ictalurus punctatus*
l: geometric mean of 0.21 and 0.37 $\mu\text{g/l}$ for *Lepomis macrochirus*

Table A8. 17: Endrin: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	0.067	alg	950
alg	10	crus	19 ^b
alg	0.10	crus	2.0
alg	100	crus	0.74 ^c
crus	0.030 ^a	crus	1.2
moll	25	crus	0.68 ^d
pisc	0.12	crus	0.24 ^e
pisc	0.19	crus	0.086 ^f
		echi	360
		moll	57 ^g
		pisc	0.60
		pisc	0.80
		pisc	0.50
		pisc	0.40 ^h
		pisc	0.60
		pisc	0.30
		pisc	0.26 ⁱ
		pisc	1.1 ^j
		pisc	0.93 ^k
		pisc	0.050
		pisc	0.094
		pisc	0.35 ^l
		pisc	2.6
		pisc	1.2
		pisc	0.63
		pisc	3.1
		pisc	0.10

All data originate from Van de Plassche et al. (1994).

a: most sensitive parameter (weight) for larvae of *Palaemonetes pugeo*

b: geometric mean of 25 and 15 $\mu\text{g/l}$ for *Calinectes sapidus*

c: geometric mean of 1.7, 0.6, and 0.4 $\mu\text{g/l}$ for *Crangon* species

d: geometric mean of 0.69, 0.63, 0.35, 0.8, and 1.2 $\mu\text{g/l}$ for different life stages of *Palaemonetes pugeo*

e: geometric mean of 0.3 and 0.2 $\mu\text{g/l}$ for *Penaeus aztecus*

f: geometric mean of 0.037 and 0.2 $\mu\text{g/l}$ for *Penaeus duorarum*

g: geometric mean of 14, 33, and 400 $\mu\text{g/l}$ for *Crassostrea virginica*

h: geometric mean of 0.36, 0.38, 0.36, 0.37, 0.34, 0.34, 1.0, and 0.34 $\mu\text{g/l}$ for different life stages of *Cyprinodon variegatus*

i: geometric mean of 0.3 and 0.23 $\mu\text{g/l}$ for *Fundulus similis*

j: geometric mean of 1.2, 1.2, 0.9, 1.1, and 1.2 $\mu\text{g/l}$ for adult *Gasterosteus aculeatus*

k: geometric mean of 4.4, 0.3, and 0.6 $\mu\text{g/l}$ for *Leiostomus xanthurus*

l: geometric mean of 0.40 and 0.3 $\mu\text{g/l}$ for *Mugil cephalus*

Table A8. 18: α -HCH: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	3300	crus	500
alg	80	pisc	2100 ^b
prot	9		
moll	20		
crus	90 ^a		
pisc	800		

All data originate from Van de Plassche et al. (1994).

a: most sensitive parameter (growth) for *Daphnia magna*

b: geometric mean of 1300 and 3500 $\mu\text{g/l}$ for *Lebistes reticulatus*

Table A8. 19: α -HCH: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]		
pisc	250		

All data originate from Van de Plassche et al. (1994).

Table A8. 20: β -HCH: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
alg	500	pisc	27 ^a
prot	83	pisc	180
crus	320		

All data originate from Van de Plassche et al. (1994).

a: parameters mortality, growth and embryonic development for *Oryzias latipes*

Table A8. 21: β -HCH: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]		
crus	10		

All data originate from Van de Plassche et al. (1994).

Table A8. 22: Lindane: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
ins	0.05	ins	0.84 ^a
ann	29	ann	98
		ann	59

All data originate from Van de Meent et al. (1990).

a: geometric mean of 0.75 and 0.95 mg/kg for *Folsomia candida*

Table A8. 23: Lindane: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
cyan	150	crus	24 ^c
alg	250	crus	6.0 ^d
alg	950	ins	2.2
alg	500	pisc	9.1
prot	660 ^a	pisc	2.9
moll	330 ^b	pisc	8.8

All data originate from Van de Plassche et al. (1994).

- a: geometric mean of 440 and 1000 µg/l for *Tetrahymena pyriformis* (parameter growth)
 b: most sensitive parameter (fecundity) for *Lymnea stagnalis*
 c: geometric mean of 54 and 11 µg/l for *Daphnia magna* (parameters reproduction and mortality)
 d: geometric mean of 4.3 and 8.3 µg/l for *Gammarus fasciatus* (parameters reproduction and mortality)

Table A8. 24: Lindane: selected data for marine water.

taxonomic group	NOEC [µg/l]	taxonomic group	NOEC [µg/l]
moll	1000	moll	5000

All data originate from Van de Plassche et al. (1994).

Table A8. 25: Carbaryl: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
bact	23000 ^a	ins	12 ^d
ann	25	ann	22 ^b
ins	1.6 ^{b,c}	ann	140 ^{b,e}
		ann	120 ^b
		ann	130 ^{b,f}
		ann	260 ^b

All data originate from Appendix 4 in Crommentuijn et al. (1997c).

- a: geometric mean of 42000 and 12500 mg/kg for *Rhizobium* species.
 b: result from deviating test
 c: geometric mean of 0.5 and 5 mg/kg for *Folsomia candida*
 d: geometric mean of 10 and 15 mg/kg for *Folsomia candida*
 e: geometric mean of 110 and 110 mg/kg for *Eisenia fetida*
 f: geometric mean of 97, 170, and 139 mg/kg for *Lumbricus terrestris*

Table A8. 26: Carbaryl: selected data for terrestrial processes.

taxonomic group	NOEC [mg/kg]		
dehy	120		

All data originate from Appendix 4 in Crommentuijn et al. (1997c).

Table A8. 27: Carbaryl: selected data for fresh water.

taxonomic group	NOEC [µg/l]	taxonomic group	NOEC [µg/l]
prot	20000	crus	10
crus	4.5	pisc	62 ^a
crus	1	moll	1000

All data originate from Appendix 2 in Crommentuijn et al. (1997c).

- a: most sensitive parameter (hatchability) for larvae of *Pimephales promelas*

Table A8. 28: Carbaryl: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
alg	100	moll	80 ^a
alg	100	moll	1000 ^b
alg	50	moll	50 ^c
alg	10	moll	1000
alg	50	moll	1
crus	0.05		

All data originate from Appendix 3 in Crommentuijn et al. (1997c).

a: most sensitive life stage (juvenile) for *Clinocardium nuttalli*

b: most sensitive parameter (embryonic development/growth) for *Crassostrea virginica*

c: most sensitive life stage (eggs) for *Mercenaria mercenaria*

Table A8. 29: Carbofuran: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
bact	11 ^a	nema	320 ^c
fung	2.4 ^b	ann	5
ann	0.5	ann	4
		ins	0.41 ^d
		ins	1.1
		ins	7.5
		ins	0.95

All data originate from Van de Plassche et al. (1994).

a: geometric mean of 2.4, 24, and 24 $\mu\text{g/l}$ for bacteria species (EC0-EC30 on agar plates considered as NOEC)

b: geometric mean of 2.4 and 2.5 $\mu\text{g/l}$ for fungi species

c: calculated from 3 LCx data for *Aphelenchus avenae* ($r^2=0.95$)

d: geometric mean of 0.75, 0.3, and 0.3 $\mu\text{g/l}$ for *Folsomia candida*

Table A8. 30: Carbofuran: selected data for terrestrial processes.

taxonomic group	NOEC [mg/kg]	taxonomic group	NOEC [mg/kg]
nitro	8.0 ^a	ure	1.7
nitro	25		

All data originate from Van de Plassche et al. (1994).

a: geometric mean of 9 and 17 mg/kg derived from two ECx values (EC31 of 17 mg/kg and EC34 of 34 mg/kg standard soil both divided by a factor of 3) for nitrogenase inhibition activity in the same soil

Table A8. 31: Carbofuran: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	9.8	ins	1.6
pisc	24.8	pisc	250
		pisc	150 ^a
		pisc	530
		pisc	480 ^b
		pisc	230 ^c
		pisc	1300 ^d
		pisc	400 ^e
		pisc	160
		amph	110

All data originate from Van de Plassche et al. (1994).

a: geometric mean of 240 and 88 $\mu\text{g/l}$ for *Lepomis macrochirus*

b: geometric mean of 380 and 600 $\mu\text{g/l}$ for *Oncorhynchus mykiss*

c: geometric mean of 240, 120 and 400 $\mu\text{g/l}$ for *Perca flavescens*

d: geometric mean of 2000, 870, and 1200 $\mu\text{g/l}$ for *Lepomis macrochirus*

e: geometric mean of 560 and 280 $\mu\text{g/l}$ for *Lepomis macrochirus*

Table A8. 32: Carbofuran: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	0.5 ^a	crus	1.5 ^{a,b}
pisc	15	crus	4.6
		pisc	390
		pisc	100

All data originate from Van de Plassche et al. (1994).

a: most sensitive life stage (zoea) of *Cancer magister*

b: most sensitive parameter (immobility)

Table A8. 33: Maneb: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]		
ann	220		

All data originate from Appendix 4 in Crommentuijn et al. (1997c).

Table A8. 34: Maneb: selected data for terrestrial processes.

taxonomic group	NOEC [mg/kg]	taxonomic group	NOEC [mg/kg]
nitr	130	N-min	31
nitr	120	N-min	120

All data originate from Appendix 4 in Crommentuijn et al. (1997c).

Table A8. 35: Maneb: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
crus	56	pisc	18 ^a

All data originate from Appendix 2 in Crommentuijn et al. (1997c).

a: most sensitive parameter (total embryotoxicity) in ELS of *Oncorhynchus mykiss*

Table A8. 36: Atrazine: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
bact	29 ^a	mac	2.9 ^{b,c}
ann	160	mac	4.6 ^{b,d}
ins	50	mac	4.6 ^{b,e}
ins	50	mac	12 ^{b,f}
fung	5 ^b	ann	40 ^b
		ann	87 ^{b,g}
		ann	23 ^b
		ann	380 ^b
		ann	65 ^b

All data originate from Appendix 4 in Crommentuijn et al. (1997c).

a: geometric mean of 17 and 50 mg/kg for nitrifying bacteria species

b: result from deviating test

c: geometric mean of 1.5 and 5.8 mg/kg for pregerminated seeds of *Avena sativa*

d: geometric mean of 2.5, 2.6 and 15 mg/kg for seeds of *Brassica rapa*

e: geometric mean of 2.5 and 8.5 mg/kg for seeds of *Lactuca sativa*

f: geometric mean of 4.2 and 32 mg/kg for seeds of *Lolium perenne*

g: geometric mean of 58 and 130 mg/kg for *Eisenia fetida*

Table A8. 37: Atrazine: selected data for terrestrial processes.

taxonomic group	NOEC [mg/kg]	taxonomic group	NOEC [mg/kg]
ATP	0.24 ^a	phos	17
dehy	1.7	phos diest	13 ^b

All data originate from Appendix 4 in Crommentuijn et al. (1997c).

a: geometric mean of 0.17 and 0.33 mg/kg for ATP content in the same soil

b: geometric mean of 5 and 33 mg/kg derived from two ECx values (EC16 of 10 mg/kg and EC21 100 mg/kg standard soil divided by a factor of 2 and 3, respectively) for phosphodiesterase activity in the same soil

Table A8. 38: Atrazine: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
cyan	270	crus	140
cyan	3	crus	1000 ^a
alg	45	crus	60 ^b
alg	110	ins	2000
alg	16	ins	110
alg	30	pisc	300
alg	40	pisc	18 ^c
alg	70	pisc	27 ^d
crus	2500	pisc	65 ^e

All data originate from Appendix 2 in Crommentuijn et al. (1997c).

a: most sensitive parameter (reproduction) for *Daphnia pulex*

b: most sensitive parameter (mortality) for *Gammarus fasciatus*

c: geometric mean of 13 and 24 $\mu\text{g/l}$ for *Ictalurus punctatus*

d: geometric mean of 15 and 48 $\mu\text{g/l}$ for *Oncorhynchus mykiss*

e: most sensitive parameter (growth) for *Salvelinus fontinalis*

Table A8. 39: Atrazine: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
alg	22 ^a	crus	80 ^d
alg	22 ^b	pisc	1900
alg	1 ^c		

All data originate from Appendix 3 in Crommentuijn et al. (1997c).

- a: most sensitive parameter (photosynthesis) for *Nitzschia sigma*
- b: most sensitive parameter (growth and photosynthesis) for *Thalassiosira fluviatilis*
- c: most sensitive parameter (mortality) for spores of *Laminaria hyperborea*
- d: most sensitive parameter (growth) for *Mysidopsis bahia*

Appendix 9 Data for other compounds used for extrapolation

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Table A9. 1: Dimethyl phthalate: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]		
ann	3200		

All data are taken from the annex to this report.

Table A9. 2: Dimethyl phthalate: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	9600	prot	540000
		alg	140000
		crus	46000
		ins	380000
		pisc	50000
		pisc	56000
		pisc	69000 ^a

All data are taken from the annex to this report.

a: geometric mean of 121 and 39 mg/l for *Pimephales promelas*

Table A9. 3: Dimethyl phthalate: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	NOEC [$\mu\text{g/l}$]
crus	10000	bact	17000 ^a
		alg	72000 ^b
		crus	69000
		crus	62000
		pisc	110000 ^c
		pisc	41000 ^d

All data are taken from the annex to this report.

a: geometric mean of 16 and 18 mg/l for *Vibrio fisheri*

b: geometric mean of 96 and 54 mg/l for *Gymnodium breve*

c: geometric mean of 100 and 115 mg/l for *Alburnus alburnus*

d: geometric mean of 29 and 58 mg/l for *Cyprinodon variegatus*

Table A9. 4: Diethyl phthalate: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]		
mac	530		

All data are taken from the annex to this report.

Table A9. 5: Diethyl phthalate: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
prot	53000	prot	130000
prot	19000	alg	16000
prot	48000	alg	45000
alg	15000	crus	69000 ^b
alg	10000	ins	130000
crus	18000 ^a	pisc	43000 ^c
		pisc	57000 ^d
		pisc	12000
		pisc	21000 ^e

All data are taken from the annex to this report.

- a: geometric mean of 25 and 13 mg/l for *Daphnia magna*
 b: geometric mean of 86, 41, 75, and 86 mg/l for *Daphnia magna*
 c: geometric mean of 110 and 16.7 mg/l for *Lepomis macrochirus*
 d: geometric mean of 53 and 61 mg/l for *Leuciscus idus melanotus*
 e: geometric mean of 16.8, 17, and 31.8 for *Pimephales promelas*

Table A9. 6: Diethyl phthalate: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	4300 ^a	pisc	29000 ^b
crus	10000		

All data are taken from the annex to this report.

- a: geometric mean of 6.1 and 3 mg/l for *Gymnodium breve*
 b: geometric mean of 29 and 30 mg/l for *Cyprinodon variegatus*

Table A9. 7: Diethyl phthalate: selected QSAR data.

taxonomic group	NOEC [mg/l]	taxonomic group	NOEC [mg/l]
bact	1100	moll	14
bact	54	crus	19
bact	150	crus	12
bact	140	ins	20
alg	140	ins	17
alg	65	pisc	7
alg	15	amph	19
fung	1200	amph	15
prot	123	amph	22
coel	15		

All data are taken from the annex to this report.

Table A9. 8: Di-iso-butyl phthalate: selected data for fresh water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
pisc	900		

All data are taken from the annex to this report.

Table A9. 9: Di-iso-butyl phthalate: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
crus	3000		

All data are taken from the annex to this report.

Table A9. 10: Di-n-butyl phthalate: selected data for terrestrial species.

taxonomic group	L(E)C50 [mg/kg]		
mac	1900		

All data are taken from the annex to this report.

Table A9. 11: Di-n-butyl phthalate: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	2800	prot	7000
alg	770 ^a	alg	400
alg	6100	alg	4200 ^c
crus	880 ^b	crus	3900 ^d
pisc	100	crus	2100
pisc	560	ins	2500 ^e
		pisc	6300
		pisc	2200
		pisc	1500 ^f
		pisc	2200 ^g
		pisc	350
		pisc	1400 ^h

All data originate from Appendix 2 in Van Wezel et al. (1999b).

- a: geometric mean of 0.21 and 2.8 mg/l for *Pseudokirchneriella subspicata*
b: geometric mean of 0.96, 1.1, 1.0, and 0.56 mg/l for *Daphnia magna*
c: geometric mean of 9.0 and 2.0 mg/l for *Scenedesmus subspicatus*
d: geometric mean of 3.7, 3.0, and 5.2 mg/l for *Daphnia magna*
e: geometric mean of 5.4, 4.0, and 0.76 mg/l for *Chironomus plumosus* (3rd – 4th instar)
f: geometric mean of 0.73, 2.1, 1.6, 2.1, and 1.6 mg/l for *Lepomis macrochirus*
g: geometric mean of 6.5, 2.6, 1.5, 1.4, and 1.6 mg/l for *Oncorhynchus mykiss*
h: geometric mean of 1.3, 4.0, 2.0, and 1.5 mg/l for *Pimephales promelas*

Table A9. 12: Di-n-butyl phthalate: selected data for marine water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
alg	280	bact	16000 ^a
		alg	53 ^b
		crus	8000
		crus	500
		crus	1700
		pisc	460 ^c

All data originate from Appendix 3 in Van Wezel et al. (1999b).

- a: geometric mean of 11 and 23 mg/l for *Vibrio fischeri*
b: geometric mean of 3.4, 20, 200, and 600 $\mu\text{g/l}$ for *Gymnodinium breve*
c: most sensitive life stage (yolk-sac fry) for *Ictalurus punctatus*

Table A9. 13: Butyl benzyl phthalate: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	290 ^a	alg	1000
		alg	600
		alg	290 ^b
		alg	600
		crus	1700 ^c
		pisc	1700 ^d
		pisc	1600 ^e
		pisc	2600 ^f

All data are taken from the annex to this report.

- a: geometric mean of 350, 260, 280, and 260 $\mu\text{g/l}$ for *Daphnia magna* (parameter reproduction)
b: geometric mean of 400 and 210 $\mu\text{g/l}$ for *Pseudokirchneriella subspicata*
c: geometric mean of 0.82 and 3.7 mg/l for *Daphnia magna*

- d: two studies for *Lepomis macrochirus*
 e: geometric mean of 0.82 and 3.3 mg/l for *Oncorhynchus mykiss*
 f: geometric mean of 1.5, 2.1 and 5.3 mg/l for *Pimephales promelas*

Table A9. 14: *Butyl benzyl phthalate: selected data for marine water.*

taxonomic group	L(E)C50 [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
crus	900	pisc	3000
pisc	510	pisc	600 ^a

All data are taken from the annex to this report.

- a: geometric mean of 550 and 660 $\mu\text{g/l}$ for *Parophrys vetulus*

Table A9. 15: *Dihexyl phthalate: selected data for fresh water.*

taxonomic group	NOEC [$\mu\text{g/l}$]		
crus	84		

All data are taken from the annex to this report.

Table A9. 16: *Diethylhexyl phthalate: selected data for species exposed via sediment.*

taxonomic group	NOEC [mg/kg]		
amph	10		

All data originate from Appendix 4 in Van Wezel et al. (1999b).

Table A9. 17: *Diethylhexyl phthalate: selected data for fresh water.*

taxonomic group	NOEC [$\mu\text{g/l}$]		
pisc	5		

All data originate from Appendix 2 in Van Wezel et al. (1999b).

Table A9. 18: *Cyclohexanone: selected data for fresh water.*

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	180000	alg	33000
cyan	52000	crus	800000
prot	570000	pisc	630000 ^a
prot	550000	pisc	580000 ^b
prot	280000		
alg	370000		

All data are taken from the annex to this report.

- a: geometric mean of 536 and 752 $\mu\text{g/l}$ for *Leuciscus idus melanotus*

- b: geometric mean of 527 and 634 $\mu\text{g/l}$ for *Pimephales promelas*

Table A9. 19: *Cyclohexanone: selected data for marine water.*

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
bact	110000		

All data are taken from the annex to this report.

Table A9. 20: Cyclohexanone: selected QSAR data.

taxonomic group	NOEC [mg/l]	taxonomic group	NOEC [mg/l]
bact	11000	moll	160
bact	280	crus	170
bact	750	crus	280
bact	830	ins	560
alg	970	ins	210
alg	770	pisc	87
alg	300	amph	240
fung	10000	amph	440
prot	1200	amph	300
coel	180		

Table A9. 21: Pyridine: selected data for terrestrial species.

taxonomic group	NOEC [mg/kg]	taxonomic group	L(E)C50 [mg/kg]
mac	50	mac	1000

All data are taken from the annex to this report.

Table A9. 22: Pyridine: selected data for fresh water.

taxonomic group	NOEC [μ g/l]	taxonomic group	L(E)C50 [μ g/l]
bact	340000	ins	230000
cyan	28000	ins	170000
prot	3900	ins	30000
prot	3500	ins	410000
prot	180000	ins	250000
alg	150000	coel	1200000
alg	280000	ann	1900000
alg	120000	ann	2400000
alg	50000	ann	1300000
		moll	350000
		crus	220000
		crus	2500000
		crus	780000 ^a
		crus	580000
		crus	180000
		pisc	94000
		amph	950000
		amph	1400000

All data are taken from the annex to this report.

a: geometric mean 240, 520, 1165, 1755, and 1130 mg/l for *Daphnia magna*

Table A9. 23: Pyridine: selected data for marine water.

taxonomic group	L(E)C50 [μ g/l]	taxonomic group	L(E)C50 [μ g/l]
bact	3300000	crus	1300000

All data are taken from the annex to this report.

Table A9. 24: Tetrahydrofuran: selected data for fresh water.

taxonomic group	NOEC [$\mu\text{g/l}$]	taxonomic group	L(E)C50 [$\mu\text{g/l}$]
bact	580000	crus	5900000
cyan	230000	pisc	2900000 ^a
prot	2900000	pisc	2200000
prot	860000		
alg	3700000		
pisc	220000		

All data are taken from the annex to this report.

a: geometric mean of 2820 and 2930 mg/l for *Leuciscus idus melanotus*

Table A9. 25: Tetrahydrofuran: selected data for marine water.

taxonomic group	L(E)C50 [$\mu\text{g/l}$]		
bact	910000		

All data are taken from the annex to this report.

Table A9. 26: Tetrahydrofuran: selected QSAR data.

taxonomic group	NOEC [mg/l]	taxonomic group	NOEC [mg/l]
bact	15000	moll	240
bact	340	crus	220
bact	910	crus	470
bact	1000	ins	970
alg	1300	ins	300
alg	1100	pisc	130
alg	480	amph	360
fung	14000	amph	750
prot	1600	amph	440
coel	250		

Table A9. 27: Tetrahydrothiophene: selected QSAR data.

taxonomic group	NOEC [mg/l]	taxonomic group	NOEC [mg/l]
bact	2200	moll	30
bact	77	crus	35
bact	210	crus	37
bact	210	ins	68
alg	230	ins	38
alg	140	pisc	16
alg	42	amph	44
fung	2200	amph	53
prot	240	amph	51
coel	32		