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INTEGRATED ENVIRONMENTAL QUALITY OBJECTIVES FOR POLYCYCLIC AROMATIC HYDROCARBONS (PAHs)

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SUMMARY

In the present report Maximum Permissible Concentrations (MPCs) are derived for 10 Polycyclic Aromatic Hydrocarbons (PAHs). The currently used MPCs presented in 'Desire for levels' (Van de Meent *et al.*, 1990) are derived from scarce laboratory studies and estimated values from 'Quantitative Structure Activity Relationships' (QSARs).

The 'new' MPCs for the considered PAHs, based on old and recent data, are derived as follows:

Aquatic environment

For the aquatic environment MPCs are derived from the available experimental data. A comparison is made of the experimental NOECs with the NOECs estimated with the QSAR-approach (Van Leeuwen *et al.*, 1992). For anthracene and benzo[*k*]fluoranthene it is concluded that the QSAR-NOECs are not comparable with the experimental NOECs. Therefore, these two PAHs can not be divided in class I (compounds with a narcotic mode of action). Apparently there is an unknown, more specific mode of action which results in higher toxicity than expected from the QSARs. For the other PAHs in the comparison it is not clear whether they do or do not act by narcosis, because there is a tendency that the experimental NOECs are lower than the QSAR estimated NOECs. Therefore, it is decided that the MPCs for the aquatic environment are calculated using the experimental data available. For 7 out of 10 PAHs (naphthalene, anthracene, phenanthrene, fluoranthene, benzo[*a*]anthracene, benzo[*k*]fluoranthene en benzo[*a*]pyrene) this results in a MPC for the aquatic environment.

For chrysene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene no experimental data are available. The MPCs for chrysene and benzo[*ghi*]perylene are calculated using the QSAR-approach (Van Leeuwen *et al.*, 1992). Because of the uncertainties in the mode of action of the selected PAHs it is decided to correct the MPCs calculated from the QSAR-NOECs, with a factor 10. For indeno[*1,2,3-cd*]pyrene the QSAR-approach (Van Leeuwen *et al.*, 1992) can not be applied because all QSAR-NOECs are estimated above 10 times the maximum water solubility. The MPC presented in 'Desire for levels' (Van de Meent *et al.*, 1990) is maintained for this PAH.

Soil/sediment

For soil and sediment the MPCs are derived from the available experimental data. This resulted in only 3 MPCs for soil for anthracene, benzo[*a*]anthracene and benzo[*a*]pyrene. Almost no experimental data are available for sediment. The three MPCs for soil are harmonized with the MPCs for the aquatic environment, using the equilibrium

partitioning method. The remaining MPCs (7 for soil (naphthalene, phenanthrene, fluoranthene, chrysene, benzo[*k*]fluoranthene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene) and 10 for sediment (naphthalene, anthracene, phenanthrene, fluoranthene, chrysene, benzo[*a*]anthracene, benzo[*k*]fluoranthene, benzo[*a*]pyrene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene) are calculated from the MPC_{water} also using the equilibrium partitioning method.

All the 'new' MPCs for the aquatic environment, based on experimental data, are lower than the MPCs presented in 'Desire for levels' (Van de Meent *et al.*, 1990). Six of the 'new' MPCs for soil (naphthalene, anthracene, phenanthrene, benzo[*a*]anthracene, benzo[*k*]fluoranthene and benzo[*a*]pyrene), are lower than the MPCs presented in 'Desire for levels' (Van de Meent *et al.*, 1990). The MPCs for fluoranthene, chrysene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene are higher. For sediment the 'new' MPCs for naphthalene, anthracene, phenanthrene, benzo[*a*]anthracene and benzo[*k*]fluoranthene, are lower than the MPCs presented in 'Desire for levels' (Van de Meent *et al.*, 1990). The MPCs for fluoranthene, chrysene, benzo[*a*]pyrene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene for sediment are higher.

It is known that PAHs can have carcinogenic and mutagenic properties. However, no method is available to incorporate these effects into the currently applied methods.

If the MPCs and NCs (negligible concentration) are compared with the natural background concentrations it is concluded that in a number of cases the NCs for soil, sediment and water and in one case the MPC for water is/are exceeded by the natural background concentration(s).

Because not all the PAHs considered have the same mode of action, it is at this moment not possible to derive a scientifically underpinned risk limit for the mixture of the 10 PAHs.

A coherence test, for harmonisation of risk limits for air, water and soil, for benzo[*a*]pyrene indicates that maintaining the concentration at the MPC_{air} level of 1 ng/m^3 will result in concentrations in soil and water that are far below the MPCs proposed.

In the following table the values are presented which can be used to set environmental quality objectives (limit and target values).

Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs). The values for water are in µg/l; the values for soil are in mg/kg (derived for standard soil containing 25% clay and 10% organic matter).

Compound	MPC (water) (µg/l)	NC (water) (µg/l)	MPC (soil) (mg/kg)	NC (soil) (mg/kg)	MPC (sediment) (mg/kg)	NC (sediment) (mg/kg)
Naphthalene	1.2 (EPA/100)	0.012	0.14 (EP)	0.0014	0.14 (EP)	0.0014
Anthracene	0.07 (EPA/100)	0.0007	0.12 (EP)	0.0012	0.12 (EP)	0.0012
Phenanthrene	0.30 (EPA/100)	0.0030	0.51 (EP)	0.0051	0.51 (EP)	0.0051
Fluoranthene	0.30 (EPA/1000)	0.0030	2.6 (EP)	0.026	2.6 (EP)	0.026
Benzo[*a*]anthracene	0.01 (EPA/1000)	0.0001	0.25 (EPA/10)	0.0025	0.36 (EP)	0.0036
Chrysene	0.34 (QSAR/A&S/10)	0.0034	10.7 (EP)	0.107	10.7 (EP)	0.107
Benzo[*k*]fluoranthene	0.04 (EPA/10)	0.0004	2.4 (EP)	0.024	2.4 (EP)	0.024
Benzo[*a*]pyrene	0.05 (EPA/100)	0.0005	0.26 (EPA/10)	0.0026	2.7 (EP)	0.027
Benzo[*ghi*]perylene	0.03 (QSAR/A&S/10)	0.0003	7.5 (EP)	0.075	7.5 (EP)	0.075
Indeno[*1,2,3-cd*]pyrene	0.04[a] (EPA/10)	0.0004	5.9 (EP)	0.059	5.9 (EP)	0.059

The extrapolation method used is placed between parenthesis

a value from 'Desire for levels' (Van de Meent *et al.*, 1990)

SAMENVATTING

In dit rapport zijn Maximaal Toelaatbare Risiconiveau's (MTR's) voor 10 Polycyclische Aromatische Koolwaterstoffen (PAK's) afgeleid. De huidige MTR's gepresenteerd in het rapport 'Streven naar waarden' (Van de Meent *et al.*, 1990) zijn gebaseerd op schaarse experimentele gegevens en 'No Observed Effect Concentrations' (NOEC's) geschat met behulp van 'Quantitative Structure Activity Relationships' (QSAR's).

De 'nieuwe' MTR's, gebaseerd op recente en oude gegevens, zijn op de volgende wijze afgeleid:

Aquatisch milieu

Voor het aquatisch milieu zijn MTR's afgeleid uit de beschikbare experimentele gegevens. Vervolgens zijn de experimentele NOEC's vergeleken met de NOEC's geschat met behulp van de QSAR-methode beschreven in Van Leeuwen *et al.* (1992). Voor anthraceen en benzo[*k*]fluorantheen blijkt uit de vergelijking van experimentele NOEC's en QSAR-NOEC's, dat deze twee PAK's niet ingedeeld kunnen worden in klasse I (stoffen met narcotiserende werking). Er is bij deze PAK's sprake van een onbekend, specifiek werkingsmechanisme hetgeen een hogere toxiciteit oplevert dan verwacht volgens de QSAR's. Voor de andere PAK's in de vergelijking is niet duidelijk of ze wel of niet een narcotiserende werking hebben, omdat er een tendens is dat de experimentele NOEC's lager zijn dan de QSAR-NOEC's. Er is daarom besloten de uiteindelijke MTR's te baseren op de beschikbare experimentele toxiciteitsgegevens. Voor 7 van de 10 PAK's (naphthaleen, anthraceen, phenanthreen, fluorantheen, benzo[*a*]anthraceen, benzo[*k*]fluorantheen en benzo[*a*]pyreen) resulteert dit in een MTR voor het aquatische milieu.

Voor de overige 3 PAK's (chryseen, benzo[*ghi*]peryleen en indeno[*1,2,3-cd*]pyreen) zijn geen experimentele gegevens beschikbaar. De MTR's voor chryseen en benzo[*ghi*] peryleen zijn berekend met behulp van de QSAR-methode (Van Leeuwen *et al.*, 1992). Omdat het niet duidelijk was uit de gemaakte vergelijking of PAK's narcotiserend werken, is besloten de MTR's voor deze PAK's te corrigeren met een extra factor 10. Voor indeno[*1,2,3-cd*]pyreen is de indicatieve MTR uit 'Streven naar waarden' (Van de Meent *et al.*, 1990) overgenomen, omdat de QSAR's uit Van Leeuwen *et al.* (1992) alle NOEC's meer dan 10 maal boven de maximale wateroplosbaarheid schat.

Bodem/sediment

Voor bodem en sediment zijn, indien mogelijk, MTR's afgeleid met behulp van de beschikbare experimentele gegevens. Doordat experimentele gegevens erg schaars zijn, is

het voor slechts 3 PAK's (anthraceen, benzo[*a*]anthraceen en benzo[*a*]pyreen) mogelijk MTR's af te leiden voor de bodem. Vervolgens zijn deze MTR's voor bodem afgestemd met die voor water met behulp van de evenwichtspartitie-methode. Voor de overige PAK's, 7 voor bodem (naphthaleen, phenanthreen, fluorantheen, chryseen, benzo[*k*]fluorantheen, benzo[*ghi*]peryleen en indeno[*1,2,3-cd*]pyreen) en 10 voor sediment (naphthaleen, anthraceen, phenanthreen, fluorantheen, chryseen, benzo[*a*]anthraceen, benzo[*a*]pyreen benzo[*k*]fluorantheen, benzo[*ghi*]peryleen en indeno[*1,2,3-cd*]pyreen) zijn MTR's afgeleid met behulp van de evenwichtspartitie-methode, waarbij de MTR's voor bodem en sediment worden berekend uit de MTR's voor het aquatische milieu.

De 'nieuwe' MTR's voor het aquatische milieu voor naphthaleen, anthraceen, phenanthreen, fluorantheen, benzo[*a*]anthraceen, benzo[*k*]fluorantheen en benzo[*a*]pyreen, gebaseerd op experimentele gegevens, zijn allemaal lager dan de waarden gepresenteerd in 'Streven naar waarden'. Zes van de 'nieuwe' MTR's voor bodem (naphthaleen, anthraceen, phenanthreen, benzo[*a*]anthraceen en benzo[*k*]fluorantheen en benzo[*a*]pyreen zijn lager dan de MTR's uit 'Streven naar waarden' (Van de Meent *et al.*, 1990). De MTR-waarden voor fluorantheen, chryseen, benzo[*ghi*]peryleen en indeno[*1,2,3-cd*]pyreen) zijn hoger. De helft van de 'nieuwe' MTR's voor sediment (naphthaleen, anthraceen, phenanthreen, benzo[*a*]anthraceen en benzo[*k*]fluorantheen) zijn lager dan de MTR's uit 'Streven naar waarden'. De MTR-waarden voor fluorantheen, chryseen, benzo[*a*]pyreen, indeno[*1,2,3-cd*]pyreen en benzo[*ghi*]peryleen zijn hoger.

Het is bekend dat PAK's in potentie carcinogeen en mutageen zijn. Er is op dit moment echter geen methodiek beschikbaar waarmee dit soort effecten in het afleiden van MTR's meegenomen kunnen worden.

Indien de MTR's en VR's (verwaarloosbaar risico) worden vergeleken met de natuurlijke achtergrond concentraties, blijkt dat in een aantal gevallen de VR's voor bodem, sediment en water en in één geval de aquatische MTR wordt overschreden door de natuurlijke achtergrondconcentratie.

Omdat niet alle PAK's hetzelfde werkingsmechanisme hebben is het op dit moment niet mogelijk een wetenschappelijk onderbouwde somnorm voor de 10 PAK's te berekenen.

Een coherentie test voor benzo[*a*]pyreen, voor harmonisatie van risikogrenzen voor lucht, water en bodem, laat zien dat het handhaven van de MTR_{lucht} (1 ng/m^3) leidt tot concentraties in bodem en water die veel lager zijn dan de in dit rapport voorgestelde MTR's.

In de bijgevoegde tabel zijn de waarden gepresenteerd die gebruikt kunnen worden voor het opstellen van grens- en streefwaarden.

Maximaal Toelaatbare Risico's (MTR's) en Verwaarloosbare Risiconiveau's (VR's). De waarden voor water zijn weergegeven in µg/l; de waarden voor bodem en sediment zijn weergegeven in mg/kg (voor standaard bodem met 25% klei en 10% organisch stof).

Stof	MTR (water) (µg/l)	VR (water) (µg/l)	MTR (bodem) (mg/kg)	VR (bodem) (mg/kg)	MTR (sediment) (mg/kg)	VR (sediment) (mg/kg)
Naphthaleen	1.2 (EPA/100)	0.012	0.14 (EP)	0.0014	0.14 (EP)	0.0014
Anthraceen	0.07 (EPA/100)	0.0007	0.12 (EP)	0.0012	0.12 (EP)	0.0012
Phenanthreen	0.30 (EPA/100)	0.0030	0.51 (EP)	0.0051	0.51 (EP)	0.0051
Fluorantheen	0.30 (EPA/1000)	0.0030	2.6 (EP)	0.026	2.6 (EP)	0.026
Benzo[*a*]anthraceen	0.01 (EPA/1000)	0.0001	0.25 (EPA/10)	0.0025	0.36 (EP)	0.0036
Chryseen	0.34 (QSAR/A&S/10)	0.0034	10.7 (EP)	0.107	10.7 (EP)	0.107
Benzo[*k*]fluorantheen	0.04 (EPA/10)	0.0004	2.4 (EP)	0.024	2.4 (EP)	0.024
Benzo[*a*]pyreen	0.05 (EPA/100)	0.0005	0.26 (EPA/10)	0.0026	2.7 (EP)	0.027
Benzo[*ghi*]peryleen	0.03 (QSAR/A&S/10)	0.0003	7.5 (EP)	0.075	7.5 (EP)	0.075
Indeno[*1,2,3-cd*]pyreen	0.04[a] (EPA/10)	0.0004	5.9 (EP)	0.059	5.9 (EP)	0.059

De gebruikte extrapolatie methode staat tussen haakjes

a waarden uit 'Streven naar waarden' (Van de Meent *et al.*, 1990)

1 INTRODUCTION

The project 'Setting integrated environmental quality objectives' started in 1989. The aim of the project is to derive environmental quality objectives for water, soil and sediment. The risk philosophy of VROM[1] (VROM, 1989) is used as the starting point. The derivation of the environmental quality objectives (limit and target values) is the responsibility of the ministry of VROM. These environmental quality objectives are based on Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs). The derivation of these risk limits is the part of the project that is performed at the RIVM[2]. MPCs are scientifically-based risk limits, no economical considerations or technical feasibility has been taken into account.

The methodology used to derive the MPCs and NCs is divided into two steps. In the first step MPCs for the mentioned compartments are derived. In the second step these MPCs are harmonized using the equilibrium partitioning method (Ep-method). MPCs are estimated using single-species toxicity data. The Negligible Concentration (NC) is set at 1% of the MPC. This percentage is established to take factors as multi chemical stress and uncertainties in risk assessment into account. The reason for harmonization is that the MPC or NC in one compartment may not lead to exceedance of the MPC or NC in one of the other compartments, due to transport of the chemical between the different compartments. A flow diagram of the different steps leading to environmental quality objectives is given in figure 1.1.

The methodology used for derivation of environmental quality objectives in this report has been presented in a number of reports published in the context of the project. The first part of the project (a), "MILBOWA"[3], resulted in the report 'Desire for levels' (Van de Meent *et al.*, 1990). In this report a methodology was proposed for deriving MPCs for several heavy metals, chlorophenols, pesticides and polycyclic aromatic hydrocarbons (PAHs). In the second part of the project (b) MPCs were derived in the sub-projects, 'trace metals'(b-1) (Van de Plassche *et al.*, 1992), 'volatile compounds'(b-2) (Van de Plassche *et al.*, 1993) and 'secondary poisoning'(b-3) (Van de Plassche, 1994).

In the present report the risk limits for the "MILBOWA" PAHs are updated. This update for PAHs is necessary because the MPCs and NCs presented in 'Desire for levels' (Van

[1] Abbreviation in Dutch for 'Ministry of Housing, Spatial Planning and the Environment'.

[2] Abbreviation in Dutch for 'National Institute of Public Health and Environment'.

[3] Abbreviation in Dutch for 'Environmental quality objectives for water and soil'.

de Meent *et al.*, 1990) are derived from scarce laboratory studies and estimated values from QSARs. Since 1989 new information on the toxicity of PAHs has become available (Hooftman, 1991; Hooftman and Evers-De Ruiter, 1992a, 1992b, 1992c and 1992d) and evaluations on the toxicity of PAHs have been performed (IPCS/EHC, in prep.). New knowledge and additional studies from 1989 to the present are taken into account to derive new risk limits for PAHs.

Although PAHs have a bioaccumulation potential, based on the high values of their n-octanol/water partition coefficient (K_{ow}), secondary poisoning is not taken into account. This decision is based on the results from literature studies performed by Neff (1979, 1985), Slooff *et al.* (1989) and Van Hattum (1995). The conclusion based on these papers is that some aquatic animals are able to accumulate PAHs, but most animals metabolise PAHs into more polar metabolites and excrete them rapidly. It is assumed and in some cases known that the metabolites formed are highly reactive, mutagenic and/or carcinogenic. However, limited information is available on this topic and it is not possible at this moment to incorporate effects as mutagenicity and carcinogenicity into the currently applied methods to derive MPCs.

Only for benzo[*a*]pyrene a risk limit for human exposure through air is available at this moment. A coherence test for benzo[*a*]pyrene will be performed using the model SIMPLE-BOX as described by Van de Plassche and Bockting (1993). For all the other PAHs critical air concentrations will be calculated according to Van de Meent (1995).

In summary, the following activities are carried out to derive the MPCs and NCs presented in this report:

a deriving MPCs for water, soil and sediment based on ecotoxicological data,
b collecting sediment-water and soil-pore water partition coefficients in order to apply the equilibrium partitioning method,
c harmonization of the MPCs and NCs for air, water, sediment and soil using the equilibrium partitioning method.

The methodology used to derive and harmonize MPCs is described in chapter 3. The MPCs based on experimental data are presented in chapter 4. In chapter 5 a comparison of experimental toxicity data with QSAR-estimated toxicity data is made. In chapter 6 the MPCs as presented in 'Desire for levels' (Van de Meent *et al.*, 1990), the MPCs based on the combined dataset containing experimental and QSAR data and a comparison of these MPCs with the MPCs derived in chapter 4 are presented. In chapter 7 the partition coefficients are presented and MPCs for soil and sediment are derived and harmonized. All the results are discussed in chapter 8, and finally, in chapter 9 the conclusions are presented.

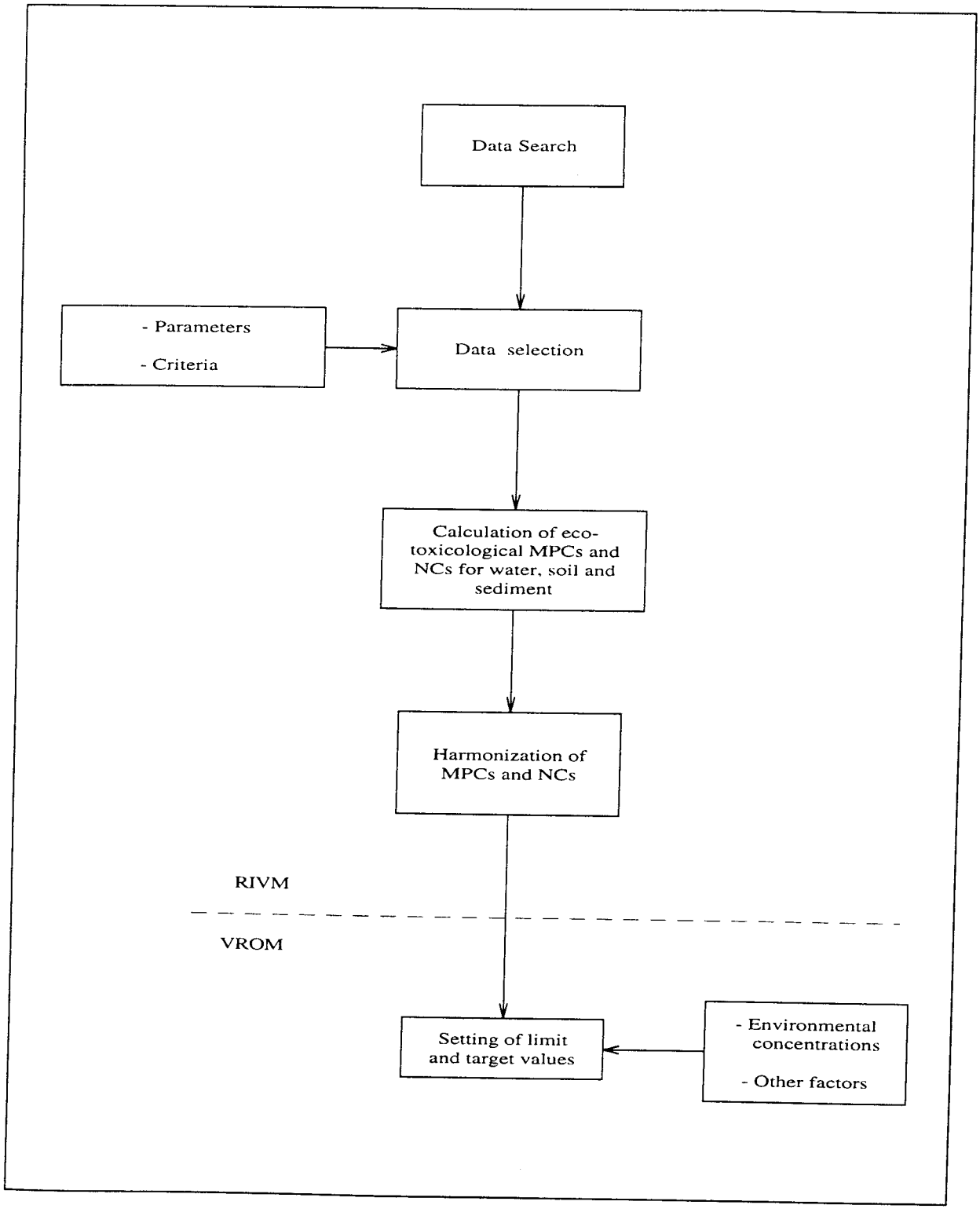


Figure 1.1 Schematic presentation of the process of setting environmental quality objectives

2 POLYCYCLIC AROMATIC HYDROCARBONS (PAHs)

The name "Polycyclic Aromatic Hydrocarbons" (PAHs) refers to a large class of organic compounds composed of two or more fused aromatic benzene rings, containing exclusively carbon and hydrogen. The main PAH pollution in the environment results from atmospheric deposition. Most PAHs are found in soil, sediment and water, which is caused by the low affinity of high molecular PAHs for air. In the atmosphere low-molecular PAHs are mainly in the gas phase and high-molecular PAHs are mainly bound to particles and aerosols. These aerosols loaded with PAHs will reach soil and water by means of wet and dry deposition, run off and direct emission (Slooff *et al.*, 1989). Because of the mutagenic and carcinogenic properties of especially PAH metabolites, PAHs have been of environmental concern since a long time.

PAHs are produced by natural processes and by human activities. Natural PAH-sources are the PAHs generated during 'natural' combustion processes like forest-fires and volcanic eruptions (Neff, 1979). Besides this PAHs are thought to be generated by organisms like plants and bacteria (literature recited in Neff, 1979 and Neff, 1985). The results of these studies are however considered contradictory (Neff, 1979; 1985). The concentrations of these natural occurring/generated PAHs are thought to be very low, in water ≤50 ng/l and in the soil ≤30 µg/kg (Geochem-Research, 1989; Slooff *et al.*, 1989).

The main sources for PAH pollution are thought to be a result of human activity. Examples are the processing of crude oil, coal and natural gas, aluminium, iron and steel production plants, heating (power plants and residual) and combustion of refuse. Other human activities like traffic and tobacco smoking also contribute to the increasing load of PAHs in the environment.

In chapter 2.1 the selected PAHs and their physical/chemical properties, molecular and structural formulas are presented. In chapter 2.2 the different modes of action for PAHs are discussed, as well as a number of processes in which metabolites and intermediates can be formed. In chapter 2.3 the carcinogenic and mutagenic effects of PAHs are discussed, and in chapter 2.4 the risks for humans are outlined. Finally in chapter 2.5 bioaccumulation in relation with secondary poisoning is discussed.

2.1 Selected PAHs

The PAHs selected for this report are the same as presented in the report 'Desire for levels' (Van de Meent *et al.*, 1990). These PAHs are naphthalene, anthracene, phenanthrene, fluoranthene, benzo[*a*]anthracene, chrysene, benzo[*k*]fluoranthene,

benzo[*a*]pyrene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene. The selection criteria are described in the RIVM report 'Integrated Criteria Document PAHs' (Slooff *et al.*, 1989).

2.1.1 Molecular and structural formulas

In table 2.1 the PAHs selected for this report are presented together with their molecular- and structural formulas and Chemical Abstracts Service registration number (CAS). PAHs are composed of carbon and hydrogen in the form of two or more aromatic benzene rings. Two aromatic rings are said to be fused when a pair of carbon atoms is shared. The resulting structure is a molecule with all the carbon and hydrogen atoms lying in a single plane. Naphthalene, consisting of two fused aromatic rings, is the smallest of the PAHs considered. Indeno[*1,2,3-cd*]pyrene, consisting of 6 fused aromatic rings, is the largest of the PAHs considered.

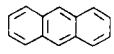
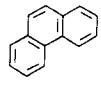
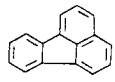
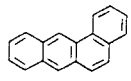
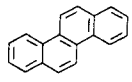
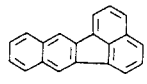
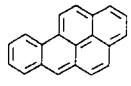
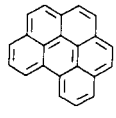
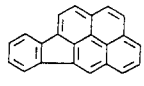
2.1.2 Physical/chemical properties

The PAHs considered can be divided into the low molecular and high molecular compounds. The cut-off point is a molecular weight of 228. Naphthalene, anthracene, phenanthrene, fluoranthene belong to the low molecular compounds and benzo[*a*]-anthracene, chrysene, benzo[*k*]fluoranthene, benzo[*a*]pyrene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene to the high molecular compounds.

PAHs are characterized by 'low to very low' water solubility and 'low to moderate' volatility. PAHs show a high affinity towards organic phases, the affinity for the water phase is low. The fraction of freely dissolved PAHs decreases rapidly with increasing hydrophobicity and with increasing concentrations of binding substrates. This is illustrated by the high partition- and sorption coefficients of PAHs for sediment and suspended matter (Slooff *et al.*, 1989).

In table 2.2 a number of physical/chemical properties for the selected PAHs are presented. (Selection criteria applied are described in the Quality Document ACT/KD/003 (ACT, 1994). The vapour pressure and Henry constant decrease with increasing molecular weight while log K_{ow} increases with increasing molecular weight. The calculated Henry constants (table 2.2) for the high molecular PAHs are lower than the measured values published in Ten Hulscher *et al.* (1992). However, the conclusion remains that high molecular PAHs are not expected to evaporate from water. The water solubility also decreases with increasing molecular weight. The water solubility of anthracene and benzo(*k*)fluoranthene are lower than expected from the range of water solubilities of the other PAHs. This deviating water solubility is reported in many publications (literature recited in Mackay *et al.*, 1992).

Table 2.1 Molecular formulas, CAS registration number and structural formulas of the selected PAHs

Name of PAH	Molecular formula	CAS registration number	Structural formula
Naphthalene	$C_{10}H_8$	91-20-3	
Anthracene	$C_{14}H_{10}$	120-12-7	
Phenanthrene	$C_{14}H_{10}$	85-01-8	
Fluoranthene	$C_{16}H_{10}$	206-44-0	
Benzo[*a*]anthracene	$C_{18}H_{12}$	56-55-3	
Chrysene	$C_{18}H_{12}$	218-01-9	
Benzo[*k*]fluoranthene	$C_{20}H_{12}$	207-08-9	
Benzo[*a*]pyrene	$C_{20}H_{12}$	50-32-8	
Benzo[*ghi*]perylene	$C_{22}H_{12}$	191-24-2	
Indeno[*1,2,3-cd*]pyrene	$C_{22}H_{12}$	193-39-5	

The half-lives of chemicals in the environment depend not only on the properties of the chemical itself, but also on the characteristics of the external environment. The factors which might influence the half-lives of chemicals are numerous. This makes it difficult to derive one reliable half-life for each compound. Because half-lives for PAHs found in the literature vary enormously, Mackay *et al.* (1992) proposed half-life classes for PAHs in the compartments water, soil and sediment. The average of these half-lives for soil are for naphthalene ± 2 months; anthracene and phenanthrene ± 8 months; fluoranthene, benzo[*a*] anthracene, chrysene, benzo[*k*]fluoranthene, benzo[*a*]pyrene ± 2 years; benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene > 2 years. These half-lives for soil will be used for calculation of critical air concentrations (see § 7.7).

Table 2.2 Physical/chemical properties

PAHs	Molecular* weight g/mol	Vapour* pressure (Pa) 25°C	Log** K_{ow} (star)	Log*** K_{ow} (ClogP)	Log**** K_{ow}	Water* solubility µg/l, 25°C	Henry***** constant 25°C
Naphthalene	128.2	10.4	3.30	3.32	3.32	31,000	$1.7*10^{-2}$
Anthracene	178.2	$1.0*10^{-3}$	4.45	4.49	4.57	45	$1.6*10^{-3}$
Phenanthrene	178.2	$2.0*10^{-2}$	4.46	4.49	4.67	1,100	$1.3*10^{-3}$
Fluoranthene	202.3	$1.2*10^{-3}$	5.16	4.95	5.22	260	$3.9*10^{-4}$
Benzo[*a*]anthracene	228.3	$2.8*10^{-5}$	5.79	5.66	5.90	11	$2.3*10^{-4}$
Chrysene	228.3	$5.7*10^{-7}$	5.73	5.66	5.79	8.8	$6.0*10^{-6}$
Benzo[*k*]fluoranthene	252.3	$5.2*10^{-8}$	6.00*	-	6.08	0.8	$6.6*10^{-6}$
Benzo[*a*]pyrene	252.3	$7.0*10^{-7}$	5.97	6.12	6.10	3.8	$1.9*10^{-5}$
Benzo[*ghi*]perylene	268.4	$2.6*10^{-9a}$	6.63	6.58	6.18	0.26	$1.1*10^{-6}$
Indeno[*1,2,3-cd*]pyrene	276[a]	$2.6*10^{-9a}$	6.4[a]	-	-	0.05[a]	$5.8*10^{-6}$

-	no data available
*	physical/chemical properties derived from Mackay *et al.* (1992)
**	star log K_{ow}-values derived from the MEDCHEM® database
***	estimated ClogP values from the MEDCHEM® database
****	'new' log K_{ow}-values (slow stirring method) from De Maagd and Sijm, 1995
*****	dimensionless Henry constant calculated according to Quality Document ACT/KD/003 (ACT,1994).
a	from (IPCS/EHC, in prep.)

The differences between the 'slow stirring' log K_{ow}-values and the star log K_{ow}-values from the MEDCHEM® database presented in table 2.2 are small. The star log K_{ow}-values derived from the MEDCHEM® database are used in this report for further calculations, because this database is considered the most reliable and complete source for deriving log K_{ow}-values. The water solubility from table 2.2 is used as a quality criterium for deriving data from toxicity studies (see §3.2.2).

2.2 Mode of action

Verhaar *et al.* (1992) classified pollutants into four classes; [1] inert chemicals, [2] less inert chemicals, [3] reactive chemicals and [4] specifically acting chemicals. Inert chemicals from class 1 are not reactive when considering overall acute effects, and do not interact with specific receptors in an organism. This type of toxicity is called baseline or minimum toxicity. In this case, in absence of all specific mechanisms of toxicity, the toxicity is determined by the chemical hydrofobicity (its log K_{ow}). The chemicals in class 2 and 3 react unselectively with certain chemical structures. The chemicals in class 4 are specifically acting chemicals that exhibit toxicity due to specific interaction with certain receptor molecules. These receptor molecules can be a wide variety of (bio)molecules such as hormones, enzymes and (poly)peptides etc. In some cases reactions with biomolecules can have other effects, for example the formation of DNA-adducts that can lead to cancer. The reaction with receptor molecules can be caused by parent compounds, metabolites or intermediates. In some cases these metabolites and/or intermediates exhibit higher reactivity and toxicity than the parent compounds.

PAHs are expected to have low acute toxicity. According to the theory of Verhaar *et al.* (1992) PAHs are divided into class 1 (baseline toxicity). From the literature however it is known that PAHs and PAH metabolites can act specifically. For example, 7,8-diol-epoxide, a metabolite of benzo[*a*]pyrene is known to have a higher carcinogenic capacity than its parent compound. For PAHs also other specific modes of actions are known for example; immunocompetence observed in *Mytilus edulis* when exposed to fluoranthene (Coles *et al.*, 1994).

There are many possible processes/routes in which reactive PAH metabolites and/or intermediates can be formed, that may be highly toxic, mutagenic or carcinogenic (Neff, 1985). For example, PAHs can be transformed, by light induced chemical (photo)oxidation or by biological transformation.

In this chapter an outline is given of processes in which metabolites and/or intermediates are formed. In chapter 2.2.1 the process of light induced photo-oxidation, and in chapter 2.2.2 the process of biotransformation is outlined.

2.2.1 Light induced photo-oxidation (Phototoxicity)

Many PAHs are known to absorb high quantities of UV-radiation (Oris *et al.*, 1984). They can be activated by various wavelengths in the UV-radiation spectra and by visible light (UV-A, 345-400 nm; UV-B, 285-345 nm; visible light, >400 nm) in aqueous, sediment

and soil media. This activation only takes place if the energy associated with the wavelength is equivalent to the difference between the energetic states of electrons in the organic molecule. In general photodynamic processes will only occur when light (visible or non visible) is absorbed. Mekenyan *et al.* (1994) developed a model which predicts phototoxicity of PAHs based on the energy stabilization of PAHs in the form of the HOMO-LUMO[4] gap. A list with the abilities of PAHs to absorb radiation is presented in table 2.3.

Table 2.3 Absorbance regions for the selected PAHs (According to Mekenyan et al., 1994)

	Absorbtion of UV-A	Absorbtion of UV-B	Absorbtion of Visible. light	Photo-induced Toxicity
Naphthalene	n	n	n	n
Anthracene	y	y	n	y
Phenanthrene	n	n	n	n
Fluoranthene	y	y	n	y
Benzo[*a*]anthracene	y	y	n	y
Chrysene	y	y	n	y
Benzo[*k*]fluoranthene	y	y	y	y
Benzo[*a*]pyrene	y	y	y	y
Benzo[*ghi*]perylene	y	y	n	y
Indeno[*1,2,3-cd*]pyrene	-	-	-	-

- no data available
y yes, absorption occurs
n no, absorption does not occur

One of the main processes which may cause phototoxicity of PAHs is as follows: PAHs absorb UV-radiation, electrons will be elevated to higher energy states and form the so called excited single state molecules. These excited single state molecules might react direct with other (bio)molecules. A second possibility is that the single state molecules can undergo a process called intersystem crossing. In this process single state molecules turn into triple state molecules, the latter being more persistent. A third possible mechanism was proposed by Landrum *et al.* (1987). They suggested that the formation of singlet oxygen was the most important mechanism. Phototoxicity can occur by one or a combination of the former mentioned processes; which of these proposed processes is the most important/likely cannot be judged at the moment.

[4] Highest Occupied Molecular Orbital - Lowest Unoccupied Molecular Orbital

Photoactivated PAH molecules may damage tissues directly or may induce redox cycling through formation of free oxygen radicals resulting in much greater toxicity under UV light. Bowling *et al.* (1983) and Newsted & Giesy (1987) stated that the photodynamic response is due to PAHs that have been assimilated by organisms rather than to phototoxic metabolites formed in the external environment. Phototoxicity of PAHs is tested in a wide range of species: for Crustacea (Holst & Giesy, 1989; Allred & Giesy, 1985; Foran *et al.*, 1991); Macrophyta (Ren *et al.*, 1994; Huang *et al.*, 1993); Pisces (Hall & Oris, 1991; Bowling *et al.*, 1983; Oris & Giesy, 1985); Algae (Gala & Giesy, 1992; Schoeny *et al.*, 1988; Cody *et al.*, 1984), Insecta (Oris *et al.*, 1984) and Oligochaete (Monson *et al.*, 1995). Newsted & Giesy (1987) stated that none of the PAHs used in their study showed phototoxicity towards *Daphnia magna* if the PAHs did not absorb UV-radiation.

Criteria have been established how to deal with literature concerning phototoxic effects (see chapter 3.2.3 Influence of light source used in toxicity tests).

2.2.2 Biotransformation of PAHs

The cytochrome P-450 Mixed Function Oxidase system (MFO system) has the capability to oxidize a wide range of chemicals. This MFO system is well developed in mammals, birds and many fish species (Walker, 1980; Varanasi *et al.*, 1986; Ahokas *et al.*, 1993). Large differences in biotransformation rates among and within invertebrate taxa exist (literature cited in Van Hattum, 1995). Biotransformation of lipophilic compounds like PAHs into more water soluble compounds is required before excretion from living organisms is possible. However, also reactive intermediates that are highly toxic, mutagenic and carcinogenic can be formed.

2.3 Carcinogenicity and mutagenicity

In the project 'Setting integrated environmental quality objectives' effects as carcinogenicity and mutagenicity are not taken into account. From several PAHs it is known that they have a carcinogenic potential. It is also known that many PAHs form metabolites which are more carcinogenic than the parent compound (for benzo[*a*]pyrene it is known that one of the metabolic products 7,8-diol-epoxide has a strong carcinogenic action). Not much information is available on the toxicity and/or carcinogenic action of the formed metabolites. It can be expected that the formation of the metabolites is species and substance dependent.

The transformation of PAHs into mutagenic and carcinogenic metabolites is caused by the

oxidative metabolism of PAHs in the MFO system. Metabolites are formed via highly electrophilic intermediate arena oxides. Some of the metabolites and intermediates can bind covalently to cellular macromolecules such as DNA, RNA and protein (Neff, 1985). It is thought that the formation of these PAH-DNA adducts are a necessary step in the carcinogenic action of these compounds (Dunn, 1991).

Benzo[*a*]pyrene could not be detected in fish by Varanasi and Stein (1991), because of extensive metabolism. However, the metabolites of benzo[*a*]pyrene (for example 7,8-diol-epoxide) were found in the fish. In this case the MFO system, responsible for detoxification, activates procarcinogenic PAHs into their ultimate reactive metabolites which may form DNA adducts (Van Schooten *et al.*, 1995). Significantly increased PAH-DNA adduct levels were observed in the liver of eel (*Anguilla*) from polluted sites in the Netherlands (Van der Oost *et al.*, 1994). Reichert *et al.* (1985) found metabolites of benzo[*a*]pyrene in tissues of *Rhepoxynius abronius* and *Eohaustorius washingtonianus*. In both species a quantifiable amount of the intermediates were covalently bound to the tissues macromolecules. Van Schooten *et al.* (1995) found significant increasing amounts of DNA adducts in earthworms (*Lumbricus terrestris*) with increasing exposure time, when exposed to PAHs in industrially contaminated soil. The same authors also found indications of DNA adducts in fish obtained from the field at PAH contaminated sites. Significant chromosome abberations where found in fresh- and saltwater fish with a LOEC of 0.1 µg/l for benzo[*a*]pyrene (recited in Slooff *et al.*, 1989).

From the above it can be expected that carcinogenic and mutagenic effects on the individual level may occur. What the effects on populations and ecosystems are is not clear. At the moment it is not possible to incorporate effects as mutagenicity and carcinogenicity into the currently applied methods.

2.4 Risks for humans

The risk of PAHs for humans has been evaluated in the framework of Intervention values (VROM, 1994) and Integrated criteria document for PAHs (Slooff *et al.*, 1989). Data on oral exposure of humans to PAHs are too restricted to form a sufficiant basis of a risk assessment for humans. The mode of action causing carcinogenicity and mutagenicity in higher animals is supposed to be the same in humans. Therefore, mutagenic and carcinogenic studies on higher animals are used for the risk assessment for humans (Vermeire *et al.*, 1991). One of the conclusions drawn in Slooff *et al.* (1989) is that PAH with 2 or 3 linear aromatic rings (naphthalene and anthracene) are not carcinogenic and that non-linear PAHs with three or more aromatic rings are supposed to be carcinogenic.

Carcinogenic PAHs
The few animal studies suitable for the risk assessment for humans concern only benzo[*a*]pyrene. An additional risk for cancer (one extra case of cancer per 10000 individuals exposed) for humans is calculated, from two mouse studies in which the mice are exposed to an oral intake of 2000-4000 ng B*a*P/kg body weight/day. Linear extrapolation is used to extrapolate this risk to total life span.

In Slooff *et al.* (1989) PAHs are classified by their relative carcinogenic potential compared to benzo[*a*]pyrene. In general this means that the carcinogenic potential of chrysene is equal (1.0) to the carcinogenic potential of B*a*P, for the other carcinogenic PAHs the potential is 0.1. The potential risk of a mixture of PAHs depends on the PAH composition and can be calculated only if the exact concentrations of the individual PAHs are available (Slooff *et al.*, 1989). This means that the risk is location dependent (Kramers and Van der Heijden, 1988). In Slooff *et al.* (1989) additivity of carcinogenic effects is assumed; the total risk is based on the sum of the carcinogenic potential with the available fractions of the individual PAHs in a mixture (recited in Vermeire *et al.*, 1991).

In Vermeire (1993) an MPC for human risk is calculated for a contaminated industrial site with a high fraction of chrysene and benzo[*a*]pyrene. The $MPC_{human\ risk}$ is 6.3 µg PAHs /kg body weight/day, for this specific situation.

2.5 Bioaccumulation in relation with secondary poisoning

Due to the high log K_{ow}-values PAHs are thought to have a potential for bioaccumulation. From the literature however, it is not clear what the exact importance of this process is in natural ecosystems. Some species accumulate PAHs and there is also information that other species are able to excrete and metabolize (biotransformation see § 3.2.2) PAHs. The excretion and metabolism is species dependent and depends strongly on the activity/availability of the MFO (Mixed Function Oxidase) system. A short overview of the results on bioaccumulation and metabolism is given below.

Van Hattum (1995) found a linear relationship between log K_{ow} and the log BCF (Bioconcentration factor) for *Asellus aquaticus*: the BCF increased with the molecular weight and K_{ow}. The BCF-values found are relatively high, leading to the conclusion that the role of metabolism (biotransformation) of PAHs for freshwater isopods seems to be limited. Curto Pons *et al.* (1993) also found that PAHs accumulate in freshwater isopods. A literature study carried out by Van Hattum (1995) shows that many invertebrate species (Crustacea, Insecta) have a potential for bioaccumulating individual PAHs, with BCF-values ranging from 40-40000 for anthracene; from 4000-25000 for phenanthrene; from

200-80000 for benzo[*a*]pyrene; from 6300-160000 for pyrene and 63000 for benzo[*a*] anthracene. For terrestrial isopods Van Brummelen *et al.* (1991) observed low bioaccumulation in field and laboratory studies.

Relatively low levels of PAH accumulation were found for vertebrates (fish, mammals and birds) due to MFO mediated biotransformation (Farrington, 1991). Ariese *et al.* (1993) found hydroxylated metabolites in the excretion products of fish. A clear biotransformation of benzo[*a*]pyrene and anthracene was observed in *Chironomus riparius* (Gerould *et al.*, 1983), whereas biotransformation was absent in the amphipod *Diporeia* spp. (Landrum, 1988) and in the oligochaete *Stylodrilus heringianus* (Frank *et al.*, 1986). Neff (1979) found that polar metabolites are excreted to water rapidly, some metabolites however, tend to be excreted more slowly to water than the parent compound (Neff, 1979; Slooff *et al.*, 1989). Slooff *et al.* (1989) concluded that the BCFs for fish and shellfish, found in experimental studies are lower than estimated values due to the relatively high rates of metabolism and excretion. De Maagd and Sijm (1995) found that benzo[*a*]pyrene, fluoranthene and benzo[*a*]anthracene were metabolized in fish, but that this was not the case for naphthalene, anthracene and phenanthrene in the same fish species (*Pimephales promelas, Poecilia reticulata* and *Brachydanio rerio*).

PAHs tend to accumulate in some species (mainly invertebrates). No data are available on accumulation in species higher in the foodchain like birds and mammals. Because it is well known that fish, birds and mammals have MFO enzyme systems which enable them to metabolize PAHs and excrete the metabolites, no special attention is paid to secondary poisoning in this report. However, the presence of the metabolites before excretion may cause other effects, which are still unclear (see also § 2.3, carcinogenicity/mutagenicity).

3 METHODOLOGY

The methodology used to derive and harmonize Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for water, sediment and soil is described in this chapter. To derive MPCs for the different compartments, toxicity data have to be searched for and evaluated. Methods for literature search and derivation of data from toxicity studies are described in chapter 3.1 and 3.2. Depending on the amount of acute and chronic toxicity data a preliminary or refined effect assessment is used to derive the MPC for the different compartments. The extrapolation methods are described in chapter 3.4. The estimation of aquatic NOECs using QSARs is described in chapter 3.5. If there are not enough toxicity data on terrestrial and sediment species the MPC for soil and sediment is estimated using aquatic toxicity data with the equilibrium partition (Ep-method; described in chapter 3.6). The Ep-method is also used to harmonize the MPCs and NCs (water and soil) based on experimental data. To be able to use the Ep-method, partition coefficients are derived from the literature (described in chapter 3.3).

3.1 Literature search

The toxicity data on single species, the soil-pore water and sediment-water partition coefficients are derived from internal and external 'Toxicology Advisory Centre' (ACT) sources. All the online research is carried out according to Quality Document ACT/KD/001 (ACT, 1994).

3.1.1 Internal ACT literature sources

The internal literature sources are:

- the documentation ('grey' literature) present at the Toxicology Advisory Centre,
- the library of the Toxicology Advisory Centre,
- cardbox literature database which contains references of articles from public literature, that have been collected and evaluated, at the Toxicology Advisory Centre, in the context of the projects 'Setting integrated environmental quality objectives' and 'Intervention values' (VROM, 1994).

3.1.2 External ACT literature sources

The external literature sources are:

- the library of the National Institute of Public Health and the Environment,
- online search in the bibliographic databases Biosis, Toxline. The online searching scheme for toxicity data and partitioning coefficients is presented in appendix 1,
- retrospective literature search using public literature and reviews as a basis.

3.2 Deriving data from toxicity studies

All the studies found are evaluated to derive NOEC and L(E)C50s for single species and microbe mediated processes. The stepwise approach used to derive these NOECs and L(E)C50s is outlined in this chapter.

3.2.1 Relevant toxicity parameters

Only toxicological criteria which may affect the species at the population level are taken into account. In general these are survival, growth and reproduction. For terrestrial studies processes as enzyme activity and microbial processes are also taken into account. Toxicity is commonly expressed as a L(E)C50 (short-term tests, duration four days or less) or NOEC (long-term, duration more than four days, with the exception of micro-organisms and algae for which a NOEC may be derived from experiments during less than four days) (Slooff, 1992).

Sometimes also other parameters are taken into account, such as behaviour of the organism. This is the case when the parameter in question is considered ecological relevant, e.g. immobility in tests with Crustaceans. Mutagenicity and carcinogenicity are not taken into account, because at this moment it is not possible to incorporate these effects in the extrapolations.

3.2.2 Quality criteria applied

A study is considered to be reliable if the design of the experiment is in agreement with international accepted guidelines such as the OECD guidelines. To judge studies which have not been performed according to these guidelines, criteria are developed at the Toxicology Advisory Centre. A summary is shown in this section, for an extensive description it is referred to the Quality Document used at the Toxicology Advisory Centre ACT/KD/003 (ACT, 1994).

- For aquatic and terrestrial studies the purity of the test substance has to be at least 80%.

- If test concentrations are analyzed, results are expressed on the basis of the measured concentrations.
- Studies with test organisms collected from polluted sites are not included.
- For aquatic studies results up to 10 times above the water solubility are considered to be acceptable. Results more than 10 times above the water solubility are not included.
- Deviating from the OECD guidelines, a maximum of 1 ml/l organic solvent is accepted for aquatic studies. Tests in which a solvent is applied have to include both solvent and test medium controls. Exceedance of the 0.1 ml/l recommended by the OECD, is reported in the footnotes of the toxicity tables.
- If in terrestrial studies a solvent is used and the test organisms are transferred to the test soil without evaporation of the solvent, the soil is not allowed to contain more than 100 mg/kg solvent. If the organisms are transferred to the test medium after evaporation, the amount of solvent used may be higher, up to 1000 mg/kg. Exceedance of the 100 mg/kg is reported in the footnotes of the toxicity tables.
- The route of exposure used for the test species in the experiment has to be in agreement with the natural route of exposure of the species considered.
- Usually the recovery of compounds has to be at least 80% for aquatic studies. Deviating from the criteria established in ACT/KD/003 (ACT, 1994) studies are used, for the 2- and 3 ring PAHs, in which less than 80% recovery is found. The measured recovery is placed in the footnotes of the toxicity tables.
- In some studies a LT50 (50% lethal time) is calculated. In general these studies are not used. Because for some PAHs not much data are available the LT50 studies are incorporated in the toxicity tables for deviating tests as an indicative value.

3.2.3 Influence of light sources used in toxicity tests

Most toxicity studies found in the literature are performed under standard laboratory conditions. In these studies animals are exposed to light regimes of 12h:12h or 16h:8h light/dark and light sources like bulbs or fluorescent lamps. It was found that PAHs showed light-induced photo oxidation (phototoxicity) when exposed to different sources of light (see chapter 2.1). It is therefore likely that phototoxicity of PAHs will occur in natural ecosystems also. This idea is supported by Landrum *et al.* (1987), who measured UV-B intensities in eutrophic surface water. In this study they found that 50% of the initial UV-B radiation was still present at a depth of 1.2 meters. Contradicting results are found in Dutch eutrophic surface water, where algae and humic substances absorb most of the UV radiation (Van Liere, *pers. comm.*; RIVM/LWD). Although it remains unclear to what extent UV radiation might penetrate into the water surface, it is very important that

the light sources used in toxicity tests are comparable to natural situations, with respect to wavelength and intensity.

Light sources as bulbs, halogen- and fluorescent lamps produce mainly UV-A and visible light and almost no UV-B. None of the mentioned commonly used artificial light sources will produce as much UV-A+B radiation as sunlight (Eggink, *pers. comm.*; RIVM/LSO). Therefore, light comparable with sunlight is only expected in studies where researchers have been paying extra attention to the light conditions in their toxicity test.

In a number of publications tests are performed in which field illumination is simulated (Hall & Oris, 1991; Holst & Giesy, 1989; Huang *et al.*, 1993). However, in most tests the specific illumination/spectrum is not specified. Therefore the following selection criteria have been established:

- Light regime used in the test should be comparable with natural situation as much as possible (see also 3.2.2). (12h:12h or 16h:8h light/dark, and clear-, half clouded and full clouded sky in short term tests).
- Light source used in the test should produce visible light, UV-A and/or UV-B radiation as close as possible to natural situation (wavelength and intensity).
- Accumulation of PAHs during a pre-incubation period in the dark is allowed, the incubation time is mentioned in the footnotes of the toxicity tables.

The studies in agreement with the criteria mentioned above are presented in the toxicity tables. If a test is not performed in agreement with these criteria, the reliability of the data is judged case by case.

3.2.4 Derivation of NOECs from the literature

Results of toxicity studies are not always expressed in a NOEC. Besides this different methods can be used to derive a NOEC. The following criteria are applied:

- If the NOEC is based on a statistical method these results are used: the highest concentration tested not differing from the control at a significance level of $P<0.05$ is regarded as the NOEC.
- If no statistical method is applied or could be used, in principle the concentration showing less than 10% effect is considered as the NOEC. A distinct concentration-effect relationship is than necessary.
- When there is a LOEC (Lowest Observed Effect Concentration) the following procedures are applied:
  a) LOEC > 10 to 20% effect: the NOEC = LOEC/2,
  b) LOEC ≥ 20% effect and a distinct concentration-effect relationship: the

EC10 is calculated or extrapolated and regarded as the NOEC,

c) LOEC ≥ 20% with no distinct concentration-effect relationship:
- LOEC 20 to 50% effect: NOEC = LOEC/3,
- LOEC ≥ 50% effect: NOEC = LOEC/10.

3.2.5 Calculation of L(E)C50s from data in the literature

If only raw data are available the LC50 is calculated according to the trimmed Spearman-Kärber method (Hamilton *et al.*, 1977/1978). EC50s are calculated using a log-logistic dose response model (Haanstra *et al.*, 1985). In most cases the raw data are not presented in the literature. In general these studies are considered reliable, because acute studies are carried out already for a long time and have been standardized to a great extent, especially in aquatic ecotoxicology.

3.2.6 Conversion of toxicity data on terrestrial/soil organisms to standard soil

Toxicity data derived from terrestrial/soil studies are converted to standard soil (e.g. 10% organic matter and 25% clay), resulting in NOECs and L(E)C50s for standard soil. For organic compounds like PAHs only the organic matter (o.m.) content is taken into account when converting NOECs and L(E)C50s. The clay content is not taken into account because this is only used to convert tests with metals to standard soil (Van de Plassche *et al.*, 1992).

For conversion of the test result to standard soil the following criteria are established:

If: % o.m. is <2%, the percentage is set at 2% o.m., followed by formula 3.1.
% o.m. is between 2%-30%, direct use of formula 3.1.
% o.m. is >30% the percentage is set at 30% o.m., followed by formula 3.1.

The criteria mentioned above are developed for species living in the soil, which are exposed to chemicals through pore water. In a number of cases species are used which live mainly on top of the soil. These species are exposed through their food. Food is considered as dead material and is described as a soil containing 30% o.m. (recited in TCB, 1992).

Formula 3.1 Conversion to standard soil

$$NOEC_{st.soil} = NOEC_{exp.} \times \frac{(10\%o.m.)}{(\%o.m._{soil/food})}$$

$NOEC_{st.\ soil}$	=	NOEC in standard soil
$NOEC_{exp.}$	=	experimental NOEC
10%o.m.	=	organic matter content of the standard soil which is 10%
$\%o.m._{soil/food}$	=	organic matter content of experimental soil or food

3.3 Derivation of partition coefficients from literature

The solid-liquid partition coefficient ($K_{p,s/l}$) describes the equilibrium distribution of a chemical over the solid phase (soil, sediment or suspended matter) and water, see formula 3.2.

Formula 3.2 Partition coefficient of equilibrium distribution between solid phase and liquid phase

$$K_{p,s/l} = \frac{C_{solid}}{C_{liquid}}$$

$K_{p,s/l}$	=	solid-liquid partition coefficient (l/kg)
C_{soil}	=	equilibrium concentration in the soil (mg/kg)
C_{water}	=	equilibrium concentration in water (mg/l)

Partition coefficients are used for two purposes:

1) If there are no terrestrial toxicity data the solid-liquid partition coefficient ($K_{p,s/l}$) is used to derive the $MPC_{soil/sed.}$ from the MPC_{water}.
2) $K_{p,s/l}$-values are used to harmonize MPCs derived from ecotoxicological data.

These $K_{p,s/l}$-values are derived from the organic carbon normalized sediment and soil-water partition coefficients (K_{oc}) which are derived by evaluating experimental studies. Procedures used and quality criteria applied for deriving organic carbon normalised

partition coefficients are described in Bockting *et al.* (1993). When no experimental data are available, the K_{oc} can be estimated using regression equations proposed by Karickhoff (1981), Gerstl (1990) and DiToro *et al.* (1991). After evaluating all the experimental studies the mean log K_{oc} of all the experimental studies is calculated. The $K_{p,s/l}$ for standard soil or sediment can be calculated using formula 3.3. The standard soil/sediment contains 10 % organic matter (is 5.88% organic carbon) and 25 % clay (see also chapter 3.2.6).

Formula 3.3 Calculation of $K_{p,s/l}$-values for standard soil/sediment from K_{oc} values

$$K_{p,s/l} = f_{oc} * K_{oc}$$

$K_{p,s/l}$	=	solid-liquid partition coefficient (l/kg)
f_{oc}	=	fraction organic carbon in standard soil (% organic carbon/100)
K_{oc}	=	organic carbon normalized partition coefficient for soil/ sediment and water (l/kg)

3.4 Extrapolation methods

The extrapolation methods used for the derivation of environmental quality objectives are the preliminary effect assessment and the refined effect assessment. The first method is applied if chronic or acute data for less than 4 species of different taxonomic groups are available. The second method is applied if chronic data for more than 4 species of different taxonomic groups are available.

In both, the preliminary effect assessment and the refined effect assessment, chronic as well as acute toxicity data are weighed over the species as follows:

- If for a single species several L(E)C50 or NOECs are available for different effect parameters the lowest is selected.
- If for a single species several L(E)C50 or NOECs are available for the same effect parameter a geometric mean is calculated.

3.4.1 Preliminary effect assessment

The preliminary effect assessment method is a modified Environmental Protection Agency (EPA) method (modification according to Van de Meent *et al.*, 1990) in which assessment

factors are applied to toxicity data. The size of this factor depends on the number and kind of the available toxicity data. The assessment factors and conditions used are shown in table 3.1 for aquatic effect assessment and in table 3.2 for terrestrial effect assessment. The outcome of the method is called an indicative MPC. The NC (Negligible Concentration) is set at 1% of the MPC. This percentage is established to take factors as multi chemical stress and uncertainties in risk assessment into account.

Table 3.1 Modified EPA-method for aquatic ecosystems

Available information	Assessment factor
lowest acute L(E)C50-value or QSAR estimate for acute toxicity	1000
lowest acute L(E)C50-value or QSAR estimate for acute toxicity for minimal algae/ crustacean/fish	100
lowest NOEC-value or QSAR estimate for chronic toxicity	10*
lowest NOEC-value or QSAR estimate for chronic toxicity for minimal algae/crustacean/ fish	10

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

Table 3.2 Modified EPA-method for terrestrial ecosystems

Available information	Assessment factor
lowest acute L(E)C50-value or QSAR estimate for acute toxicity	1000
lowest acute L(E)C50-value or QSAR estimate for acute toxicity for three representatives of microbe mediated processes, earthworms or arthropods and plants	100
lowest NOEC-value or QSAR estimate for chronic toxicity	10*
lowest NOEC-value or QSAR estimate for chronic toxicity for three representatives of microbe mediated processes, earthworms or arthropods and plants	10

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

3.4.2 Refined effect assessment

The statistical extrapolation method used for derivation of environmental quality objectives in the Netherlands, is based on the assumption that the sensitivities of species in an ecosystem can be described by a statistical frequency distribution. For a detailed overview of the theory and the statistical adjustments since its introduction, reference is made to the

original literature (Kooijman, 1987; Van Straalen and Denneman, 1989; Wagner and Løkke, 1991; Aldenberg and Slob, 1993).

The protection level of the MPC is set at a level that protects 95% of all the species and microbial processes in an ecosystem. This 95% protection level or Hazardous Concentration for 5% of the species (HC5) can be calculated with a 50% and 95% confidence level (Aldenberg and Slob, 1993). The ratio between the 50% and 95% confidence is used to indicate the uncertainty in the estimation of the MPC at the 95% protection level.

The method of Aldenberg and Slob (1993) assumes that the NOECs used for calculation fit the log-logistic distribution. For checking this assumption the data available are tested statistically with the so called empirical distribution function (EDF): Kolmogorov-Smirnov D*sqrt(n) test. If the NOECs are not log-logistically distributed at a significance level of 1% and there are no reasons for leaving out outliers the calculated MPC is used, mentioning the non log-logistically distribution in a note. The NC (Negligible Concentration) is set at 1% of the MPC.

3.5 QSAR-approach

With the QSAR-approach it is possible to derive NOECs from QSARs for different aquatic organisms. These NOECs can be used as input data for the extrapolation method of Aldenberg and Slob (1993) in order to calculate the MPC_{water}. The approach can only be used for chemicals that act by narcosis. The QSARs used are derived from Van Leeuwen *et al.* (1992) and are expressed as log NOEC = a log K_{ow} + b. Van Leeuwen *et al.* (1992) obtained QSARs from literature and applied acute - chronic ratios to transform these QSARs for acute or chronic lethal effects into QSARs for chronic sublethal effects.

In this report the QSAR-approach is used to decide whether PAHs can be considered as chemicals that act by narcosis. For a more detailed description of the QSAR selection criteria see Van Leeuwen *et al.* (1992).

3.6 Equilibrium partitioning

The equilibrium partition method (Ep-method) was originally proposed by Pavlou and Weston (1984) to develop sediment quality criteria. The concept has been described in detail by Shea (1988) and DiToro *et al.* (1991). The method attempts to model the tendency of a chemical to move from one environmental compartment to another. Solid-

liquid partition coefficients ($K_{p,s/l}$) describe the equilibrium distribution of a chemical over a solid phase (soil, sediment or suspended matter) and water (see formula 3.2).

The Ep-method is used for two purposes:
1) when no soil/sediment data are available (§ 3.6.1),
2) for harmonization of the MPC_{soil} and/or $MPC_{sediment}$ (§ 3.6.2).

3.6.1 Calculation of MPC soil/sediment from MPC water

When no data for terrestrial or sediment dwelling organisms are available the Ep-method can be used to calculate a concentration in soil ($MPC_{soil/sed.}$) from a concentration in water (MPC_{water}) (see formula 3.4).

Two important assumptions are made when applying this method:
1) uptake of substances is mainly through the pore water,
2) the sensitivity of terrestrial and aquatic species is comparable.

Formula 3.4 Calculation of MPC soil/sediment from MPC water

$$MPC_{soil/sed.} = MPC_{aq.} * K_{p,s/l}$$

$MPC_{soil/sed.}$	=	Maximum Permissible Concentration in soil/sediment (mg/kg, dry soil or sediment)
$MPC_{aq.}$	=	Maximum Permissible Concentration in water derived from toxicity data (mg/l)
$K_{p,s/l}$	=	solid-liquid partition coefficient (l/kg)

3.6.2 Harmonization

The reason for harmonization is that the MPC or NC in one compartment may not lead to exceedance of MPC or NC in one of the other compartments, due to transport of the chemical between the different compartments. Formula 3.4 can also be used to harmonize independently derived MPCs for water and soil. However, if no toxicity data are available for soil and sediment organisms, harmonization of MPCs for the different compartments is impossible. In that case the equilibrium partitioning method can be used only as an indirect method to derive soil/ sediment MPCs based on aquatic ecotoxicological data.

Although low molecular PAHs can also be present in the gas phase, no harmonization with the air compartment can be performed. There is no information available to derive MPCs for organisms exposed through the air. However, critical air concentrations will be calculated, using the methodology as described in Van de Meent (1995).

4 MPCs FOR AQUATIC ENVIRONMENT BASED ON EXPERIMENTAL DATA

In chapter 4.1 the availability of fresh- and saltwater toxicity data is described. A comparison of fresh- and saltwater toxicity data is made in chapter 4.2. Finally, in chapter 4.3 the MPCs based on experimental data are presented.

4.1 Availability of aquatic toxicity data

The aquatic toxicity data found in the literature are presented in appendix 2 and 3 for freshwater and saltwater organisms, respectively. In this report a number of studies mentioned in Slooff *et al.* (1989) are left out because these studies are not in agreement with the quality criteria (ACT/KD/003 (ACT, 1994)) used in this report. Especially several studies with Algae are rejected because the test durations are too short (e.g. 1-4 hours). Therefore the dataset of this report and the dataset in Slooff *et al.* (1989) are different in some aspects. In some cases however, the rejected studies are used for indicative purposes (Appendix 2 and 3, evaluated but rejected).

Freshwater organisms:
For approximately half of the selected PAHs acute and chronic toxicity data are available; for 5 out of 10 PAHs acute and 6 out of 10 PAHs chronic data. For chrysene, benzo-[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene no useful experimental aquatic toxicity data were found. Most studies concern toxicity of naphthalene, anthracene and phenanthrene. The datasets for the other PAHs are small.

For anthracene, phenanthrene and fluoranthene a number of new toxicity studies are available. Most of these studies concern phototoxicity of the PAHs, for anthracene McCloskey & Oris, 1991; Foran *et al.*, 1991; Holst & Giesy, 1989; Gala & Giesy, 1992 and Huang *et al.*, 1993. For phenanthrene Huang *et al.* (1993) and for fluoranthene Ren *et al.* (1994). For phenanthrene, fluoranthene, benzo[*k*]fluoranthene and benzo[*a*]pyrene chronic 'Early Life Stage' (ELS) fish tests and for phenanthrene and chrysene chronic *Daphnia* tests are available. These ELS- and chronic Daphnia tests were carried out by TNO[5] (Hooftman, 1991; Hooftman & Evers de Ruiter, 1992a, 1992b, 1992c and 1992d) on behalf of the ministry of VROM[6] and RIZA[7]. This research was initiated because little

[5] Abbreviation in Dutch for 'Institute of Applied Scientific Research'.

[6] Abbreviation in Dutch for 'Ministry of Housing, Spatial Planning and the Environment'.

[7] Abbreviation in Dutch for 'Institute for Inland Water Management and Waste Water Treatment'.

chronic toxicity data were available in 1990 (Desire for levels; Van de Meent *et al.*, 1990). In spite of these new studies, still few data are available.

Saltwater organisms:
The number of data available for saltwater organisms is much lower than the number of data available for freshwater organisms. For 3 out of 10 PAHs acute and 2 out of 10 PAHs chronic data are available. As was found for freshwater organisms, most data were found for naphthalene and phenanthrene. For anthracene, benzo[*a*]anthracene, chrysene, benzo[*k*]fluoranthene, benzo[*a*]pyrene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene no experimental saltwater toxicity data were found.

4.2 Comparison fresh- and saltwater toxicity data

In general, the data sets for all PAHs are small. Therefore it is not possible to compare the sensitivities of fresh- and saltwater organisms on the basis of NOECs. Only for naphthalene enough experimental L(E)C50s are available to make a comparison (see figure 4.1).

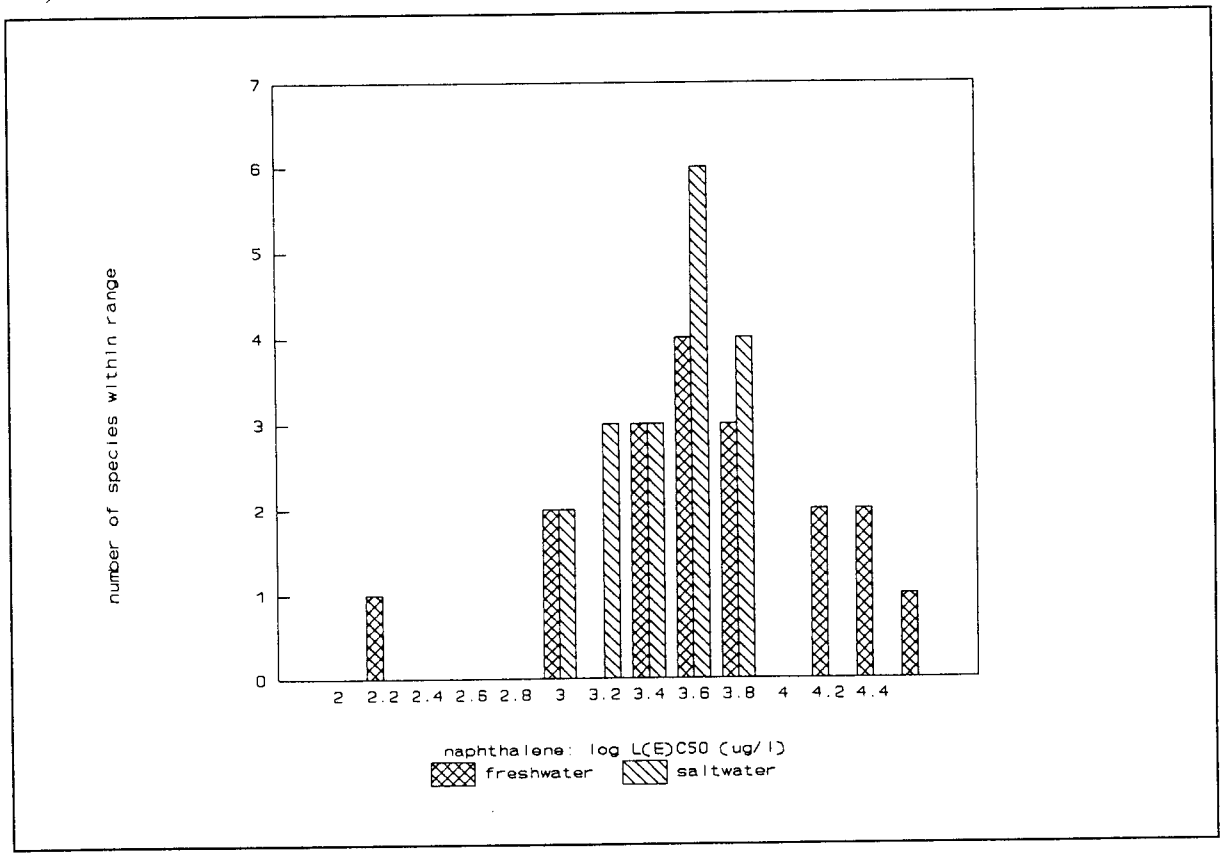


Figure 4.1 Naphthalene; distribution of L(E)C50s for fresh- and saltwater organisms

From figure 4.1 it can be concluded that the sensitivities of fresh- and saltwater organisms for naphthalene are comparable. A comparison on the basis of a t-test showed no significant difference (P>0.05). Although the comparison of naphthalene is the only comparison possible, it is not expected that the sensitivities of fresh- and saltwater organisms for the other PAHs will give different results. Therefore it is assumed that the sensitivities of fresh- and saltwater organisms for all PAHs are not different and that it is justified to calculate MPCs for the aquatic environment combining fresh- and saltwater data.

4.3 MPCs based on experimental data

As was described in chapter 3.4 only one value per species is used in the extrapolations to derive MPCs. Therefore a selection of data used in the extrapolation is made from the data presented in appendix 2 and 3.

The MPCs presented in table 4.1 are derived using the data selected for extrapolation (see appendix 6). All MPCs are calculated using the preliminary effect assessment method (modified EPA-method), because not enough chronic toxicity data are available to use the refined effect assessment method (Aldenberg and Slob, 1993). The $MPC_{freshwater}$, $MPC_{saltwater}$ and $MPC_{combined}$ (fresh- and saltwater) are shown. For each of the PAHs separately an explanation is given how the MPC is derived.

Naphthalene

The $MPC_{freshwater}$ for naphthalene is calculated using the preliminary effect assessment method (modified EPA-method). An assessment factor of 100 is applied on the lowest LC50 available, because organisms of taxonomic groups Algae, Crustacea and Pisces are available. This results in a $MPC_{freshwater}$ of 1.2 µg/l.

The $MPC_{saltwater}$ for naphthalene is also calculated using the modified EPA-method. An assessment factor of 1,000 is applied on the lowest LC50 available. Resulting in a $MPC_{saltwater}$ of 0.75 µg/l. An assessment factor of 100, instead of a factor 1,000 on saltwater data, is not applied in this case, because it can be concluded from a deviating saltwater Algae test that it is not inconceivable that Algae have a similar sensitivity as the other taxonomical groups available.

The $MPC_{combined}$ is the same as the $MPC_{freshwater}$ despite that the $MPC_{saltwater}$ is lower. Combining the fresh- and saltwater data results in an assessment factor of 100 instead of 1,000 on the saltwater toxicity data because now data are available for the taxonomical groups Algae, Crustacea and Pisces.

Table 4.1 MPCs for aquatic organisms based on experimental data

compound	$MPC_{freshwater}$ (µg/l)	$MPC_{saltwater}$ (µg/l)	$MPC_{combined}$ (µg/l)	Lowest NOEC (µg/l)	Lowest L(E)C50 (µg/l)
Naphthalene	1.2 (EPA/100)	0.75 (EPA/1000)	1.2 (EPA/100)	21	120
Anthracene	0.07 (EPA/100)	-	0.07 (EPA/100)	1.67[a]	6.9[b]
Phenanthrene	0.30 (EPA/100)	6.0 (EPA/100)	0.30 (EPA/100)	32	30
Fluoranthene	1.2 (EPA/10)	0.30 (EPA/1000)	0.30 (EPA/1000)	12[c]	300
Benzo[*a*]anthracene	0.01 (EPA/1000)	-	0.01 (EPA/1000)	-	10
Chrysene	-	-	-	-	-
Benzo[*k*]fluoranthene	0.04 (EPA/10)	-	0.04 (EPA/10)	0.36[d]	-
Benzo[*a*]pyrene	0.05 (EPA/100)	-	0.05 (EPA/100)	6.3	5.0
Benzo[*ghi*]perylene	-	-	-	-	-
Indeno[*1,2,3-cd*]pyrene	-	-	-	-	-

The extrapolation method used is placed between parenthesis

- no data available
- a geometric mean of 5 NOECs (reproduction) for *Daphnia magna*; 4.5, 2.2, 1.9, 1.1 and 0.63 µg/l (see appendix 2 and 6)
- b geometric mean of 8 L(E)C values for *Lepomis spec.*; 1.3, 8.0, 3.8, 8.3, 2.8, 12, 18 and 26 µg/l (see appendix 2 and 6)
- c geometric mean of 2 NOECs (growth) for *Brachydanio rerio*; 6.9 and 22 µg/l (see appendix 2 and 6)
- d geometric mean of 2 NOECs (growth) for *Brachydanio rerio*; 0.27 and 0.48 µg/l (see appendix 2 and 6)

Anthracene

The $MPC_{freshwater}$ for anthracene is calculated using the preliminary effect assessment method (modified EPA-method). An assessment factor of 100 is applied on the geometric mean of 8 LC50s for Pisces. This factor is used although no acute data for Algae and Crustacea are available. However, if the chronic NOECs, for Algae and Crustacea, are converted into L(E)C50s (acute and chronic ratio's; factor 3 for Algae and a factor 10 for Crustacea) it is clear that Algae and Crustacea are less or comparable sensitive with Pisces. Therefore a factor 100 is used instead of the factor 1,000 expected from the acute data. This results in a MPC of 0.07 µg/l.

Because there are no saltwater toxicity data available for anthracene, the $MPC_{combined}$ is the same as the $MPC_{freshwater}$.

Phenanthrene

The $MPC_{freshwater}$ for phenanthrene is calculated using the preliminary effect assessment method (modified EPA-method). An assessment factor of 100 is applied on the lowest LC50 value available. This results in a MPC of 0.3 µg/l.

The $MPC_{saltwater}$ for phenanthrene is also calculated using the modified EPA-method. An

assessment factor of 100 is applied on the geometric mean of two EC50s, which results in a MPC of 6.0 µg/l. The assessment factor of 100, instead of a factor 1,000, on fresh- and saltwater data is applied although no toxicity data for Algae are included in the dataset of this report (appendix 2 and 3). From Slooff *et al.* (1989) however, it can be concluded that Algae are not among the most sensitive species for phenanthrene. The quality of these Algae studies is questionable, but they are considered adequate for indicative purposes.
The $MPC_{combined}$ is the same as the $MPC_{freshwater}$ which is 0.3 µg/l.

Fluoranthene
The $MPC_{freshwater}$ for fluoranthene is calculated using the preliminary effect assessment method (modified EPA-method). An assessment factor of 10 is applied on the geometric mean of 2 NOECs for Pisces. This results in a MPC of 1.2 µg/l.
The $MPC_{saltwater}$ for fluoranthene is also calculated using the preliminary effect assessment method. An assessment factor of 1,000 is applied on the lowest LC50 available, which results in a MPC of 0.3 µg/l.
The $MPC_{combined}$ is the same as the $MPC_{saltwater}$, which is 0.3 µg/l.

Benzo[a]anthracene
The $MPC_{freshwater}$ for benzo[*a*]anthracene is calculated using the preliminary effect assessment method (modified EPA-method). An assessment factor of 1,000 is applied on the lowest LC50 available. This results in a MPC of 0.01 µg/l.
Because there are no saltwater toxicity data available for benzo[*a*]anthracene the $MPC_{combined}$ is the same as the $MPC_{freshwater}$.

Chrysene
No experimental data are available to derive a MPC.

Benzo[k]fluoranthene
The $MPC_{freshwater}$ for benzo[*k*]fluoranthene is calculated using the preliminary effect assessment method (modified EPA-method). An assessment factor of 10 is applied on the geometric mean of 2 NOECs for Pisces. This results in a MPC of 0.04 µg/l.
Because there are no saltwater toxicity data available the $MPC_{combined}$ is the same as the $MPC_{freshwater}$, which is 0.04 µg/l.

Benzo[a]pyrene
The $MPC_{freshwater}$ for benzo[*a*]pyrene is calculated using the preliminary effect assessment method (modified EPA-method). An assessment factor of 100 is applied on the lowest LC50 available. The assessment factor 100 instead of 1,000 is justified because a chronic NOEC for Pisces is available. From this NOEC it can be concluded that Pisces are expected to be less sensitive than Crustacea and Algae. This results in a MPC of 0.05 µg/l.

Because there are no saltwater toxicity data available the $MPC_{combined}$ is the same as the $MPC_{freshwater}$.

Benzo[ghi]perylene
No experimental data are available to derive a MPC.

Indeno[1,2,3-cd]pyrene
No experimental data are available to derive a MPC.

5 COMPARISON OF QSAR DATA WITH EXPERIMENTAL DATA

According to the theory of Verhaar *et al.* (1992) PAHs can be classified into class 1 (narcotic mode of action or baseline toxicity). Van Leeuwen *et al.* (1992) presented QSAR estimates for toxicity of narcotic chemicals for 19 species of different taxonomic groups. To check if these QSAR estimated NOECs (see appendix 7) describe the toxicity of PAHs according to Verhaar *et al.* (1992), a comparison is made with the available experimental NOECs found in the literature (see appendix 2 and 3).

The results of this comparison are presented in table 5.1. In order to express the differences between the experimental and QSAR estimated NOECs a factor is used. In this factor the QSAR estimated NOECs are divided by the experimental NOECs. The experimental NOECs and QSAR-NOECs used in the comparison are based on the same toxicity parameters. The QSARs for *Brachydanio rerio* and *Pimephales promelas* are the same. In some cases more than 1 experimental NOEC is available. In this case the NOECs are presented as a range.

Table 5.1 Comparison of QSAR data and experimental data

compound	taxonomic group	species	NOEC (QSAR)* (µg/l)	$NOEC_{(range)}$ (exp.)** (µg/l)	factor (QSAR/exp.)
Naphthalene	Pisces	*Pimephales promelas*[a]	770	450	1.7
Anthracene	Algae	*Selenastrum capricornutum*[b]	120	1.5-8.7	14-80
	Crustacea	*Daphnia magna*[c]	84	0.63-4.5	19-133
Phenanthrene	Crustacea	*Daphnia magna*[c]	82	18-180	0.5-4.6
	Pisces	*Brachydanio rerio*[a]	105	32-56	1.9-3.3
Fluoranthene	Pisces	*Brachydanio rerio*[a]	29	6.9-22	1.3-4.2
Chrysene	Crustacea	*Daphnia magna*[c]	5	≥1.4	≤3.6
Benzo[*k*]fluoranthene	Pisces	*Brachydanio rerio*[a]	6.8	0.27-0.48	14-25
Benzo[*a*]pyrene	Pisces	*Brachydanio rerio*[a]	7.2	6.3	1.1

* predicted NOECs according to Van Leeuwen *et al.*, 1992

** toxicity data from current report, see appendix 2 and 3.

a equation used to calculate the NOEC (growth) values: log NOEC = -0.87*(log K_{ow}) + (-2.35), (r^2=0.90;n=27)

b equation used to calculate the NOEC (growth) values: log NOEC = -1.00*(log K_{ow}) + (-1.71), (r^2=0.93;n=10)

c equation used to calculate the NOEC (reproduction) values: log NOEC = -1.04*(log K_{ow}) + (-1.70), (r^2=0.98; n=17)

For naphthalene, phenanthrene, fluoranthene, chrysene and benzo[*a*]pyrene the experimental NOECs presented in table 5.1 there is an observable tendency that experimental NOECs are lower, except for one *Daphnia* study for phenanthrene resulting in the factor 0.5.

For anthracene and benzo[*k*]fluoranthene the experimental NOECs clearly deviate from the QSAR predicted NOECs. This deviation may be explained by phototoxicity. According to the HOMO-LUMO theory of Mekenyan *et al.* (1994) anthracene and benzo[*k*]fluoranthene are among the most phototoxic PAHs. From the experimental data in appendix 2 and 3 however, this is not evident. It seems that even in the tests in which no specific attention is paid to phototoxicity, anthracene is more toxic than expected from the structure. Probably a none specified, specific mode of action causes higher toxicity for these two PAHs.

For benzo[*a*]anthracene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene no experimental NOECs are available to compare with the QSAR estimated NOECs.

6 'OLD' AND 'NEW' QSAR MPCs AND A COMPARISON

In chapter 6.1 the currently used MPCs are presented, as derived in 'Desire for levels' (Van de Meent *et al.*, 1990). In chapter 6.2 the MPCs based on the combined dataset of experimental- and QSAR-data from Van Leeuwen *et al.*, 1992, are presented. Finally, in chapter 6.3 a comparison is made between the MPCs based on experimental data, the MPCs derived from QSAR/NOECs and experimental NOECs combined and the MPCs from 'Desire for levels' (Van de Meent *et al.*, 1990).

6.1 MPCs for aquatic environment from 'Desire for levels' (Van de Meent *et al.*, 1990)

The MPCs for the aquatic environment for PAHs in 'Desire for levels' (Van de Meent *et al.*, 1990) are derived from QSARs available at that moment:

De Wolf *et al.* (1988) derived a QSAR for the water flea (*Daphnia magna*):

log NOEC (mmol/l) = -0.99 log K + 4.16 (r=0.97; s=0.50; n=10)

Van Leeuwen *et al.* (1990) derived a QSAR for fish (*Pimephales promelas*):

log NOEC (mmol/l) = -0.90 log K + 3.80 (r=0.96; s=0.33; n=30)

In 'Desire for levels' (Van de Meent *et al.*, 1990) a comparison was made between the NOECs calculated with the QSARs (see above) and the experimental NOECs available at that time. The conclusion of this comparison was that the experimental NOECs were a factor 3-10 lower. Because the QSARs were selected as the basis for determining risk levels the MPCs derived from the QSARs were corrected with a factor 5. This factor 5 was applied in addition to a factor 10 (modified EPA-method) on the lowest QSAR estimated NOEC available for *Daphnia* or *Pimephales*. This resulted in a MPC for the aquatic environment.

The MPCs for the aquatic environment proposed in 'Desire for levels' (Van de Meent *et al.*, 1990) are presented in table 6.1. together with the QSAR-NOECs for *Daphnia magna* and *Pimephales promelas* (De Wolf *et al.*, 1988; Van Leeuwen *et al.*, 1990).

Table 6.1 MPCs from 'Desire for levels' (Van de Meent et al., 1990)

compound	NOEC (QSAR) *Daphnia magna* (µg/l)	NOEC (QSAR) *Pimephales promelas* (µg/l)	MPC * (QSAR) (µg/l)
Naphthalene	634	572	10
Anthracene	90	100	2
Phenanthrene	90	100	2
Fluoranthene	26	33	0.5
Benzo[*a*]anthracene	9.4	13	0.2
Chrysene	9.4	13	0.2
Benzo[*k*]fluoranthene	4.2	6.3	0.1
Benzo[*a*]pyrene	4.2	6.3	0.1
Benzo[*ghi*]perylene	1.2	2.0	0.02
Indeno[*1,2,3-cd*]pyrene	1.8	3.0	0.04

* All MPCs are calculated using the modified EPA-method; EPA/10 with an extra factor 5

6.2 MPCs based on the combined dataset of QSAR- and experimental data for the aquatic environment

In table 6.2 MPCs are presented which are based on the combined dataset of the estimated QSAR-NOECs (Van Leeuwen *et al.*, 1992, see appendix 7) and the experimental NOECs. For selection of the QSAR-NOECs a limit of 10 times the maximum water solubility is used. All NOECs exceeding this limit are rejected (see chapter 3.2.2). If for the same species a QSAR-NOEC and an experimental NOEC is available, the latter is preferred. No MPCs for anthracene and benzo[*k*]fluoranthene are calculated using the QSAR-approach, because from the comparison in chapter 5 it is evident that there probably is a none specified, specific mode of action that causes higher toxicity for these two PAHs.

The number of QSAR-NOECs included in the dataset to derive the MPC depends on the water solubility of the PAHs. In general it can be concluded from table 6.2 that with increasing hydrofobicity and molecular mass the number of useable QSAR-NOECs decreases. For indeno[*1,2,3,-cd*]pyrene no MPC based on the QSAR-approach is calculated because all QSAR estimated NOECs are more than 10 times above the maximum water solubility (see table 2.2). The MPC for benzo[*ghi*]perylene, derived from QSAR-NOECs, is slightly above the maximum water solubility, which is 0.26 µg/l.

From the MPCs in table 6.2 it can be seen that the MPCs decrease with increasing molecular weight and decrease with decreasing water solubility (for physical/chemical properties, see table 2.2).

Table 6.2 MPCs based on QSAR-approach (Van Leeuwen et al., 1992)

compound	no. NOEC (exp.) (n)	no. NOEC (QSAR) (n)	tot. no. NOEC (exp.+QSAR) (n)	MPC* (µg/l)	
Naphthalene	5	18	23	99	(4.6)
Phenanthrene	5	15	20	25	(3.7)
Fluoranthene	2	16	18	6.9	(4.6)
Benzo[*a*]anthracene	0	12	12	2.7	(3.2)
Chrysene	0	11	11	3.4	(2.8)
Benzo[*a*]pyrene	1	9	10	2.0[a]	(2.7)
Benzo[*ghi*]perylene	0	5	5	0.33	(4.2)
Indeno[*1,2,3-cd*]pyrene	0	0	0	-	-

* MPCs calculated with the refined effect assessment (Aldenberg and Slob, 1993); between parenthesis: ratio between $MPC_{50\% \text{ confidence}}$ and $MPC_{95\% \text{ confidence}}$

a no logistic distribution (Kolmogorov-Smirnov D*sqrt(n) test)

6.3 Comparison of MPCs for the aquatic environment based on experimental data, combined dataset of exp./QSAR data and the data from 'Desire for levels'

In table 6.3 the MPCs based on experimental data ($MPC_{combined}$ from chapter 4.3), the MPCs based on the combined dataset of experimental- and QSAR-data (chapter 6.2) and the MPCs from 'Desire for levels' (Van de Meent *et al.*, 1990) (chapter 6.1) are summarized.

From table 6.3 it can be seen that the MPCs derived using the QSAR-approach from Van Leeuwen *et al.*, 1992 are higher than the MPCs derived using the QSARs presented in 'Desire for levels' (Van de Meent *et al.*, 1990). The reason for this deviation is the applied extrapolation method. The MPCs derived from the new QSAR-method are extrapolated with the refined effect assessment method (Aldenberg and Slob, 1993). The MPCs from 'Desire for levels' (Van de Meent *et al.*, 1990) are calculated using the preliminary effect assessment method (modified EPA-method). In 'Desire for levels' (Van de Meent *et al.*, 1990) the MPCs are corrected with an extra factor 5, on top of the factor 10 prescribed by the modified EPA-method. The reason for this extra factor is the difference (factor 3-10) between the experimental NOECs and the NOECs estimated with the QSARs from De Wolf *et al.* (1988) and Van Leeuwen *et al.* (1990).

The NOECs estimated with the QSAR-method (Van Leeuwen *et al.*, 1992) seem to be comparable with the available experimental NOECs for 5 out of 7 PAHs (see chapter 5). The factor 3-10 observed in 'Desire for levels' (Van de Meent *et al.*, 1990) is not found in

the present report. The differences found in the present report (chapter 5) are smaller (factor 0.5-4.6).

Table 6.3 Summary of the MPCs for the aquatic environment

compound	MPC_{water} (experimental) (µg/l)	MPC_{water}* (exp. + QSAR) (µg/l)	MPC_{water}** (Desire for levels)) (µg/l)
Naphthalene	1.2 (EPA/100)	99	10
Anthracene	0.07 (EPA/100)	-	2
Phenanthrene	0.30 (EPA/100)	25	2
Fluoranthene	0.30 (EPA/1000)	6.9	0.5
Benzo[*a*]anthracene	0.01 (EPA/1000)	2.7	0.2
Chrysene	-	3.4	0.2
Benzo[*k*]fluoranthene	0.04 (EPA/10)	-	0.1
Benzo[*a*]pyrene	0.05 (EPA/100)	2.0	0.1
Benzo[*ghi*]perylene	-	0.33	0.02
Indeno[*1,2,3-cd*]pyrene	-	-	0.04

- no data available
* MPCs calculated with the refined effect assessment (Aldenberg and Slob, 1993)
** All MPCs are calculated using the modified EPA-method; EPA/10 with an extra factor 5

The MPCs derived from experimental data are low compared to the MPCs from the QSAR-approach (Van Leeuwen *et al.*, 1992) and the QSARs from Van Leeuwen *et al.* (1990) and De Wolf *et al.* (1988). For most experimental MPCs these low values are partly caused by the high extrapolation factors used in the preliminary effect assessment method.

The main question to be answered at this moment is whether to use the experimental data or the combined dataset of experimental and QSAR predicted NOECs (Van Leeuwen *et al.*, 1992) to derive MPCs for the aquatic environment.

In the project 'Setting environmental quality objectives' MPCs are based on experimental data as much as possible. In order to achieve this a large number of quality criteria are applied, to guarantee the quality of the studies used. The QSAR-approach however, is a method that estimates toxicity from the structure and physical-chemical properties of the compounds in question. From the comparison between experimental NOECs and the QSAR estimated NOECs (chapter 5) it is evident that some PAHs do not act by narcosis (anthracene and benzo[*k*]fluoranthene). For the other PAHs it is not clear whether they do or do not act by narcosis. The differences found in the comparison in the present report (chapter 5) are a factor 0.5-4.6. Biologically a maximum factor 4.6 is not much. However, from the comparison it is also obvious that there is a tendency that experimental NOECs

are lower than the QSAR estimated NOECs. Apparently the QSAR-method underestimates the toxicity of the PAHs with a maximum factor of 4.6, when compared to the experimental NOECs. The conclusion is that it can not be excluded that there is a specific mode of action for these PAHs. Therefore it is decided to prefer the experimental toxicity data above QSAR estimated data to derive the 'final' MPCs for the aquatic environment. This results in 7 MPCs for the aquatic environment for, naphthalene, anthracene, phenanthrene, fluoranthene, benzo[*a*]anthracene, benzo[*k*]fluoranthene and benzo[*a*]pyrene.

Besides the uncertainties in the QSAR-approach it is known that PAHs have a carcinogenic and mutagenic potential. There are also effects found on the immune-system, which is reported by Coles *et al.* (1994). Apparently there are many different modes of action concerning PAHs that have effects on organisms, which forces to be precautious.

For chrysene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene no experimental data are available. For indeno[*1,2,3-cd*]pyrene the QSAR-approach (Van Leeuwen *et al.*, 1992) can not be applied because all NOECs are estimated more than 10 times above the maximum water solubility (see chapter 6.2). Therefore, it is decided to use the MPC presented in 'Desire for levels' (Van de Meent *et al.*, 1990) for indeno[*1,2,3-cd*]pyrene. For chrysene and benzo[*ghi*]perylene MPCs are calculated (table 6.2) using the QSAR-approach (Van Leeuwen *et al.*, 1992), these 'new' QSAR determined MPCs are preferred above the 'old' QSAR determined MPCs (Van de Meent *et al.*, 1990). The problem that remains however are the uncertainties in the QSAR-approach discussed earlier. Therefore it is decided to correct the MPCs calculated with the QSAR-approach (Van Leeuwen *et al.*, 1992), for chrysene and benzo[*ghi*]perylene by applying an extra factor 10.

In table 6.4 the 'final' MPCs for the aquatic environment are presented.

Table 6.4 Summary of the MPCs for the aquatic environment

compound	MPC_{water} (final) (µg/l)
Naphthalene	1.2 (EPA/100)
Anthracene	0.07 (EPA/100)
Phenanthrene	0.30 (EPA/100)
Fluoranthene	0.30 (EPA/1000)
Benzo[*a*]anthracene	0.01 (EPA/1000)
Chrysene	0.34 (QSAR/A&S/10)
Benzo[*k*]fluoranthene	0.04 (EPA/10)
Benzo[*a*]pyrene	0.05 (EPA/100)
Benzo[*ghi*]perylene	0.03 (QSAR/A&S/10)
Indeno[*1,2,3-cd*]pyrene	0.04[a] (EPA/10)

The extrapolation method used is placed between parenthesis

a from 'Desire for levels' (Van de Meent *et al.*, 1990)

7 MPCs FOR SOIL AND SEDIMENT BASED ON EXPERIMENTAL DATA

In this chapter the MPCs for soil and sediment are presented. In chapter 7.1 the availability of data is described for both the toxicity- and log K_{oc} data. In chapter 7.2 the log K_{oc}s and the $K_{p,s/l}$-values calculated from these log K_{oc}s are presented. In chapter 7.3 the MPCs for soil based on experimental data are presented. In chapter 7.4 the MPCs for soil and sediment are calculated from the MPC_{water} applying the equilibrium partitioning method, for those substances for which no experimental data are available. The MPCs for soil are harmonized in chapter 7.5 and in chapter 7.6 the 'final' MPCs for soil and sediment are summarized. Finally, in chapter 7.7 critical air concentrations are calculated.

7.1 Availability of soil, sediment and log K_{oc} data

Soil toxicity data:
The soil toxicity data found are presented in appendix 4. The total number of soil toxicity studies found in the literature is very limited. For only 3 PAHs (anthracene, benzo [*a*]anthracene and benzo[*a*]pyrene) reliable data were found.

Sediment toxicity data:
Almost no experimental sediment toxicity data are available. Only for fluoranthene a number of sediment studies are available. A number of crustaceans and a insect were tested in water sediment systems, with the use of natural sediments (Suedel *et al.*, 1993 and Swartz *et al.*, 1990) with a %om of 0.68-0.85 and artificial sediments (DeWitt *et al.*, 1989) with a %om of 29.4. The L(E)C50 values for the crustaceans *Daphnia magna, Eohaustorius estuarius, Hyalella azteca* and *Rhepoxynius abronius* (Suedel *et al.*, 1993; DeWitt *et al.*, 1992 and Swartz *et al.*, 1990) ranged between 2 and 21 mg/kg sediment and between 3 and 9 mg/kg sediment for the insect *Chironomus tentans* (Suedel *et al.*, 1993). The toxicity for the same species based on porewater and the water above the sediment ranged, for the crustaceans between 3 and 240 µg/l and for the insect between 30 and 250 µg/l. It is however, not possible to use the experimental sediment toxicity data for fluoranthene to derive a MPC for sediment, because no evaluation criteria for sediment studies exist at the moment.

Log K_{oc}s:
The experimental log K_{oc}s found in the literature are presented in appendix 5. For naphthalene and anthracene a relatively large dataset of experimental log K_{oc}s is available. For all other PAHs less log K_{oc}s are available, but for all PAHs at least two experimental log K_{oc}s are present.
If the log K_{oc}s based on experiments with sediment are compared with log K_{oc}s on the

basis of experiments with soil for naphthalene (figure 7.1) and anthracene (appendix 5), it can be concluded that sediment log K_{oc}s seem to be higher.

The log K_{oc}s for all higher molecular PAHs are based solely on sediment based values (Evers & Smedes, 1993; Kayal & Conell, 1990; Van Hattum, 1995) under varying conditions. The results from Kayall and Conell (1990) and Van Hattum (1995) are based on experiments in which field contaminated sediments are used. It can be expected that PAHs are bound more strongly to the organic matter of the sediments, because of the rather long presence of the PAHs in the sediment.

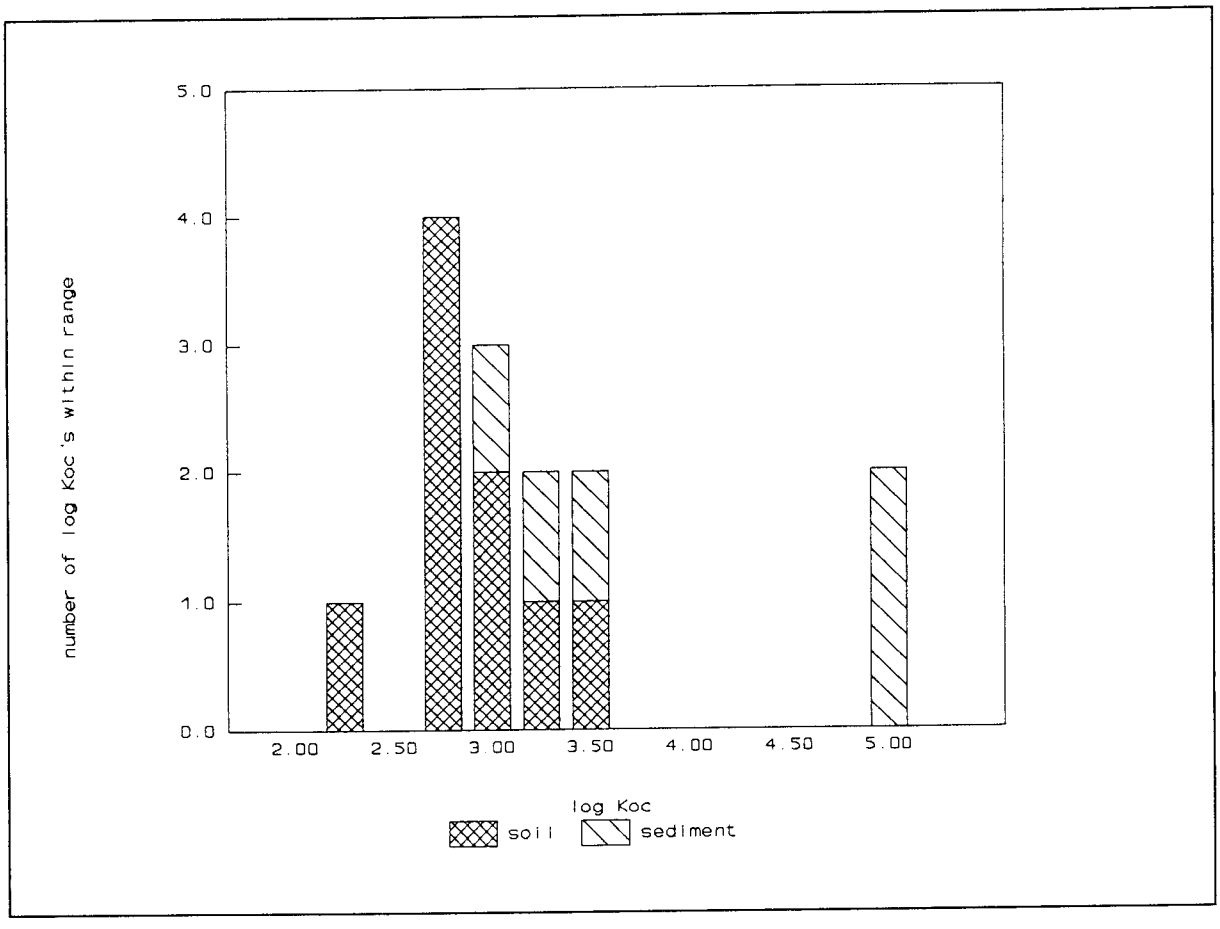


Figure 7.1 Comparison of soil and sediment derived log K_{oc}s for naphthalene

In the study performed by Evers and Smedes (1993) the "co-solvent method" is applied. Especially for very hydrophobic compounds it is assumed that this method gives a better estimation for a log K_{oc} than other methods. This co-solvent method is also used in the study performed by Nkedi-Kizza *et al.* (1985) with soil samples. In this study the co-solvent log K_{oc} is comparable with the available log K_{oc}s.

7.2 $K_{p,s/l}$-values for standard soil

The average of the experimental log K_{oc}s found in the literature is calculated and normalized for standard soil/sediment. The standard soil/sediment contains 10 % organic matter (is 5.88% organic carbon) and 25 % clay (see also chapter 3.2.6). The experimental log K_{oc}s used for calculation can be found in appendix 5.

In table 7.1 the available average experimental log K_{oc}s are presented. The experimental log K_{oc}s are divided in soil- and sediment log K_{oc}s. Also mentioned in the table are the sediment log K_{oc}s from Evers & Smedes (1993) derived using the co-solvent method.

Table 7.1 Experimental log K_{oc}s for soil and sediment

compound	Average exp. log K_{oc} total dataset	Average exp. log K_{oc} Sediment	exp. log K_{oc}* Sediment co-solvent	Average exp. log K_{oc} batch exp. sed.+soil	Average exp. log K_{oc} Soil
Naphthalene	3.16 (±0.77,n=15)	3.73 (±0.92,n=6)	-	3.16 (±0.77,n=15)	2.78 (±0.34,n=9)
Anthracene	4.73 (±0.87,n=11)	5.65 (±0.87,n=4)	5.57	4.65 (±0.88,n=10)	4.20 (±0.13,n=7)
Phenanthrene	5.06 (±0.83,n=6)	5.05 (±0.84,n=6)	5.32	5.01 (±0.92,n=5)	-
Fluoranthene	5.38 (±1.07,n=6)	6.02 (±0.54,n=4)	5.88	5.28 (±1.17,n=5)	4.11 (±0.014,n=2)
Benzo[*a*]anthracene	6.59 (±0.64,n=4)	6.59 (±0.64,n=4)	7.02	6.44 (±0.70,n=3)	-
Chrysene	6.42 (±0.46,n=4)	6.42 (±0.46,n=4)	6.77	6.30 (±0.49,n=3)	-
Benzo[*k*]fluoranthene	6.81 (±0.96,n=4)	6.81 (±0.96,n=4)	7.84	6.46 (±0.81,n=3)	-
Benzo[*a*]pyrene	6.84 (±0.85,n=4)	6.84 (±0.85,n=4)	7.72	6.55 (±0.75,n=3)	-
Benzo[*ghi*]perylene	7.38 (±1.10,n=2)	7.38 (±1.10,n=2)	8.15	6.60 (n=1)	-
Indeno[*1,2,3-cd*]pyrene	7.52 (±1.30,n=2)	7.52 (±1.30,n=2)	8.44	6.60 (n=1)	-

Standard deviation (SD) and number of data are placed between parenthesis

- no data available
* co-solvent method, Evers & Smedes (1993)

It must be remarked here that the average experimental log K_{oc}s for the high molecular PAHs are based on only four or two experimental values, in which sediment is used (see appendix 5, and table 7.1). Since the average log K_{oc}s for all higher molecular PAHs are based solely on sediment based values of Evers & Smedes (1993), Kayal & Conell (1990) and Van Hattum (1995), it is expected that this results in high average log K_{oc}s.

In general it can be concluded from the dataset that experimental sediment log K_{oc}s are higher than the average soil log K_{oc}s (Fig 7.1, table 7.1). If the sediment log K_{oc}s from Evers & Smedes (1993) (co-solvent method, table 7.1) are compared with the sediment values of Kayal & Conell (1990) and Van Hattum (1995) it is clear that these values are

much higher (see appendix 5). The reason why the co-solvent method results in higher values than the values derived from batch experiments is the fact that conventional batch methods might overestimate the biological availability of the substance, because a certain amount is bound to organic and colloidal material in the water phase. On the other hand it is not exactly known which part of the substance, organic or colloidal bound, is biological available. Because of the small dataset it is difficult to decide whether the higher log K_{oc}s for sediment are a result of sediment characteristics or experimental conditions used.

In table 7.2 the average (experimental) log K_{oc}, the estimated log K_{oc}s according to Karickhoff (1981), Gerstl (1990) and DiToro *et al.* (1991) are presented.

Table 7.2 Estimated log K_{oc} values compared to experimental log K_{oc}s

compound	Average exp. log K_{oc} total dataset	estimated log K_{oc}*	estimated log K_{oc}**	estimated log K_{oc}***
Naphthalene	3.16 (±0.77, n=15)	2.92	3.56	3.30
Anthracene	4.73 (±0.87, n=11)	4.06	4.44	4.45
Phenanthrene	5.06 (±0.83, n=6)	4.06	4.45	4.46
Fluoranthene	5.38 (±1.07, n=6)	4.76	5.00	5.16
Benzo[*a*]anthracene	6.59 (±0.64, n=4)	5.38	5.46	5.79
Chrysene	6.42 (±0.46, n=4)	5.32	5.42	5.73
Benzo[*k*]fluoranthene	6.81 (±0.96, n=4)	5.59	5.62	6.00
Benzo[*a*]pyrene	6.84 (±0.85, n=4)	5.56	5.60	5.97
Benzo[*ghi*]perylene	7.38 (±1.10, n=2)	6.21	6.10	6.63
Indeno[*1,2,3-cd*]pyrene	7.52 (±1.30, n=2)	5.98	5.93	6.40

Standard deviation (SD) and number of data are placed between parenthesis

The log K_{ow} used is the MEDCHEM® star value (see table 2.2)

* estimated log K_{oc} according to Karickhoff, 1981; log K_{oc} = 0.989 * log K_{ow} - 0.346
** estimated log K_{oc} according to Gerstl, 1990; log K_{oc} = 0.762 * log K_{ow} + 1.051
*** estimated log K_{oc} according to DiToro *et al.*, 1991; log K_{oc} = log K_{ow};

If the estimated log K_{oc}s (from table 7.2) are compared with the average experimental log K_{oc}s it can be seen that the log K_{oc}s of the PAHs with lower molecular weights are comparable (naphthalene, anthracene, phenanthrene and fluoranthene) with the estimated ones. The average experimental log K_{oc}s for PAHs with higher molecular weights, (benzo[*a*]anthracene, chrysene, benzo[*k*]fluoranthene, benzo[*a*]pyrene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene) are more than one log unit higher than the estimated values from Karickhoff (1981), Gerstl (1990) and DiToro *et al.* (1991).

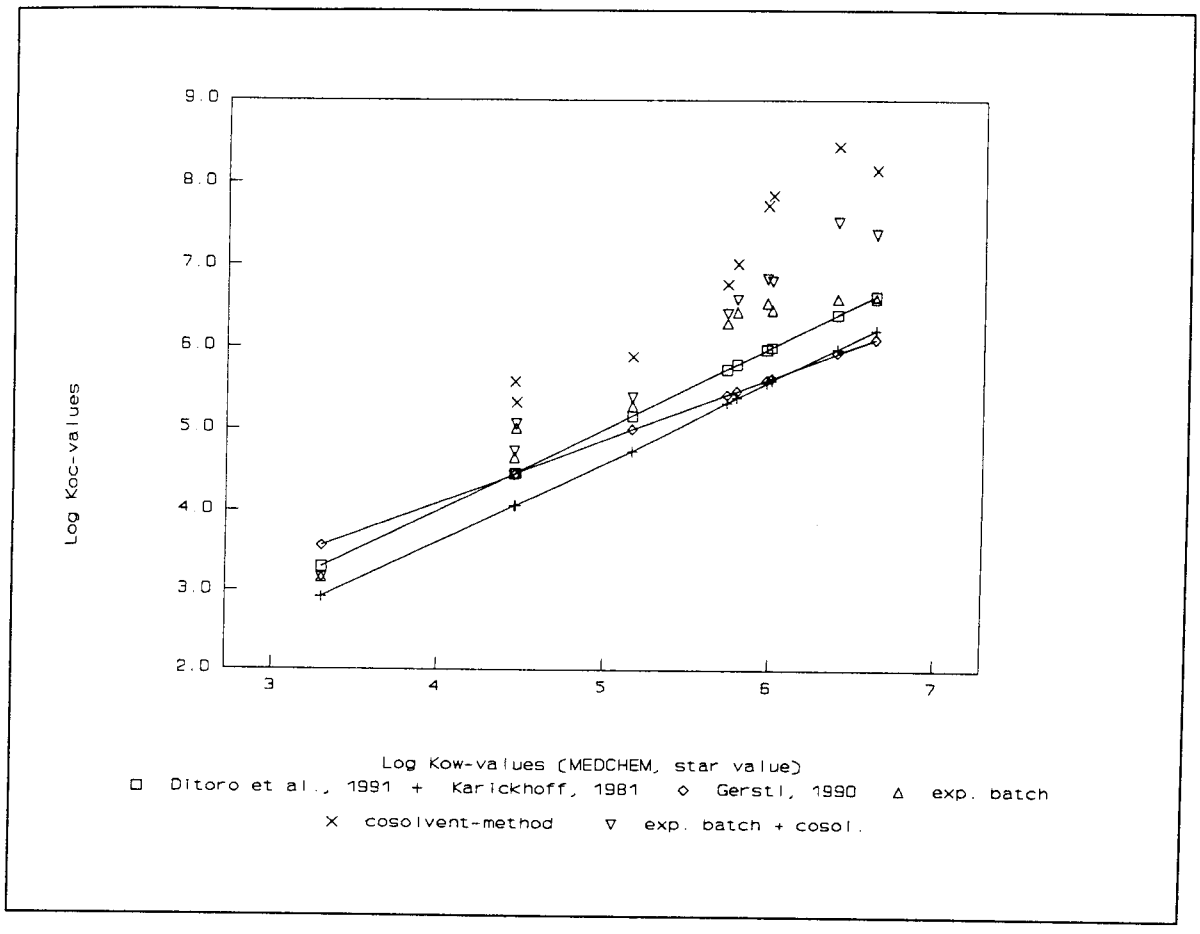


Figure 7.2 Comparison of all available log K_{oc}s.

In figure 7.2 the relationships between the log K_{ow}-star-values from the MEDCHEM® database and the estimated and experimental log K_{oc}s from table 7.1 and 7.2 are given.

The log K_{oc} values using the co-solvent method are higher than all other log K_{oc} values (experimental and estimated) for the PAHs considered. The estimated log K_{oc} values using Karickhoffs equation are the lowest for all PAHs considered and comparable with the 'Gerstl log K_{oc}s' in the higher log K_{ow} region. The estimated log K_{oc} values using Gerstl are comparable with the experimental log K_{oc}s in the low log K_{ow} region.

Although experimental data are normally preferred above estimated values it is clear from table 7.2 (column 1) that the experimental values have large variations, which makes it difficult to judge whether it is valid to use these values for equilibrium partitioning. Because the reliability of the experimental data remains unclear and the estimated data from Karickhoff (1981) and Gerstl (1990) seem to be low compared with the experimental data in the low log K_{ow} region, it is decided to use the log K_{oc}s from DiToro *et al.* (1991) to calculate the $K_{p,s/l}$-values (see table 7.3). The log K_{oc}s from DiToro present a middle

course between 'high' experimental values and 'low' estimated values.

In table 7.3 the calculated (standard soil/sediment corrected) log $K_{p,s/l}$-values for the different PAHs are presented. The $K_{p,s/l}$-values are calculated according to formula 3.3 (see chapter 3.3), using the estimated log K_{oc}s according to DiToro *et al.* (1991).

Table 7.3 $K_{p,s/l}$-values based on K_{oc} values

compound	estimated log K_{oc}*	log $K_{p,s/l}$ st.soil
Naphthalene	3.30	2.07
Anthracene	4.45	3.22
Phenanthrene	4.46	3.23
Fluoranthene	5.16	3.93
Benzo[*a*]anthracene	5.79	4.56
Chrysene	5.73	4.49
Benzo[*k*]fluoranthene	6.00	4.77
Benzo[*a*]pyrene	5.97	4.74
Benzo[*ghi*]perylene	6.63	5.40
Indeno[*1,2,3-cd*]pyrene	6.40	5.17

* calculated log K_{oc} according to DiToro *et al.*, 1991; log K_{oc} = log K_{ow}; log K_{ow}s used are the MEDCHEM® star log K_{ow}-values (see table 2.2)

7.3 MPCs for soil based on experimental data

The MPCs for standard soil are calculated using the toxicity data (corrected for standard soil) presented in appendix 6 (data used for extrapolation). Only for anthracene, benzo[*a*]anthracene and benzo[*a*]pyrene MPCs can be derived based on experimental data. These MPCs are calculated using the preliminary effect assessment method (modified EPA-method). The $MPCs_{soil}$ based on experimental data are presented in table 7.4.

Table 7.4 MPC_{soil} based on experimental data (standard soil)

compound	MPC_{soil} (experimental data) (mg/kg)	Lowest L(E)C50 (mg/kg)	Lowest (NOEC) (mg/kg)
Anthracene	0.15 (EPA/1000)	150	-
Benzo[*a*]anthracene	0.25 (EPA/10)		2.5
Benzo[*a*]pyrene	0.26 (EPA/10)	-	2.6

Below an explanation is given of how the experimental MPCs for soil are derived:

Anthracene
The MPC_{soil} for anthracene is calculated using the preliminary effect assessment method. A factor 1,000 is applied on the lowest EC50 available. This results in a MPC_{soil} of 0.15 mg/kg (see table 7.4).

Benzo[a]anthracene
The MPC_{soil} for benzo[*a*]anthracene is calculated using the preliminary effect assessment method. A factor 10 is applied on the lowest NOEC available. This results in a MPC_{soil} of 0.25 mg/kg.

Benzo[a]pyrene
The MPC_{soil} for benzo[*a*]pyrene is calculated using the preliminary effect assessment method. A factor 10 is applied on the lowest NOEC available. This results in a MPC_{soil} of 0.26 mg/kg.

7.4 Calculation of MPC soil and sediment from the MPC_{water} using the equilibrium partitioning method

In table 7.5 the MPCs for soil and sediment are calculated from the 'final' MPC_{water} (table 6.4) using the equilibrium partitioning method. The $K_{p,s/l}$-values used are derived from table 7.3. The MPCs are calculated according to formula 3.4 (see chapter 3.5.1).

Table 7.5 Calculation of MPC soil and sediment from MPC_{water} using the Ep-method

compound	$MPC_{(water)}$ (final) (µg/l)	log $K_{p,s/l}$ ($l*kg^{-1}$)	MPC soil and sediment Ep-method (mg/kg)
Naphthalene	1.2 (EPA/100)	2.07	0.14
Anthracene	0.07 (EPA/100)	3.22	0.12
Phenanthrene	0.30 (EPA/100)	3.23	0.51
Fluoranthene	0.30 (EPA/1000)	3.93	2.6
Benzo[*a*]anthracene	0.01 (EPA/1000)	4.56	0.36
Chrysene	0.34 (QSAR/A&S/10)	4.49	10.7
Benzo[*k*]fluoranthene	0.04 (EPA/10)	4.77	2.4
Benzo[*a*]pyrene	0.05 (EPA/100)	4.74	2.7
Benzo[*ghi*]perylene	0.03 (QSAR/A&S/10)	5.40	7.5
Indeno[*1,2,3-cd*]pyrene	0.04 (EPA/10)	5.17	5.9

The extrapolation method used is placed between parenthesis

7.5 Harmonization of MPCs for soil based on experimental data

In table 7.6 the MPC_{soil} based on equilibrium partitioning (Ep) method and the MPC_{soil} based on experimental data for anthracene, benzo[*a*]anthracene and benzo[*a*]pyrene are presented.

Table 7.6 Harmonization of MPC_{soil} based on experimental data

compound	MPC_{soil} (Ep-method) (mg/kg)	MPC_{soil} (ecotoxicological data) (mg/kg)
Anthracene	0.12 (EP)	0.15 (EPA/1000)
Benzo[*a*]anthracene	0.36 (EP)	0.25 (EPA/10)
Benzo[*a*]pyrene	2.7 (EP)	0.26 (EPA/10)

The used extrapolation method is placed between parenthesis

Anthracene
The experimental MPC for soil for anthracene is approximately the same as the MPC_{soil} when calculated with the equilibrium partitioning method. The MPC calculated with the equilibrium partitioning method is the lowest value and is used as the 'final' MPC for soil.

Benzo[a]anthracene
The experimental MPC for soil for benzo[*a*]anthracene is approximately the same as the MPC_{soil} when calculated with the equilibrium partitioning method. The experimental MPC is the lowest value and is used as the 'final' MPC for soil.

Benzo[a]pyrene
The experimental MPC_{soil} for benzo[*a*]pyrene differs a factor 10 with the MPC_{soil} calculated with the Ep-method. The experimental MPC_{soil} is the lowest value and is used as the 'final' MPC for soil.

7.6 Summary of the MPCs for soil and sediment

In table 7.7 the 'final' MPCs for soil and sediment are presented together with MPCs for soil/sediment from 'Desire for levels' (Van de Meent *et al.*, 1990).

Table 7.7 Final MPCs soil and sediment

compound	$MPC_{soil/sed.}$* (desire for levels) (mg/kg)	$MPC_{soil\ and\ sediment}$ (EP-method) (mg/kg)	MPC_{soil} (ecotoxicological data) (mg/kg)	MPC_{soil} (final) (mg/kg)	$MPC_{sediment}$ (final) (mg/kg)
Naphthalene	1.3 (EP)	0.14 (EP)	-	0.14 (EP)	0.14 (EP)
Anthracene	5.2 (EP)	0.12 (EP)	0.15 (EPA/1000)	0.12 (EP)	0.12 (EP)
Phenanthrene	4.6 (EP)	0.51 (EP)	-	0.51 (EP)	0.51 (EP)
Fluoranthene	1.6 (EP)	2.6 (EP)	-	2.6 (EP)	2.6 (EP)
Benzo[*a*]anthracene	2.0 (EP)	0.36 (EP)	0.25 (EPA/10)	0.25 (EPA/10)	0.36 (EP)
Chrysene	2.0 (EP)	10.7 (EP)	-	10.7 (EP)	10.7 (EP)
Benzo[*k*]fluoranthene	2.5 (EP)	2.4 (EP)	-	2.4 (EP)	2.4 (EP)
Benzo[*a*]pyrene	2.5 (EP)	2.7 (EP)	0.26 (EPA/10)	0.26 (EPA/10)	2.7 (EP)
Benzo[*ghi*]perylene	2.0 (EP)	7.5 (EP)	-	7.5 (EP)	7.5 (EP)
Indeno[*1,2,3-cd*]pyrene	2.5 (EP)	5.9 (EP)	-	5.9 (EP)	5.9 (EP)

The used extrapolation method is placed between parenthesis

* MPCs from 'Desire for levels' (Van de Meent *et al.*, 1990)

Six of the MPCs for soil are lower than the MPCs from 'Desire for levels' (Van de Meent *et al.*, 1990) (naphthalene, anthracene, phenanthrene, benzo[*a*]anthracene, benzo[*k*] fluoranthrene and benzo[*a*]pyrene), for the remaining PAHs these values are higher (fluoranthene, chrysene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene).
Half the MPCs for sediment calculated with the Ep-method are lower than the MPCs from 'Desire for levels' (Van de Meent *et al.*, 1990) (naphthalene, anthracene, phenanthrene, benzo[*a*]anthracene and benzo[*k*]fluoranthrene), for the remaining PAHs these values are higher (fluoranthene, chrysene, benzo[*a*]pyrene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene). Because the experimental MPCs for the aquatic environment in this report are lower than the MPCs for the aquatic environment derived from the QSARs in 'Desire for levels' (Van de Meent *et al.*, 1990), one would expect that this would result in MPCs for soil that are all lower than the MPCs for soil in 'Desire for levels' (Van de Meent *et al.*, 1990). However, this is not the case because the log K_{oc}s used in this report are higher than the log K_{oc}s used in 'Desire for levels' (Van de Meent *et al.*, 1990).

The MPCs for benzo[*a*]pyrene for soil and sediment differ approximately a factor 10. The reason is that the sediment MPC is calculated with the Ep-method and is not harmonized because no experimental sediment data are available. The MPC for soil for benzo[*a*]pyrene is harmonized with the available experimental soil data, resulting in the factor 10 difference.

7.7 Critical air concentrations

Steady-State soil/air Concentration Ratios (SSCR) for all the PAHs are calculated using the SIMPLE-BOX model as described by Van de Meent (1993). The SIMPLE-BOX model is a model that is often referred to as the Mackay-type: it is a multimedia fate model in which the environmental compartments are represented by homogenous boxes. For an extensive description of the model reference is made to Van de Meent (1993) and Van de Meent and De Bruijn (1995).

From this SSCR it is possible to calculate a Critical Air Concentration using formula 7.1. The meaning of this Critical Air Concentration ($CRITCONC_{air}$) is that the concentration in soil would become equal to the Maximum Permissible Concentration if the concentration in air would be maintained at the Critical Air Concentration.

Formula 7.1 Calculation of Critical Air Concentrations

$$CritCONC_{air} = MPC_{soil} / SSCR_{soil/air}$$

$CritCONC_{air}$	= critical concentration in air in g/m3
MPC_{soil}	= maximum Permissible Concentration in soil in g/kg (dry weight)
$SSCR_{soil/air}$	= steady State Concentration Ratio soil/air in m3/kg (dry weight)

The calculations are performed in the same way as described in Van de Meent *et al.* (1995) for pesticides. For each of the PAHs considered the substance specific characteristics as molecular weight, vapour Pressure, log K_{ow} (star value) and water solubility from table 2.2 are used as input. Besides this the Melting Point and DT50 in soil from Mackay *et al.* (1992) are used. The only difference with the calculations in Van de Meent *et al.* (1995) is the fraction leaching from the soil, which was assumed 0.9 in the case of the pesticides (Van de Meent, 1995). In the calculations for PAHs a fraction leaching of 0.4 is assumed. A first comparison of results using both fractions showed that the outcome was not influenced by this change.

The Steady-State soil/air Concentration Ratios (SSCR) and critical air concentrations for all the PAHs are listed in table 7.8. In the calculations it is assumed that the main emission route is through the air (the primary compartment) and that natural soil is the compartment of focus (secondary compartment). This secondary compartment is only loaded indirectly via the primary compartment, the air.

Table 7.8 Calculation of Critical Air Concentrations for the PAHs considered

	MPC_{soil} (mg/kg)	$SSRC_{(soil-air)}$ $m^3/kg(dry)$	Critical air conc. g/m^3
Naphthalene	0.14 (EP)	$9.99*10^{-1}$	$1.4*10^{-4}$
Anthracene	0.12 (EP)	$1.40*10^{+1}$	$8.6*10^{-6}$
Phenanthrene	0.51 (EP)	$1.50*10^{+1}$	$3.3*10^{-6}$
Fluoranthene	2.6 (EP)	$2.00*10^{+2}$	$1.3*10^{-5}$
Benzo[*a*]anthracene	0.25 (EPA/10)	$1.10*10^{+3}$	$2.2*10^{-7}$
Chrysene	10.7 (EP)	$8.10*10^{+3}$	$7.8*10^{-7}$
Benzo[*k*]fluoranthene	2.4 (EP)	$1.00*10^{+4}$	$2.4*10^{-7}$
Benzo[*a*]pyrene	0.26 (EPA/10)	$8.20*10^{+3}$	$3.2*10^{-8}$
Benzo[*ghi*]perylene	7.5 (EP)	$1.10*10^{+4}$	$4.7*10^{-7}$
Indeno[*1,2,3-cd*]pyrene	5.9 (EP)	$1.00*10^{+4}$	$5.8*10^{-7}$

The used extrapolation method is placed between parenthesis

The coherence criterion can only be tested for benzo[*a*]pyrene. This is done by comparing the concentration at steady state in the secondary compartments (soil and water) with the MPC proposed in that compartment. The MPC_{air} for benzo[*a*]pyrene is 1 ng/m^3 (VROM, 1994; Janus *et al.*, 1994) and is based on epidemiological studies (Slooff *et al.*, 1989). The analysis indicates that maintaining the concentration at the MPC_{air} level will result in concentrations in soil and water of 0.000032 mg/l and 0.0082 mg/kg respectively which is far below the MPCs proposed. The concentration in water is calculated using the $SSCR_{water}$, which is $3.2*10^{+1}$ m^3/l.

8 DISCUSSION

In this chapter a number of subjects are discussed, starting with the availability of data (see chapter 8.1). In chapter 8.2 a number of special PAH properties are discussed in relation with the derivation of the MPCs. In chapter 8.3 the derivation of the 'final' MPCs is discussed. In chapter 8.4 the subject combination toxicity is discussed. Finally, in chapter 8.5 the MPCs and NCs are compared with the available data on natural background concentrations.

8.1 Data availability

In order to derive reliable risk levels data availability is a very important item. In the present report the risk levels for "the MILBOWA" PAHs are updated. This update for PAHs is necessary because MPCs and NCs presented in 'Desire for levels' (Van de Meent *et al.*, 1990) have been derived from scarce laboratory studies and estimated values from QSARs.

Aquatic toxicity data
Most of the new published studies focus on the phenomenon of light induced photo-oxidation (phototoxicity). These studies are taken into account according to the criteria established in chapter 3.2.2. For a number of PAHs (e.g. phenanthrene, fluoranthene, benzo[*k*]fluoranthene, chrysene, benzo[*a*]pyrene and benzo[*ghi*]perylene) TNO carried out chronic 'Early Life Stage' ELS tests with fishes (Hooftman, 1991; Hooftman & Evers de Ruiter, 1992a; 1992b; 1992c; 1992d). The results of these tests are used, but a few studies were not in agreement with the quality criteria established in the project 'Setting environmental quality objectives'(ACT, 1994). Although the research carried out by TNO results in extra chronic toxicity data for a number of PAHs, there are still not enough chronic toxicity data available to use the refined effect assessment method (Aldenberg & Slob, 1993). Especially studies with Algae are lacking in most cases.

Soil and sediment data
The total number of soil toxicity studies, concerning PAHs is very limited. For only 3 PAHs reliable toxicity data were found. Almost no sediment toxicity studies are found in the literature.

Log K_{oc}s
For naphthalene, anthracene, phenanthrene and fluoranthene a relatively large data set is available. For all other PAHs at least two experimental log K_{oc} value are available.

8.2 Special PAHs properties

Volatility

A few of the low molecular weight PAHs are moderately volatile, in a number of cases this may result in low recoveries of the test substances in laboratory tests. This is also experienced by Hooftman, 1991; Hooftman & Evers de Ruiter, 1992a; 1992b; 1992c and 1992d); it seemed very hard to maintain constant exposure concentrations in their experiments. Especially for naphthalene volatility seems to be a very important loss-factor. From the acute toxicity results for this PAH it can be seen that in most closed static- and closed continuous flow culture systems resulted in higher toxicity (see appendix 2). Since not enough data are available to test if these observations are significant it remains unclear if special attention has to be paid to the volatility of low molecular PAHs. If however volatility is important one should follow the procedures described in Van de Plassche *et al.* (1993), where MPCs for volatile compounds are derived for water, soil, sediment and air (see also chapter 8.3, critical air concentrations). In this report all studies are judged case by case if volatility influences the test concentrations.

Water solubility

Most PAHs have very low to moderate low water solubility. In many cases large amounts of solvents are used in toxicity tests with substances with low water solubility. This is also the case with many studies concerning PAH toxicity. For this reason many studies are rejected.

Log K_{oc}s

Most PAHs are extreme hydrophobic which causes problems when deriving reliable log K_{oc}s. Therefore the co-solvent technique is applied in order to measure log K_{oc}s in a way that there is a higher correlation between hydrophobicity and log K_{oc}s. For a number of PAHs this co-solvent method is used. For soil this does not result in higher log K_{oc}s (Nkedi-Kizza *et al.*, 1985), for sediment however this results in high log K_{oc}s (Evers & Smedes, 1993). From our dataset it seems that log K_{oc}s for sediment are higher than log K_{oc}s for soil. It is not possible to decide whether this is a result of experimental conditions or a difference between partitioning of compounds in sediment or soil. Kile *et al.* (1995) found that sediment K_{oc}s, for nonpolar organic pollutants, were twice as high as the soil K_{oc}s. They suggest that the process that converts eroded soils into bed sediments causes a change in the organic matter properties. More experimental results are necessary to determine if the sediment and soil log K_{oc}s for PAHs are different.

Normally experimental data are preferred above estimated values. The experimental values have large variations, which makes it difficult to judge whether it is valid to use these values for equilibrium partitioning. Because the reliability of the experimental data

remains unclear and the estimated data from Karickhoff (1981) and Gerstl (1990) seem to be low compared with the experimental data in the low log K_{ow} region, it is decided to use the log K_{oc}s from DiToro *et al.* (1991) to calculate the $K_{p,s/l}$-values. The log K_{oc}s from DiToro present a middle course between 'high' experimental values and 'low' estimated values.

Light induced photo-oxidation (phototoxicity)
As mentioned earlier, UV- and a large part of the visible light in the Dutch eutrophic waters is absorbed by humic substances. It is therefore not very likely that the degree of phototoxicity seen in laboratory tests will have the same impact in field situations. Unfortunately there are practically no field tests available to validate this approach. One of the field studies in which significant phototoxicity of PAHs is observed, is a study with the oligochaete *Lumbriculus variegatus* (Monson *et al.*, 1995). The conclusion in this paper is that disregarding phototoxic effects may provide values that are substantially underprotective for benthic communities. In a comparable field study with *Ceriodaphnia dubia* enhanced toxicity was observed in the presence of sunlight relative to shaded conditions (Ireland *et al.*, 1993; cited in Monson *et al.*, 1995). The conclusion is that phototoxicity is probably an important toxicity mechanism in the laboratory and in some field situations. It should also be remarked that it is not possible to relate the higher toxicity of anthracene and benzo[*k*]fluoranthene to a phototoxic mode of action in this report.

It should be stressed here that field evaluations are necessary to be able to quantify aspects as phototoxicity.

Carcinogenicity and mutagenicity
It can be expected that carcinogenic and mutagenic effects on the individual level may occur. The impact of these effects on populations and ecosystems are however, not clear. At the moment is not possible to incorporate these effects into the currently applied methods.

Bioaccumulation and secondary poisoning
Although PAHs tend to accumulate in some species (mainly invertebrates), no data are available on accumulation in species higher in the foodchain like birds and mammals. Because it is well known that fish, birds and mammals have MFO enzyme systems which enables them to metabolize and thereafter excrete PAHs and/or PAH metabolites no special attention is paid to secondary poisoning in this report. However, the effects of the metabolites before excretion may cause other effects, which are still unclear (see also § 2.3, carcinogenicity/mutagenicity).

8.3 Maximum Permissible Concentrations

Aquatic environment

The question whether to use the experimental data or QSAR predicted NOECs to derive MPCs remains a difficult question. The MPCs derived from the experimental data are low when compared with the MPCs presented in 'Desire for levels' (Van de Meent *et al.*, 1990) and the MPCs estimated with the QSAR-approach from Van Leeuwen *et al.* (1992). The MPCs estimated with this QSAR-method are higher than the MPCs presented in 'Desire for levels' (Van de Meent *et al.*, 1990). One of the reasons for the high (experimental) MPCs are the high extrapolation factors used, when applying the modified EPA-method. The MPCs estimated with the 'new' QSAR-method are calculated using the refined effect assessment method. The QSAR estimated MPCs presented in 'Desire for levels' (Van de Meent *et al.*, 1990) were adjusted with a factor 5, because the experimental NOECs available at that time were a factor 3-10 lower than the QSAR-NOECs.

The reliability of the experimental MPCs is not doubted since they are derived from studies which are evaluated using a large number of quality criteria. The QSAR-approach from Van Leeuwen *et al.* (1990) and the QSARs from De Wolf *et al.*, 1988 and Van Leeuwen *et al.*, 1990 are methods that estimate toxicity from the structure and physical-chemical properties of the compound in question. From the comparison between experimental NOECs and the 'new' QSAR estimated NOECs (chapter 5) it is evident that some PAHs do not act by narcosis (anthracene and benzo[*k*]fluoranthene). For the other PAHs in the comparison it is not clear whether they do or do not act by narcosis. From the comparison it is also obvious that there is a tendency that experimental NOECs are lower than the QSAR estimated NOECs. It is not inconceivable that the QSAR-method underestimates the toxicity of the PAHs. It is therefore decided to prefer the experimental data above the QSAR-data to derive the 'final' MPCs for the aquatic environment. This results in 7 'final' MPCs for the aquatic environment for, naphthalene, anthracene, phenanthrene, fluoranthene, benzo[*a*]anthracene, benzo[*k*]fluoranthene and benzo[*a*]pyrene.

For chrysene, benzo[*ghi*]perylene and indeno[*1,2,3-cd*]pyrene no experimental data are available. For indeno[*1,2,3-cd*]pyrene the QSAR-approach (Van Leeuwen *et al.*, 1992) can not be applied because all NOECs are estimated more than 10 times above the maximum water solubility. Therefore, it is decided to use the MPC presented in 'Desire for levels' (Van de Meent *et al.*, 1990) for indeno[*1,2,3-cd*]pyrene. For chrysene and benzo[*ghi*] perylene MPCs are calculated (table 6.2) using the QSAR-approach (Van Leeuwen *et al.*, 1992), these 'new' QSAR determined MPCs are preferred above the 'old' QSAR determined MPCs (Van de Meent *et al.*, 1990). Because of the discussed uncertainties in the QSAR-approach it is decided to correct these MPCs (chrysene and benzo[*ghi*]perylene)

with a factor 10. Although there is no scientific basis to use this factor, it is decided in absense of better knowledge, to apply the factor 10.

Soil and sediment
Almost all MPCs for soil are based on equilibrium partitioning because no experimental dat are available. Only for anthracene, benzo[*a*]anthracene and benzo[*a*]pyrene MPCs for soil are derived from experimental data. All the MPCs for sediment are based on the Ep-method.

The MPCs for benzo[*a*]pyrene for soil and sediment are different. The reason is that the sediment MPC is calculated with the Ep-method and is not harmonized because no experimental sediment data are available. The MPC for soil for benzo[*a*]pyrene is harmonized with the available experimental soil data.

Air
Only for benzo[*a*]pyrene the coherence criterion is tested. The conclusion is that maintaining the concentration at the MPC_{air} level (benzo[*a*]pyrene) will result in steady state concentrations in soil and water that are lower than the proposed MPCs in these compartments.

8.4 Combination toxicity

Not much data on combination toxicity of PAHs are available. In a study with *Daphnia magna* exposed to combinations of phenanthrene, anthracene, naphthalene and acenaphtene antagonistic effects were found using the concentration addition model (Munoz *et al.*: cited in Hensbergen and Van Gestel, 1995). From a study performed with *Brachydanio rerio* exposed to different PAHs Hooftman *et al.* (1993: cited by Hensbergen and Van Gestel, 1995) concluded that the PAHs studied act additive. This conclusion is however doubted by Hensbergen and Van Gestel (1995) because of the use of NOECs as scalars and the use of test concentrations in the vicinity of maximum solubility.

In a literature study performed by Hensbergen and Van Gestel (1995) a procedure was proposed to incorporate combination toxicity in risk limits. According to the authors it is necessary to know the toxicity of each of the substances of a mixture for different species and the fraction of each of the substances in this mixture. An important assumption in this procedure is that the substances in the mixture have the same mode of action.

According to the Hensbergen and Van Gestel (1995) it is however at this moment, due to lack of data, not possible to propose a risk limit for soil, for a combination of the 10

PAHs in this report. Besides this from the comparison of QSAR-data and experimental data in chapter 5 of the present report it is concluded that not all the PAHs considered have the same mode of action. Because of these reasons it is at this moment not possible to derive a scientifically underpinned risk limit for the 10 PAHs combined. It is only possible to calculate the combination toxicity for the PAHs that are known to have the same mode of action. With the results in this report however, this is not possible.

8.5 Natural background concentrations

In table 8.1 a comparison is made between the MPCs, NC-values and the natural background concentrations for water and soil.

Aquatic environment

If the background concentrations as presented in 'Desire for levels' (Van de Meent *et al.*, 1990) (table 8.1) for PAHs are compared with the NC- and MPCs derived in this report, it is clear that for a number of PAHs the NC-values and one MPC are exceeded by the available natural background concentrations. These background concentrations are derived from a literature study carried out by Geochem-Research, (1989).

Table 8.1 Comparison of MPCs and NCs for water and soil with natural background concentrations

compound	MPC $_{(water)}$ (µg/l)	NC $_{(water)}$ (µg/l)	Backgr.# conc. $_{water}$ in solution (µg/l)	MPC $_{(soil)}$ (mg/kg)	NC $_{(soil)}$ (mg/kg)	Backgr.## conc. $_{soil}$ (mg/kg)
Naphthalene	1.2	0.012	-	0.14[a]	0.0014	-
Anthracene	0.07	*0.0007*	0.004	0.12[a]	*0.0012*	0.006
Phenanthrene	0.30	*0.003*	0.05	0.51[a]	*0.005*	0.078
Fluoranthene	0.30	*0.003*	0.009	2.6[a]	0.026	0.122
Benzo[*a*]anthracene	0.01	*0.0001*	0.0002	0.25	*0.0025*	0.033
Chrysene	0.34	0.0034	0.001	10.7[a]	0.107	-
Benzo[*k*]fluoranthene	0.04	0.0004	0.0004	2.4[a]	*0.024*	0.043
Benzo[*a*]pyrene	0.05	0.0005	0.0003	0.26	0.0026	-
Benzo[*ghi*]perylene	0.03	0.0003	0.00006	7.5[a]	0.075	-
Indeno[*1,2,3-cd*]pyrene	0.04	0.0004	-	5.9[a]	0.059	-

a based on equilibrium partitioning
BC MPC or NC exceeded by the natural Background concentration (*BC*)
Geochem-Research (1989)
Van Brummelen *et al.*, in press; estimated natural background concentration (Noord-Hollands duinreservaat)

Soil

Van Brummelen *et al.* (in press) obtained estimated natural background concentrations by fitting PAH loads as a function of the distance from a blast furnace plant. The values presented in table 8.2 are based on these estimates (recalculated for standard soil). If the background concentrations for the individual PAHs are compared with the NCs and MPCs derived in this report, it is seen that for all the PAHs for which background concentrations are available the NCs are exceeded by the available natural background concentrations. For the values in table 8.2 and the values given by Faber and Heijmans (submitted) it is questionable if these values can be considered as natural background concentrations because contamination from anthropogenic sources can not be excluded.

In table 8.2 a comparison is made between the MPCs, NC-values and the natural background concentrations for sediment.

Sediment

If the background concentrations for sediment as presented in 'Desire for levels' (Van de Meent *et al.*, 1990) (table 8.2) for PAHs are compared with the NC- and MPCs derived in this report, it is seen that for two PAHs the NC-values are exceeded by the available natural background concentrations. These background concentrations are derived from a literature study carried out by Geochem-Research (1989). The values derived from this literature study are based on measurements of pre-anthropogenic sediments, which are considered uncontaminated (Van de Meent *et al.*, 1990). Other results available are the measurements of Directorate-General of public Works and Water Management (DGW, 1992). The results of background concentration in saltwater sediments were comparable with the concentrations from Geochem-Research (1989). The results of the measured values of the Province Zuid-Holland (Naald, 1990) are not considered being natural background concentrations, because contamination can not be excluded.

It must be stressed however that the comparison of the derived MPCs and NCs, for soil, sediment and water, with the mentioned background concentration is not based on an extensive update of literature on this subject. It should also be mentioned that the background concentration presented in tables 8.1-8.3 are average values. These average values are the mean values from ranges of measured natural background concentrations. These ranges show the uncertainties in the average natural background concentrations measured in the environment. For example the (aquatic) natural background concentration for phenanthrene is 0.05 µg/l, calculated from the range 0.0098-0.098 µg/l and 0.0004 µg/l for benzo[*k*]fluoranthene calculated from the range 0.00008-0.0008 µg/l.

Table 8.2 Comparison of MPCs and NCs for sediment with natural background concentrations

compound	MPC (sediment) (mg/kg)	NC (sediment) (mg/kg)	Backgr.# conc. sediment (mg/kg)
Naphthalene	0.14[a]	0.0014	-
Anthracene	0.12[a]	*0.0012*	0.002
Phenanthrene	0.51[a]	*0.005*	0.03
Fluoranthene	2.6[a]	0.026	0.01
Benzo[*a*]anthracene	0.36[a]	0.0036	0.001
Chrysene	10.7[a]	0.107	0.005
Benzo[*k*]fluoranthene	2.4[a]	0.024	0.005
Benzo[*a*]pyrene	2.7[a]	0.027	0.004
Benzo[*ghi*]perylene	7.5[a]	0.075	0.003
Indeno[*1,2,3-cd*]pyrene	5.9[a]	0.059	-

a based on equilibrium partitioning
BC MPC or NC exceeded by the natural Background concentration (*BC*)
Geochem-Research (1989); natural background conc. in pre-anthropogenic sediment from the river Rhine

At the moment there is a discussion how to deal with natural background concentrations in the framework of the derivation of environmental quality objectives for metals. In previous reports risk limits are set equal to the natural background concentrations available if the risk limit exceeds the natural background concentration. A new methodology on how to integrate natural background concentrations into the derivation of risk limits will become available (Struijs *et al.*, in prep).

Besides the 10 PAHs selected for this report many other 'natural occurring' PAHs are found in the environment. For example fluorene, pyrene, coronene and benzo[*b*]fluoranthene. In some cases the background concentrations of these PAHs are higher than the background concentrations of the 10-PAHs considered (Van Brummelen *et al.*, in press; DGW (1992)).

9 CONCLUSIONS

Data availability

- Although new aquatic toxicity data are available, the number of reliable toxicity data for most PAHs is still very disappointing. Therefore all experimental aquatic MPCs are calculated using the preliminary effect assessment method.

- The number of reliable soil toxicity data is very low. Only three MPCs for soil are based on experimental data. Almost no sediment data are available.

- The number of log K_{oc} studies for the high molecular PAHs is very low.

Log K_{oc}s

- From the results presented in this report it seems that sediment log K_{oc}s are higher than soil log K_{oc}s. More insight in differences between sediment and soil derived log K_{oc}s is necessary.

Special PAH properties

- Low water solubility of most PAHs causes rejection of many toxicity studies.

- Phototoxicity may be a significant consideration for organisms exposed to PAHs in laboratory situations, but is not expected to have the same impact in field situations. To validate this assumption, actual field experiments are necessary.

- From a comparison of QSAR-NOECs with experimental NOECs it is concluded that anthracene and benzo[*k*]fluoranthene are much more toxic than expected. Apparently a specific none specified mode of action causes higher toxicity.

- It is not possible at the moment to incorporate effects as carcinogenicity and mutagenicity into the risk assessment methods applied.

Derivation of MPCs

- The use of experimental data for derivation of MPCs leads to MPCs that are lower than the MPCs presented in 'Desire for levels' (Van de Meent *et al.*, 1990).

- From the results in this report it seems that the 'new' QSAR-approach from Van Leeuwen *et al.* (1992) results in estimated NOECs which are more than 10 times the maximum water solubility for PAHs with high molecular weight and low water solubility.

- The 'new' QSAR-approach (Van Leeuwen *et al.*, 1992) results in higher MPC-values for PAHs than the QSAR-method applied in 'Desire for levels' (Van de Meent *et al.*, 1990).

- The MPC_{air} for benzo[*a*]pyrene leads to steady state concentrations in soil and water that are lower than the proposed MPCs in these compartments.

Combination toxicity

- In the present report it is concluded that not all the PAHs considered have the same mode of action. Therefore, it is at this moment not possible to derive a scientifically underpinned risk limit for the 10 PAHs combined.

Critical air concentrations

- A coherence test for benzo[*a*]pyrene indicates that maintaining the concentration at the MPC_{air} level 1 ng/m^3 will result in concentrations in soil and water that are far below the MPCs proposed.

Background concentrations

- For a number of PAHs the NC-values for soil, sediment and water and for one PAH the MPC_{water} are/is exceeded by the natural background concentrations. These natural background concentrations are the same values as presented in 'Desire for levels' (Van de Meent *et al.*, 1990). It must be stressed however that the comparison of the derived MPCs and NCs with the natural background concentrations is not based on an extensive update of literature on this subject. A more extended research concerning background concentrations is necessary.

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APPENDICES

Appendix 1 Online searching scheme for fresh-, saltwater, soil/sediment and log K_{oc} values

name of compound	molecular formula	CAS reg. nr.	online aquatic fresh/salt	online soil	online $K_{p,s/l}$
Naphthalene	$C_{10}H_8$	91-20-3	>11/92	>11/92	>11/92
Anthracene	$C_{14}H_{10}$	120-12-7	" "	" "	" "
Phenanthrene	$C_{14}H_{10}$	85-01-8	" "	" "	" "
Fluoranthene	$C_{16}H_{10}$	206-44-0	" "	" "	" "
Benzo[*a*]anthracene	$C_{18}H_{12}$	56-55-3	" "	" "	" "
Chrysene	$C_{18}H_{12}$	218-01-9	" "	" "	" "
Benzo[*k*]fluoranthene	$C_{20}H_{12}$	207-08-9	" "	" "	" "
Benzo[*a*]pyrene	$C_{20}H_{12}$	50-32-8	" "	" "	" "
Benzo[*ghi*]perylene	$C_{22}H_{12}$	191-24-2	" "	" "	" "
Indeno[*1,2,3-cd*]pyrene	$C_{22}H_{12}$	193-39-5	" "	" "	" "

The online searching period for the IPCS/EHC (in prep.), according to BKH (P. Okkerman *pers. comm.*), is 1988-(november)1992. This document is considered a reliable review for retrieving data from the literature. The online research carried out at the National Institute for Public Health and Environment is started at 11/1992.

Appendix 2 Freshwater toxicity data

In this appendix toxicity data for freshwater organisms are presented in three different tables:
- table 2.1.x: chronic toxicity data: NOECs,
- table 2.2.x: acute toxicity data: L(E)C50s,
- table 2.3.x: data from deviating toxicity tests.

Legend:

organism	Species used in the test, followed by age, length, weight and/or life stage
A	Y test substance analysed in test solution N test substance not analysed in solution
test type	S: static; R: renewal; CF: continuous flow; IF: Intermittent flow $_c$: closed testvessels
test water	am : artificial medium; tw : tap water; nw : natural water; rw : reconstituted water;
test sustance purity	percentage active ingredient; anal. : analytical grade; tech. : technical grade; high : high but unknown purity
exposure time	min: minute(s); h: hour(s); d: day(s); w: week(s); m: month(s);
results	> and ≥ value indicated is highest concentration used in the test. < and ≤ value indicated is lowest concentration used in the test.
α	given value based on measured concentrations
-	no information available

Content:

2.1.5 Benzo[*k*]fluoranthene
2.1.6 Benzo[*a*]pyrene

acute toxicity data (table 2.2.x)
2.2.1 Naphthalene
2.2.2 Anthracene
2.2.3 Phenanthrene
2.2.4 Benzo[*a*]anthracene
2.2.5 Benzo[*a*]pyrene

data from deviating toxicity tests (table 2.3.x)
2.3.1 Naphthalene
2.3.2 Anthracene
2.3.3 Phenanthrene
2.3.4 Fluoranthene
2.3.5 Chrysene
2.3.6 Benzo[*a*]pyrene
2.3.7 Benzo[*ghi*]perylene

Table 2.1.1 : Chronic toxicity of naphthalene to freshwater organisms: NOECs

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l	Reference
Pisces										
Pimephales promelas, embryo/larvae	Y	CF	-	rw	7.9-8.0	535-596	30 d	NOEC	450[a]	DeGraeve *et al.*, 1982
Pimephales promelas, embryo/larvae	Y	CF	-	rw	7.9-8.0	535-596	30 d	NOEC	1,800[b]	DeGraeve *et al.*, 1982
Pimephales promelas, embryo/larvae	Y	CF	-	rw	7.9-8.0	535-596	30 d	NOEC	450[c]	DeGraeve *et al.*, 1982
Sarotherodon mossambicus, 18 g	N	R	-	tw	7.6	235	12 w	NOEC	2,300[d]	Dange & Masurekar, 1982

a hatchability; unclear dose response curve, 14% effect at 450 µg/l; solvent is methanol, <0.4 ml/l; lowest oxygen conc. in test 4.9 mg/l
b mortality; solvent is methanol, <0.4 ml/l; lowest oxygen conc. in test 4.9 mg/l
c length and weight growth; solvent is methanol, <0.4 ml/l; lowest oxygen conc. in test 4.9 mg/l
d growth measured as wet weight

Table 2.1.2 : Chronic toxicity of anthracene to freshwater organisms: NOECs

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l	Reference
Macrophyta										
Lemna gibba	Y	S	-	am	-	-	8 d	NOEC	300[1a]	Huang *et al.*, 1993
Algae/Chlorophyta										
Selenastrum capricornutum	Y	S	99.9%	am	7.5	-	22 h	NOEC	1.5[b] α	Gala & Giesy, 1992
Selenastrum capricornutum	Y	S	99.9%	am	7.5	-	22 h	NOEC	2.5[b] α	Gala & Giesy, 1992
Selenastrum capricornutum	Y	S	99.9%	am	7.5	-	22 h	NOEC	2.3[b] α	Gala & Giesy, 1992
Selenastrum capricornutum	Y	S	99.9%	am	7.5	-	22 h	NOEC	8.7[b] α	Gala & Giesy, 1992
Selenastrum capricornutum	Y	S	99.9%	am	7.5	-	22 h	NOEC	7.8[b] α	Gala & Giesy, 1992
Selenastrum capricornutum	Y	S	99.9%	am	7.5	-	24 h	NOEC	1.7[c] α	Gala & Giesy, 1992
Selenastrum capricornutum	Y	S	99.9%	am	7.5	-	24 h	NOEC	2.7[c] α	Gala & Giesy, 1992
Selenastrum capricornutum	Y	S	99.9%	am	7.5	-	24 h	NOEC	2.2[c] α	Gala & Giesy, 1992
Selenastrum capricornutum	Y	S	99.9%	am	7.5	-	24 h	NOEC	2.5[c] α	Gala & Giesy, 1992
Selenastrum capricornutum	Y	S	99.9%	am	7.5	-	24 h	NOEC	3.9[c] α	Gala & Giesy, 1992
Crustacea										
Daphnia magna	Y	R	anal.	am	8.1	230	21 d	NOEC	2.2[d] α	Foran *et al.*, 1991
Daphnia magna	Y	R	anal.	am	8.1	230	21 d	NOEC	4.1[d] α	Foran *et al.*, 1991
Daphnia magna	Y	R	anal.	am	8.1	230	21 d	NOEC	2.2[e] α	Foran *et al.*, 1991
Daphnia magna	Y	R	anal.	am	8.1	230	21 d	NOEC	2.2[f] α	Foran *et al.*, 1991
Daphnia magna	Y	R	anal.	am	8.1	230	21 d	NOEC	1.9[g] α	Foran *et al.*, 1991
Daphnia magna	Y	R	anal.	am	8.1	230	21 d	NOEC	4.5[h] α	Foran *et al.*, 1991
Daphnia magna	Y	R	anal.	am	8.1	230	21 d	NOEC	2.2[i] α	Foran *et al.*, 1991
Daphnia magna	Y	R	anal.	am	8.1	230	21 d	NOEC	1.9[j] α	Foran *et al.*, 1991
Daphnia magna	Y	R	anal.	am	8.1	230	21 d	NOEC	1.1[k] α	Holst & Giesy, 1989
Daphnia magna	Y	R	anal.	am	8.1	230	21 d	NOEC	0.63[l] α	Holst & Giesy, 1989

1 above water solubility, which is 45 µg/l, at 25°C

a growth; NOEC=EC10; light regime: (constant light 'cool white fluorescent lamps', producing UV-A + UV-B); ratio visible:UV-A:UV-B is 100:10:1 based on the number of photons, total intensity 40 $\mu mol*m^{-2}sec^{-1}$, this is comparable with natural sunlight (spectrum + intensity)

b growth rate; light regime: (constant light with 'white fluorescent bulbs', used with a filter to eliminate UV-A+B (<390nm)), (UV-A with increasing intensity from the first to the fifth downwards produced by blacklights, the intensity of the UV-A in the tests was 765, 410, 406, 218 and 125 $\mu W/cm^2$, UV-B radiation was filtered from the blacklight spectrum; actual conc. 70% of nominal conc. at t=0, and 50% after the renewal period of 8 h, the results are presented as the calculated values between t=0 and t=8 h; during each renewal the conc. new substance is added to derive the initial nominal conc.

c primary production; light regime: (constant light with 'white fluorescent bulbs', used with a filter to eliminate of UV-A+B (<390nm)), (UV-A with increasing intensity from the first to the fifth downwards produced by 'blacklights', the intensity of the UV-A in the tests was 765, 410, 406, 218 and 125 $\mu W/cm^2$, UV-B radiation was filtered from the blachlight spectrum; actual conc. 70% of nominal conc. at t=0, and 50% after the renewal period of 8 h, the results are presented as the calculated average between t=0-8 h according to a first order kinetics loss model; NOEC=EC10

d growth measured as intrinsic rate of increase; no UV-radiation; visible light by 'white fluorescent lamps'; light regime: 16 h light and 8 h dark

e growth measured as intrinsic rate of increase; UV-radiation at 31 $\mu W/cm^{-2}$; ratio UV-A:UV-B is 8:1; visible light by 'white fluorescent lamps'; light regime: 16 h light and 8 h dark

f growth measured as intrinsic rate of increase; UV-radiation at 60 $\mu W/cm^{-2}$; ratio UV-A:UV-B is 8:1; visible light by 'white fluorescent lamps'; light regime: 16 h light and 8 h dark

g growth measured as intrinsic rate of increase; UV-radiation at 117 $\mu W/cm^{-2}$; ratio UV-A:UV-B is 8:1; visible light by 'white fluorescent lamps'; light regime: 16 h light and 8 h dark

h reproduction; UV-radiation at 31 $\mu W/cm^{-2}$; ratio UV-A:UV-B is 8:1; visible light by white fluorescent lamps; light regime: 16 h light and 8 h dark

i reproduction; UV-radiation at 60 $\mu W/cm^{-2}$; ratio UV-A:UV-B is 8:1; visible light by white fluorescent lamps; light regime: 16 h light and 8 h dark

j reproduction; UV-radiation at 117 $\mu W/cm^{-2}$; ratio UV-A:UV-B is 8:1; visible light by white fluorescent lamps; light regime: 16 h light and 8 h dark

k reproduction measured as total number neonates afther 6 broods; no UV-radiation; visible light by 'white fluorescent lamps'; light regime: 16 h light and 8 h dark; NOEC=LOEC/2, 6% effect at 2.1 µg/l; the 6% is significant when compared with the control

l reproduction measured as total number neonates afther 6 broods; UV-radiation at 117 $\mu W/cm^{-2}$; ratio UV-A:UV-B is 8:1; visible light by 'white fluorescent lamps'; light regime: 16 h light and 8 h dark; NOEC=LOEC/3, 23% effect at 1.9 µg/l

Table 2.1.3 : Chronic toxicity of phenanthrene to freshwater organisms: NOECs

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l		Reference
Macrophyta											
Lemna gibba	Y	S	-	am	-	-	8 d	NOEC	600[a]		Huang *et al.*, 1993
Crustacea											
Daphnia magna	N	R	-	-	-	-	21 d	NOEC	180[b]		Hooftman & Evers-de Ruiter, 1992c
Daphnia magna	N	IF	-	-	-	-	21 d	NOEC	18[b]		Hooftman & Evers-de Ruiter, 1992c
Daphnia magna	N	IF	-	-	-	-	21 d	NOEC	56[c]		Hooftman & Evers-de Ruiter, 1992c
Daphnia magna	N	IF	-	-	-	-	21 d	NOEC	32[d]		Hooftman & Evers-de Ruiter, 1992c
Daphnia pulex, <24 h	Y	R	-	tw	6.9-7.5	41-50	7-11 w	NOEC	110[e]	α	Geiger & Buikema, 1982
Daphnia pulex, <24 h	Y	R	-	tw	6.9-7.5	41-50	7-11 w	NOEC	60[f]	α	Geiger & Buikema, 1982
Pisces											
Brachydanio rerio	N	R	-	-	-	-	21 d	NOEC	32[g]		Hooftman & Evers-de Ruiter, 1992c
Brachydanio rerio	N	R	-	-	-	-	21 d	NOEC	56[h]		Hooftman & Evers-de Ruiter, 1992c
Brachydanio rerio	N	R	-	-	-	-	21 d	NOEC	≥56[i]		Hooftman & Evers-de Ruiter, 1992c

a growth; NOEC=EC10; light regime: (constant light 'cool white fluorescent lamps', producing UV-A + UV-B); ratio visible:UV-A:UV-B is 100:10:1 based on the number of photons, total intensity 40 µmol*$m^{-2}sec^{-1}$, this is comparable with natural sunlight (spectrum + intensity)

b reproduction

c mortality

d growth

e reproduction as number of broods per animal, and number of death young per brood per animal; exposure time is total life-time; light regime 16 h light and 8 h dark, by 'cool white fluorescent bulbs'

f growth measured as the length of the first brood animals; exposure time is total life-time; light regime 16 h light and 8 h dark, by 'cool white fluorescent bulbs'

g length growth

h growth measured as wet weight

i mortality/hatching

Table 2.1.4 : Chronic toxicity of fluoranthene to freshwater organisms: NOECs

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l	Reference
Macrophyta										
Lemna gibba	Y	R	-	am	-	-	8 d	NOEC	200[a]	Ren *et al.*, 1994
Pisces										
Brachydanio rerio, eggs	Y	IF	96%	rw	7.3-7.8	210	41 d	NOEC	69[b] α	Hooftman & Evers-de Ruiter, 1992a
Brachydanio rerio, eggs	Y	IF	96%	rw	7.3-7.8	210	41 d	NOEC	6.9[c] α	Hooftman & Evers-de Ruiter, 1992a
Brachydanio rerio, eggs	Y	IF	96%	rw	7.3-7.8	210	41 d	NOEC	22[d] α	Hooftman & Evers-de Ruiter, 1992a

a growth; NOEC=EC10; light regime: (constant light 'cool white fluorescent lamps', prucing UV-A + UV-B); ratio visible:UV-A:UV-B is 100:10:1 based on the number of photons, total intensity 40 µmol*$m^{-2}sec^{-1}$, this is comparable with natural sunlight (spectrum + intensity)

b mortality of young fish; actual conc. of the substance 27-76%, average 48%; highest conc. (180 µg/l) is tested in separate test

c growth measured as fish length; actual conc. of the substance 27-76%, average 48%; highest conc. (180 µg/l) tested in separate test

d same as c, but growth measured as wet weight

Table 2.1.5 : Chronic toxicity of benzo[*k*]fluoranthene to freshwater organisms: NOECs

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l		Reference
Pisces											
Brachydanio rerio, eggs	Y	IF	100%	rw	7.9-8.2	206	6 w	NOEC	0.48[a]	α	Hooftman & Evers-de Ruiter, 1992b
Brachydanio rerio, eggs	Y	IF	100%	rw	7.9-8.2	206	6 w	NOEC	0.27[b]	α	Hooftman & Evers-de Ruiter, 1992b
Brachydanio rerio, eggs	Y	IF	100%	rw	7.9-8.2	206	6 w	NOEC	0.48[c]	α	Hooftman & Evers-de Ruiter, 1992b

a mortality of young fish; actual conc. 36-109% of initial conc., average 72%
b growth measured as fish length; actual conc. 36-109% of initial conc., average 72%
c same as b, but now growth measured as wet-weight

Table 2.1.6 : Chronic toxicity of benzo[*a*]pyrene to freshwater organisms: NOECs

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l	Reference
Pisces										
Brachydanio rerio	Y	-	-	-	-	-	42 d	NOEC	6.3[1] α	TNO, 1993

1 above the water solubility, which is 3.8 µg/l at 25°C

Table 2.2.1 : Acute toxicity of naphthalene to freshwater organisms: L(E)C50s

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l	Reference
Algae/Chlorophyta										
Chlorella vulgaris	N	S	-	-	-	-	48 h	EC50	33,000[1a]	Kauss & Hutchinson, 1975/ Basis-Document RIVM for PAHs, 1989
Mollusca										
Physa gyrina, 7.5 mm, 0.057 g	Y	S_c	-	nw	7.8	140	48 h	LC50	5,000	Milleman *et al.*, 1984
Crustacea										
Daphnia magna	Y	S	-	tw	8.0-8.6	-	48 h	LC50	3,400[b]	Crider *et al.*, 1982
Daphnia magna, 1.5 mm, 4-6 d	N	S_c	≥97%	am	6.0-7.0	-	48 h	LC50	16,600	Bobra *et al.*, 1983
Daphnia magna, <24 h	N	S_c	≥97%	rw	-	-	48 h	EC50	2,200[c]	Munoz & Tarazona, 1993
Daphnia magna, adult, mixed age	N	S	-	nw	7.6	134	48 h	LC50	22,600[d]	Eastmond *et al.*, 1984
Daphnia magna, 24 h	Y	S_c	-	nw	7.8	140	48 h	EC50	2,200[e]	Milleman *et al.*, 1984
Daphnia pulex, <24 h	N	S	≥96%	rw	-	170	48 h	EC50	4,700[f]	Smith *et al.*, 1988
Daphnia pulex, 1.9-2.1 mm	N	S_c	-	nw	7.5	-	96 h	LC50	1,000[g]	Trucco *et al.*, 1983
Daphnia pulex, young	Y	S	-	tw	6.8-7.5	43-48	48 h	LC50	3,400[h] α	Geiger & Buikema, 1981
Daphnia pulex, neonates	Y	S	-	tw	7.2	43	48 h	LC50	3,400[h] α	Geiger & Buikema, 1982
Insecta										
Chironomus attenuattus, 4 th. instar	N	S	-	tw	7.9-8.3	-	24 h	LC50	13,000	Darville & Wilhm, 1984
Chironomus tentans, 4 th. instar	Y	S_c	-	nw	7.8	140	48 h	EC50	2,800[e]	Milleman *et al.*, 1984
Tanytarsus dissimilis, 4 th. instar	N	S	-	tw	7.9-8.3	-	48 h	LC50	12,600	Darville & Wilhm, 1984
Pisces										
Micropterus salmoides, eggs 2-4 h post spawning	Y	CF	-	am	7.4-8.1	86-116	96 h	LC50	680	Milleman *et al.*, 1984
Oncorhynchus mykiss, eggs 20 min. post fertilization	Y	CF	-	am	7.4-8.1	86-116	96 h	LC50	120	Milleman *et al.*, 1984
Pimephales promelas, 34 d	N	S	98%	-	7.4	44	96 h	LC50	6,100	Geiger *et al.*, 1985
Pimephales promelas, 1-2 months, 0.27 g, 28 mm	Y	S_c	-	nw	7.8	140	96 h	LC50	2,000[e]	Milleman *et al.*, 1984

1 above water solubility, which is 31,000 µg/l, at 25°C

a growth; original data not available
b test performed in the dark
c immobility; solvent is methanol, max. 2 ml/l; minimal oxygen conc. 2 mg/l
d solvent is acetone + surfactant triton X-100, 0.5 ml/l and 0.5 mg/l respec.; oxygen conc. ca. 3.9 mg/l
e immobility; solvent methanol , 1ml/l
f immobility; solvent is acetone, 0.5 ml/l
g light regime is 12 h light and 12 h dark, with mixed fluorescent and natural light
h solvent is methanol, <0.4 ml/l; lowest oxygen conc. in test 4.9 mg/l

Table 2.2.2 : Acute toxicity of anthracene to freshwater organisms: L(E)C50s

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l		Reference
Pisces											
Lepomis macrochirus, juvenile, 0.8 g, 3.1 cm	Y	CF	tech.	tw	7.7	326	5 d	LC50	1.3[a]	α	McCloskey & Oris, 1991
Lepomis macrochirus, juvenile, 0.8 g, 3.1 cm	Y	CF	tech.	tw	7.7	326	5 d	LC50	8.0[b]	α	McCloskey & Oris, 1991
Lepomis macrochirus, juvenile, 0.8 g, 3.1 cm	Y	CF	tech.	tw	7.7	326	5 d	LC50	3.8[c]	α	McCloskey & Oris, 1991
Lepomis macrochirus, juvenile, 0.8 g, 3.1 cm	Y	CF	tech.	tw	7.7	326	5 d	LC50	8.3[d]	α	McCloskey & Oris, 1991
Lepomis macrochirus, juvenile, 0.5-1 g, 2-3 cm	Y	CF	tech.	tw	8.2	328	6 d	LC50	2.8[e]		Oris & Giesy, 1985
Lepomis spec., juvenile, 0.5-1 g, 2-3 cm	Y	CF	tech.	tw	8.2	328	6 d	LC50	12[f]		Oris & Giesy, 1985
Lepomis spec., juvenile, 0.5-1 g, 2-3 cm	Y	CF	tech.	tw	8.2	328	6 d	LC50	18[g]		Oris & Giesy, 1985
Lepomis spec., juvenile, 0.5-1 g, 2-3 cm	Y	CF	tech.	tw	8.2	328	6 d	LC50	26[e]		Oris & Giesy, 1985
Insecta											
Aedes aegypti, third instar	Y	R	-	am	-	-	48 h	LC50	27[h]		Oris *et al.*, 1984

a constant illumination;, UV A+B and visible light, spectrum 91 % equal to natural sunlight; UV-A and -B intensities are 108 and 6.7 µW/cm^2; total intensity approximately equal to 0.5 and 1.0 meter depth in an eutrophic lake; 24 h pre-exposure to anthracene; 20 °C temperature

b as a, except the temperature is 20°C, and oxygen conc. is 8.1 mg/l

c as a, except the temperature is 30°C, and oxygen conc. is 6.9 mg/l

d as a, except the temperature is 30°C, and oxygen conc. is 8.1 mg/l

e 48 h pre-exposure to anthracene in the dark, followed by 96 h anthrancene + UV exposure; light regime is 24 h light during 96 h exposure; simulated sunlight produced by white and ultraviolet fluorescent bulbs; UV-B intensity is 15 µW/cm^2

f as e, except UV-B intensity is 170 µW/cm^2

g as e, except UV-B intensity is 70 µW/cm^2

h 24 h pre-exposure to anthracene in the dark, followed by 24 h anthrancene + UV exposure; light regime is 24 h light during 24 h UV + anthracene exposure; simulated sunlight (half clouded sky) bulbs; UV-B intensity is 15 µW/cm^2

Table 2.2.3 : Acute toxicity of phenanthrene to freshwater organisms: L(E)C50s

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l	Reference
Crustacea										
Daphnia magna, 1.5 mm, 4-6 d	N	S_c	≥97%	am	6.0-7.0	-	48 h	LC50	1,200[1]	Bobra *et al.*, 1983
Daphnia magna, <24 h	N	S_c	≥97%	rw	-	-	48 h	EC50	380[a]	Munoz & Tarazona, 1993
Daphnia magna, adult, mixed age	N	S	-	nw	7.6	134	48 h	LC50	840[b]	Eastmond *et al.*, 1984
Daphnia magna, 24 h	Y	S_c	-	nw	7.8	140	48 h	EC50	700[c]	Milleman *et al.*, 1984
Daphnia pulex, <24 h	N	S	≥96%	rw	-	170	48 h	EC50	350[d]	Smith *et al.*, 1988
Daphnia pulex, <24 h	N	S	≥96%	rw	-	hard	48 h	EC50	730[d]	Passino & Smith, 1987
Daphnia pulex, 1.9-2.1 mm	N	S_c	-	nw	7.5	-	96 h	LC50	100[e]	Trucco *et al.*, 1983
Daphnia pulex, young	Y	S	-	tw	6.8-7.5	43-48	48 h	LC50	1,140[1] α	Geiger & Buikema, 1981
Pisces										
Micropterus salmoides, eggs 2-4 h post spawning	Y	CF	-	am	7.4-8.1	86-116	96 h	LC50	250	Milleman *et al.*, 1984
Oncorhynchus mykiss, eggs 20 min. post fertilization	Y	CF	-	am	7.4-8.1	86-116	96 h	LC50	30	Milleman *et al.*, 1984

1 above water solubility, which is 1,100 µg/l, at 25°C

a immobility; solvent is methanol, max. 2 ml/l; oxygen conc. min. 2 mg/l
b solvent is acetone + surfactant triton X-100, 0.5 ml/l and 0.5 mg/l respec., lightregime 16 h light and 8 h dark; oxygen conc. ca. 3.9 mg/l
c immobility
d immobility; solvent is acetone, 0.5 ml/l
e light regime is 12 h light and 12 h dark, with mixed fluorescent and natural light; animals also exposed during the 24 h period

Table 2.2.4 : Acute toxicity of benzo[*a*]anthracene to freshwater organisms: L(E)C50s

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l	Reference
Crustacea										
Daphnia pulex, 1.9-2.1 mm	N	S_c	-	nw	7.5	-	96 h	LC50	10[a]	Trucco *et al.*, 1983

a light regime is 12 h light and 12 h dark, with mixed fluorescent and natural light

Table 2.2.5 : Acute toxicity of benzo[*a*]pyrene to freshwater organisms: L(E)C50s

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l	Reference
Algae/Chlorophyta										
Scenedesmus capricornutum	N	S	≥99%	am	-	-	72 h	EC50	5.0[1a]	Schoeny *et al.*, 1988
Selenastrum capricornutum	N	S	≥99%	am	-	-	72 h	EC50	15[1a]	Schoeny *et al.*, 1988
Crustacea										
Daphnia pulex, 1.9-2.1 mm	N	S_c	-	nw	7.5	-	96 h	LC50	5.0[1b]	Trucco *et al.*, 1983

1 above water solubility, which is 3.8 µg/l, at 25°C

a growth; light conditions: 16 h light and 8 h dark, illumination with 'white light'
b light regime is 12 h light and 12 h dark, with mixed fluorescent and natural light

Table 2.3.1 : Values from deviating freshwater tests for naphthalene

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l	Reference
Crustacea										
Daphnia magna, 4-6 d	N	CF_c	≥97%	am	6.0-7.0	-	48 h	LC50	4,700[a]	Abernethy *et al.*,1986
Daphnia pulex, <24 h	Y	R	-	tw	6.9-7.5	41-50	1 w	LC50	19,600[b]	Geiger *et al.*, 1980
Insecta										
Somatochlora cingulata	N	-	-	-	-	-	96 h	LC50	1,000-2,500[c]	Correa & Coler, 1983
Amphibia										
Xenopus laevis, larvae	Y	CF	tech.	tw	7.0-7.1	-	96 h	LC50	2,100[d] α	Edmisten & Bantle, 1982
Pisces										
Oreochromis mossambicus	N	R	-	-	-	-	96 h	LC50	7,900	Dange, 1986
Pimephales promelas, embryo/larvae	Y	CF	-	rw	7.9-8.0	535-596	30 d	LC50	1,600[e]	DeGraeve *et al.*, 1982

a solvent is ethanol, 9.5 ml/l, this solvent conc. caused no effects on *Daphnia*; high loss of compound, actual concentrations not mentioned
b light regime 16 h light and 8 h dark, at 1086 lux; results expressed as 57% of the water soluble fraction, solubility in test water is 34,000 µg/l
c data from range finding test prior to a oxygen uptake test
d solvent is ethanol, 0.8-1.9 ml/l; lightregime 12 h light and 12 h dark
e solvent is acetone, amount unknown

Table 2.3.2 : Values from deviating freshwater tests for anthracene

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l	Reference
Crustacea										
Daphnia magna, mature	N	S	anal.	tw	-	-	2 h	LC50	20[a]	Kagan *et al.*, 1985
Daphnia magna, 4-6 d	N	CF_c	≥97%	am	6.0-7.0	-	48 h	LC50	36[b]	Abernethy *et al.*, 1986
Daphnia magna, <24 h	N	S_c	≥97%	rw	-	-	48 h	EC50	80-110[1c]	Munoz & Tarazona, 1993
Insecta										
Aedes aegypti, <8 h	N	S	anal.	-	-	-	<24 h	LC50	150[1d]	Kagan *et al.*, 1985
Pisces										
Pimephales promelas, 5 cm, 0.8 g	N	S	anal.	-	-	-	25 h	LC50	360[1e]	Kagan *et al.*, 1985
Pimephales promelas, eggs	Y	CF	anal.	-	8.0	184	8 w	NOEC	6.7[m] α	Hall & Oris, 1991
Pimephales promelas, eggs	Y	CF	anal.	-	7.9	191	11 w	NOEC	11.6[m] α	Hall & Oris, 1991

1 above water solubility, which is 45 µg/l, at 25°C

a exposure: 1 h. in the dark followed by 1 h. irradiation with 13 W/m^2

b test conducted in the dark

c immobility; solvent is methanol, max. 2 ml/l; oxygen conc. min. 2 mg/l

d exposure: ca. 12 h. in the dark followed by 1 h. irradiation with 13 W/m^2, mortality recorded several hours later than the irradiation period

e exposure: ca. 0.5 h. in the dark followed by 0.5 h. irradiation with 7.5 W/m^2, mortality recorded 24 h later

f hatching succes; female and male animals where exposed for 8 and 11 w to anthracene, hatching was observed with eggs produced during the 8 and 11 weeks period; the concs. in the first 8 weeks where 6 and 12 µg/l and 12 and 20 µg/l in last 3 weeks; hatching was observed in water without anthracene; light regime 16 h light and 8 h dark in the 8 and 11 weeks period; light regime during hatching 16 h light and 8 dark with additional UV-A (68 $\mu W/m^{-2}$) and UV-B (6.7 $\mu W/m^{-2}$), this is 91% of the natural light conditions; hatching of eggs without the additional UV radiation showed no increase in hatching succes.

Table 2.3.3 : Values from deviating freshwater tests for phenanthrene

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l	Reference
Algae										
Anabaena flos-aqua	Y	S	-	am	-	-	2 w	NOEC	600	Slooff *et al.*, 1989
Selenastrum capricornutum	Y	S	-	am	-	-	4 h	EC50	900	Slooff *et al.*, 1989
Nitzschia palea	Y	S	-	am	-	-	4 h	EC50	900	Slooff *et al.*, 1989
Crustacea										
Daphnia magna, 4-6 d	N	CF_c	≥97%	am	6.0-7.0	-	48 h	LC50	210[a]	Abernethy *et al.*, 1986

a test performed in the dark

Table 2.3.4 : Values from deviating freshwater tests for fluoranthene

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l		Reference
Algae											
Anabaena flos-aqua	Y	S	-	am	-	-	2 w	EC10	50		Slooff *et al.*, 1989
Selenastrum capricornutum	N	-	-	-	-	-	96 h	EC50	54,000		Slooff *et al.*, 1989
Crustacea											
Daphnia magna, mature	N	S	anal.	tw	-	-	2 h	LC50	4[a]		Kagan *et al.*, 1985
Daphnia magna, <48 h	Y	S	-	nw	7.0	120	10 d	EC50	100[b]	α	Suedel *et al.*, 1993
Hyalella azteca, 0.6-1.0 mm	Y	S	-	nw	7.0	120	10 d	EC50	45[b]	α	Suedel *et al.*, 1993
Insecta											
Aedes aegypti, <8 h	N	S	anal.	-	-	-	<24 h	LC50	12[c]		Kagan *et al.*, 1985
Chironomus tentans, second instar, 10-12 d	Y	S	-	nw	7.0	120	10 d	EC50	32[b]	α	Suedel *et al.*, 1993
Pisces											
Pimephales promelas, 5 cm, 0.8 g	N	S	anal.	-	-	-	25 h	LC50	200[d]		Kagan *et al.*, 1985

a exposure: 1 h. in the dark followed by 1 h. irradiation with 13 W/m^2; contineously exposed to the substance
b solvent is aceton amount unknown
c exposure: ca. 12 h. in the dark followed by 1 h. irradiation with 13 W/m^2, mortality recorded several hours later than the irradiation period; contineously exposed to the substance
d exposure: ca. 0.5 h. in the dark followed by 0.5 h. irradiation with 7.5 W/m^2, mortality recorded 24 h later; contineously exposed to the substance

Table 2.3.5 : Values from deviating freshwater tests for chrysene

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l		Reference
Crustacea											
Daphnia magna, neonates	Y	R	-	tw	7.5	363	48 h	LT50	0.7[a]	α	Newsted & Giesy, 1987
Daphnia magna, <24 h	Y	IF	99-100%	rw	7.3-8.1	212	21 d	NOEC	≥1.4[b]	α	Hooftman, 1991
Daphnia magna, <24 h	Y	IF	99-100%	rw	7.3-8.1	212	21 d	NOEC	≥1.4[c]	α	Hooftman, 1991

a LT50 study; only 1 conc. tested; actual conc. is 67% of initial conc.; light regime 24 h light; 24 h pre-exposure with PAHs buth without UV-radiation; light intensity during test period, UV-A = 120 µW/cm^2 and UV-B = 25 µW/cm^2; UV-A and UV-B ratio = 4.12:1

b mortality, actual conc. 41-81% of initial conc., average 58%

c reproduction, actual conc. 41-81% of initial conc., average 58%

Table 2.3.6 : Values from deviating freshwater tests for benzo[*a*]pyrene

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l	Reference
Algae/Chlorophyta										
Selenastrum capricornutum	N	S	≥99%	am	-	-	96 h	EC50	2.5[a]	Cody *et al.*, 1984
Selenastrum capricornutum	N	S	≥99%	am	-	-	96 h	NOEC	10[1b]	Cody *et al.*, 1984

1 above the water solubility, which is 3.8 µg/l at 25°C

a growth; solvent is ethylene glycol monomethyl ether (EGME), 4 ml/l; light conditions: 16 h light and 8 h dark, illumination with 'black light' with an energy output of $5.7*10^{-3}$ W/m^2 at 380 nm

b growth; solvent is ethylene glycol monomethyl ether (EGME), 4 ml/l; light conditions: 16 h light and 8 h dark, illumination with 'cool white fluorescent light' with an energy output of $1.3*10^{-4}$ W/m^2 at 380 nm

Table 2.3.7 : Values from deviating freshwater tests for benzo[*ghi*]perylene

Organism	A	Test type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exp. time	Crite-rion	Result µg/l		Reference
Pisces											
Pimephales promelas, larvae	Y	R	high.	tw	-	-	96 h	LC20	0.15[a]	α	Oris & Giesy, 1987

a LT50 study, no lethal time found, at the end of the test period (96 h) 20% effect was found; simulated sunlight, UV-A at 95 µW/m^2 and UV-B at 20 µW/m^2; 24 h preincubation with toxicant without light; actual conc. 75% of initial, only 1 conc. tested

Appendix 3 Saltwater toxicity data

In this appendix toxicity data for saltwater organisms are presented in three different tables:
- table 3.1.x: chronic toxicity data: NOECs,
- table 3.2.x: acute toxicity data: L(E)C50s,
- table 3.3.x: data from deviating toxicity tests.

Legend:

organism	species used in the test, followed by age, length, weight and/or life stage
A	Y test substance analysed in test solution N test substance not analysed in solution
test type	S: static; R: renewal; CF: continuous flow; IF = Intermittent flow $_c$ = closed testvessels
test sustance purity	percentage active ingredient; anal. : analytical grade; tech. : technical grade; high : high but unknown purity
test water	am = artificial medium; tw = tap water; nw = natural water rw = reconstituted water;
exposure time	min: minute(s); h: hour(s); d: day(s); w: week(s); m: month(s)
results	> and ≥ value indicated is highest concentration used in the test. < and ≤ value indicated is lowest concentration used in the test.
α	given value based on measured concentrations
-	no information available

Content:

acute toxicity data (table 3.2.x)

3.2.1 Naphthalene

3.2.2 Phenanthrene

3.2.3 Fluoranthene

data from deviating toxicity tests (table 3.3.x)

3.3.1 Naphthalene

3.3.2 Anthracene

3.3.3 Phenanthrene

3.3.4 Fluoranthene

Table 3.1.1 : Chronic toxicity of naphthalene to saltwater organisms: NOECs

Organism	A	Test type	Test sub. purity	Test water	pH	Salinity ‰	Exp. time	Crite-rion	Result µg/l		Reference
Crustacea											
Cancer magister, zoeae	Y	R	anal.	nw	-	29-34	9 w	NOEC	21[a]		Caldwell, 1977
Pisces											
Oncorhynchus gorbuscha, juvenile, 0.33 g, 3.2 cm	Y	CF	-	nw	-	28	5 w	NOEC	120[b]	α	Moles & Rice, 1983
Oncorhynchus gorbuscha, juvenile, 0.33 g, 3.2 cm	Y	CF	-	nw	-	28	5 w	NOEC	560[c]	α	Moles & Rice, 1983
Oncorhynchus kisutch, fry, 1.0 g	Y	CF	-	nw	-	-	5 w	NOEC	370[d]	α	Moles *et al.*, 1981

a duration of larval development, significant reduction in the first three larval instars; light regime is 13 h light and 11 h dark; larvae obtained from an alaskan female crab, no effects on the same crab species obtained from Oregon

b growth measured as body wet weight

c growth measured as body length

d same as in note a and b, and body dry weight

Table 3.1.2 : Chronic toxicity of phenanthrene to saltwater organisms: NOECs

Organism	A	Test type	Test sub. purity	Test water	pH	Salinity ‰	Exp. time	Crite-rion	Result µg/l	Reference
Crustacea										
Rhithropanopeus harrissi, zoeae	N	R	-	am	-	25	1 w	NOEC	150[a]	Laughlin & Neff, 1979

a mortality; same NOEC with a salinity 15 ppm; light regime 12 h light and 12 h dark; temperature 20°C

Table 3.2.1 : Acute toxicity of naphthalene to saltwater organisms: L(E)C50s

Organism	A	Test type	Test sub. purity	Test water	pH	Salinity ‰	Exp. time	Crite-rion	Result µg/l		Reference
Mollusca											
Callinectes sapidus, adult, 50-227 g	Y	CF	anal.	nw	-	10	48 h	LC50	2,900[a]	α	Sabourin, 1982
Callinectes sapidus, adult, 50-227 g	Y	CF	anal.	nw	-	20	48 h	LC50	2,200[a]	α	Sabourin, 1982
Callinectes sapidus, adult, 50-227 g	Y	CF	anal.	nw	-	30	48 h	LC50	2,000[a]	α	Sabourin, 1982
Annelida											
Neanthes arenaceodentata	Y	S	≥98%	am	-	32	96 h	LC50	3,800[b]		Rossi & Neff, 1978
Crustacea											
Artemia salina, nauplii	Y	S	≥98%	am	8.5-8.7	32	24 h	EC50	3,200[c]	α	Foster & Tullis, 1984
Calanus finmarchicus, adult	Y	S_c	>97%	nw	-	33	96 h	LC50	1,400[d]	α	Falk-Petersen *et al.*, 1982
Elasmopus pectenicrus, adult	N	R	-	nw	-	30	96 h	LC50	2,700		Lee & Nicol, 1978
Eurytemora affinis	Y	S_c	≥99%	nw	-	20	24 h	LC50	3,800[e]		Ott *et al.*, 1978
Hemigrapsus nudus	N	CF	-	nw	-	28-29	8 d	LC50	1,100[f]		Gharrett & Rice, 1987
Hemigrapsus nudus	N	CF	-	nw	-	28-29	8 d	LC50	2,100[f]		Gharrett & Rice, 1987
Hemigrapsus nudus	N	CF	-	nw	-	28-29	8 d	LC50	2,800[f]		Gharrett & Rice, 1987
Neomysis americana	Y	CF	-	am	-	-	96 h	LC50	1,300[g]	α	Smith & Hargreaves, 1983
Neomysis americana	Y	CF	-	am	-	-	96 h	LC50	850[h]	α	Smith & Hargreaves, 1983
Pisces											
Fundulus heteroclitus, 8.2 cm	Y	R	-	nw	7.6	15	96 h	LC50	5,300[i]		DiMichele & Taylor, 1978
Gadus morhua, eggs	Y	S	>97%	nw	-	33	96 h	LC50	750[d]	α	Falk-Petersen *et al.*, 1982
Metapenaeus monocerus, juvenile	N	R	-	nw	7.5	18	96 h	LC50	4,200[j]		Deshmukh *et al.*, 1985
Metapenaeus monocerus, juvenile	N	R	-	nw	7.5	18	96 h	LC50	5,700[j]		Deshmukh *et al.*, 1985
Metapenaeus monocerus, juvenile	N	R	-	nw	7.5	18	96 h	LC50	5,500[j]		Deshmukh *et al.*, 1985

a constant illumination
b strong decrease in test conc. LC50 as the initial actual conc.; solvent is acetone, 1 ml/l
c immobility; constant illumination; EC50 is the geom. mean between the nominal and the 24 h measured conc.; actual conc. 67% of initial conc.
d actual conc. circa 33% of initial conc.
e solvent is methanol, max. 0.4 ml/l

f different tidal schedules, with different % exposure to air; 0% (1,100 µg/l), 33% (2,100 µg/l) and 66% (2,800 µg/l); animals from field population acclimated for 1 month
g solvent is ethanol, amount unknown; temperature 15 °C; actual conc. ca. 55% of initial conc.
h solvent is ethanol, amount unknown; temperature 25 °C; actual conc. ca. 55% of initial conc.
i light regime 14 h light and 10 h dark; estimated with Spearman and Karber
j temperature 30°C, which is the summer temperature for this species; LC50s at 20°C(winter) and 25°C(monsoon) are 5,700 µg/l and 5,500 µg/l

Table 3.2.2 : Acute toxicity of phenanthrene to saltwater organisms: L(E)C50s

Organism	A	Test type	Test sub. purity	Test water	pH	Salinity ‰	Exp. time	Crite-rion	Result µg/l	Reference
Annelida										
Neanthes arenaceodentata	Y	S	≥98%	am	-	32	96 h	LC50	600[a]	Rossi & Neff, 1978
Crustacea										
Artemia salina, nauplii	N	CF_c	≥97%	-	-	30	24 h	LC50	680[b]	Abernethy *et al.*, 1986
Artemia salina, nauplii	Y	S	≥98%	am	8.5-8.7	32	24 h	EC50	520[c] α	Foster & Tullis, 1984

a solvent is acetone, 1 ml/l
b test conducted in the dark
c immobility; constant illumination; EC50 is the geom. mean between the nominal and the 24 h measured conc.

Table 3.2.3 : Acute toxicity of fluoranthene to saltwater organisms: L(E)C50s

Organism	A	Test type	Test sub. purity	Test water	pH	Salinity ‰	Exp. time	Crite-rion	Result µg/l		Reference
Annelida											
Neanthes arenaceodentata	Y	S	≥98%	am	-	32	96 h	LC50	300[a]	α	Rossi & Neff, 1978

a decrease in test conc., actual conc. ca. 40% of initial conc.; solvent is acetone, 1 ml/l

Table 3.3.1 : Values from deviating saltwater tests for naphthalene

Organism	A	Test type	Test sub. purity	Test water	pH	Salinity ‰	Exp. time	Crite-rion	Result µg/l	Reference
Bacteriophyta										
Photobacterium phosphoreum	N	S	anal.	am	-	-	30 min	EC50	2,600[a]	Arfsten *et al.*, 1994
Photobacterium phosphoreum	N	S	anal.	am	-	-	30 min	EC50	3,000[b]	Arfsten *et al.*, 1994
Algae/Rhodophyta										
Champia parvula	N	R	-	am	-	30	11-14 d	NOEC	<350[c]	Thursby *et al.*, 1985
Crustacea										
Artemia salina, nauplii	N	CF_c	≥97%	-	-	30	24 h	LC50	11,000[d]	Abernethy *et al.*, 1986
Cancer magister, zoeae	Y	R	anal.	nw	-	29-34	9 w	NOEC	>170[e]	Caldwell, 1977
Cancer magister, zoeae	Y	R	anal.	nw	-	29-34	9 w	NOEC	>130[e]	Caldwell, 1977
Palaemonetes pugio	Y	S	-	nw	-	20	24 h	LC50	2,600	Anderson *et al.*, 1974
Parhyale hawaiensis, adult	N	S	-	nw	-	30	24 h	LC50	17,500[f]	Lee & Nicol, 1978
Parhyale hawaiensis, adult	N	S_c	-	nw	-	30	24 h	LC50	6,200[f]	Lee & Nicol, 1978
Penaeus aztecus	Y	S	-	nw	-	20	24 h	LC50	2,500	Anderson *et al.*, 1974
Pisces										
Cyprinodon variegatus	Y	S	-	nw	-	20	24 h	LC50	2,400	Anderson *et al.*, 1974
Oncorhynchus gorbuscha, fry	Y	S	-	nw	-	27	24 h	LC50	900	Thomas & Rice, 1979

a fluorescense; solvent is ethanol at 20 ml/l (ca. 2%), solvent caused no significant effects at this conc.; light regime is 30 min. dark

b fluorescense; solvent is ethanol at 20 ml/l (ca. 2%), solvent caused no significant effects at this conc.; light regime is 30 min. light; light source with UV-A+B, total irradiation 400-800 $\mu W/cm^2$, for 30 min.

c growth; light regime 16 h light and 8 h dark, with an intensity of 75-80 $\mu E\ m^{-2}*s^{-1}$, produced by 'cool-white fluorescent light'; no naphthalene found at the end of the test

d constant exposure in the dark

e mortality; light regime is 13 h light and 11 h dark; larvae obtained from an Alaskan female crab (NOEC = 130 µg/l) and from an Oregon female crab (NOEC = 170 µg/l)

f antibiotics (penicillin 25 mg/l and streptomycin 50 mg/l) added to all conc. including controls, 100% survival in controls

Table 3.3.2 : Values from deviating saltwater tests for anthracene

Organism	A	Test type	Test sub. purity	Test water	pH	Salinity $^{o}/_{oo}$	Exp. time	Crite-rion	Result µg/l	Reference
Bacteriophyta										
Photobacterium phosphoreum	N	S	anal.	am	-	-	30 min	EC50	11[a]	Arfsten *et al.*, 1994
Crustacea										
Artemia salina, nauplii	N	CF_c	≥97%	-	-	30	24 h	LC50	>50[b]	Abernethy *et al.*, 1986
Artemia salina	N	S	anal.	-	-	-	3 h	LC50	20[c]	Kagan *et al.*, 1985

a fluorescense; solvent is ethanol at 20 ml/l (ca. 2%), solvent caused no significant effects at this conc.; light regime is 30 min. light; light source with UV-A+B, total irradiation 400-800 µW/cm^2, for 30 min.

b test performed in the dark

c exposure: 2 hr. in the dark followed by 1 hr. irradiation with 13 W/m^2

Table 3.3.3 : Values from deviating saltwater tests for phenanthrene

Organism	A	Test type	Test sub. purity	Test water	pH	Salinity ‰	Exp. time	Crite-rion	Result µg/l	Reference
Bacteriophyta										
Photobacterium phosphoreum	N	S	anal.	am	-	-	30 min	EC50	310[a]	Arfsten *et al.*, 1994
Photobacterium phosphoreum	N	S	anal.	am	-	-	30 min	EC50	210[b]	Arfsten *et al.*, 1994

a fluorescense; solvent is ethanol at 20 ml/l (ca. 2%), solvent caused no significant effects at this conc.; light regime is 30 min. dark

b fluorescense; solvent is ethanol at 20 ml/l (ca. 2%), solvent caused no significant effects at this conc.; light regime is 30 min. light; light source with UV-A+B, total irradiation 400-800 µW/cm^2, for 30 min.

Table 3.3.4 : Values from deviating saltwater tests for fluoranthene

Organism	A	Test type	Test sub. purity	Test water	pH	Salinity $^{o}/_{oo}$	Exp. time	Crite-rion	Result µg/l	Reference
Bacteriophyta										
Photobacterium phosphoreum	N	S	anal.	am	-	-	30 min	EC50	470[a]	Arfsten *et al.*, 1994
Crustacea										
Artemia salina, eggs	N	S	anal.	-	-	-	3 h	LC50	40[b]	Kagan *et al.*, 1985

1 above water solubility, which is 260 µg/l, at 25°C

a fluorescense; solvent is ethanol at 20 ml/l (ca. 2%), solvent caused no significant effects at this conc.; light regime is 30 min. light; light source with UV-A+B, total irradiation 400-800 µW/cm^2, for 30 min.

b exposure: 2 hr. in the dark followed by 1 hr. irradiation with 13 W/m^2

Appendix 4 Soil toxicity data

In this appendix toxicity data for soil organisms are presented in four different tables:
- table 4.1.x: chronic toxicity data: NOECs,
- table 4.2.x: acute toxicity data: L(E)C50s,
- table 4.3.x: toxicity to soil microbial processes and enzymatic activity,
- table 4.3.x: data from deviating toxicity tests.

Legend:

organism/process	species tested, followed by age, length, weight and/or life stage; microbial process or enzymatic activity in question
A	Y test substance analysed in test soil N test substance not analysed in test soil
art. soil	artificial soil
% organic-matter (%om)	% organic matter (if presented in % organic carbon a factor of 1.7 was used to calculate % om)
exposure. time (exp. time)	min. : minute(s); h: hours; d: days; w: week(s); m: month(s)
standard soil (st. soil)	(10 % om and 25% clay)
results	> and ≥ value indicated is highest concentration used in the test. < and ≤ value indicated is lowest concentration used in the test.
α	given value based on measured concentrations
-	no data available

Content:

Table 4.1.1 : Chronic toxicity of benzo[*a*]anthracene to soil organisms

Organism/process	Soil type	pH	% O.m.	% Clay	Temp. °C	Exp. time	Criterion	Result test soil (mg/kg d.w.)	Result stand. soil (mg/kg d.w.)	Reference
Crustacea										
Oniscus assellus, 6-10 mg	-	-	>90%	-	20	47 w	NOEC	7.5[a]	2.5 α	Van Brummelen *et al*, submitted

a route of exposure is through food, mixture of poplar-, maple- and birch-leaves (3:2:1; ±90%), added with 10% DOKO dog food at a ratio of; parameters, female freshweight; purity of substance is 99%

Table 4.1.2 : Chronic toxicity of benzo[*a*]pyrene to soil organisms

Organism/process	Soil type	pH	% O.m.	% Clay	Temp. °C	Exp. time	Criterion	Result test soil (mg/kg d.w.)	Result stand. soil (mg/kg d.w.)	Reference
Annelida										
Enchytraeus crypticus	-	-	3.9	-	20-25	30 d	NOEC	3.4[a]	8.7	Achazi *et al.*, 1995
Eisenia f. fetida	-	-	3.9	-	20	28 d	NOEC	1.0[b]	2.6	Achazi *et al.*, 1995
Crustacea										
Oniscus assellus, 2.82 mg	-	-	>90%	-	20	9 w	NOEC	32[c]	11	Van Brummelen & Stuijfzand, 1993
Porcellio scaber, 8.52 mg	-	-	>90%	-	20	9 w	NOEC	32[c]	11	Van Brummelen & Stuijfzand, 1993
Porcellio scaber, adult males	-	-	>90%	-	17	4 w	NOEC	25[d]	8.3	Van Straalen & Verweij, 1991

a reproduction; NOEC=LOEC/3, 24% effect at 10.1 mg/kg

b survival; NOEC=LOEC/10, 51% effect at 10 mg/kg; reproduction; NOEC=LOEC/10, 90% effect at 10 mg/kg

c route of exposure is through food, mixture of poplar leaves and DOKO dog at a ratio of (9:1, dry weight); parameters, dry- and freshweight and length growth; purity of substance is 98%; light regime is 12 h light and 12 h dark

d route of exposure is through food; food is poplar leaves; parameters, length growth; light regime is 12 h light and 12 h dark; females showed no growth effect even at the highest concentration, which is 125 mg/kg

Table 4.2.1 : Acute toxicity of anthracene to soil organisms

Organism/process	Soil type	pH	% O.m.	% Clay	Temp. °C	Exp. time	Criterion	Result test soil (mg/kg d.w.)	Result stand. soil (mg/kg d.w.)	Reference
Macrophyta										
Avena sativa	sandy loam	5.5	2	-	23-35	14 d	LC50	530	2600	Mitchell *et al.*, 1988
Avena sativa	sandy loam	5.5	2	-	23-35	14 d	EC50	30[a]	150	Mitchell *et al.*, 1988
Cucumis sativus	sandy loam	5.5	2	-	23-35	14 d	EC50	720[a]	3600	Mitchell *et al.*, 1988

a growth as post emergence of seedlings; according to OECD 208

Table 4.3.1 : Values from deviating soil test for naphthalene

Organism/process	Soil type	pH	% O.m.	% Clay	Temp. °C	Exp. time	Criterion	Result test soil (mg/kg d.w.)	Result stand. soil (mg/kg d.w.)	Reference
Macrophyta										
Lactuca sativa	loam	7.5	1.4	12	21	7 d	EC50	±100[a]	±500	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	1.4	12	21	7 d	EC50	>100[a]	>500	Hulzebos *et al.*, 1993
Microbial processes										
CO_2-evolution	silt loam	7.3	3.0	13	25	80 d	NOEC	≥25[b]	≥83	Kirchman *et al.*, 1991

a shoot growth; ca. 50% recovery at the end of the test; light regime, 16 h light and 8 h dark, at an intensity of 6,500 lux produced by fluorescent bulbs
b purity of naphthalene unknown; after 10 days ca. 10% of the initial conc. was disapeared; no significant effects during the 80 day testperiod

Table 4.3.2 : Values from deviating soil test for anthracene

Organism/process	Soil type	pH	% O.m.	% Clay	Temp. °C	Exp. time	Criterion	Result test soil (mg/kg d.w.)	Result stand. soil (mg/kg d.w.)	Reference
Macrophyta										
Cucumis sativus	sandy loam	5.5	2	-	23-35	14 d	LC50	>1000[a]	>5000	Mitchell *et al.*, 1988
Glycine max	sandy loam	5.5	2	-	23-35	14 d	LC50	>1000[a]	>5000	Mitchell *et al.*, 1988
Banksia ericifolia	sandy loam	5.5	2	-	23-35	14 d	LC50	>1000[a]	>5000	Mitchell *et al.*, 1988
Casuarina distyla	sandy loam	5.5	2	-	23-35	14 d	LC50	>1000[a]	>5000	Mitchell *et al.*, 1988
Eucalyptus eximia	sandy loam	5.5	2	-	23-35	14 d	LC50	>1000[a]	>5000	Mitchell *et al.*, 1988
Glycine max	sandy loam	5.5	2	-	23-35	14 d	EC50	>1000[b]	>5000	Mitchell *et al.*, 1988
Banksia ericifolia	sandy loam	5.5	2	-	23-35	14 d	EC50	>1000[b]	>5000	Mitchell *et al.*, 1988
Casuarina distyla	sandy loam	5.5	2	-	23-35	14 d	EC50	>1000[b]	>5000	Mitchell *et al.*, 1988
Eucalyptus eximia	sandy loam	5.5	2	-	23-35	14 d	EC50	>1000[b]	>5000	Mitchell *et al.*, 1988

a highest measured conc.

b growth as post emergence of seedlings; according to OECD 208; highest measured conc.

Table 4.3.3 : Values from deviating soil test for phenanthrene

Organism/process	Soil type	pH	% O.m.	% Clay	Temp. °C	Exp. time	Criterion	Result test soil (mg/kg d.w.)	Result stand. soil (mg/kg d.w.)	Reference
Annelida										
Eisenia fetida	art.soil	-	10	20	-	21 d	EC50	240[a]	240	Bowmer *et al.*, 1993
Isopoda										
Folsomia candida	art.soil	-	10	20	20	28 d	LC50	150[b]	150	Bowmer *et al.*, 1993
Folsomia candida	art.soil	-	10	20	20	28 d	NOEC	75[c]	75	Bowmer *et al.*, 1993

a cocoon production; recovery only 5-10% at the end of the 21 d period; according to OECD 207
b according to OECD 207; test carried out in the dark
c reproduction; according to OECD 207; test carried out in the dark

Table 4.3.4 : Values from deviating soil test for chrysene

Organism/process	Soil type	pH	% O.m.	% Clay	Temp. °C	Exp. time	Criterion	Result test soil (mg/kg d.w.)	Result stand. soil (mg/kg d.w.)	Reference
Annelida										
Eisenia fetida	art.soil	-	10	20	-	14 d	LC50	>1000[a]	>1000	Bowmer *et al.*, 1993

a according to OECD 207

Table 4.3.5 : Values from deviating soil test for benzo[*a*]pyrene

Organism/process	Soil type	pH	% O.m.	% Clay	Temp. °C	Exp. time	Criterion	Result test soil (mg/kg d.w.)	Result stand. soil (mg/kg d.w.)	Reference
Isopoda										
Porcellio scaber, 8.52 g	-	-	>90%	-	20	9 w	NOEC	>320[a]	>110	Van Brummelen & Stuijfzand, 1993

a route of exposure is through food, mixture of poplar leaves and DOKO dog at a ratio of (9:1, dry weight); parameters, dry- and freshweight and length growth; purity of substance is 98%; light regime is 12 h light and 12 h dark

Appendix 5 Raw data on partition coefficients

In this appendix data on soil-water and sediment-pore water partiton coefficients are presented

Legend:

solid/water	solid water ratio used in experiment
mass balance	Y: checked whether total amount of substance analysed in different compartments equals total amount added at start of experiment, N: no check
equilibrium time	time after substance added before concentrations are analysed in different compartments

Content:

Table 5.1: raw data on equilibrium partition coefficients of selected polycyclic aromatic hydrocarbons

testsubstance	soil type	% oc	pH	CEC mmol/kg	solid/water g/l	mass bal.	equil. time	log K_{oc}	reference
naphthalene									
	quartz sand	1.80	-	-	88-175	Y	3 h	2.12	Barrett *et al.*, 1994
	soil sorbent	3.70	-	-	88-175	Y	3 h	3.27	Barrett *et al.*, 1994
	clay loam	1.42	5.91	124	-	N	-	2.64	Kishi *et al.*, 1990
	light clay	1.51	5.18	132	-	N	-	2.92	Kishi *et al.*, 1990
	light clay	3.23	5.26	283	-	N	-	2.87	Kishi *et al.*, 1990
	sandy loam	7.91	5.41	263	-	N	-	2.62	Kishi *et al.*, 1990
	clay loam	10.40	4.89	350	-	N	-	2.73	Kishi *et al.*, 1990
	soil	1.6	5.7	-	1.2-50	N	48 h	3.15	Podoll *et al*, 1989
	silt loam	1.94	-	-	±10-800	N	24 h	2.67[b]	Fu & Luthy, 1986
	sediment	2.70	-	-	-	-	-	3.08	De Maagd & Sijm, 1995
	sediment	3.38	7.8	-	200	N	3 h	5.00[a]	Kayal & Connell, 1990
	sediment	2.9	-	-	0.4	Y	24 h	3.24	Voice *et al.*, 1983
	sediment	3.8	-	-	0.4	Y	24 h	3.34	Voice *et al.*, 1983
	sediment	4.02	-	-	4.55-180	N	2 h	2.93	Vowles & Mantoura, 1987
	sediment	5.55[a]	-	-	-	Y	-	4.8[a]	Van Hattum, 1995
anthracene									
	clay loam	2.23	6.0	372E+3	400-440	N	20 h	4.32[b]	Rao *et al.*, 1990
	soil EPA2	2.40	7.9	142.9	-	N	24 h	4.10	Shimizu & Liljestrand, 1991
	soil EPA16	1.20	6.5	105	-	N	24 h	4.11	Shimizu & Liljestrand, 1991
	soil EPA22	1.67	7.55	85.3	-	N	24 h	4.10	Shimizu & Liljestrand, 1991
	soil EPA23	2.38	6.7	311.5	-	N	24 h	4.10	Shimizu & Liljestrand, 1991
	sandy clay loam	3.9	7.3	218	500	N	24 h	4.36[c]	Nkedi-Kizza *et al.*, 1985
	sandy clay loam	3.9	7.3	218	500	N	24 h	4.33[c]	Nkedi-Kizza *et al.*, 1985
	sediment	2.7	-	-	-	-	-	4.57	De Maagd & Sijm, 1995
	sediment	-	-	-	10	Y	72 h	5.93[d]	Evers & Smedes, 1993
	sediment	3.38	7.8	-	200	N	3 h	5.76[a]	Kayal & Connell, 1990
	sediment	5.5[a]	-	-	-	N	-	6.7[a]	Van Hattum, 1995
phenanthrene									
	sediment (25-29 cm)	5.23	-	-	0.5	N	30 h	4.30	Chin & Gschwend, 1992
continued ↓	sediment	4.02	-	-	4.55-180	N	2 h	4.26	Vowles & Mantoura, 1987

Table 5.1: (continued)

testsubstance	soil type	% oc	pH	CEC mmol/kg	solid/water g/l	mass bal.	equil. time	log K_{oc}	reference
phenanthrene									
	sediment	3.38	7.8	-	200	N	3 h	6.12[a]	Kayal & Connell, 1990
	sediment	-	-	-	10	Y	72 h	5.69[d]	Evers & Smedes, 1993
	sediment	5.55[a]	-	-	-	N	-	5.9[a]	Van Hattum, 1995
	sediment	2.7	-	-	-	-	-	4.45	De Maagd & Sijm, 1995
fluoranthene									
	sand (synthetic)	1.5	-	-	-	N	24 h	4.12	Rebhun *et al.*,1992
	sand (synthetic)	2.0	-	-	-	N	24 h	4.10	Rebhun *et al.*,1992
	sediment	2.7	-	-	-	-	-	5.32	De Maagd & Sijm, 1995
	sediment	3.38	7.8	-	200	N	3 h	6.38[a]	Kayal & Connell, 1990
	sediment	-	-	-	10	Y	72 h	6.12[d]	Evers & Smedes, 1993
	sediment	5.5[a]	-	-	-	-	-	6.5[a]	Van Hattum, 1995
benzo[*a*]anthracene	sediment	3.38	7.8	-	200	N	3 h	6.30[a]	Kayal & Connell, 1990
	sediment	-	-	-	10	Y	72 h	7.36[d]	Evers & Smedes, 1993
	sediment	5.5[a]	-	-	-	-	-	7.2[a]	Van Hattum, 1995
	sediment	2.7	-	-	-	-	-	5.83	De Maagd & Sijm, 1995
chrysene	sediment	3.38	7.8	-	200	N	3 h	6.27[a]	Kayal & Connell, 1990
	sediment	-	-	-	10	Y	72 h	7.18[d]	Evers & Smedes, 1993
	sediment	5.5[a]	-	-	-	-	-	6.8[a]	Van Hattum, 1995
	sediment	2.7	-	-	-	-	-	5.83	De Maagd & Sijm, 1995
benzo[*k*]fluoranthene	sediment	3.38	7.8	-	200	N	3 h	5.99[a]	Kayal & Connell, 1990
	sediment	-	-	-	10	Y	72 h	8.50[d]	Evers & Smedes, 1993
	sediment	5.5[a]	-	-	-	-	-	7.4[a]	Van Hattum, 1995
	sediment	2.7	-	-	-	-	-	5.99	De Maagd & Sijm, 1995

continued ↓

Table 5.1: (continued)

testsubstance	soil type	% oc	pH	CEC mmol/kg	solid/water g/l	mass bal.	equil. time	log K_{oc}	reference
benzo[*a*]pyrene	sediment	3.38	7.8	-	200	N	3 h	6.26[a]	Kayal & Connell, 1990
	sediment	-	-	-	10	Y	72 h	8.37[d]	Evers & Smedes, 1993
	sediment	5.5[a]	-	-	-	-	-	7.4[a]	Van Hattum, 1995
	sediment	2.7	-	-	-	-	-	5.98	De Maagd & Sijm, 1995
benzo[*ghi*]perylene	sediment	-	-	-	10	Y	72 h	8.70[d]	Evers & Smedes, 1993
	sediment	5.5[a]	-	-	-	-	-	6.6[a]	Van Hattum, 1995
indeno[*1,2,3-cd*]-pyrene	sediment	-	-	-	10	Y	72 h	8.95[d]	Evers & Smedes, 1993
	sediment	5.5[a]	-	-	-	-	-	6.3[a]	Van Hattum, 1995

a no batch experiment, mean value of different field contaminated sediments
b estimated using linear regression with data for different co-solvent fractions
c co-solvent method; intercept (log Kp for solvent conc.=0) estimated from given graphic.
d co-solvent method; 'true K_{oc}" extrapolated to 100% water; without influence of "third phase" material
e test with sediment; K_{oc} is calculated for the lowest concentration maesured in the interstitial water.

Appendix 6 Experimental data used for extrapolation

Toxicity data used for extrapolation methods; freshwater organisms (NOEC and L(E)C50s in µg/l)

compound	taxonomic group	Statistical extrapol. NOEC	$EPA_{-method}$ L(E)C50	$EPA_{-method}$ NOEC
Naphthalene	Pisces		120	
Anthracene	Pisces		6.9[a]	
Phenanthrene	Pisces		30	
Fluoranthene	Pisces			12[b]
Benzo[*a*]anthracene	Crustacea		10	
Benzo[*k*]fluoranthene	Pisces			0.36[c]
Benzo[*a*]pyrene	Crustacea		5	

a Geometric mean of 8 LC50s for *Lepomis spec.*; 1.3, 8.0, 3.8, 8.3, 2.8, 12, 18, and 26 µg/l.
b Geometric mean of 2 NOECs (growth) for *Brachydanio rerio*; 6.9 and 22 µg/l.
c Geometric mean of 2 NOECs (growth) for *Brachydanio rerio*; 0.27 and 0.48 µg/l.

Toxicity data used for extrapolation methods; saltwater organisms (NOEC and L(E)C50s in µg/l)

compound	taxonomic group	Statistical extrapol. NOEC	$EPA_{-method}$ L(E)C50	$EPA_{-method}$ NOEC
Naphthalene	Pisces		750	
Phenanthrene	Crustacea		595[a]	
Fluoranthene	Annelida		300	

a Geometric mean of 1 LC50 and 1 EC50 (immobility) value for *Artemia salina*; 680 and 520 µg/l.

Toxicity data used for extrapolation methods; salt- and fresh water organisms combined (NOEC and L(E)C50s in µg/l)

compound	taxonomic group	Statistical extrapol. NOEC	$EPA_{-method}$ L(E)C50	$EPA_{-method}$ NOEC
Naphthalene	Pisces		120	
Anthracene	Pisces		6.9[a]	
Phenanthrene	Pisces		30	
Fluoranthene	Annelida		300	
Benzo[*a*]anthracene	Crustacea		10	
Benzo[*k*]fluoranthene	Pisces			0.42[b]
Benzo[*a*]pyrene	Crustacea		5	

a Geometric mean of 8 LC50s for *Lepomis spec.*; 1.3, 8.0, 3.8, 8.3, 2.8, 12, 18, and 26 µg/l.
b Geometric mean of 2 NOECs (growth) for *Brachydanio rerio*; 0.27 and 0.48 µg/l.

Toxicity data (standard soil) used for extrapolation methods; soil organisms (NOEC and L(E)C50s in mg/kg)

compound	taxonomic group	Statistical extrapol. NOEC	$EPA_{-method}$ L(E)C50	$EPA_{-method}$ NOEC
Anthracene	Macrophyta		150	
Benzo[*a*]anthracene	Crustacea			2.5
Benzo[*a*]pyrene	Annelida			2.6

Appendix 7 Experimental data and QSAR data (combined dataset) used for extrapolation.

Toxicity data used for extrapolation methods; fresh- and saltwater organisms NOECs in mg/l,

SUBSTANCE: naphthalene

experimental data

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Pisces			
Pimephales promelas	0.45	*Sarotherodon mossambicus*	2.3
Oncorhynchus gorbuscha	0.26[a]	*Oncorhynchus kisutch*	0.37
Crustacea			
Cancer magister	0.021		

a Geometric mean of 2 NOECs (growth); 0.12 and 0.56 mg/l.

derived from QSARs (Van Leeuwen *et al.*, 1992)

log K_{ow} 3.30
MW(g) 128.20

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Bacteria			
Clostridium botulinum	129.4	*Bacillus subtilus*	9.2
Pseudomonas putida	24.9	*Photobacterium phosphoreum*	22.1
Fungi			
Saccharomyces cerevisiae	152.7		
Algae			
Skeletonema costatum	20.5	*Scenedesmus subspicatus*	7.2
Selenastrum capricornutum	1.3		
Protozoa			
Tetrahymena pyriformis	15.4		
Coelenterates			
Hydra oligactis	1.7		
Molluscs			
Lymnaea stagnalis	1.5		

continued ↓

derived from QSARs (Van Leeuwen *et al.*, 1992) continued

log K_{ow} 3.30
MW(g) 128.20

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Arthropods			
Nitocra spinipes	2.5	*Daphnia magna*	0.95
Aedes aegypti	1.4	*Culex pipiens*	1.9
Fish			
Pimephales promelas/ Brachydanio rerio	0.770[a]		
Amphibia			
Ambystoma mexicanum	2.1	*Rana temporaria*	1.1
Xenopus laevis	2.2		

a this QSAR-NOEC is replaced by the available experimental NOEC for this species.

Toxicity data used for extrapolation methods; fresh- and saltwater organisms NOECs in mg/l,

SUBSTANCE: phenanthrene

experimental data

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Macrophyta			
Lemna gibba	0.60		
Crustacea			
Daphnia magna	0.032	*Daphnia pulex*	0.060
Rhithropanopeus harrissi	0.15		
Pisces			
Brachydanio rerio	0.042[a]		

a Geometric mean of 2 NOECs (growth); 0.032 and 0.056 mg/l.

derived from QSARs (Van Leeuwen *et al.*, 1992)

log K_{ow} 4.46
MW(g) 178.20

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Bacteria			
Clostridium botulinum	-	*Bacillus subtilus*	2.326
Pseudomonas putida	6.259	*Photobacterium phosphoreum*	4.990
Fungi			
Saccharomyces cerevisiae	-		
Algae			
Skeletonema costatum	4.166	*Scenedesmus subspicatus*	1.012
Selenastrum capricornutum	0.121		
Protozoa			
Tetrahymena pyriformis	2.5288		
Coelenterates			
Hydra oligactis	0.2319		
Molluscs			
Lymnaea stagnalis	0.216		
Arthropods			
Nitocra spinipes	0.429	*Daphnia magna*	0.082[a]
Aedes aegypti	0.107	*Culex pipiens*	0.273

continued ↓

derived from QSARs (Van Leeuwen *et al.*, 1992) continued

log K_{ow} 4.46
MW(g) 178.20

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Fish			
Pimephales promelas/ Brachydanio rerio	0.105[a]		
Amphibia			
Ambystoma mexicanum	0.273	*Rana temporaria*	0.083
Xenopus laevis	0.280		

- above 10 times the maximum water solubility and therefore rejected
a this QSAR-NOEC is replaced by the available experimental NOEC for this species.

Toxicity data used for extrapolation methods; fresh- and saltwater organisms NOECs in mg/l,

SUBSTANCE: fluoranthene

experimental data

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Macrophyta			
Lemna gibba	0.20		
Pisces			
Brachydanio rerio	0.0123[a]		

a Geometric mean of 2 NOECs (growth); 0.0069 and 0.022 mg/l.

derived from QSARs (Van Leeuwen *et al.*, 1992)

log K_{ow} 5.16
MW(g) 202.30

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Bacteria			
Clostridium botulinum	-	*Bacillus subtilus*	0.941
Pseudomonas putida	2.533	*Photobacterium phosphoreum*	1.893
Fungi			
Saccharomyces cerevisiae	-		
Algae			
Skeletonema costatum	1.482	*Scenedesmus subspicatus*	0.287
Selenastrum capricornutum	0.027		
Protozoa			
Tetrahymena pyriformis	0.791		
Coelenterates			
Hydra oligactis	0.066		
Molluscs			
Lymnaea stagnalis	0.061		
Arthropods			
Nitocra spinipes	0.138	*Daphnia magna*	0.017
Aedes aegypti	0.021	*Culex pipiens*	0.077
Fish			
Pimephales promelas/ Brachydanio rerio	0.029[a]		

continued ↓

derived from QSARs (Van Leeuwen *et al.*, 1992) continued

log K_{ow} 5.16
MW(g) 202.30

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Amphibia			
Ambystoma mexicanum	0.075	*Rana temporaria*	0.016
Xenopus laevis	0.075		

- above 10 times the maximum water solubility and therefore rejected
a this QSAR-NOEC is replaced by the available experimental NOEC for this species.

Toxicity data used for extrapolation methods; fresh- and salt water organisms NOECs in mg/l, derived from QSARs (Van Leeuwen *et al.*, 1992)

SUBSTANCE: benzo[*a*]anthracene

log K_{ow} 5.79
MW(g) 228.30

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Bacteria			
Clostridium botulinum	-	*Bacillus subtilus*	-
Pseudomonas putida	-	*Photobacterium phosphoreum*	-
Fungi			
Saccharomyces cerevisiae	-		
Algae			
Skeletonema costatum	-	*Scenedesmus subspicatus*	0.093
Selenastrum capricornutum	0.072		
Protozoa			
Tetrahymena pyriformis	-		
Coelenterates			
Hydra oligactis	0.021		
Molluscs			
Lymnaea stagnalis	0.020		
Arthropods			
Nitocra spinipes	0.050	*Daphnia magna*	0.004
Aedes aegypti	0.005	*Culex pipiens*	0.025
Fish			
Pimephales promelas/ Brachydanio rerio	0.009		
Amphibia			
Ambystoma mexicanum	0.024	*Rana temporaria*	0.004
Xenopus laevis	0.023		

- above 10 times the maximum water solubility and therefore rejected

Toxicity data used for extrapolation methods; fresh- and saltwater organisms NOECs in mg/l, derived from QSARs (Van Leeuwen *et al.*, 1992)

SUBSTANCE: chrysene

log K_{ow} 5.73
MW(g) 228.30

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Bacteria			
Clostridium botulinum	-	*Bacillus subtilus*	-
Pseudomonas putida	-	*Photobacterium phosphoreum*	-
Fungi			
Saccharomyces cerevisiae	-		
Algae			
Skeletonema costatum	-	*Scenedesmus subspicatus*	-
Selenastrum capricornutum	0.0083		
Protozoa			
Tetrahymena pyriformis	-		
Coelenterates			
Hydra oligactis	0.0240		
Molluscs			
Lymnaea stagnalis	0.0224		
Arthropods			
Nitocra spinipes	0.0561	*Daphnia magna*	0.0050
Aedes aegypti	0.0057	*Culex pipiens*	0.0282
Fish			
Pimephales promelas/ Brachydanio rerio	0.0106		
Amphibia			
Ambystoma mexicanum	0.0267	*Rana temporaria*	0.0044
Xenopus laevis	0.0258		

- above 10 times the maximum water solubility and therefore rejected

Toxicity data used for extrapolation methods; fresh- and saltwater organisms NOECs in mg/l,

SUBSTANCE: benzo[*a*]pyrene

experimental data

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Pisces			
Brachydanio rerio	0.0063		

derived from QSARs (Van Leeuwen *et al.*, 1992)

log K_{ow} 5.97
MW(g) 252.30

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Bacteria			
Clostridium botulinum	-	*Bacillus subtilus*	-
Pseudomonas putida	-	*Photobacterium phosphoreum*	-
Fungi			
Saccharomyces cerevisiae	-		
Algae			
Skeletonema costatum	-	*Scenedesmus subspicatus*	-
Selenastrum capricornutum	0.0053		
Protozoa			
Tetrahymena pyriformis	-		
Coelenterates			
Hydra oligactis	0.0165		
Molluscs			
Lymnaea stagnalis	0.0154		
Arthropods			
Nitocra spinipes	-	*Daphnia magna*	0.0031
Aedes aegypti	0.0034	*Culex pipiens*	0.0194

continued ↓

derived from QSARs (Van Leeuwen *et al.*, 1992) continued

log K_{ow} 5.97
MW(g) 252.30

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Fish			
Pimephales promelas/ Brachydanio rerio	0.0072[a]		
Amphibia			
Ambystoma mexicanum	0.0181	*Rana temporaria*	0.0027
Xenopus laevis	0.0173		

- above 10 times the maximum water solubility and therefore rejected
a this QSAR-NOEC is replaced by the available experimental NOEC for this species.

Toxicity data used for extrapolation methods; fresh- and saltwater organisms NOECs in mg/l, derived from QSARs (Van Leeuwen *et al.*, 1992)

SUBSTANCE: benzo[*ghi*]perylene

log K_{ow} 6.63
MW(g) 268.40

Species	NOEC (mg/l)	Species	NOEC (mg/l)
Bacteria			
Clostridium botulinum	-	*Bacillus subtilus*	-
Pseudomonas putida	-	*Photobacterium phosphoreum*	-
Fungi			
Saccharomyces cerevisiae	-		
Algae			
Skeletonema costatum	-	*Scenedesmus subspicatus*	-
Selenastrum capricornutum	0.0012		
Protozoa			
Tetrahymena pyriformis	-		
Coelenterates			
Hydra oligactis	-		
Molluscs			
Lymnaea stagnalis	-		
Arthropods			
Nitocra spinipes	-	*Daphnia magna*	0.0007
Aedes aegypti	0.0007	*Culex pipiens*	-
Fish			
Pimephales promelas/ Brachydanio rerio	0.0020		
Amphibia			
Ambystoma mexicanum	-	*Rana temporaria*	0.0005
Xenopus laevis	-		

- above 10 times the maximum water solubility and therefore rejected

Appendix 8 References

References for log K_{oc}s

References

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