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Maximum Permissible Concentrations and Negligible Concentrations for aniline derivatives

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This research was carried out on behalf and for the account of the Directorate General for Environmental Protection, Directorate of Chemicals, External Safety and Radiation Protection in the framework of the project "Setting integrated environmental quality objectives", project no. 601501.

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Preface

This report contains results carried out in the framework of the project "Setting Integrated Environmental Quality Objectives". The results have been discussed in an advisory group. The members are M. Beek (National Institute of Inland Water Management), M.M.H.E. van den Berg (Health Council of the Netherlands), T. Crommentuijn (National Institute of Public Health and the Environment), C. Denneman (Ministry of Housing, Spatial Planning and the Environment), J. Deneer (Winand Staring Centre for Integrated Land, Soil and Water Research), J. Faber (Institute for Forestry and Nature Research), M. Janssen (National Institute of Public Health and the Environment), D. Sijm (National Institute of Public Health and the Environment), J. Struijs (National Institute of Public Health and the Environment), M.E.J. van der Weiden (Ministry of Housing, Spatial Planning and the Environment), J. van Wensem (Technical Soil Protection Committee) and A.P. van Wezel (National Institute of Public Health and the Environment).

CONTENTS

SUMMARY

This report contains Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for chloro- (CAs), nitro- (NAs) and methylsubstituted anilines (MAs). It is written within the context of the project "Setting Integrated Environmental Quality Objectives" of the Ministry of Housing, Spatial Planning and the Environment (VROM). In combination with additional information, MPCs and NCs enables VROM to set Environmental Quality Objectives (EQOs).

Aniline derivatives have frequently been measured in Dutch surface waters during the last decade. In principle, MPCs are derived for the anilines measured in the environment, which are chloroanilines, (chloro)nitroanilines and (chloro)methylanilines. Since the amount of ecotoxicity data was expected to be low, a compilation was made of all possible isomers of the groups of anilines mentioned above. Furthermore, an attempt was made to derive "group MPCs" as far as possible. This term refers to MPCs which are derived for selected groups of isomers by combining all available toxicity data on a class of isomers and, subsequently, applying an extrapolation method. When applying this method, we assume that isomers have the same mode of action, and that the effects are considered additive in the case of an organism being exposed simultaneously to more than one isomer. The MPC derived in this way can, subsequently, be used for the sum of the individual compounds included in a group value. For example, if 2-CA and 3-CA are detected simultaneously in water, the sum of the concentration of both compounds may be related to the MPC_{water}.

The derivation of MPCs and NCs is restricted by the lack of ecotoxicological data. The values for the compartments are derived as follows:

- *water*: Only the MPCs for monochloroanilines (MCAs), dichloroanilines (DCAs), nitroanilines (NAs), methylanilines (MAs) and dimethylanilines (DMAs) are derived by statistical extrapolation. For nitro-phenylanilines (N-PA) only marine water data are available on which the modified EPA-method is applied.
- *soil*: Only for CAs reliable toxicity data are available. However, only the MPCs for MCAs and DCAs are derived by statistical extrapolation. For trichloroanilines (TCAs), tetrachloroanilines (TeCAs) and pentachloroaniline (PCA) MPCs are derived by the modified EPA-method. For chloro-nitroanilines (C)NAs) and chloro-methylanilines (C)MAs MPCs are derived using the equilibrium partitioning method.
- *sediment*: All MPCs are derived by the equilibrium partitioning method since no toxicity data on sediment dwelling organisms are available.

The MPCs and NCs derived are compared to actual concentrations in Dutch surface waters using recent data from the 'Institute for Inland Water Management and Waste Water Treatment (RIZA)' and the 'Association of Rhine and Meuse Water Supply Companies (RIWA)'. It appears that only a fraction of the considered compounds are regularly measured and detected in surface waters.

MPCs and NCs are compared to the sum of the measured concentrations of a group of isomers. It is found that none of the derived MPC_{water}s is exceeded by the actual concentrations measured during 1995/96. However, with the exception of DMA all NCs are exceeded by the actual concentrations. No data on soil and sediment concentrations are available.

Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for water, soil and sediment.

Substance	MPC_{water} (µg/l)		NC_{water} (µg/l)	MPC_{soil} (µg/kg)		NC_{soil} (µg/kg)	MPC_{sed} (µg/kg)		NC_{sed} (µg/kg)
MCA	2.0	A&S[a]	0.02	5100	A&S	51	40	EP	0.4
DCA	3.0	A&S	0.03	7800	A&S	78	120	EP	1.2
TCA	6.0	EPA/100	0.06	420	EP	4.2	420	EP	4.2
PCA	0.1	EPA/100	0.001	60	EP	0.6	60	EP	0.6
MA	10	A&S	0.10	30	EP	0.3	30	EP	0.3
DMA	50	A&S	0.50	350	EP	3.5	350	EP	3.5

a extrapolation method: A&S= Statistical extrapolation; EPA=modified EPA-method/extrapolation factor; EP=Equilibrium Partitioning

SAMENVATTING

In dit rapport zijn Maximaal Toelaatbare Risiconiveaus (MTR's) en Verwaarloosbare Risicioniveaus (VR's) voor chloor-, nitro- en methylgesubstitueerde anilines afgeleid. Het rapport is geproduceerd in het kader van het project "Integrale Normstelling Stoffen (INS)" van het Ministerie voor Volkshuisvesting, Ruimtelijke Ordening en Milieubeheer (VROM). Op basis van de MTR's en VR's en aanvullende informatie kunnen door VROM normen worden opgesteld.

Aniline derivaten zijn de afgelopen tien jaar regelmatig aangetoond in zoete oppervlaktewateren, zodat de keuze van de stoffen in de eerste plaats is gebaseerd op het voorkomen in het milieu. Daarbij was de keuze gericht op chlooranilines, (chloor)-nitroanilines en (chloor)methylanilines. Omdat de te verwachten hoeveelheid ecotoxiciteits-data gering is, is een overzicht gemaakt van alle isomeren van deze stofgroepen. Er is geprobeerd zo veel mogelijk "groep-MTR's" af te leiden. Dit betekent dat één waarde kan worden toegepast voor een groep van isomeren. Dit is gedaan door de toxiciteitsdata van b.v. alle monochlooranilines te combineren en vervolgens een extrapolatie-methode toe te passen. Hiervoor is aangenomen dat isomeren hetzelfde werkingsmechanisme bezitten en dat effecten additief zijn, in het geval een organisme tegelijkertijd is blootgesteld aan meer dan één isomeer. Een groep MTR kan worden toegepast op de som van de isomeren binnen een groep waarvoor een groep MTR is afgeleid. Bijvoorbeeld, als 2-chlooraniline (2-CA) en 3-chlooraniline (3-CA) tegelijkertijd zijn aangetoond in water, kan de som van de concentraties worden gerelateerd aan de groep MTR voor monochlooranilinen.

Het aantal toxiciteitsdata beperkte de betrouwbaarheid van de MTR's en VR's. De waarden zijn als volgt afgeleid:

- *water*: Alleen de MTR's voor monochlooranilines (MCA's), dichlooranilines (DCA's), nitroanilines (NA's), methylanilines (MA's) en dimethylanilines (DMA's) zijn afgeleid via statistische extrapolatie. Voor nitro-phenylanilinen (N-PA) zijn alleen zoutwater-data beschikbaar, waarop de aangepaste EPA-methode is toegepast.
- *bodem*: Alleen voor CA's zijn betrouwbare data gevonden. Alleen de MTR's voor MCA's en DCA's zijn met statistische extrapolatie afgeleid. MTR's voor trichlooranilines (TCA's), tetrachlooranilines (TeCA's) en pentachlooraniline (PCA's) zijn afgeleid met de aangepaste EPA-methode, MTR's voor chloor-nitroanilines (C)NA's) en chloor-methylanilines (C)MA's) zijn afgeleid met de evenwichtspartitie methode.
- *sediment*: Alle MTR's zijn afgeleid met de evenwichtspartitie methode, aangezien geen data voor sediment organismen zijn gevonden.

De MTR's en VR's zijn vergeleken met recent gemeten concentraties van het 'Rijksinstituut voor 'Integraal Zoetwaterbeheer en Afvalwaterbehandeling (RIZA)' en de 'Samenwerkende Rijn- en Maaswaterleidingsbedijven (RIWA)'. Maar een fractie van de behandelde stoffen wordt regelmatig gemeten dan wel aangetoond. Bij de vergelijking is bij voorkeur van de som van de gemeten concentraties van de isomeren uitgegaan.

Recent gemeten concentraties in 1995-96 in Nederlandse oppervlaktewateren blijken de afgeleide MTR's niet te overschrijden. Behalve voor DMA overschrijden de gemeten concentraties wel de afgeleide VR's. Data over gehaltes van anilines in bodem en sediment zijn niet beschikbaar.

Maximaal Toelaatbare Risiconiveau's (MTR's) en Verwaarloosbare Risiconiveau's (VR's) voor water, bodem en sediment.

Substance	MPC_{water} (µg/l)		NC_{water} (µg/l)	MPC_{bodem} (µg/kg)		NC_{bodem} (µg/kg)	MPC_{sed} (µg/kg)		NC_{sed} (µg/kg)
MCA	2.0	A&S[a]	0.02	5100	A&S	51	40	EP	0.4
DCA	3.0	A&S	0.03	7800	A&S	78	120	EP	1.2
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PCA	0.1	EPA/100	0.001	60	EP	0.6	60	EP	0.6
MA	10	A&S	0.10	30	EP	0.3	30	EP	0.3
DMA	50	A&S	0.50	350	EP	3.5	350	EP	3.5

a extrapolatie methode: A&S= statistische extrapolatie; EPA=gemodifieceerde EPA-methode/extrapolatiefactor; EP=evenwichts-partitie-methode

1. INTRODUCTION

The project "Setting Integrated Environmental Quality Objectives" was started in 1989 by the Directorate-General for the Environment. It is focused on the derivation of concentration limits for the compartments air, water, sediment and soil for a great number of compounds and is based on the risk philosophy of the Ministry of Housing, Spatial Planning and Environment (VROM, 1989). The setting of the environmental quality objectives (EQOs) is the responsibility of this ministry. The method used in this project consists in general of deriving Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for different environmental compartments. The derivation of these risk limits is the part of the project which is performed at the National Institute of Public Health and the Environment (RIVM).

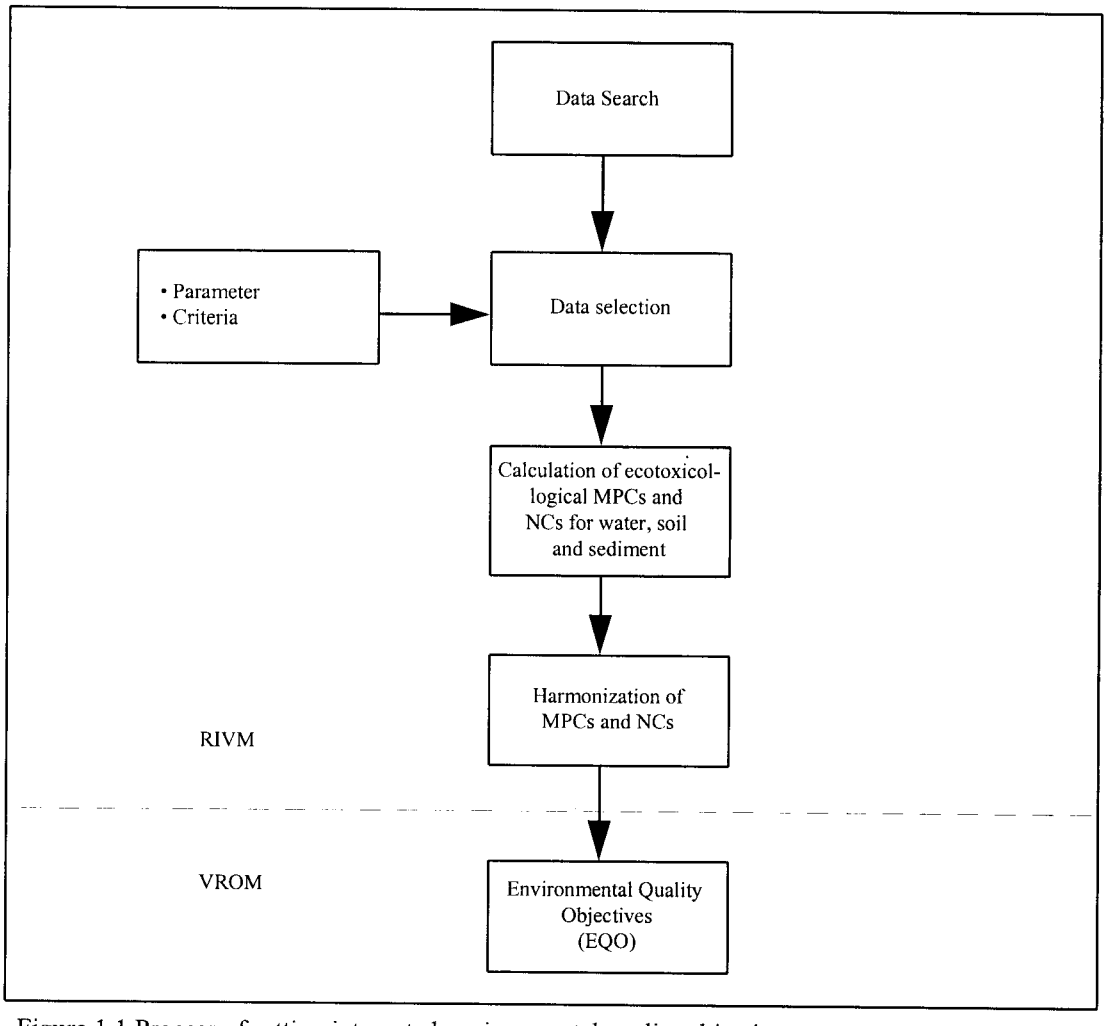

Figure 1.1 Process of setting integrated environmental quality objectives.

Two steps are necessary for deriving the mentioned risk limits (Figure 1.1). First, MPCs for the environmental compartments are derived. Subsequently, in the second step, these MPCs are harmonised (by applying the equilibrium partitioning method (EP-method) or multi-media

fate models like Simple-Box (Van de Meent, 1993). The MPCs are derived on the basis of single-species toxicity data.
Species may encounter multi-chemical stress in water and/or soils and sediments. Therefore, the NC is set at 1% of the MPC to take this factor into account. Due to intercompartimental transport of chemicals, MPCs or NCs in one compartment may exceed the values for another. For that reason the values are harmonised.
Hitherto, the methodology for deriving MPCs and NCs is presented and applied in several reports published within this project. In the first part of the project (a) "MILBOWA", MPCs for heavy metals, chlorophenols, pesticides and polycyclic aromatic hydrocarbons (PAHs) are presented in 'Desire for levels', (Van der Meent *et al.*, 1990). The MPCs and NCs for PAHs were updated by Kalf *et al.* (1995). Within several sub-projects of the second part (b), MPCs were derived for 'trace metals' (Van de Plassche *et al.*, 1992), 'volatile compounds' (Van de Plassche *et al.*, 1993) and 'substances with a potential for secondary poisoning' (Van de Plassche, 1994). MPCs for metals are updated by Crommentuijn *et al.* (1997a), MPCs for a large group of pesticides are derived by Crommentuijn *et al.* (1997b).

In the context of the present report MPCs and NCs are derived for a number of anilines. The following groups of derivates are considered:

- chloroanilines
- (chloro)nitroanilines
- (chloro)methylanilines

These compounds are mainly chosen based on their occurrence in the environment. Since the amount of toxicity data is expected to be low for most of the compounds all possible isomers of these groups are summarised according to the list of commercial chemical substances (EINECS). This results in a list of about 70 compounds. However, it is not our aim to derive MPCs for all compounds individually. To be able to use quality objectives it is desirable to derive as much as possible group values since that will increase the applicability. In the following the group values are referred to as 'group MPCs'. These group MPCs are derived by combining all available toxicity data on a group of isomers, e.g. monosubstituted chloroanilines, and applying an extrapolation method. The MPC derived in this way can subsequently be used for each of the individual compounds included in a group value. This means that for each individual isomer of a group the same MPC can be used. For applying this method it is assumed that isomers have the same mode of action and that the effects are considered additive in the case an organism is exposed simultaneously to more than one isomer (Denneman and Van Gestel, 1990).

With the exception of chloroanilines no quality criteria for aniline derivates have been set earlier. Slooff *et al.* (1991) proposed indicative Maximum Acceptable Risk Levels (MARs) for chloroanilines. These risk levels will be compared with the MPCs derived in this report.

Based on the fact that most compounds have relatively low log K_{ow}-values (Table 2.1) strong bioaccumulation is not expected, and therefore no attention is paid to the bioaccumulative behaviour and secondary poisoning (see paragraph 2.7).

From the literature it is furthermore found that anilines are not readily biodegraded (BUA 1988; Struijs *et al.*, 1983; Wellens, 1990; SIDS, 1995; BUA, 1996). For choroanilines indications are found that they undergo biotransformation in fish (De Wolf *et al.*, 1993; De Wolf *et al.*, 1994).

Although several anilines are classified as possible carcinogenic to humans (IARC, 1993) these issues are not included in this report. This is based on the fact that at this moment no suitable procedure is available to include mutagenicity and carcinogenity into the currently applied methodology for the derivation of MPCs and NCs. Besides that it is uncertain how species are affected at the population level. Evaluation of data on carcinogenic and mutagenic effects for humans, which was conducted in the context of another RIVM project, revealed that only few data are available (Janssen *et al.*, 1997), so at present it is not possible to include a profound human risk evaluation.

The following steps will be conducted to derive the MPCs and NCs which are presented in this document:

- deriving MPCs and NCs for water, soil and sediment based on experimental literature data
- collecting sediment water and soil pore water partition coefficients for applying the equilibrium partitioning method
- harmonisation of the MPCs and NCs for water, sediment and soil by using the equilibrium partitioning method.

In chapter 2 an overview is given of the physical-chemical properties together with the mode of action and the bioaccumulative behaviour of the concerned anilines. In chapter 3 the method of deriving and harmonising MPCs and NCs is described, followed by a presentation of the MPCs based on experimental data for the aquatic environment in chapter 4. In chapter 5 the derivation of MPCs for soil and sediment based on experimental data are presented. In chapter 6 the derivation and calculation of soil sorption coefficients (log K_{oc}) is outlined, followed by the derivation of MPCs for soil and sediment based on equilibrium partitioning using soil water partition coefficients (K_p) in chapter 7. The results will be discussed in chapter 8 together with a comparison of the derived MPCs with measured concentrations of anilines in the environment. Finally, the conclusions are presented in chapter 9.

2. ANILINES

In this chapter some aspects concerning the selected compounds are summarised. In paragraph 2.1 the chemical structure and the terminology of the anilines is outlined followed by the choice of compounds in paragraph 2.2. In paragraph 2.3 the physical-chemical properties are summarised together with data on biodegradability. The use of anilines and the pathways into the environment are presented in paragraph 2.4 The biotransformation of anilines will be outlined in paragraph 2.5. The mode of action is presented in paragraph 2.6 followed by a description of the bioaccumulative behaviour in paragraph 2.7.

2.1 Chemical structure and terminology

The CAS-registration numbers together with the molecular and structural formulas are listed in Appendix 1. The name 'aniline' refers to a compound consisting of an aromatic benzene ring with one hydrogen atom substituted by an amino group (NH_2) (Figure 2.1). Substitutions can occur in all positions within the benzene ring. The position number is determined by the position of the amino group which is considered to be situated in position 1. Position 2, 3, and 4 also refer to as *ortho*, *meta* and *para* position, respectively. Hydrogen atoms can be substituted among others by halogenids or functional groups (alkyl-, nitro-, hydroxyl group etc.) Substitutions also occur at the nitrogen atom of the amino group in the case of methylanilines. The nomination 'N-methylaniline' or 'N,N-dimethylaniline' refers to mono- or dimethylic substitution, respectively, within the amino group.

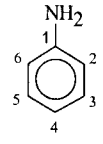

Figure 2.1 Structure of aniline

2.2 Choice of compounds

The following groups of aniline derivatives are considered:

- chloroanilines
- (chloro-)nitroanilines
- (chloro-)methylanilines

The choice of the compounds is mainly based on their occurrence in the environment. They are detected in surface waters like Rhine and Meuse during the last ten years (Venema, 1990; Barreveld, 1991; Heymen, 1992; Van Genderen *et al.*, 1994; RIWA, 1995a; RIWA, 1995b; RIWA, 1996a; RIWA, 1996b). Since it was expected that the amount of toxicity data available is low an inventarisation is made of all possible isomers of the above mentioned chemical groups according to the list of commercial chemical substances (EINECS) (Table 2.1). Moreover, it is assumed that isomers with similar structure show similar toxicity. To be able to derive group values all toxicity data available are collected for all the compounds not

only depending on their occurrence in the environment, but also to receive a broader range of underlying data to derive (group) MPCs. It is found, that only a small number of anilines actually occur in the environment (Table 2.1).
As mentioned before 'group MPC' refers to *one* risk limit for a group of similar substances. It can be applied to the sum of the concentration of the isomers which occur simultaneously in the environment.

2.3 Physical-chemical properties and degradability

The physical-chemical properties of the anilines and abbreviations are listed in Table 2.1. The data are mainly derived from the ASTER-database. Since the values in the data base are expressed in units other than it is required according to the quality document (CSR, 1996) they had to be recalculated. The compounds for which data are found have a low to moderate water solubility. The n-octanol water partition coefficients are used for calculation of the soil sorption coefficients (log K_{oc}). Experimental values obtained by the slow-stirring method (De Bruijn *et al.*, 1989) are preferred (CSR, 1996). If no experimental data are available the "star values" from the MEDCHEM database are used. In case these data are also not available the log K_{oc}s are calculated with the ClogP values from the ASTER database. Based on the magnitude of the Henry constant evaporation of anilines from the water phase is not considered to be an important process when MPCs are derived. The pK_b values are calculated with the pK_a values from the ASTER database.

To ensure that the toxicity is exerted by the parent compound the (bio)degradability has to be taken into account. Especially compounds with a half-life of less than a few hours are of particular concern since the toxicity is probably exerted by their metabolites (CSR, 1996). In the following paragraph a short overview is given on the degradability of the anilines.
Several authors reported no degradability of 2-CA, (Struijs *et al.*, 1983; Canton *et al.*, 1985; MITI, 1992), whereas BUA (1994) recorded a potential degradability of this compound as well as for 3-CA. Janicke and Hilge (1980) reported resistance to biodegradation for 4-CA, 3,4- and 3,5-DCA and 2,4,6-TCA. MITI (1992) and BUA (1996) reported no degradation within 2 and 4 weeks of several DCAs, respectively. According to the former 2,4,6-TCA is not degradable within a period of 4 weeks. No degradation data on TeCA are found. These compounds are not expected to degrade rapidly (Peijnenburg, personal communication). The mono-substituted NAs are not degradable (Pitter, 1976; Urano and Kato, 1986; Wellens, 1990). No degradability of 2-chloro-4-nitro-aniline (2-C-4-NA) and 2-nitro-4-chloroaniline (2-N-4-CA) was reported by Struijs *et al.* (1983), Canton *et al.* (1985) and MITI (1992). Data on MAs revealed for 2-MA a degree of degradation of 65% within 14 days (MITI, 1992) and 96% within 11 days (Wellens, 1990). Almost no degradation of 3-MA (0-1%) and 4-MA (1%) is reported in MITI (1992), whereas Wellens (1990) found 94% degradation of 4-MA within 8 days. In the literature the data on degradability of CMAs present a wide range, varying from 0% (MITI, 1992) to 100% (BUA, 1990) within two weeks. In the SIDS document (1995) no degradation up to 35 days is reported of 4-N-PA.

Table 2.1 Physical-chemical properties of substituted aniline derivates. Compounds which are marked with an "x" have been found in Dutch surface waters within the last two years.

Substance		Abbreviation	Molecular[a] weight (g/mol)	Vapour[a] pressure (Pa,25°C)	log[b] K_{ow}	log[c] K_{ow} (star)	log[d] K_{ow} (ClogP)	Water[a] solubility (mg/l, 25°C)	Henry[e] constant (25°C)	pK_b[f]
2-chloroaniline	x	2-CA	127.58	33.3	1.93	1.90	1.93	3730	4.60e-4	11.35
3-chloroaniline	x	3-CA	127.58	11.2	1.91	1.88	1.93	3730	1.55e-4	11.35
4-chloroaniline	x	4-CA	127.58	62.2	1.88	1.88	1.91	1380	2.33e-3	10.11
2,3-dichloroaniline		2,3-DCA	162.02	8.6	2.86	2.86	2.79	471	1.19e-3	12.42
2,4-dichloroaniline	x	2,4-DCA	162.02	0.9	2.91	2.91	2.79	214	2.75e-4	12.04
2,5-dichoroaniline		2,5-DCA	162.02	2.12	2.92	2.92	2.79	280	4.95e-4	12.42
2,6-dichloroaniline	x	2,6-DCA	162.02	2.12	2.82	2.82	2.79	352	3.94e-4	13.28
3,4-dichloroaniline	x	3,4-DCA	162.02	2.12	-	2.69	2.79	181	7.66e-4	11.18
3,5-dichloroaniline	x	3,5-DCA	162.02	0.34	-	2.90	2.79	269	8.26e-5	11.55
2,3,4-trichloroaniline		2,3,4-TCA	196.46	0.04	3.68	3.69	3.58	30	1.06e-4	13.11
2,3,5-trichloroaniline		2,3,5-TCA	196.46	-	-	-	-	-	-	-
2,4,5-trichloroaniline	x	2,4,5-TCA	196.46	0.17	3.69	3.69	3.58	17	7.93e-4	13.11
2,4,6-trichloroaniline		2,4,6-TCA	196.46	0.29	3.69	3.69	3.58	26	8.84e-4	13.97
3,4,5-trichloroaniline		3,4,5-TCA	196.46	-	-	-	-	-	-	-
2,3,4,5-tetrachloroaniline		2,3,4,5-TeCA	230.90	0.03	4.57	4.57	4.33	1.5	1.86e-3	14.17
2,3,5,6-tetrachloroaniline		2,3,5.6-TeCA	230.90	0.03	4.46	4.46	4.33	2.1	1.33e-3	15.41
pentachloroaniline		PCA	265.34	7.34e-4	5.08	-	5.08	2.5e-2	3.14e-3	16.10
2-nitroaniline		2-NA	138.13	0.06	-	1.85	1.78	2430	1.66e-6	14.37
3-nitroaniline		3-NA	138.13	0.29	-	1.37	1.37	3450	4.73e-6	11.55
4-nitroaniline		4-NA	138.13	0.29	-	1.39	1.31	1740	9.39e-6	13.05
4-nitro-N-phenylaniline		4-N-NPA	214.2	7.42e-5	-	3.74	4.01	2.6	2.50e-6	-
2-nitro-N-phenylaniline		2-N-NPA	214.2	7.42e-5	-	-	4.48	2.6	2.50e-6	-
2,4-dinitroaniline		2,4-DNA	183.12	1.25e-4	-	1.72*	1.84	6100	1.52e-9	18.00
2,6-dinitroaniline		2,6-DNA	183.12	1.25e-4	-	1.79	1.84	600	1.52e-8	19.33
3,5-dinitroaniline		3,5-DNA	183.12	1.25e-4	-	1.89	1.37	1300	6.96e-9	13.68
2-chloro-4-nitroaniline		2-C-4-NA	172.6	0.05	-	-	2.17	470	6.59e-6	13.02
2-chloro-5-nitroaniline		2-C-5-NA	172.6	0.05	-	-	2.17	430	7.30e-6	13.48
2-chloro-6-nitroaniline		2-C-6-NA	172.6	-	-	-	-	-	-	-
2-nitro-3-chloroaniline		2-N-3-CA	172.6	-	-	-	-	-		-
2-nitro-4-chloroaniline		2-N-4-CA	172.6	0.05	-	2.72	2.64	110	2.84e-5	12.94
2-nitro-5-chloroaniline		2-N-5-CA	172.6		-		-	-	-	-
3-nitro-4-chloroaniline		3-N-4-CA	172.6	0.05	-	2.06	1.89	1180	2.64e-6	12.24
2,4-dichloro-6-nitroaniline		2,4-DC-6-NA	207.0		-	3.33*	-	-	-	-
2,5-dichloro-4-nitroaniline		2,5-DC-4-NA	207.0	7.41e-3	-	2.68	-	50	1.14e-5	16.04
2,6-dichloro-4-nitroaniline		2,6-DC-4-NA	207.0	7.41e-3	-	2.79*	2.96	12	4.98e-5	16.91
3,4-dichloro-6-nitroaniline		3,4-DC-6-NA	207.0	-	-	-	-	-	-	-
4,6-dinitro-2-chloroaniline		4,6-DN-2-CA	217.6	2.05e-5	-	2.63	-	60	2.91e-8	19.93
2,6-dinitro-4-chloroaniline		2,6-DN-4-CA	217.6	2.05e-5	-	2.63	-	78	2.31e-8	20.02
2-methylaniline	x	2-MA	107.2	42.25	-	1.32	1.56	8340	2.19e-5	9.71
3-methylaniline	x	3-MA	107.2	36.65	-	1.40	1.56	8340	1.90e-4	9.25
4-methylaniline	x	4-MA	107.2	44.65	-	1.39	1.56	5750	3.36e-4	9.02
N-methylaniline		N-MA	107.2	109.70	-	1.66	1.64	6790	6.99e-4	
N,N-dimethylaniline		N,N-DMA	121.2	133.29	-	2.31	2.34	1110	5.90e-3	8.94
N,2-dimethylaniline		N,2-DMA	121.2	138.62	-	2.16	2.29	1140	5.95e-3	-
N,3-dimethylaniline		N,3-DMA	121.2	138.62	-	2.14*	2.29	1140	5.95e-3	-
N,4-dimethylaniline		N,4-DMA	121.2	138.62	-	2.15	2.29	1140	5.95e-3	-
2,3-dimethylaniline		2,3-DMA	121.2	33.72	-	1.81*	2.21	1660	9.93e-4	9.54
2,4-dimethylaniline		2,4-DMA	121.2	135.95	-	1.68	2.21	1660	4.00e-3	9.30
2,5-dimethylaniline		2,5-DMA	121.2	135.95	-	1.83	2.21	1660	4.00e-3	9.54
2,6-dimethylaniline		2,6-DMA	121.2	47.98	-	1.84	2.21	1660	1.41e-3	10.00
3,4-dimethylaniline		3,4-DMA	121.2	2.99	-	1.86*	2.21	970	1.50e-4	8.84
3,5-dimethylaniline		3,5-DMA	121.2	33.72	-	1.91*	2.21	1660	9.93e-4	9.07
N,N,2-trimethylaniline		N,N,2-TMA	135.2	133.29	-	2.85	2.99	235	3.09e-2	9.29
N,N,3-trimethylaniline		N,N,3-TMA	135.2	83.97	-	2.80	2.99	177	2.59e-2	8.73
N,N,4-trimethylaniline		N,N,4-TMA	135.2	27.86	-	2.81	2.99	177	8.58e-3	8.46
2,3,4-trimethylaniline		2,3,4-TMA	135.2	-	-	-	-	-	-	-
2,4,5-trimethylaniline		2,4,5-TMA	135.2	-	-	-	-	-	-	-
2,4,6-trimethylaniline		2,4,6-TMA	135.2	2.04	-	2.31*	2.86	116	9.56e-4	9.59
3,4,5-trimethylaniline		3,4,5-TMA	135.2	-	-	2.31*	-	-	-	-
2-chloro-4-methylaniline		2-C-4-MA	141.6	29.59	-	-	2.58	730	2.31e-3	10.95
2-chloro-5-methylaniline		2-C-5-MA	141.6	-	-	-	-	-	-	-
2-chloro-6-methylaniline		2-C-6-MA	141.6	43.85	-	-	2.58	730	3.43e-3	11.64
3-chloro-2-methylaniline		3-C-2-MA	141.6	11.69	-	-	2.58	730	9.14e-4	10.77
3-chloro-4-methylaniline		3-C-4-MA	141.6	54.52	-	2.41*	2.58	730	4.26e-3	10.08
5-chloro-2-methylaniline		5-C-2-MA	141.6	54.52	-	-	2.58	730	4.26e-3	10.77
4-chloro-N-methylaniline		4-C-N-MA	141.6	-	-	2.66*	-	-	-	-
4-chloro-2-methylaniline		4-C-2-MA	141.6	29.06	-	-	2.58	700	2.37e-3	10.40
3-chloro-N,N-dimethylaniline		3-C-N,N-DMA	155.6	33.59	-	3.22*	3.22	105	2.01e-2	13.11
2,6-dichloro-3-methylaniline		2,6-DC-3-MA	176.0	0.88	-	-	3.44	63	9.90e-4	10.22

- no data available

a physical/chemical properties derived/recalculated from the ASTER-database

b according to De Bruijn *et al.* (1989)

c star log K_{ow} -values derived from the MEDCHEM®-database (* estimated values)

d derived from the ASTER database

e dimensionless Henry-constant calculated according to the quality document (CSR, 1996)

f calculated with pK_as

As a consequence it is assumed that toxic effects which are reported in the evaluated studies are caused by the parent compound. No special attention is paid to the toxic effects of the metabolites.

2.4 Use of anilines and pathways into the environment

No natural sources are known for these compounds. Mono- (MCAs) and dichloroanilines (DCAs) are produced through hydrogenation of chloro-nitrobenzene. Trichloroanilines (TCAs) are synthesised by direct chlorination of aniline. Nitroanilines (NAs) and chloro-nitroanilines (CNAs) are manufactured by ammonolysis of the corresponding chloro-nitrobenzenes. 4-nitro-N-phenylaniline (4-N-NPA) is synthesised through condensation of 4-chloro-nitrobenzene with aniline (BGC, 1994). Methylanilines (MAs) are produced by methylation of aniline. Corresponding chloro-nitrotoluenes serve as precursors for chloro-methylanilines (CMAs) (BUA, 1997).

Table 2.2 Application of several aniline derivates in the Netherlands and world-wide.

Substance	application in the Netherlands	application world-wide	Reference
2-CA	azoic dyes (possible)	pesticides, azoic dyes, solvents, standard in colorimeters and intermediary chemicals	Slooff *et al.* (1991)
3-CA	pesticides, pharmac. prod., pigments (100-1000 t/y)	pesticides, pigments, and pharmac. prod. and intermediary chemicals	Slooff *et al.* (1991)
4-CA	pesticides, pharmac. prod., pigments (100-1000 t/y)	pesticides, azoic dyes, pigments, pharmac. prod. and intermediary chemicals	Slooff *et al.* (1991)
2,3-DCA	none	none (no industrial significance)	Slooff *et al.* (1991)
2,4-DCA	none	pigments	Slooff *et al.* (1991)
2,5-DCA	none	pigments	Slooff *et al.* (1991)
2,6-DCA	none	pigments	Slooff *et al.* (1991)
3,4-DCA	pesticides	pesticides	Slooff *et al.* (1991)
3,5-DCA	none	pesticides	Slooff *et al.* (1991)
2-NA	unknown	intermediate for rubber chemicals, dyes, pigments and pesticides	BUA, 1988
4-NA	unknown	intermediate for rubber chemicals, dyes, pigments and pesticides (5200 t in 1983 in Western-Europe)	BUA, 1995a
2-C-4-NA	unknown	dyes, intermediate for pesticides (ca. 1350 t in Germany /y)	BUA, 1993
3-MA	unknown	intermediates for dye, chemicals and pharmac. (1000-1200 t/y in Germany)	BUA, 1997
N,N-DMA	unknown	acid scavenger for synthesis of penicillin derivates; intermediate for dyes, photo chemicals and pharmac.	BUA, 1995b
3-C-4-MA	unknown	(intermediate for) pesticides, intermediate for dyes, and pharmaceuticals (2700 t in Western-Europe in 1985)	BUA, 1990
3-C-2-MA	unknown	unknown	BUA, 1990
5-C-2-MA	unknown	unknown	BUA, 1990

In Table 2.2 the application and the amount of several aniline derivates in the Netherlands and world-wide are listed. Depending on the application aniline derivates are released via different pathways into the environment.

MCAs and DCAs can be expected to enter the environment as impurities of crop protection agents. Caused by degradation and washing-out processes an indirect introduction of these compounds can occur into the water. E.g., 3-CA is formed through degradation of

chloropropham[a], 4-CA is a metabolite of diflubenzuron[a] and monolinuron[a] (Venema, 1990). 3,4-DCA is formed through degradation of diuron[a] and linuron[a]. Pentachloroaniline (PCA) can enter the environment through biodegradation or conversion of the pesticide quintozene[b] (TAH, 1990). Data on emission of other CAs (TCAs, TeCAs) are not available.
(Chloro)nitroanilines and (chloro)methylanilines (C)MAs) enter the environment mainly through discharge of wastewater and the use of pesticides (BUA, 1988; BUA, 1995a; BUA, 1990; BUA, 1997). However, also no data on emission of these compounds in the Netherlands are available.

2.5 Biotransformation

An organism has two major ways to eliminate a chemical once it has entered the body: excretion of the parent compound or biotransformation (Van Leeuwen and Hermens, 1995). The latter is considered as an enzyme-catalysed conversion which alters, in particular lipophilic, substances in more water-soluble forms, which enables an organism to excrete them at a higher rate. The most common biotransformation reactions are among others hydroxylation, epoxidation, dealkylation and certain conjugation reactions.
For aromatic compounds such as polycyclic aromatic hydrocarbons (PAHs) it is found that during transformation metabolites can be formed which are more toxic than the parent compound (Neff, 1979; Neff, 1985). In the literature it is found that anilines mainly react as methaemoglobin formers. Oxidation of the amino group or (in the case of nitroanilines) reduction of the nitro group results in the formation of phenylhydroxylamine. Divalent iron in haemoglobin is oxidised to methaemoglobin, which is incapable of transferring oxygen. As a consequence of long exposure extramedullary hematopoiesis can occur due to hypoxia in liver and spleen of mammals (BUA, 1993; BUA 1995a).
Several authors investigated the biotransformation in fish of mono-, di- and trichloroanilines and nitroanilines. In fish acetylation is the main route of biotransformation of chloroanilines (Zok *et al.*, 1991). For *meta*- and *para*-substituted chloroanilines higher biotransformation rates are reported in *Brachydanio rerio* (Zok *et al.*, 1991) and in *Poecilia reticulata* (De Wolf *et al.*, 1993) than for *ortho*-substituted anilines. Zok *et al.* (1991) found elimination rates of 100% for 3-CA and 3,4-DCA, 65%, 26% and 17% for 4-CA, 2,4-CA and 2-CA, respectively, within 24 hours. No biotransformation are found for 2-NA and 4-NA. De Wolf *et al.* (1993) reported biotransformation of TCAs in *Poecilia reticulata*.
According to Zok *et al.* (1991) biotransformation of lower-substituted anilines has no effect on the toxicity (2-CA, 3-CA, 4-CA, 3,4-DCA, 2-NA, 3-NA, 4-NA), because the metabolites formed act in the same unspecified way as the parent compounds. However, these authors do not exclude the possibility of the occurrence of long-term effects caused by the metabolites. De Wolf *et al.* who investigated the biotranformation of higher chlorinated anilines (De Wolf *et al.*, 1989; De Wolf *et al.*, 1992c; De Wolf *et al.*, 1993) assumed that the biotransformation potential is related to the chemical structure. Anilines which are substituted in one or both *ortho*-position(s) are less biotransformable than other isomers, probably due to steric hindrance. The same authors also found a higher BCF for 2,3,4,5-TeCA in fish at high

[a] permitted in the Netherlands (Gewasbeschermingsgids, 1996)
[b] not permitted in the Netherlands (Gewasbeschermingsgids, 1996)

concentrations than at low concentrations. They assumed, if biotransformation plays a role in the elimination, that the increase could be explained by the saturation of biotransformation-related enzyme systems by the compound, resulting in a lower elimination rate. Another explanation for the increase could be the toxic influence of the compound on the biotransformation system, also resulting in a lower overall elimination rate. De Wolf *et al.* (1992b) related the toxicity of 2,3,4,5-TeCA to its biotransformation potential. They found a decrease in lethal body burden (LBB) with time, which they suggested to be related to a time-dependent formation of toxic metabolites.
From the above it can be concluded that some aniline derivates undergo biotransformation in fish, depending on the concentration and the exposure time. These species may be at risk in the case they are exposed to these chemicals for a prolonged time.
However, no data on biotransformation in relation to toxicity are available for other (aquatic) organisms.

2.6 Mutagenicity and Carcinogenicity

Although some anilines are known to have a mutagenic and/or carcinogenic potential these effects are not taken into account within the project 'Setting Integrated Environmental Quality Objectives', since it remains unclear whether species are affected at the population level. Mutagenic and carcinogenic effects of anilines are evaluated within the assessment procedure of the possible risks for humans. In the context of the 'Intervention Value project' it is aimed to derive *maximum permissible risk levels* for chloroanilines based on carcinoginicity in humans (Janssen *et al.*, 1997). Due to the lack of appropriate toxicity data no limit values could be derived for DCAs, TCAs, TeCAs and PCAs. For MCAs an oral excess 10^{-4} life-time tumour risk of 0.9 µg/kg bw is derived (chance of 1 to 10000 to develop a tumour when exposed to 0.9 µg/kg bw for life).

2.7 Bioaccumulation and secondary poisoning

Organic substances with a high n-octanol water partition coefficient (log K_{ow} > 5) are considered to have a bioaccumulative potential (CSR, 1996). Uptake of these substances might have serious consequences for higher members of the food chain, like birds and mammals. As a consequence, not only direct but also indirect effects have to be taken into account when quality objectives are derived.
In general, anilines have a weak to moderate bioaccumulative potential. With the exception of 2-CA no experimental determined bioconcentration factors (BCFs) of MCAs are found. According to MITI (1992) 2-CA bioaccumulates weakly in fish (<14-32 l/kg). For DCAs BCFs are reported in the range of 4-95 l/kg in *Cyprinus carpio*, *Brachydanio rerio* and *Oncorhynchus mykiss* (BUA, 1996). BCFs in fish reported for TCAs range from 34 to 147 l/kg (MITI, 1992; De Wolf *et al.*, 1992a). Data on bioaccumulation of TeCAs in the literature are limited. De Wolf *et al.* (1992a[c], 1992b[c]; 1994) experimentally determined BCFs in *Poecilia reticulata* ranging from 125-330 l/kg. BCFs are reported for mono-NAs ranging from 4.4-10 l/kg, 12.9 l/kg for 2,4-DNA, and for 4-chloro-2-nitroaniline (4-C-2-NA) ranging from

[c] BCFs recalculated on the basis of wet weight

8.0-13.4 l/kg (Zok *et al.*, 1991; Kalsch *et al.*, 1991; MITI, 1992, BUA 1995a). Canton *et al.* (1985) theoretically determined a BCF of 33 l/kg for 2-C-4-NA. In the SIDS document (1991) a BCF of 580 l/kg in fish is reported for 4-N-NPA. BCFs reported for fish for MAs and DMAs range from <1.7 to 10.1 l/kg (MITI, 1992). Data on CMAs are lacking. However, in the literature it is assumed that these compounds do not bioaccumulate due to their low log K_{ow}-values (BUA, 1990).

Calculation of the BCF for PCA based on a QSAR derived by Veith *et al.* (1979) results a BCF of more than 4100 l/kg. However, in the literature experimentally determined BCFs are reported up to 510 l/kg for PCA (De Wolf *et al.*, 1992a[d]). This indicates that the BCF calculated based on log K_{ow} could be overestimated, especially in the case when chemicals undergo biotransformation, which is found for higher chlorinated anilines in fish (De Wolf *et al.*, 1993; De Wolf *et al.*, 1994).

As a consequence no further attention is paid to the possible effects to mammals and birds due to secondary poisoning.

[d] BCFs recalculated on the basis of wet weight

3. METHODOLOGY

In this chapter the methodology of deriving Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (NCs) for water, sediment and soil is described. In order to set these criteria ecotoxicological data for the different environmental compartments have to be collected and evaluated. The method of data search, data evaluation, and data selection is summarised in paragraph 3.1, 3.2 and 3.3, respectively. For deriving MPCs and NCs two different extrapolation methods are applied depending on the amount of toxicity data. These extrapolation methods are described in paragraph 3.4. Some aspects concerning the derivation of the MPC_{water} are outlined in paragraph 3.5. The methodology for the derivation of group MPCs is briefly described in paragraph 3.6. Paragraph 3.7 describes the derivation of partition coefficients from the literature. If no sufficient data for soil and sediment species are available MPCs are estimated using the Equilibrium Partitioning method (EP-method) (paragraph 3.8). Some aspects concerning the critical air concentrations are outlined in paragraph 3.9.

3.1 Literature search

All toxicity data are obtained from external and internal 'Centre for Substances and Risk Assessment' (CSR) sources. On-line search is conducted according to the quality document CSR/P/001 (CSR, 1997).

3.1.1 Internal literature sources

The following internal literature sources are used:

- the library of the CSR
- the cardbox literature database containing articles form public literature, which have been collected and evaluated within the project 'Setting Integrated Environmental Quality Objectives' and 'Intervention Values'
- 'grey' literature (summaries, non-published documents), which is present in the documentation of the CSR

3.1.2 External literature sources

The external literature sources are:

- the library of the National Institute for Public Health and the Environment
- on-line search in the databases Biosis and Toxline
  retrospective search based on public literature and reviews

3.2 Deriving data from toxicity studies

For deriving NOECs and $L(E)C_{50}$ single species tests and tests concerning microbial processes are evaluated. In this paragraph the stepwise procedure for deriving these data is presented.

3.2.1 Relevant toxicity criteria

Relevant toxicity parameters are those which affect species at the population level. These are survival, growth and reproduction. For terrestrial species also microbe mediated processes and enzyme activities are taken into account. In general toxicity is expressed as acute $L(E)C_{50}$ or chronic NOECs. The consideration of acute or chronic test depends on the species which is tested. E.g., a 16-h test with Protozoans is considered acute and a fish test enduring 28 d is considered chronic. In the case of micro-organisms or algae NOECs may be derived from tests lasting less than four days (Slooff, 1992). A more detailed description is given in the quality document (CSR, 1996).

In some cases other parameters than population parameters, e.g. behaviour, may also be used for deriving NOECs or $L(E)C_{50}$. This is the case if the parameter in question is considered as ecological relevant, e.g. immobility in tests with crustaceans. At this moment no methodology is available to evaluate studies in which carcinogenicity and mutagenicity is taken as endpoint. It is still uncertain whether species are affected at the level of the population. Therefore, these parameters are not taken into account.

3.2.2 Quality criteria

A study is considered reliable if it is conducted according to international accepted guidelines such as the OECD guidelines. Within the Centre of Substances and Risk Assessment criteria have been developed to judge studies that deviate from that guidelines. In the following the quality criteria applied for derivation NOECs and $L(E)C_{50}$ are summarised. For an extensive description see the quality criteria (CSR, 1996):

- Substance purity has to be at least 80 %.
- Studies using animals from polluted sites are rejected.
- In aquatic studies results more than 10 times the substance solubility are not included
- Solvent use: a maximum of 1 ml/l organic solvents is accepted (OECD 0.1 mg/l). Exceedance of the value in the OECD guidelines has to be mentioned in a footnote of the toxicity tables.
- Using solvents in terrestrial studies: if solvent was not allowed to evaporate from soil medium before test animals are transferred, solvent concentration may not exceed 100 mg/kg. If transferred after evaporation concentration may reach up to 1000 mg/kg. Exceedance of 100 mg/kg is mentioned in a footnote.
- In aquatic studies the recovery of a compound has to be at least 80 %.

3.2.3 Derivation of NOECs from the literature

In chronic studies the results are not always expressed as NOECs. In some cases only the raw data of chronic studies are presented. Different methods can be used to derive a NOEC:

- Results are used if the NOEC is based on a statistical method: the lowest concentration exhibiting no significant effect ($p < 0.05$) is considered the NOEC.

- No statistical method is applied: the concentration showing less than 10% effect is considered the NOEC, provided that a clear concentration-effect relationship is available.
- In case of a LOEC (Lowest Observed Effect Concentration) the following criteria are applied:
  1. LOEC > 10 - 20% effect: NOEC = LOEC/2,
  2. LOEC ≥ 20% effect and a distinct concentration-effect relationship: EC_{10} is calculated or extrapolated and regarded the NOEC,
  3. LOEC ≥ 20% with no concentration-effect relationship:
     - LOEC 20 - 50% effect: NOEC=LOEC/3,
     - LOEC ≥ 50% Effect: NOEC = LOEC/10.

3.2.4 Calculation of L(E)C_{50}s from literature data

Based on raw data an LC_{50} can be calculated according to the trimmed method of Spearman-Kärber (Hamilton *et al.*, 1977/78). EC_{50} is calculated with a log-logistic dose-response model (Haanstra *et al.*, 1985). It should be mentioned that in most studies raw data are not presented. Nevertheless, it is assumed that acute toxicity tests are conducted according to standardised methods.

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

Toxicity data from terrestrial/soil studies are converted to soil with standard organic matter and clay content (e.g. 10% organic matter, 25% clay). For organic compounds such as anilines only the organic matter content is taken into account in this recalculation. The clay content is only used when results of tests with (heavy) metals have to be converted to standard soil (Van de Plassche *et al.*, 1992).
Conversion has to be conducted according to the following criteria:

- if % o.m. < 2%, the percentage is set at 2% o.m. followed by the formula in Table 3.1,
- if % o.m. is between 2-30%, use formula in Table 3.1,
- if % o.m. > 30% the percentage is considered 30%, following the formula in Table 3.1.

Table 3.1 Conversion to standard soil.

$$NOEC/LC50_{st.soil} = NOEC/LC50_{exp} \times \frac{(10\%o.m.)}{(\%o.m._{soil,food})}$$

$NOEC/LC50_{st.\ soil}$	=	NOEC or LC50 in standard soil
$NOEC/LC50_{exp.}$	=	experimental NOEC or LC50
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

The criteria above are set for species living in the soil and which are exposed to contaminants through pore water. In studies concerning species living on the surface these species are exposed to chemicals through food. Food is considered dead material and is described as soil containing 30% o.m.

3.3 Data selection

Raw toxicity data derived from the literature are evaluated and summarised in Appendix 2 to Appendix 5. For each substance, separate tables for chronic and acute data are given. In the table for aquatic species the result of the toxicity study (in mg/l) is presented together with the experimental conditions: species, if the test substance is analysed, test type, testwater, pH and hardness of the testwater, duration of the experiment, the criterion (NOEC or $L(E)C_{50}$) and the reference study. In the table for marine species the hardness is replaced by the salinity.
In the table for terrestrial species and microbial and enzymatic processes the result of the toxicity test is presented as mg/kg, together with the experimental condition: the species used or process studied, soil type, pH, organic matter content and clay content of the soil, temperature and exposure time, the criterion and the reference of the study.

3.4 Extrapolation methods

Two extrapolation methods for deriving environmental quality objectives are applied. First, the preliminary method which is used when chronic or acute toxicity data for species of less than four taxonomic groups are available, and second, the refined assessment, which is applied when chronic data for species of at least four different taxonomic groups are available. In both assessment methods chronic and acute data are considered as follows:

- if for a single species several NOECs or $L(E)C_{50}$ are found for *different* effect parameters the lowest is selected;
- if for a single species several NOECs or $L(E)C_{50}$ are found for the *same* effect parameter the geometric mean is calculated.

Table 3.2 Modified EPA-method for aquatic and terrestrial ecosystems

Available information	Assessment factor
Aquatic ecosystems	
lowest acute $L(E)C_{50}$-value or QSAR estimate for acute toxicity	1000
lowest acute $L(E)C_{50}$-value or QSAR estimate for acute toxicity for minimal algae/crustaceans/pisces	100
lowest NOEC-value or QSAR estimate for chronic toxicity	10*
lowest NOEC-value or QSAR estimate for minimal algae/crustaceans/pisces	10
Terrestrial ecosystems	
lowest acute $L(E)C_{50}$-value or QSAR estimate for acute toxicity	1000
lowest acute $L(E)C_{50}$-value or QSAR estimate for acute toxicity for three representatives of microbial processes, earth-worms or arthropods and plants	100
lowest NOEC-value or QSAR estimate for chronic toxicity	10*
lowest NOEC-value or QSAR estimate for three representatives of microbial processes, earthworms or arthropods and plants	10

* value is subsequently compared to the calculated value based on the lowest $L(E)C_{50}$, the lower is selected.

3.4.1 Preliminary assessment (modified EPA-method)

In this method, which was developed by the Environmental Protection Agency and modified by Van de Meent *et al.* (1990), assessment factors are applied to toxicity data. The order of

magnitude of the assessment factor depends on the number and kind of toxicity data available. Table 3.2 shows the assessment factors and the conditions for aquatic and terrestrial effect assessment. The NC is set at 1% of the MPC to take factors as multi-chemical stress and other uncertainties into account.

3.4.2 Refined effect assessment

A detailed description of the theory and the statistical background of this method is given in the literature (Kooijman, 1987; Van Straalen and Denneman, 1989; Aldenberg and Slob, 1993). This method is based on the assumption that the sensitivities of species within an ecosystem follows a statistical distribution.
The MPC is derived in such a way that 95% of the species and microbial processes within an ecosystem are protected. This 95% protection level, also referred to as the Hazardous Concentration for 5% of the species (HC_5), can be calculated with the 50% and 95% confidence level according to Aldenberg and Slob (1993). The ratio between the 50% and 95% confidence indicates uncertainties in the estimation of the MPC at the 95% protection level.
The method of Aldenberg and Slob (1993) assumes that the NOECs are following a log-logistic distribution. This can be tested with the Kolmogorov-Smirnov D*sqrt(n) which evaluates such distribution.

3.5 Derivation of the MPC_{water}

Within the procedure to set EQOs in general one MPC for freshwater and marine water is derived. Only if it can be proven that differences in sensitivity exist between freshwater and marine water two values are derived. If it is not possible to compare sensitivities it is assumed that there are no differences and one value is derived. As mentioned before data on marine water toxicity are very limited.

3.6 Derivation of group MPCs

One basic consideration for the decision to derive group MPCs instead of individual values is the toxic behaviour of the compounds. It is assumed that substances with similar structure have similar toxicity. From the literature it is found that the toxicity of anilines depends on the position of the substitution group and the degree of substitution (Zok *et al.*, 1991; De Wolf *et al.*, 1992c) (see paragraph 4.3.1). Consequently, to derive an MPC for a group of isomers the data are compared, to evaluate if there are differences in toxicity between the related compounds. If there are differences an MPCs is derived for each isomer individually according to the method described above. Subsequently, if no differences in toxicity between isomers are found all toxicity data for a group of isomers can be pooled and an MPC should be derived according to the method described above.
The methodology used here to derive a group MPC is different from the methodology to derive MPCs for di-, tri- and tetrachlorobenzenes in Van de Plassche and Bockting (1993). In that document the MPCs for the isomers are derived individually and, subsequently, the geometric mean of the MPCs is considered the final MPC.

The group MPC derived here can be used for the sum of the individual compounds included in a group value. E.g., if 2-CA and 3-CA are detected simultaneously in water, the sum of the concentration can be related to the group MPC_{water}.

3.7 Derivation of partition coefficients from the literature

The soil water partition coefficient (K_p) describes the ratio of the distribution of a compound between the solid (soil, sediment or suspended matter) and liquid phase (Table 3.3). It can be calculated from the organic carbon normalised soil water partition coefficient (log K_{oc}), which is derived from experimental studies. Bockting *et al.* (1993) evaluated and complemented a great amount of experimental log K_{oc}-values. They also set procedures and quality criteria for deriving experimental partition coefficients. Log K_{oc}-values can also be estimated by regression equations, when experimental data are lacking (Sabljic *et al.*, 1995). After the evaluation of all studies concerning log K_{oc}-values the mean log K_{oc} is calculated. The K_p for standard soil can be estimated using the formula in Table 3.4. (standard soil: 10% o.m., is 5.88% organic carbon; 25% clay).

Table 3.3 Partition coefficient of equilibrium between solid phase and liquid phase.

$$K_p = \frac{C_{solid}}{C_{liquid}}$$

K_p	=	solid water partition coefficient (l/kg)
C_{solid}	=	equilibrium concentration in the soil (mg/kg)
C_{liquid}	=	equilibrium concentration in the water (mg/l)

Table 3.4 Calculation of K_p-values for standard soil/sediment from K_{oc}-values.

$$K_p = f_{oc} \times K_{oc}$$

K_p	=	solid liquid partition coefficient (l/kg)
K_{oc}	=	org. carbon normalised partition coefficient for soil/sediment and water (l/kg)
f_{oc}	=	fraction organic carbon in standard soil (% organic carbon/100)

3.8 Equilibrium-partitioning method (EP-method)

The equilibrium-partitioning method was first used by Pavlou and Weston (1984) with the aim of developing sediment quality criteria. The principle has been described by Di Toro *et al.* (1991). The partition coefficient K_p (Table 3.4) describes the equilibrium distribution of a compound over the solid and aqueous phase. First, it is applied when there are no soil/sediment data available for terrestrial or soil-dwelling species and, secondly, for harmonisation of MPC_{soil} and/or $MPC_{sed.}$. Harmonisation prevents from exceedance of MPCs or NCs in one compartment compared to another by taking intercompartimental exchange processes into account.

For applying the EP-method several assumptions have to be made. Firstly, it is assumed that bioavailability and toxicity are closely related to the pore water concentration; Secondly, the

sensitivity of aquatic organisms and organisms living in sediment is equal; Thirdly, an equilibrium exists between the pore water and the chemicals sorbed to particulate sediment organic carbon and these concentrations can be described by a partition coefficient (K_{oc}).
The assumptions above lead to the conclusion that the exposure in an aquatic system is comparable to a sediment water system, which could be described by the EP-method. However, in the literature these assumptions are points of discussion. E.g., bioavailability and toxicity of a substance decreases with increasing time that the substance remains in the soil (Alexander, 1995; Belfroid *et al.*, 1996). Not taking this phenomenon, called 'ageing', into account lead to overestimation of the risk, in the case the sorption coefficient K_p is based on the K_{ow} or derived from a short term laboratory study. The bioavailability seems also to be dependent on the class of chemical. Inn addition, whether or not an equilibrium is reached will be determined by the habitat and physiology of an organism (Van Brummelen *et al.*, 1996) and its capability of biotransformation (Belfroid *et al.*, 1996).
These points of discussion mentioned above imply that there is not always an equilibrium situation between environmental compartments, which introduces an additional uncertainty in risk assessment. Due to the lack of data it is difficult to determine the deviation from equilibrium caused by the above mentioned processes. It should be stressed, however, that MPCs represent a potential risk to be used as general risk limit. Site-specific conditions should be included when actual risks are evaluated.
For terrestrial and sediment organisms the same assumptions are used when applying the equilibrium partitioning method, i.e. the concentration of the substance in the pore water is most relevant for bioavailability and toxicity. Van Gestel and Ma (1990) concluded that the soil pore water concentrations is of primary importance for the exposure of earthworms to 2,4-DCA.
The MPC for soil and sediment dwelling species can be calculated by equilibrium partitioning using the formula in Table 3.5.

Table 3.5 Calculation of $MPC_{soil/sed.}$ from MPC_{water}

$$MPC_{soil/sed.} = MPC_{aq.} \times K_p$$

$MPC_{soil/sed.}$	=	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	=	solid-water partition coefficient (l/kg)

3.9 Critical air concentrations

No data on emission of anilines into the air are available for the Netherlands. These compounds are not expected to evaporate significantly from water or soil due to their low vapour pressure and Henry's constant (Table 2.1). Even above fungicide plants or fields treated with crop protection agents no significant amounts of anilines are detected (BUA, 1991; BUA, 1995a). Also the evaporation from the aqueous phase is expected to be insignificant as a possible transportation process (BUA, 1995a). From the above it can be concluded that transport through air is no significant route and therefore, no critical air concentrations are calculated for the anilines.

4. DERIVING MPCS FOR THE AQUATIC ENVIRONMENT BASED ON EXPERIMENTAL DATA

In paragraph 4.1, the availability of fresh- and marine water data is discussed for chloroanilines, (chloro)nitroanilines and (chloro)methylanilines. A comparison of freshwater and marine water data will be made in paragraph 4.2. As mentioned previously it will be evaluated whether individual or group MPCs will be derived. This is paragraph 4.3. The derivation of individual values is presented in Appendix 8.

4.1 Availability of freshwater and marine water toxicity data

4.1.1 Chloroanilines

The toxicity data found on freshwater organisms are presented in Appendix 2 followed by the data on marine water organisms in Appendix 3. The largest quantity of data is found for this group of aniline derivates. However, the number of useful studies is small. Concerning freshwater studies, most data are found for 2,4-DCA and 3,4-DCA, no data at all are available for 2,3-DCA, 2,3,5-TCA and 3,4,5-TCA, respectively. For 2,3-DCA, 2,4,6-TCA, 2,3,4-TCA and 2,3,5,6-TeCA only acute data are found.

Table 4.1. Number of chronic freshwater studies per taxonomic group per compound. Ba= bacteriophyta, Pr=protozoa, Al=algae, Ma=macrophyta, Co=coelenterata, Ro=rotatoria, Mo= mollusca, Cr=crustaceans, In=insecta, Pi=pisces, Am=amphibia.

	Ba	Pr	Al	Ma	Co	Ro	Mo	Cr	In	Pi	Am
2-CA			1					1			
3-CA			1					1		1	
4-CA	1		1					1		2	
2,4-DCA	2		2	1	1		1	1	1	3	1
2,6-DCA	1		2								
3,4-DCA		2	2			1	1	2	1	4	
3,5-DCA										1	
2,4,5-TCA										1	
2,3,4,5-TeCA										2	
PCA										1	

As far as marine water studies are concerned, data are even more limited. Some studies which have been found in reviews had to be rejected since the original references could not obtained. As a consequence only for 3,4-DCA chronic and acute marine water studies are available.
In Table 4.1 the number of chronic freshwater studies per taxonomic group are presented for the different compounds. As it is clear from this table, for 3,5-DCA, 2,4,5-TCA, 2,3,4,5-TeCA and PCA the evaluated studies concern only one taxonomic group, furthermore, in the case of 3,5-DCA and PCA test results for only one species are found.
To illustrate the scarcity of toxicity data in general, the number of chronic and acute data for 2,4-DCA and 3,4-DCA are presented in Figure 4.1. From this figure it is clear that the total amount of toxicity data, presented as NOECs and L(E)C_{50}, is low even for the two selected compounds.

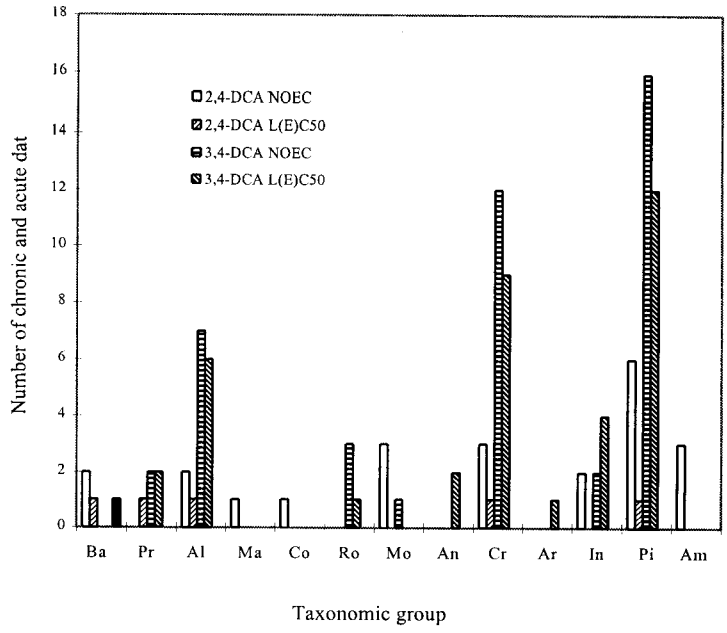

Figure 4.1. Total number of chronic (NOEC) and acute (L(E)C50) freshwater data for 2,4-DCA and 3,4-DCA. Ba=Bacteriophyta, Pr= protozoa, Al=algae, Ma=macrophyta, Co=coelenterata, Ro=rotatoria, Mo=mollusca, An=annelida, Cr=crustaceans, Ar=arachnida, In=insecta, Pi=pisces, Am=amphibia.

4.1.2 (Chloro)nitroanilines

The freshwater and marine water toxicity data found for (chloro)nitroanilines are presented in Appendix 2 and Appendix 3. For these compounds the lowest quantity of data is found. Only for eight compounds of this group of aniline derivates (Table 2.1) reliable toxicity data are found. In particular, studies on chloronitroanilines are very limited, moreover, only for 2-C-4-NA, 4-C-2-NA and 2,4-DC-4-NA (acute) toxicity data on aquatic organisms are found. With the exception of 2-N-NPA and 4-N-NPA no marine water data on nitroanilines are available. Within chronic studies bacteriophyta (1 species), protozoa (3 species), algae (4 species) and crustaceans (1 species) are tested. Acute studies are found for bacteriophyta (2 species), algae (1 species), crustaceans (2 species) and pisces (6 species). A number of studies found are deviating and are not taken into account when an MPC is derived. These studies are listed in Appendix 6.

4.1.3 (Chloro)methylanilines

The amount of both chronic and acute freshwater studies concerning (chloro)methylanilines is very limited. For only 11 compounds out of 31 (Table 2.1) reliable studies are found. Moreover, data on the chloro-substituted MAs are not available (Figure 4.2). A considerable amount of studies is found to be deviating (Appendix 6). That includes also 5 compounds (N,2-DMA; N,3-DMA; 2,5- and 2,6-DMA; 4-C-2-MA) for which no other toxicity are obtained from the literature.

As it is clear from Figure 4.2 more acute data than chronic data on methylanilines are found in the literature. Concerning marine water studies only for one compound (3-C-4-MA) toxicity data are found.

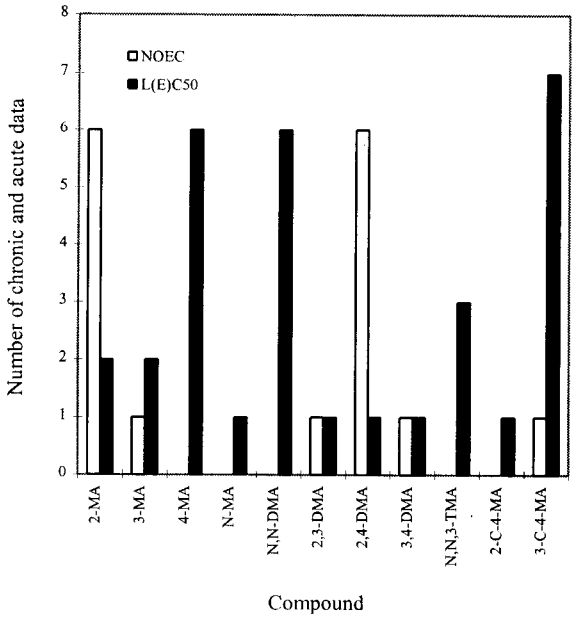

Figure 4.2 Comparison of chronic (NOEC) and acute (L(E)C50) freshwater data on (chloro)methylanilines.

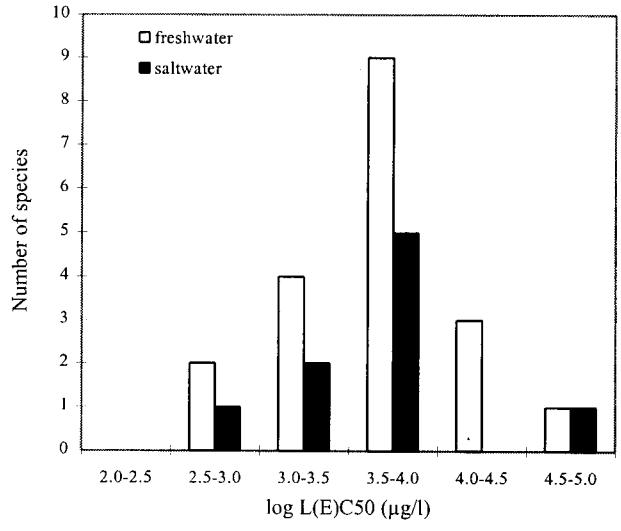

Figure 4.3 Comparison of acute freshwater and marine water toxicity data on 3,4-DCA.

4.2 Comparison of freshwater and marine water toxicity data

The only compound for which sufficient data on freshwater and marine water organisms are found is 3,4-DCA. In Figure 4.3 the sensitivity of freshwater and marine water species to 3,4-

DCA, expressed as the log $L(E)C_{50}$, is compared. It can be concluded that there is no difference in sensitivity between the species. This is confirmed by a Duncan t-test which shows no significant difference between the data ($p>0.05$). Despite the fact that the data set is very small, it is assumed that these findings hold for all the compounds concerned in this document.

4.3 Derivation of MPC_{water} based on experimental data

In paragraph 4.3.1 the decision to derive group MPCs or individual values will be discussed, followed by a discussion of the influence of the degree of substitution on the toxicity. In paragraph 4.3.3 the methodology of the derivation of the group MPC_{water} will be outlined. Subsequently, the derivation of MPCs will be presented for chloroanilines, (chloro)-nitroanilines and (chloro)methylanilines in paragraph 4.3.4, 4.3.5 and 4.3.6, respectively.

4.3.1 Group MPCs or individual MPCs

The decision to derive group MPCs instead of individual MPCs is mainly based on the toxic behaviour of the compounds. An important assumption, when group values are derived, is, that isomers have comparable toxicity. However, indications are found that the toxicity of an isomer depends on the position at which the substitution occurs. This position determines whether or not a compound is biotransformed. De Wolf *et al.* (1992c) concluded that the rate of biotransformation of chlorinated anilines in *Poecilia reticulata* is in a qualitative sense related to the structure of a substance. These authors found biotransformation of 3,4,5-TCA, 2,3,4-TCA and 2,4,5-TCA, but no biotransformation of di-*ortho* substituted anilines such as 2,4,6TCA, 2,3,4,6 TeCA and PCA. Zok *et al.* (1991) stated that biotransformation in the *ortho* position is sterically hindered. Moreover, nitro and chloro substituents in the *meta* and *para* may inactivate the amino group by their electronic influence. This might be responsible for the fact that biotransformation is faster in the *meta* position than in the *ortho* and *para* position. If one can assume that the toxicity of an isomer depends on the capability of biotransformation at a certain position, it can be concluded from the above that aniline substituted in the *ortho* position are more toxic than the corresponding isomers. In spite of this, such tendency can not be confirmed when the available toxicity data are compared. E.g. monochloroanilines which are substituted in the *para* position appear to be more toxic to the green algae *Scenedesmus subspicatus* than corresponding isomers substituted in the *ortho* or *meta* position (Schmidt and Schnabl, 1988). These authors found 8-d-NOECs for growth of 0.03, 3.9 and 4.1 mg/l for 4-CA, 2-CA and 3-CA, respectively. Such results are not found for other species. Kühn *et al.* (1989a) found 21-d NOECs of 0.03, 0.01 and 0.01 mg/l for reproduction of *Daphnia magna* after exposure to 2-, 3- and 4-CA, respectively. Zok *et al.* (1991) found only small differences in the toxicity of these compounds to the freshwater species *Brachydanio rerio*. According to these authors 2-CA is the most toxic (96h-LC_{50}: 5.2 mg/l compared to 19 mg/l for 3-CA and 35 mg/l for 4-CA). The same authors also found only small differences in toxicity of mononitroanilines to *B. rerio*. Maas-Diepeveen and Van Leeuwen (1986) exposed *D. magna* to 2-, 3- and 4-MA and found 48h-LC_{50} of 0.52, 0.15 and 0.20 mg/l, respectively.

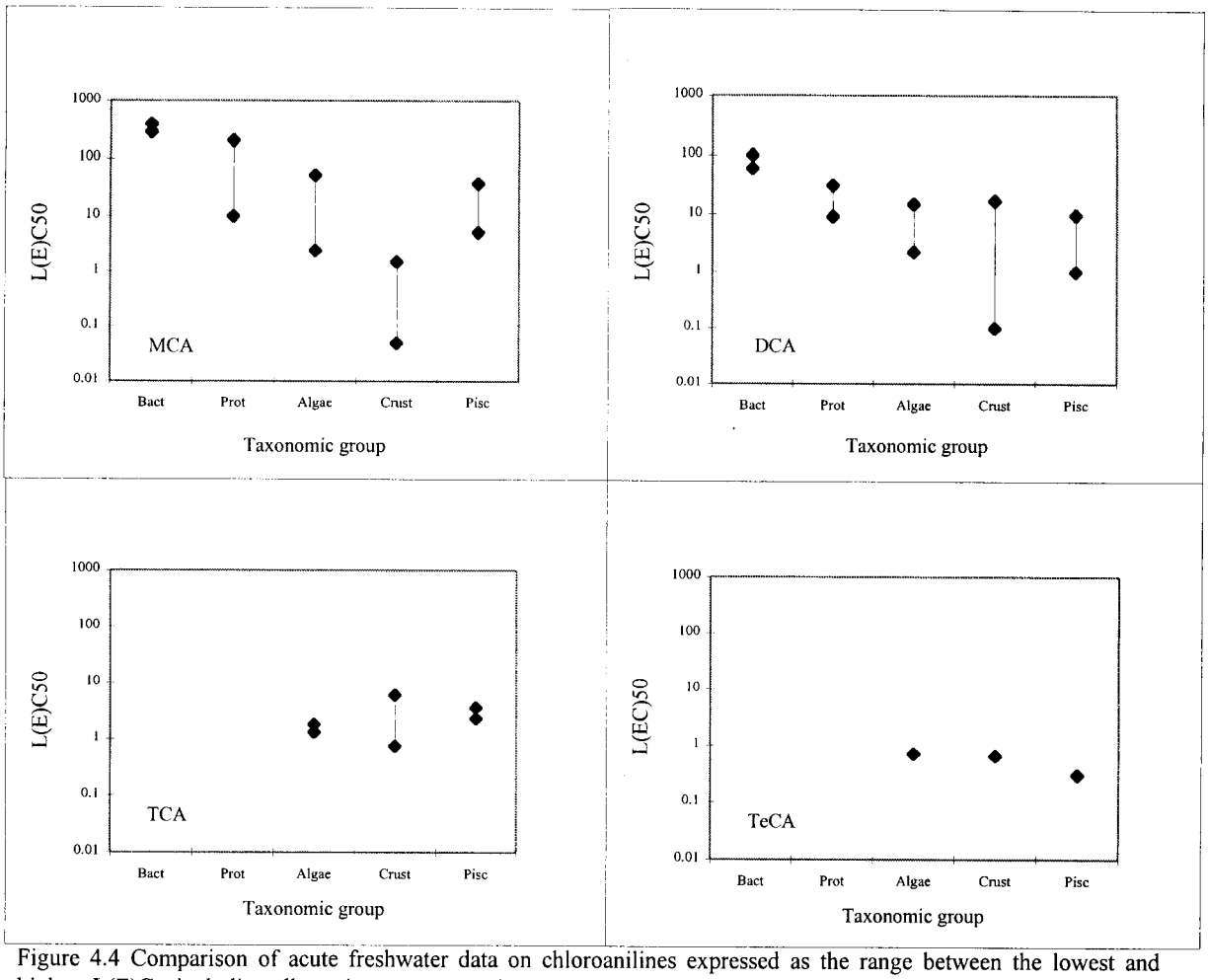

Figure 4.4 Comparison of acute freshwater data on chloroanilines expressed as the range between the lowest and highest L(E)C_{50} including all species per taxonomic group.

4.3.2 Toxicity in relation to the degree of substitution

From the literature only little evidence is found that the toxicity increases with increasing degree of substitution. Van Leeuwen *et al.* (1990) found NOECs ranging from 1.0, 0.32, 0.056, 0.032 and 0.01 for 3-MCA, 3,5-DCA, 2,4,5-TCA, 2,3,4,5-TeCA and PCA, respectively, for the survival, hatching and growth of *B. rerio*. Hermens *et al.* (1984) found 14-d LC_{50} for *P. reticulata* for MCAs ranging from 6.3-26 mg/l, for DCAs ranging from 1.7-6.3 mg/l, for TCAs from 1.4-2.0 mg/l and for TeCA 0.4 mg/l.

This can, however, not be confirmed when a broader range of toxicity data and more species are compared. In Figure 4.4 acute freshwater toxicity data for MCAs, DCAs, TCAs and TeCAs, presented as a range between the lowest and highest L(E)C_{50} found for all species within a taxonomic group, are compared (acute data on PCA are not available). From this figure it is difficult to conclude whether there is a positive relationship between the degree of chlorination and the toxicity of the CAs. Especially for the higher substituted anilines this appears partly due to the small data set. Therefore no factor to relate the toxicity to the degree of substitution is used to derive MPCs and the MPCs are derived based on experimental data.

4.3.3 Methodology to derive a group MPC

In a first step MPCs are derived for every compound individually. Since only one value per species is used for deriving MPCs, a selection has to be made from the data which are listed in Appendix 2 and Appendix 3. First, the $MPC_{freshwater}$ and $MPC_{saltwater}$ are derived. In a second step, freshwater and marine water data are combined to derive an MPC_{water}. They are presented in Appendix 9. A detailed description of the derivation of individual MPCs is presented in Appendix 8, together with the experimental data which are used for extrapolation of the individual MPCs.
To derive a MPC for a group of isomers chronic and acute toxicity data are pooled regardless of the substituted position. Afterwards, the $MPC_{freshwater}$, $MPC_{saltwater}$ and MPC_{water} are derived following the procedure described above. All data which are used for extrapolation group MPCs are listed in Appendix 10.

4.3.4 Chloroanilines

In the following paragraph group MPCs are derived for the mono-, di-, tri-, tetra- and pentachloroaniline(s).

Monochloroanilines
Applying statistical extrapolation an $MPC_{freshwater}$ of 0.002 mg/l for MCAs is derived, which is a factor 5 lower than the lowest NOEC. Since no marine water data on MCAs are found the group MPC_{water} is assumed to be the same as the $MPC_{freshwater}$ (Table 4.2).

Dichloroanilines
Applying statistical extrapolation results in an $MPC_{freshwater}$ of 0.006 mg/l. That value is a factor 3 larger than the lowest NOEC. Applying the same method on the combined freshwater and marine water data revealed a MPC_{water} of 0.003 mg/l, which is in the same order of magnitude as the MPC_{water} found for MCAs (Table 4.2).

Trichloroanilines
No sufficient data on TCAs are available to apply statistical extrapolation. The group $MPC_{freshwater}$ for TCAs is calculated by applying a factor 10 on the lowest NOEC resulting in a value of 0.006 mg/l. Due to the lack of marine water data the $MPC_{freshwater}$ is considered the MPC_{water} (Table 4.2).

Tetrachloroanilines
The calculation of the $MPC_{freshwater}$ for TeCAs results in a value of 0.003 mg/l by applying a factor 100 on the lowest $L(E)C_{50}$ for algae, crustaceans and pisces. The $L(E)C_{50}$ is used since less than three NOECs for algae, crustaceans and fish are available. As for TCAs the $MPC_{freshwater}$ is considered the MPC_{water} (Table 4.2).

Pentachloroaniline

No acute data for PCA are found in the literature. In principle following the criteria in Table 3.2 a factor 10 should be applied. Since only one NOEC on freshwater toxicity is available it is decided, deviating from these criteria to apply a factor 100. This factor is also applied within the derivation of a PNEC[d], when one NOEC for either fish or *Daphnia* is available (TGD, 1996). The resulting value of 0.0001 mg/l is considered the MPC_{water} (Table 4.2).

Table 4.2 Group MPCs for chloroanilines for aquatic organisms and the lowest NOEC and $L(E)C_{50}$. MPC_{water}s are derived by combining freshwater and marine water toxicity data.

Substance	$MPC_{freshwater}$ (mg/l)		$MPC_{saltwater}$ (mg/l)		MPC_{water} (mg/l)		Lowest NOEC (mg/l)	Lowest $L(E)C_{50}$ (mg/l)
MCA	0.002	A&S[c]	-	-	0.002	A&S	0.01	0.1[b]
DCA	0.006	A&S	0.0003[a]	EPA/10	0.003	A&S	0.002	0.1
TCA	0.006	EPA/10	-	-	0.006	EPA/10	0.056	0.73
TeCA	0.003	EPA/100	-	-	0.003	EPA/100	0.032	0.3
PCA	0.0001	EPA/100	-	-	0.0001	EPA/100	0.01	-

- no data available
a calculated MPC solely based on marine water data for 3,4-DCA
b geometric mean of 3 $L(E)C_{50}$ *D. magna* (4-CA): 0.05; 0.31; 0.11 mg/l
c extrapolation method: A&S= Statistical extrapolation; EPA=modified EPA-method/extrapolation factor; EP=Equilibrium Partitioning

4.3.5 (Chloro)nitroanilines

In the following paragraph the MPC_{water}s are derived for nitroanilines and chloro-substituted nitroanilines. As for chloroanilines it is attempted to combine data to derive one group MPC.

Nitroanilines

Since 8 NOECs are available on mono-substituted NAs statistical extrapolation is applied which results in a group $MPC_{freshwater}$ of 0.3 mg/l. That value is a factor 1.3 lower than the lowest NOEC. The $MPC_{freshwater}$ is considered the MPC_{water} since no marine water data are available.

No reliable freshwater data are available for the N-NPA. The $MPC_{saltwater}$ is derived by applying a factor 1000 on the lowest $L(E)C_{50}$. This results in a value of 0.003 mg/l, which is considered the MPC_{water} (Table 4.3).

2,4-DNA is the only dinitrosubstituted aniline derivative for which reliable toxicity data are found. Applying a factor 1000 on the lowest $L(E)C_{50}$ a $MPC_{freshwater}$ of 0.01 mg/l is obtained, which is a factor 10 lower than the lowest NOEC. The $L(E)C_{50}$ is used since less than three NOECs for algae, crustaceans and fish are available. The $MPC_{freshwater}$ is considered the MPC_{water} (Appendix 9).

Since no further toxicity data on dinitroanilines are obtained from the literature the MPC_{water} for 2,4-DNA is proposed as the group MPC_{water} for all DNAs (Table 4.3).

Chloronitroanilines

The MPC_{water} for monochloronitroanilines (CNA) is derived by applying a factor 1000 on the lowest $L(E)C_{50}$ found for 2-C-4-NA and 4-C-2-NA, resulting in a value of 0.003 mg/l. The

[d] abbreviation for 'Predicted No Effect Concentration'

MPC_{water} calculated for 2,4-DC-4-NA is considered the MPC_{water} for all and dichloro-nitroanilines (DCNA) (Table 4.3).

Table 4.3 Group MPCs for (chloro)nitroanilines for aquatic organisms and the lowest NOEC and $L(E)C_{50}$. MPC_{water}s are derived by combining freshwater and marine water toxicity data.

Substance	$MPC_{freshwater}$ (mg/l)		$MPC_{saltwater}$ (mg/l)		MPC_{water} (mg/l)		Lowest NOEC (mg/l)	Lowest $L(E)C_{50}$ (mg/l)
NA	0.34	A&S[b]	-		0.34	A&S	0.4	0.98
N-NPA	-	-	0.003	EPA/1000	0.003	EPA/1000	-	3.0[a]
DNA	0.01	EPA/1000	-		0.01	EPA/1000	0.1	9.6
CNA	0.003	EPA/1000	-		0.003	EPA/1000	-	3.2
DCNA	0.002	EPA/1000	-		0.002	EPA/1000	-	2.1

- no data available
a geometric mean of 5 EC_{50} luminescence *V. fischeri*: 7.7, 9.8, 1.0, 1.6, 1.9 mg/l
b extrapolation method: A&S= Statistical extrapolation; EPA=modified EPA-method/extrapolation factor; EP=Equilibrium Partitioning

4.3.6 (Chloro)methylanilines

In the following text the group MPC_{water} are derived for methylanilines and chloro-substituted methylanilines. The procedure is already described above. The individual MPCs are presented in Appendix 9. The group values are summarised in Table 4.4.

Monomethylanilines

The $MPC_{freshwater}$ is derived by statistical extrapolation and results in a value of 0.01 mg/l, which is the same as the lowest NOEC. That MPC is also considered the MPC_{water} since no marine water data are available (Table 4.4).

Table 4.4 Group MPCs for (chloro)methylanilines for aquatic organisms and the lowest NOEC and $L(E)C_{50}$. MPC_{water}s are derived by combining freshwater and marine water toxicity data .

Substance	$MPC_{freshwater}$ (mg/l)		$MPC_{saltwater}$ (mg/l)		MPC_{water} (mg/l)		Lowest NOEC (mg/l)	Lowest $L(E)C_{50}$ (mg/l)
MA	0.01	A&S[c]	-		0.01	A&S	0.01	0.15
DMA	0.05	A&S	-		0.05	A&S	0.05[a]	9.9
TMA	0.05	EPA/1000	-		0.05	EPA/1000	-	50[b]
CMA	0.001	EPA/1000	0.005	EPA/1000	0.001	EPA/1000	1.0	0.6

- no data available
a geometric mean 2 NOECs reproduction *D. magna*: 0.016; 0.16 mg/l
b geometric mean 3 LC50s *P. promelas*: 53; 52; 46 mg/l
c extrapolation method: A&S= Statistical extrapolation; EPA=modified EPA-method/extrapolation factor; EP=Equilibrium Partitioning

Dimethylanilines

Statistical extrapolation is applied to calculate the $MPC_{freshwater}$. Extrapolation results in a value of 0.05 mg/l, which is in the same order of magnitude as the lowest NOEC found for DMAs. Due to the lack of marine water data the $MPC_{freshwater}$ is considered the MPC_{water} (Table 4.4).

Trimethylanilines

A factor 1000 is applied on the lowest $L(E)C_{50}$ found for N,N,3-TMA. This results in an $MPC_{freshwater}$ of 0.05 mg/l (Appendix 9). The $MPC_{freshwater}$ is considered the MPC_{water}.

Although the data set of TMAs is very limited, the MPC_{water} for N,N,3-TMA is also proposed as the group MPC_{water} for TMAs (Table 4.4).

Chloromethylanilines

The $MPC_{freshwater}$ is obtained by applying a factor 1000 on the lowest $L(E)C_{50}$ found for 2-C-4-MA and 3-C-4-MA, resulting in a value of 0.001 mg/l. The $L(E)C_{50}$ is used since less than three NOECs for algae, crustaceans and fish are available. The $MPC_{saltwater}$ is 0.005 mg/l, also derived with the modified EPA-method (factor 1000). Combining all freshwater and marine water data and applying a factor 1000 on the lowest $L(E)C_{50}$ results in a MPC_{water} of 0.001 mg/l. The latter is a factor 1100 lower than the lowest NOEC (Table 4.4).

5. DERIVING MPCS FOR SOIL BASED ON EXPERIMENTAL DATA

In paragraph 5.1 the availability of soil toxicity data together with log K_{oc}s for chloroanilines, (chloro)nitroanilines and (chloro)methylanilines is discussed. In paragraph 5.2 the derivation of MPCs for soil based on toxicity data is presented. The group values are presented in this chapter, for the individual values it is referred to Appendix 11.

5.1 Availability of soil toxicity data

5.1.1 Chloroanilines

Toxicity data on soil organisms are presented in Appendix 4 followed by the data on microbial and enzymatic processes in Appendix 5. The overall quantity of data is low. The amount of chronic data is shown in Figure 5.1. From this figure it is clear that the number of taxonomic groups tested within chronic studies, is also low. No data on soil toxicity at all are available for 2,5-, and 2,6-DCA, 2,3,4-, 2,3,5- and 3,4,5-TCA. For 3-CA only acute data are found in the literature. In particular, for the higher chlorinated isomers (TCAs, TeCAs, PCA) only one NOEC is found.

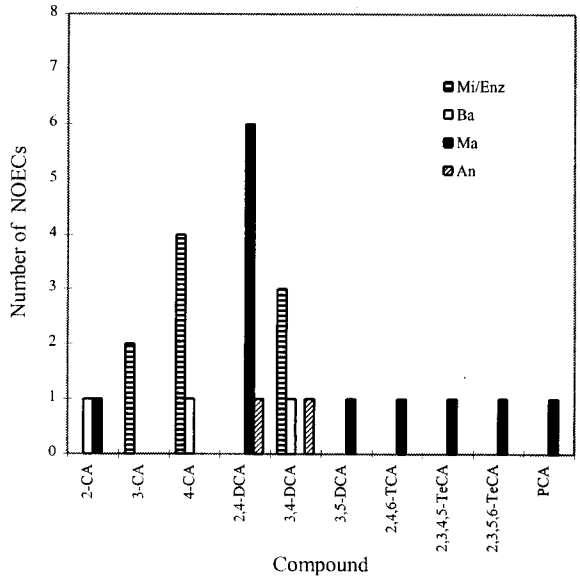

Figure 5.1 Number of chronic soil toxicity data. Mi/Enz=microbial and enzymatic activity, Ba=Bacteriophyta, Ma=Macrophyta, An=Annelida.

5.1.2 (Chloro)nitroanilines

No reliable data on soil toxicity are available on (chloro)nitroanilines. A considerable amount of studies is found using the agar-plating method, which is considered an unnatural growth medium (CSR, 1996). Moreover, it is difficult to derive soil concentrations from the results of such studies. Therefore, these studies are not included in the evaluation.

5.1.3 (Chloro)methylanilines

No toxicity data on terrestrial organisms or microbial/enzymatic processes are found for these compounds.

5.2 Derivation of MPCs for soil based on experimental data

Within the derivation of the MPC_{soil} it is intended to derive an MPC for soil organisms ($MPC_{species}$) and for microbial/enzymatic processes ($MPC_{processes}$) individually, based on the data which are listed in Appendix 4 and Appendix 5. In principle for determination of the 'final' MPC_{soil} preference is then given to the lowest value. However, the reliability of the two values has to be taken into account, which is determined by the amount of data which is used for extrapolation. When the reliability is comparable and comparable methods are used, the lower value is chosen. For anilines all MPCs are based on a small dataset, therefore it is judged on a case-by-case basis which MPC is selected.

5.2.1 Chloroanilines

Similar to aquatic toxicity data, it is intended to derive group MPCs for mono-, di- tri- and tetrachloronanilines. Data for extrapolation of the group MPCs are presented in Appendix 13. In Appendix 11 the derivation of the MPCs for the individual compounds is presented together with the data used for extrapolation. The individual MPCs are listed in Appendix 12.

Monochloroanilines

The $MPC_{species}$ is derived by applying a factor 1000 on the geometric mean of 6 $L(E)C_{50}$s for *L. sativa*, which leads to a value of 0.1 mg/kg. Since NOECs for 5 different microbial/enzymatic processes are available statistical extrapolation is applied. This results is an $MPC_{processes}$ of 5.1 mg/kg. The latter is considered as the MPC_{soil} (Table 5.1).

Table 5.1 Group MPCs using experimental data (species and microbe-mediated processes) for chloroanilines and the lowest NOEC and $L(E)C_{50}$.

Substance	$MPC_{species}$ (mg/kg)		$MPC_{processes}$ (mg/kg)		MPC_{soil} (mg/kg)	Lowest NOEC (mg/kg)	Lowest $L(E)C_{50}$ (mg/kg)
MCA	0.10	EPA/1000[h]	5.1	A&S	5.1	13	103[a]
DCA	0.13	EPA/1000	7.8	A&S	7.8	24[g]	125[b]
TCA	0.13	EPA/1000	-	-	0.13	50	125[c]
TeCA	0.17	EPA/1000	-	-	0.17	28[e]	167[d]
PCA	1.50	EPA/1000	-	-	1.5	50	1500[f]

- no data available
a geometric mean 6 EC_{50} growth *L. sativa*: 85; 75; 140; 115; 156; 74 mg/kg
b geometric mean 7 EC_{50} growth *L. sativa*: 160; 145; 120; 368; 90;80; 65 mg/kg
c geometric mean 2 EC_{50} growth *L. sativa*: 135; 115 mg/kg
d geometric mean 2 EC_{50} growth *L. sativa*: 235; 120 mg/kg
e geometric mean 2 NOECs growth *L. sativa*: 50; 16 mg/kg
f geometric mean 2 LC_{50} *L. rubellus*: 2200; 1000 mg/kg
g geometric mean 4 NOECs *L. sativa*: 86; 50; 16; 5 mg/kg
h extrapolation method: A&S= Statistical extrapolation; EPA=modified EPA-method/extrapolation factor; EP=Equilibrium Partitioning

Dichloroanilines

Applying a factor 1000 on the geometric mean of 7 $L(E)C_{50}$ for *L. sativa* an $MPC_{species}$ is derived of 0.1 mg/kg. Based on chronic data for four different microbial/enzymatic processes

the group $MPC_{processes}$ is derived by statistical extrapolation. That leads to a value of 7.8 mg/kg which is considered the MPC_{soil} (Table 5.1).

Trichloroanilines

The $MPC_{species}$ is calculated with the EPA-method by applying a factor 1000 on the lowest $L(E)C_{50}$ found for TCAs, since less than three NOECs for representatives of earthworms, arthropods and plants are available. That leads to an $MPC_{species}$ of 0.13 mg/kg (Table 5.1).

Tetrachloroanilines

A factor 1000 is applied on the lowest $L(E)C_{50}$ found for TeCAs, since less than three NOECs for representatives of earthworms, arthropods and plants are available. This results in an $MPC_{species}$ of 0.17 mg/kg (Table 5.1).

Pentachloroaniline

The MPCspecies for PCA is calculated based on the lowest $L(E)C_{50}$, by applying a factor 1000, since less than three NOECs for representatives of earthworms, arthropods and plants are available. That leads to an $MPC_{species}$ of 1.5 mg/kg (Table 5.1).

6. DERIVING SOIL WATER PARTITION COEFFICIENTS (LOG K_{OC})

In the case experimental data on soil/sediment toxicity are lacking the $MPC_{soil/sed.}$ can be derived from the MPC_{water} with the soil water partition coefficient (K_p, paragraph 3.4). This coefficient can be calculated from the organic carbon normalised soil-water partition coefficient (log K_{oc}), also referred to as the soil sorption coefficient. The log K_{oc}-values can be derived from experimental studies, which is preferred within setting quality objectives for soil and sediment. When more than one value is available for one compound the (geometric) mean of the log K_{oc}s is calculated. The log K_{oc} can further be calculated by Quantitative Structure-Activity Relationships (QSAR). In this paragraph the availability and derivation of experimental log K_{oc}s will be discussed in paragraph 6.1 followed by the calculation of log K_{oc}s in paragraph 6.2.

6.1 Log K_{oc}s based on experimental studies

The log K_{oc}s for the concerned compounds which are based on experimental studies together with the experimental conditions are presented in Appendix 7. These values are derived according to Bockting *et al.* (1993) who described procedures and quality criteria for the derivation of partition coefficients. The total quantity of data is very low. Again, for CAs most values are found.

6.2 Calculation of log K_{oc}s

Numerous authors have written about the prediction of the soil sorption coefficient from the n-octanol water partition coefficient (log K_{ow}) and other parameters (Briggs, 1981; Karickhoff, 1981; Gerstl, 1990; Gerstl, 1990; Sekusak and Sabljic, 1992; Meylan *et al.*, 1992; Sabljic *et al.* 1995). The relationships (QSARs) between the parameters are calculated based on various data sets by using linear regression.

Table 6.1 QSARs applied for calculation the log K_{oc} (Sabljic *et al.*, 1995).

Substance	QSAR
Chloroanilines (Chloro)methylanilines	$\log K_{oc}=0.85+0.62\times\log K_{ow}$ [a], $r^2=0.808$, n=20
Mononitro(chloro)anilines	$\log K_{oc}=0.90+0.63\times\log K_{ow}$ [b], $r^2=0.744$, n=54
Di-/trinitro(chloro)anilines	$\log K_{oc}=1.92+0.38\times\log K_{ow}$ [c], $r^2=0.817$, n=20

a Sabljic *et al.*, (1995): equation 10
b Sabljic *et al.*, (1995): equation 4
c Sabljic *et al.*, (1995): equation 12

The log K_{ow}-log K_{oc}-relationships are frequently used because of their simplicity and because they appear to predict the soil sorption coefficient reasonably well (Bockting *et al.*, 1993).

Recently Sabljic *et al.* (1995) developed QSARs for prediction of the log K_{oc} for anilines and dinitroanilines from the log K_{ow} (Table 6.1). According to Sabljic (pers. communication) the QSARs presented in Table 6.1 are applied to calculate the log K_{oc}.
As mentioned in paragraph 2.3 experimental log K_{ow}s obtained by the slow-stirring method (De Bruijn *et al.*, 1989) are preferred (CSR, 1996). If no experimental data are available the "star values" from the MEDCHEM database are used. In case these data are also not available the log K_{oc}s are calculated with the ClogP values from the ASTER database.
The experimental data are presented in Appendix 7. The calculated log K_{oc} values are presented in Table 6.2. They are expressed as the geometric mean of the calculated values within a group of derivates (Appendix 7). Comparison of both experimental and QSAR-based log K_{oc}s revealed a weak correlation (r^2=0.79, n=18).

Table 6.2 Calculated log K_{oc}-values.

Substance	log K_{oc}	stdev	(n)
MCA	2.02	0.21	(3)
DCA	2.62	0.05	(6)
TCA	3.14	0.01	(3)
TeCA	3.65		(2)
PCA	4.00		(1)
NA	1.86	0.17	(3)
N-NPA	3.48		(2)
DNA	2.60	0.04	(3)
TNA	2.92		(1)
CNA	2.33	0.18	(4)
DCNA	2.74	0.22	(3)
DNCA	2.92		(1)
MA	1.74	0.09	(4)
DMA	2.07	0.13	(10)
TMA	2.47	0.18	(5)
CMA	2.54	0.22	(9)

7. DERIVING MPCS FOR SOIL AND SEDIMENT BASED ON EQUILIBRIUM PARTITIONING

In the previous chapter the calculation of log K_{oc} values based on the relationship between the soil sorption coefficient and the n-octanol water partition coefficient is described. In the following these calculated coefficients will be used to derive MPCs for soil and sediment based on equilibrium partitioning (EP-method). In paragraph 7.1 the calculation of the soil water partition coefficient K_p is described. In paragraph 7.2 the calculated MPCs for soil and sediment is presented together with the harmonisation of the MPCs for soil and sediment.

7.1 Calculation of the soil water partition coefficient (K_p)

As mentioned in paragraph 3.4 the soil water partition coefficient can be used for two purposes, first, to derive $MPC_{soil/sed.}$ in the case experimental data are lacking, and second, to harmonise MPC for soil and/or sediment. The method for calculating the K_p is already described previously. The calculated soil water partition coefficients are listed in Table 7.1 together with the log K_{oc}s. In the project 'Intervention Values' also log K_{oc}s for chloroanilines have been derived (Kreule and Swartjes, 1997). These values are also listed in Table 7.1. Since these values are used to derive intervention values and show only small differences from the calculated log K_{oc}s they will be used for further calculations of the soil water partition coefficients and harmonisation, with the exception of the log K_{oc} for PCA. For this compound the calculated log K_{oc} will be maintained. The coefficients are corrected for standard soil/sediment. The standard soil/sediment contains 10% organic matter (5.88% organic carbon) and 25% clay.

Table 7.1 Soil sorption coefficients (log K_{oc}) and soil water partition coeffiecients (log K_p).

Substance	log K_{oc}[a]		log K_p	
MCA	2.02	*2.54**	0.79	*1.31**
DCA	2.62	*2.85**	1.39	*1.62**
TCA	3.14	*3.08**	1.91	*1.85**
TeCA	3.65	*3.84**	2.42	*2.61**
PCA	4.00*	*4.62*	2.77*	*3.39*
NA	1.86		0.63	
N-NPA	3.48		2.25	
DNA	2.60		1.37	
TNA	2.92		1.69	
CNA	2.33		1.10	
DCNA	2.74		1.51	
DNCA	2.92		1.69	
MA	1.74		0.51	
DMA	2.07		0.84	
TMA	2.47		1.24	
CMA	2.54		1.31	

a log K_{oc}s from Kreule and Swartjes (1997) and the log K_p calculated based on these values are printed italic

* values used for further calculation

7.2 MPCs for soil and sediment using equilibrium partitioning and harmonisation

Calculation of $MPC_{soil/sed.}$

In Table 7.2 the calculated MPC for soil and sediment using equilibrium partitioning method are presented. The method is described in paragraph 3.5. The K_p-values are derived from Table 7.1. The MPC_{water}s are derived from toxicological data (chapter 4).

Table 7.2 Calculation of the $MPC_{soil/sed.}$ with the equilibrium partitioning method.

Substance	MPC_{water} (mg/l)		log K_p	$MPC_{soil/sed.}$ (mg/kg)	
MCA	0.002	A&S	1.31	0.04	EP
DCA	0.003	A&S	1.62	0.12	EP
TCA	0.006	EPA/10	1.85	0.42	EP
TeCA	0.003	EPA/100	2.61	1.22	EP
PCA	0.0001	EPA/100	2.77	0.06	EP
NA	0.34	A&S	0.63	1.45	EP
N-NPA	0.003	EPA/1000	2.25	0.53	EP
DNA	0.01	EPA/1000	1.37	0.23	EP
CNA	0.003	EPA/1000	1.10	0.04	EP
DCNA	0.002	EPA/1000	1.51	0.06	EP
MA	0.01	A&S	0.51	0.03	EP
DMA	0.05	A&S	0.84	0.35	EP
TMA	0.05	EPA/1000	1.24	0.87	EP
CMA	0.001	EPA/1000	1.31	0.02	EP

- no data available
extrapolation method is placed behind the MPC

Harmonisation of MPC for soil and sediment based on experimental data

For determining the final MPC_{soil}, in general preference is given to the lowest one, as this prevents exceeding the level in one compartment by maintaining the level in another. Nevertheless, the reliability of an MPC has to be taken into account, which is related to the amount of data and to the extrapolation method. Only if both MPC_{water} and MPC_{soil} are based on a large data set (preferably at least 4 chronic values) a direct comparison of MPC_{soil} based on ecotoxicological data and MPC_{soil}(EP-method) is possible and the lower one should be chosen.

In Table 7.3 the MPC_{soil} calculated with the EP-method and MPC_{soil} based on experimental data are presented. Due to the lack of sediment toxicity data the MPCs, which are calculated using the EP-method are considered the $MPC_{sed.}$. Moreover, the MPC_{soil} and $MPC_{sed.}$ are the same in the case no soil toxicity data are available. In the case toxicity data for soil are available it is decided per compound, which MPC_{soil} -based on toxicological data or on the EP-method- is considered as the final MPC_{soil}.

Since both the MPC_{soil} for MCAs and DCAs are derived by statistical extrapolation these values are chosen as the final MPC_{soil} for these compounds.

The data set for TCAs for water and soil toxicity is limited. Therefore, the MPC based on the EP-method is considered the MPC_{soil}, as the MPC_{water} is derived by applying a factor 10 unlike the MPC_{soil}, which is derived by applying a factor 1000.

The MPC_{soil} for TeCAs differ more than a factor 7 from each other. Since data for both water and soil are limited for these compounds and the partition coefficient is QSAR based, the MPC based on soil toxicity data is considered the MPC_{soil}.
The MPC_{soil} for pentachloroaniline based on the EP-method is a factor 25 lower than the MPC_{soil} based on ecotoxicological data. The MPC_{water} is based on one chronic value on which a factor 100 is applied, unlike the MPC_{soil}, which is based on the lowest $L(E)C_{50}$s (factor 1000). Because of the large difference between the MPCs and the large safety factor which is used to derive the MPC_{soil} based on ecotoxicological data, the MPC_{soil} based on the EP-method is considered as the final MPC_{soil}.

Table 7.3 Harmonisation of the MPC_{soil} for chloroanilines based on experimental data.

Substance	$MPC_{soil/sed.}$ (mg/kg) (EP-method)		MPC_{soil} (mg/kg) (ecotox. data)		MPC_{soil} (mg/kg) (final value)		$MPC_{sed.}$ (mg/kg) (final value)	
MCA	0.04	EP[a]	5.1	A&S	5.1	A&S	0.04	EP
DCA	0.12	EP	7.8	A&S	7.8	A&S	0.12	EP
TCA	0.42	EP	0.13	EPA/1000	0.42	EP	0.42	EP
TeCA	1.22	EP	0.17	EPA/1000	0.17	EPA	1.22	EP
PCA	0.06	EP	1.50	EPA/1000	0.06	EP	0.06	EP
NA	1.45	EP	-	-	1.45	EP	1.45	EP
N-NPA	0.53	EP	-	-	0.53	EP	0.53	EP
DNA	0.23	EP	-	-	0.23	EP	0.23	EP
CNA	0.04	EP	-	-	0.04	EP	0.04	EP
DCNA	0.06	EP	-	-	0.06	EP	0.06	EP
MA	0.03	EP	-	-	0.03	EP	0.03	EP
DMA	0.35	EP	-	-	0.35	EP	0.35	EP
TMA	0.87	EP	-	-	0.87	EP	0.87	EP
CMA	0.02	EP	-	-	0.02	EP	0.02	EP

- no data available

a extrapolation method: A&S= Statistical extrapolation; EPA=modified EPA-method/extrapolation factor; EP=Equilibrium Partitioning

8. DISCUSSION

In the following chapter a number of subjects are discussed. The derivation of individual and group MPCs depending on the chemical structure is outlined in paragraph 8.1. The use of Quantitative Structure-Activity Relationships (QSAR) to determine the toxicity of anilines is discussed in paragraph 8.2. The MPCs for water and soil are discussed in paragraph 8.2, followed by a comparison of the MPCs and NCs to data from (semi)field studies and measured environmental concentrations in paragraph 8.3.

8.1 Derivation of MPCs depending on the chemical structure

As outlined in paragraph 4.3.1, no clear relationship is found between the position of substitution and the toxicity of a compound. From the literature various results are found concerning the toxicity of isomers. 4-CA is slightly more toxic to the green algae *S. subspicatus* than 2-CA and 3-CA (Schmidt and Schnabl, 1988). Small differences in toxicity of these compounds to *C. pyrenoidosa* are found by Maas-Diepeveen and Van Leeuwen (1986). MCAs show no difference in chronic toxicity to *Daphnia* (Kühn *et al.*, 1989a). Small differences in toxicity are also found for MAs (Hermens *et al.*, 1984; Maas-Diepeveen and Van Leeuwen, 1986).
From the above it is obvious that there is no clear evidence that the toxicity is influenced by the structure of an isomer. It should be stressed here, however, that this assumption is not based on any statistical method. Nevertheless, the group MPCs within this report are derived not depending on which position within the aromatic ring a substitution occurs.
Comparing all acute toxicity data on CAs no evidence is found that the toxic behaviour of a compound is influenced by the degree of substitution (Figure 4.4). From the literature only limited toxicity data are found which indicate such relationship (Hermens *et al.*, 1984; Van Leeuwen *et al.*, 1990).

8.2 Toxicity of anilines based on Quantitative Structure-Activity Relationships (QSARs)

According to Verhaar *et al.* (1992) chemicals are ranked into 4 classes: 1) inert chemicals; 2) less inert chemicals; 3) reactive chemicals and 4) chemicals with a specific mode of action. The mode of action of *inert chemicals*, also referred to as class 1 chemicals, is called apolar narcosis and is considered to be an expression as a result of a non-specific mode of action. This so called base-line toxicity is solely depending on the hydrophobicity (log K_{ow}) of a compound. For such compounds Quantitative Structure Activity Relationships (QSARs) can be used to estimate the toxicity of compounds for aquatic organisms (Van Leeuwen *et al.*, 1992).
Anilines with more than three chlorine substituents (e.g. TeCA, PCA) are classified as class 1 chemicals. Anilines with one nitro substituent and/or one to three chlorine substituents and/or alkyl substituents are considered as *less inert chemicals* or class 2 chemicals, which act by polar narcosis (Verhaar *et al.*, 1992). They are expected to have a higher acute toxicity compared to chemicals exhibiting baseline toxicity.
Such distinction, class 2 chemical exhibiting a higher toxicity than class 1 chemicals, is found by Vaes *et al.* (in press), who investigated the toxicity of nineteen chemicals based on their n-

octanol water partition coefficient. The author stated that the interpretation of toxicity data can strongly depend on the choice of the partition coefficient. Because, if the toxicity of the same compounds is related to the membrane water partitioning coefficient (log K_{DMPC}) the distinction disappeared. The author concluded that the classification of class 1 and class 2 chemicals based on the log K_{ow} is probably more a result of the use of the wrong parameter than of the difference in intrinsic toxicity. Urrestarazu Ramos *et al.* (in prep.) used besides log K_{ow} hydrogen bonding capacity descriptors (Q^-, Q^+, ε_{HOMO}, ε_{LUMO}) to build QSARs for the acute toxicity of narcotics. They concluded that the toxicity of apolar and polar narcotics is caused by the same mode of action.
From the above it can be concluded that QSARs are available to estimate the aquatic toxicity of anilines, which are classified as apolar and polar narcotics. However, due to the lack of capacity descriptors it is not possible to include these estimations in the present report.

Table 8.1 Comparison MPCs for chloroanilines with indicative maximum acceptable risk levels (iMARs) from Slooff *et al.* (1991).

Substance	MPC_{water} (mg/l)	$iMAR_{water}$ (mg/l)	MPC_{soil} (mg/kg)	$iMAR_{soil}$ (mg/kg)
MCA	0.002	0.02	5.1	1.2-5.0
DCA	0.006	0.005	7.8	0.5-5.0
TCA	0.006	0.002	0.13	5.0
TeCA	0.003	0.0005	0.17	1.6-5.0
PCA	0.0001	0.0002	1.50	0.1

In the past Slooff *et al.* (1991) used QSARs based on the hydrophobicity to derive indicative maximum acceptable risk levels (iMARs) for CAs for water (Table 8.1). For the estimation one QSAR derived for *Poecilia reticulate* and one for *Photobacteria* are used. The ratios between the chloroanilines, based on the geometric mean of these QSARs, are applied on the MAR_{water}[e] for 2,4-DCA. Based on this QSARs the authors found a inverse relationship between the iMAR and the degree of substitution.
Compared to the $iMAR_{water}$s the MPC_{water}s for DCAs, TCAs and PCA are in the same order of magnitude, whereas the MPC_{water} for MCAs is a factor 10 lower and for TeCAs a factor 6 higher than the corresponding iMAR (Table 8.1). The $iMAR_{soil}$ from Slooff *et al.* (1991) are all derived by the modified EPA-method. Unlike the $iMAR_{water}$ they show no relationship to the degree of substitution (Table 8.1). MPC_{soil}s for MCAs and DCAs are in the same order of magnitude as the $iMAR_{soil}$s, for TCA and TeCA the MPC_{soil} are a factor 38 and 10-29, respectively, lower and for PCA a factor 15 higher than the $iMAR_{soil}$s.

8.3 Maximum permissible concentrations for water, soil and sediment

Aquatic environment
The MPC for the aquatic environment are calculated based on experimental data. A QSAR-approach to estimate the MPC is not applied due to the lack of time and data. Therefore, in the case when there are no toxicity data available (TNA, DNCA) no MPC could be derived. As mentioned previously group MPCs are derived. All MPCs are derived based on at least one

[e] unlike iMAR derived by statistical extrapolation

toxic value. For that reason, the resulting risk limit is considered to be representative for a group of isomers, for which the data set is limited.

Soil and sediment
Except for chloroanilines the MPCs for soil are calculated by EP-method. MPCs for sediment are all calculated by the EP-method. The MPC_{soil} for CAs are harmonised because experimental data are available. When MPC_{soil}s based on ecotoxicological data and on the EP-method are harmonised the lower one is not necessarily chosen. The method of extrapolation is taken into account. If a MPC_{soil} is estimated by statistical extrapolation that value is preferred, even when it appears to be larger than the MPC derived by the EP-method as it is the case of MCA and DCA.

8.4 MPCs in relation to data from (semi)field studies and measured environmental concentrations

8.4.1 Data from (semi)field studies

The derived MPCs are compared to toxicity data obtained from outdoor artificial stream experiments (Mitchell, 1992; Girling *et al.*, 1992). Within these experiments several macro-invertebrates are exposed to 3,4-DCA in a constant flow system. Mitchell (1992) exposed organisms to 4 measured concentrations of 0.07, 0.24, 0.8 and 2.4 mg/l (cf nominal concentrations of 0.1, 0.3, 1.0, 3.0 mg/l). Girling *et al.* (1992) exposed *Onchorhynchus mykiss* to seven (measured) concentrations ranging from 0.45 to 4700 µg/l. The flow system is created by pumping water from a natural calcareous stream through a stainless-steel channel. The compound is added continuously.
For *Gammarus pulex* a 28-d-NOEC (neonate growth) of 0.07 mg/l and for the growth of 3rd instar *Chironomus riparus* a 28-d-NOEC of 0.8 mg/l is found (Mitchell, 1992). These values are a factor 23 and 270, respectively, larger than the group MPC_{water} derived for dichloroanilines. Notice here, that toxicity values of *one* compound are related to the group MPC_{water}. Compared to the individual MPC_{water} for DCAs the NOECs are a factor 88 and 1000 larger, respectively. Girling *et al.* (1992) found a 18-d-NOEC (mortality eggs) for *O. mykiss* of 0.002 mg/l. This is almost the same values as the derived group MPC_{water} for dichloroanilines, but is still a factor 2.5 higher than the MPC derived for 3,4-DCA (Appendix 9).
In field studies natural processes, e.g. sorption to organic matter, may influence the bioavailability of a compound. As a consequence, in (semi)field studies a higher dose is required to find the same effect. Although, the data set from field studies found is limited to one compound, it shows that the derived MPCs (group and individual value) are lower than the NOECs found in these studies. However, it should be kept in mind that the magnitude of the extrapolation factor depends on the amount of laboratory data available. Also the amount

Table 8.2 Median and maximum concentrations of several anilines during 1995/96 in Rijn, Maas and Ysselmeer (RIWA, 1995a, 1995b; RIWA, 1996a, 1996b).

	median (number of measurements) and maximum concentration (µg/l)													
	Rijn 1995		Maas 1995				Rijn 1996		Maas 1996				Ysselmeer 1996	
	Lobith		Eijsden		Keizersveer		Lobith		Eijsden		Keizersveer		Andijk[a]	
Substance	med. (n)	max.	med. (n)	max.	med. (n)	max.	med. (n)	max.	med. (n)	max.	med. (n)	max.	mean (n)	max.
2-CA	0.06 (13)	0.21	< (13)	<	< (13)	0.01	-	-	-	-	-	-	-	-
3-CA	-	-	-	-	-	-	-	-	<	<	-	-	-	-
4-CA	-	-	-	-	-	-	-	-	<	<	-	-	-	
2,4-DCA	-	-	-	-	-	-	-	-	<	<	-	-	-	
2,6-DCA	-	-	-	-	-	-	-	-	<	<	-	-	-	
3,4-DCA	0.07 (13)	0.16	0.08 (13)	0.31	0.06 (13)	0.21	0.06 (14)	0.27	< (14)	0.56	< (12)	0.68	< (5)	0.08
3,5-DCA	< (13)	0.20	< (12)	0.10	< (13)	0.26	-	-	-	-	-	-	-	-
2,4,5-TCA	0.15 (13)	0.96	< (13)	0.12	< (13)	0.16	0.23 (14)	0.45	<	<	<	<	0.10 (5)	0.14
2-MA	< (12)	0.20	< (13)	0.37	0.01 (13)	0.10	< (14)	0.23	< (14)	0.43	<	0.20	<	<
3-MA	-	-	-	-	-	-	-	-	< (13)	0.39	-	-	-	-
4-MA	0.11 (13)	0.27	< (13)	0.04	< (13)	0.80	-	-	-	-	-	-	-	-

- no data available

< below limit of quantification: 2-CA 0.01-0.05 µg/l; 3-CA 0.10 µg/l; 4-CA 0.05 µg/l; 2,4-DCA 0.05 µg/l; 2,6-DCA 0.5 µg/l; 0.01-0.05 µg/l; 3,5-DCA 0.01 µg/l; 2,4,5-TCA 0.05 µg/l; 2-MA 0.01-0.20 µg/l; 3-MA 0.05 µg/l; 4-MA 0.01 µg/l.

a no median concentration in reference

of field studies is too limited to draw solid conclusions, because it cannot be excluded that other organisms than the ones used in the field studies are more sensitive.

8.4.2 Measured environmental concentrations of anilines

Anilines have been most extensively monitored during the last 15 years. However, data on measured concentrations of aniline derivates in the Dutch environment are limited and related to freshwater. No data are found on the occurrence in marine water, soil or sediment.
As mentioned before only a fraction of the compounds listed in Table 2.1 are actually detected in the environment. Especially chloroanilines have been found. Measurements of MCAs, DCAs and one TCA at different locations during 1990 revealed concentrations up to a maximum of 0.19 µg/l[f] for DCAs (Venema *et al.*, 1990). PCA, which is a metabolite of quintozene, is found once at a concentration of 0.01 µg/l (Phernambucq *et al.* 1996). NAs and MAs have been less frequently monitored. Maximum concentration found for NAs are 4.1 µg/l[g] (Barreveld, 1991). Concentrations found for MAs and DMAs never exceed 0.8 and 0.4 µg/l, respectively (Phernambucq *et al.*, 1996).
In Table 8.2 an overview is given of measured concentrations of anilines at different locations in the Netherlands during 1995 and 1996 presented as the median and maximum concentration. The number of substances which are monitored regularly is low. 3,4-DCA and 2,4,5-TCA are the most frequent detected compounds at the different locations.

8.4.3 MPCs and NCs in relation to environmental concentrations

The small amount of toxicity data and the fact that only a few substances listed in Table 2.1 actually occur in the environment, has consequences for the derivation of the MPCs for water and soil. It is questionable whether it is necessary or useful to derive risk limit for compounds which do not enter the environment. Therefore, in the following only these substances are considered for which environmental data are found.
CAs are mainly detected, but almost no data are found for higher chlorinated anilines, however. NAs are incidentally detected, though these data are not up-to-date. No data on higher substituted NAs and CNAs are available. MAs and DMAs are repeatedly found in surface waters, no data are obtained for higher substituted MAs and CMAs.
In Table 8.3 environmental concentrations of anilines are compared to the MPCs and NCs derived within the present report. For comparison, these values are used which are obtained from measurements preferably during the last two years. The most recent data are obtained from the annual reports from the 'Association of Rhine and Meuse Water Supply Companies'

[f] sum of the concentrations found for DCAs
[g] considered is the sum of the maximum concentrations found

(RIWA, 1995a; 1995b; RIWA, 1996a; 1996b), which conducts monthly measurements at different locations in Netherlands mainly along the rivers Rijn and Maas and the Ysselmeer. Although data on PCA and DMAs are not up-to-date they are included in Table 8.3. For comparison with the group MPCs, maximum measured concentrations (from the same location) are summed in the case data on several isomers are available (Table 8.2).

Table 8.3 Comparison of MPCs and NCs with (summed) measured environmental concentrations.

Substance	MPC_{water} (µg/l)	NC_{water} (µg/l)	conc. water (µg/l)	MPC_{soil} (µg/kg)	NC_{soil} (µg/kg)	MPC_{sed} (µg/kg)	NC_{sed} (µg/kg)
MCA	2.0	0.02	0.21[a]	5100	51	30	0.3
DCA	3.0	0.03	0.68[b]	7800	78	120	1.2
TCA	6.0	0.06	0.96[c]	420	4.2	420	4.2
PCA	0.1	0.001	0.01[d]	1500	15	60	0.6
MA	10	0.10	0.90[e]	30	0.3	30	0.3
DMA	50	0.50	0.4[d]	350	3.5	350	3.5

a (sum of) maximum measured concentration on MCAs
b (sum of) maximum measured concentration on DCAs
c (sum of) maximum measured concentration on TCAs
d observation in 1993 (Phernambucq *et al.*, 1996)
e (sum of) maximum measured concentration on MAs

It should be mentioned here that the values listed in Table 8.3 are referring to the concentration of one isomer in the case of MCAs, DCAs, TCAs and DMAs and two isomers in the case of MAs. From a methodological point of view it is desirable to have more underlying data to obtain a realistic picture whether or not the environmental concentrations are critical.

In Table 8.3 the MPCs for soil and sediment are also included. Since no data on concentrations of anilines in these compartments are available it could not be judged whether the derived MPCs for sediment and soil are protective.

The MPC_{water} derived in this document are a factor 4-125 larger than the measured maximum concentrations (Table 8.3). The derived NC_{water}s for MCAs, DCAs, TCAs and PCA are a factor 9-22 lower than the maximum concentrations found. The NC_{water} for DMA is a factor 1.3 larger than the maximum concentration. On the basis of this preliminary comparison it seems that at present there is no inadmissible risk on aquatic organisms exerted by aniline derivates.

9. CONCLUSIONS

Data availability

The largest amount of toxicity data is found for the group of chloroanilines. Even for this group the data set is limited especially when marine water and soil toxicity data are concerned. Only for MCAs and DCAs the MPC_{water} and MPC_{soil} are derived by statistical extrapolation. No sediment data are found.

The number of experimental log K_{oc} studies is very low for chloroanilines. No soil sorption data are found on other compounds. Therefore, log K_{oc}s are estimated by QSARs proposed by Sabljic *et al.* (1995).

Derivation of MPCs

The derivation of the MPCs is seriously hampered by lack of toxicity data, in particular for the higher substituted anilines.

Since a great amount of structurally similar compound is concerned group MPCs are derived group of isomers providing a same mode of action. These MPCs can be related to the sum of the individual compounds included in a group value.

The MPC_{water} in this document deviate up to a factor 10 from the $iMAR_{water}$s derived by Slooff *et al.* (1991), while the MPC_{soil} deviate a factor 10-38 from $iMAR_{soil}$s. Since in particular the MPC_{water}s are based on a greater dataset these values are considered more reliable than the $iMAR_{water}$s according to Slooff *et al.* (1991).

Environmental concentrations

Data on the occurrence of anilines in the environment are very limited and mainly concern the great rivers. Moreover, only a small amount of substances is found in the environment. When the risk limits are related to these environmental data it can be concluded that the group MPCs are not exceeded by (summed) measured concentrations. Related to the occurrence in the environment it can be furthermore concluded, that the derivation of MPCs is necessary only for a small number of anilines (Table 8.3).

On the basis of this preliminary comparison it seems that at present aquatic organisms are not at risk. Since no data on soil and sediment concentrations are available no judgement can be made whether or not the derived MPCs and NCs for soil and sediment are exceeded by actual concentrations.

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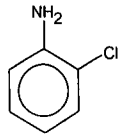
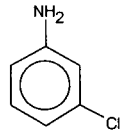
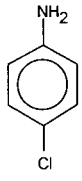
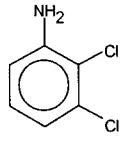
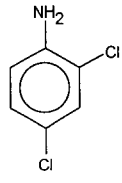
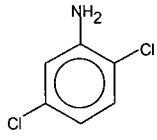
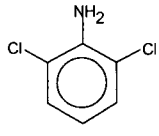
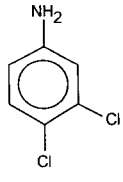
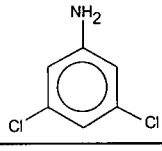
APPENDICES

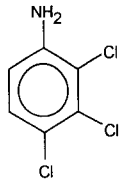
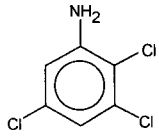
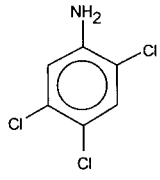
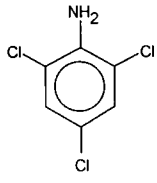
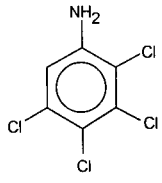
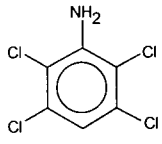
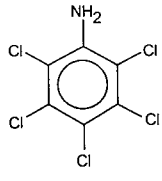
Appendix 1. CAS-registration numbers, molecular and structural formulae of the selected anilines.

Chloroanilines

Name	Cas.No.	Molecular formula	Structural formula
2-chloroaniline	95-95-1	C_6H_6ClN	
3-chloroaniline	108-42-9	C_6H_6ClN	
4-chloroaniline	106-47-8	C_6H_6ClN	
2,3-dichloroaniline	608-27-5	$C_6H_5Cl_2N$	
2,4-dichloroaniline	554-00-7	$C_6H_5Cl_2N$	
2,5-dichoroaniline	95-82-9	$C_6H_5Cl_2N$	
2,6-dichloroaniline	608-31-1	$C_6H_5Cl_2N$	
3,4-dichloroaniline	95-76-1	$C_6H_5Cl_2N$	
3,5-dichloroaniline	626-43-7	$C_6H_5Cl_2N$	

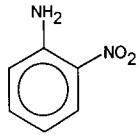
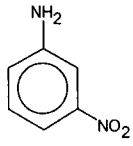
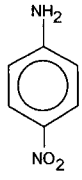
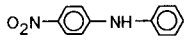
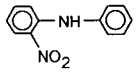
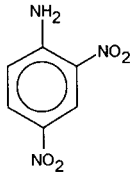
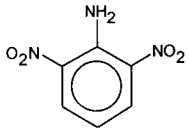
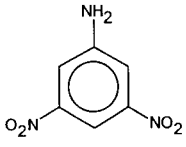
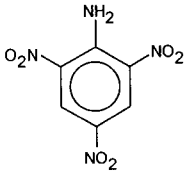
Appendix 1 continued CAS-registration numbers, molecular and structural formulae of the selected anilines.

Chloroanilines

Name	Cas.No.	Molecular formula	Structural formula
2,3,4-trichloroaniline	634-93-5	$C_6H_4Cl_3N$	
2,3,5-trichloroaniline	18487-39-3	$C_6H_4Cl_3N$	
2,4,5-trichloroaniline	636-30-6	$C_6H_4Cl_3N$	
2,4,6-trichloroaniline	634-93-5	$C_6H_4Cl_3N$	
2,3,4,5-tetrachloroaniline	634-83-3	$C_6H_3Cl_4N$	
2,3,5,6-tetrachloroaniline	3481-20-7	$C_6H_3Cl_4N$	
pentachloroaniline	527-20-8	$C_6H_2Cl_5N$	

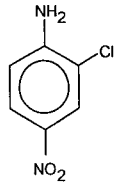
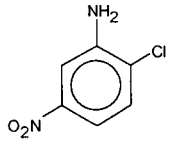
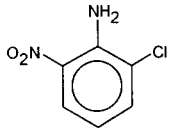
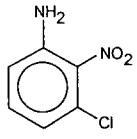
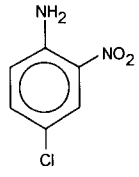
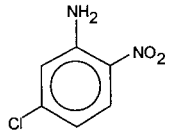
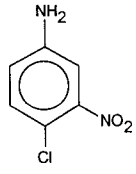
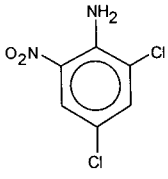
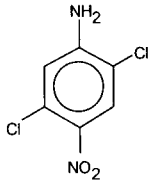
Appendix 1 continued CAS-registration numbers, molecular and structural formulae of the selected anilines.

(Chloro)nitroanilines

Name	Cas.No.	Molecular formula	Structural formula
2-nitroaniline	88-74-4	$C_6H_6N_2O_2$	
3-nitroaniline	99-09-2	$C_6H_6N_2O_2$	
4-nitroaniline	100-01-6	$C_6H_6N_2O_2$	
4-nitro-N-phenylaniline	836-30-6	$C_{12}H_{10}N_2O_2$	
2-nitro-N-phenylaniline	119-75-5	$C_{12}H_{10}N_2O_2$	
2,4-dinitroaniline	97-02-9	$C_6H_5N_3O_4$	
2,6-dinitroaniline	606-22-4	$C_6H_5N_3O_4$	
3,5-dinitroaniline	618-87-1	$C_6H_5N_3O_4$	
2,4,6-trinitroaniline	489-98-5	$C_6H_4N_4O_6$	

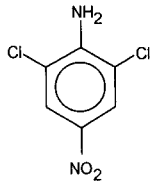
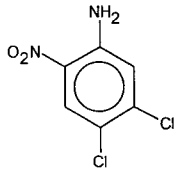
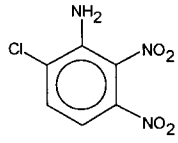
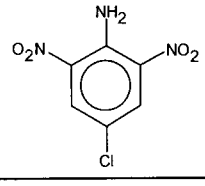
Appendix 1 continued CAS-registration numbers, molecular and structural formulae of the selected anilines.

(Chloro)nitroanilines

Name	Cas.No.	Molecular formula	Structural formula
2-chloro-4-nitroaniline	121-87-9	$C_6H_5ClN_2O_2$	
2-chloro-5-nitroaniline	6283-25-6	$C_6H_5ClN_2O_2$	
2-chloro-6-nitroaniline	769-11-9	$C_6H_5ClN_2O_2$	
2-nitro-3-chloroaniline	59483-54-4	$C_6H_5ClN_2O_2$	
2-nitro-4-chloroaniline	89-63-4	$C_6H_5ClN_2O_2$	
2-nitro-5-chloroaniline	1635-61-6	$C_6H_5ClN_2O_2$	
3-nitro-4-chloroaniline	635-22-3	$C_6H_5ClN_2O_2$	
2,4-dichloro-6-nitroaniline	2683-43-4	$C_6H_4Cl_2N_2O_2$	
2,5-dichloro-4-nitroaniline	6627-34-5	$C_6H_4Cl_2N_2O_2$	

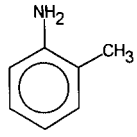
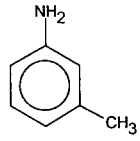
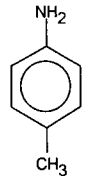
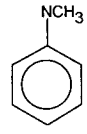
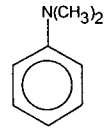
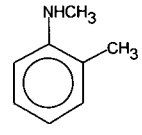
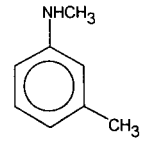
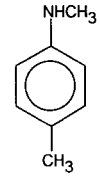
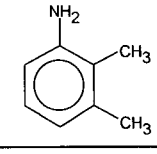
Appendix 1 continued CAS-registration numbers, molecular and structural formulae of the selected anilines.

(Chloro)nitroanilines

Name	Cas.No.	Molecular formula	Structural formula
2,6-dichloro-4-nitroaniline	99-30-9	$C_6H_4Cl_2N_2O_2$	
3,4-dichloro-6-nitroaniline	6641-64-1	$C_6H_4Cl_2N_2O_2$	
2,4-dinitro-6-chloroaniline	3531-19-9	$C_6H_4ClN_3O_4$	
2,6-dinitro-4-chloroaniline	5388-62-5	$C_6H_4ClN_3O_4$	

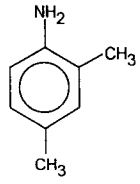
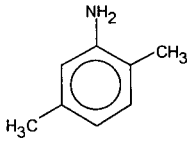
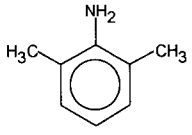
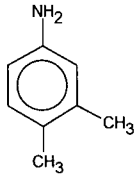
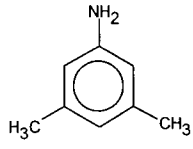
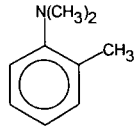
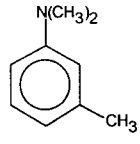
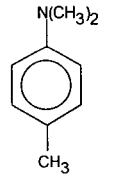
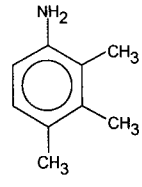
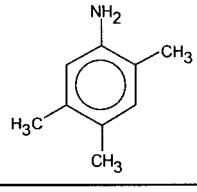
Appendix 1 continued CAS-registration numbers, molecular and structural formulae of the selected anilines.

(Chloro)methylanilines

Name	Cas.No.	Molecular formula	Structural formula
2-methylaniline	95-53-4	C_7H_9N	
3-methylaniline	108-44-1	C_7H_9N	
4-methylaniline	106-49-0	C_7H_9N	
N-methylaniline	100-61-8	C_7H_9N	
N,N-dimethylaniline	121-69-7	$C_8H_{11}N$	
N,2-dimethylaniline	611-21-2	$C_8H_{11}N$	
N,3-dimethylaniline	696-44-6	$C_8H_{11}N$	
N,4-dimethylaniline	623-08-5	$C_8H_{11}N$	
2,3-dimethylaniline	87-59-2	$C_8H_{11}N$	

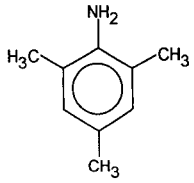
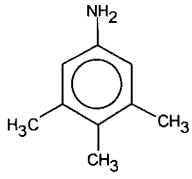
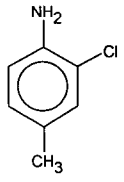
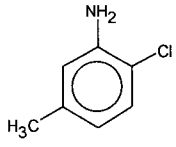
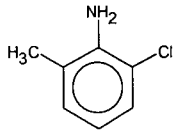
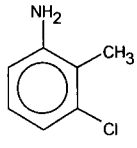
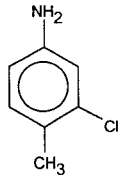
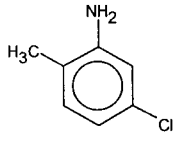
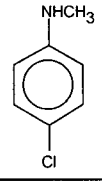
Appendix 1 continued CAS-registration numbers, molecular and structural formulae of the selected anilines.

(Chloro)methylanilines

Name	Cas.No.	Molecular formula	Structural formula
2,4-dimethylaniline	95-68-1	$C_8H_{11}N$	
2,5-dimethylaniline	95-78-3	$C_8H_{11}N$	
2,6-dimethylaniline	87-62-7	$C_8H_{11}N$	
3,4-dimethylaniline	95-64-7	$C_8H_{11}N$	
3,5-dimethylaniline	108-69-0	$C_8H_{11}N$	
N,N,2-trimethylaniline	609-72-3	$C_9H_{13}N$	
N,N,3-trimethylaniline	121-72-2	$C_9H_{13}N$	
N,N,4-trimethylaniline	99-97-8	$C_9H_{13}N$	
2,3,4-trimethylaniline	1467-35-2	$C_9H_{13}N$	
2,4,5-trimethylaniline	137-17-7	$C_9H_{13}N$	

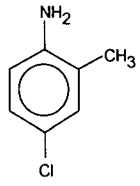
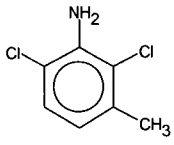
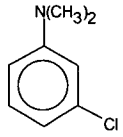
Appendix 1 continued CAS-registration numbers, molecular and structural formulae of the selected anilines.

(Chloro)methylanilines

Name	Cas.No.	Molecular formula	Structural formula
2,4,6-trimethylaniline	88-05-1	$C_9H_{13}N$	
3,4,5-trimethylaniline	1639-31-2	$C_9H_{13}N$	
2-chloro-4-methylaniline	615-65-6	C_7H_8ClN	
2-chloro-5-methylaniline	95-81-8	C_7H_8ClN	
2-chloro-6-methylaniline	87-63-8	C_7H_8ClN	
3-chloro-2-methylaniline	87-60-5	C_7H_8ClN	
3-chloro-4-methylaniline	95-74-9	C_7H_8ClN	
5-chloro-2-methylaniline	95-79-4	C_7H_8ClN	
4-chloro-N-methylaniline	932-96-7	C_7H_8ClN	

Appendix 1 continued CAS-registration numbers, molecular and structural formulae of the selected anilines.

(Chloro)methylanilines

Name	Cas.No.	Molecular formula	Structural formula
4-chloro-2-methylaniline	95-69-2	C_7H_8ClN	
2,6-dichloro-3-methylaniline	64063-37-2	$C_7H_7Cl_2N$	
3-chloro-N,N-dimethylaniline	6848-13-1	$C_8H_{10}ClN$	

Legend of Appendix 2 to Appendix 6.

organisms	Species used in the test, if available followed by: age, size, weight or life stage	
A	Y	test substance analysed in test solution
	N	test substance not analysed in solution or no data
test type	S	static
	R	renewal
	CF	continuous flow
test water	am	artificial medium
	tw	tap water
	nw	natural water
	rw	reconstituted water
test substance purity	percentage active ingredient (%)	
	anal	analytical grade
	tech	technical grade
	high	high but unknown purity
exposure time	h	hour(s)
	d	day(s)
	w	week(s)
	m	month(s)
	CLC	complete life cycle
	ELS	early life stage
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	

Appendix 2. Chronic freshwater toxicity data.

2-chloroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Scenedesmus subspicatus	N	S	-	am	7.0	60	8 d	NOEC	3.9[a]	Schmidt and Schnabl, 1988
Crustaceans										
Daphnia magna	Y	R	-	am	8.0	-	21 d	NOEC	0.032[b]	Kühn *et al.*, 1989a

a growth; reported EC10 is considered to be equal to the NOEC
b parent mortality, reproduction rate, appearance of first offspring

3-chloroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Scenedesmus subspicatus	N	S	-	am	7.0	60	8 d	NOEC	4.1[a]	Schmidt and Schnabl, 1988
Crustaceans										
Daphnia magna	Y	R	-	am	8.0	-	21 d	NOEC	0.013[b]	Kühn *et al.*, 1989a
Pisces										
Brachydanio rerio, ELS test	Y	R	98	rw	8.0-8.2	210	28 d	NOEC	1.0[c]	Van Leeuwen *et al.*, 1990

a growth, the reported EC10 is considered to be equal to the NOEC
b reproduction rate and appearance of first offspring
c survival; hatching; growth

Appendix 2 continued. Chronic freshwater toxicity data.

4-chloroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Pseudomonas putida	N	S	-	-	-	-	16 h	NOEC	72	Knie *et al.*, 1983
Algae										
Chlorophyta										
Scenedesmus subspicatus	N	S	-	am	7.0	60	8 d	NOEC	0.03[h]	Schmidt and Schnabl, 1988
Scenedesmus subspicatus	N	S	98	am	-	-	96 h	NOEC	0.4[g]	Geyer *et al.*, 1985
Crustaceans										
Daphnia magna	Y	R	-	am	8.0	-	21 d	NOEC	0.01[a,b]	Kühn *et al.*, 1989a
Pisces										
Brachydanio rerio, 6 m	N	CF	> 99	tw	7.3	360	CLC	NOEC	0.2[e]	Bresch *et al.*, 1990
Brachydanio rerio, 6 m	N	CF	> 99	tw	7.3	360	CLC	NOEC	0.013[f]	Bresch *et al.*, 1990
Oryzias latipes, 0-3 d larvae	Y	CF	99.9	nw	7.9	45.8	28 d	NOEC	8.2[c]	Holcombe *et al.*, 1995
Oryzias latipes, 0-3 d larvae	Y	CF	99.9	nw	7.9	45.8	28 d	NOEC	0.75[d]	Holcombe *et al.*, 1995

a reproduction rate
b appearance of first offspring
c mortality
d growth, NOEC=LOEC/3 (33% effect)
e fertilization rate in F1 and F2 generation, egg release in both generations was lower at all concentrations (NOEC < 0.04 mg/l)
f number of eggs; NOEC=LOEC/3
g growth
h growth, the reported IC10 is considered to be equal to the NOEC

Appendix 2 continued. Chronic freshwater toxicity data.

2,4-dichloroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l		Reference
Bacteriophyta											
Pseudomonas fluorescens	N	S	-	am	-	81	7 h	NOEC	10[a]		Slooff and Canton, 1983
Cyanophyta											
Microcystis aeruginosa	N	S	-	am	-	24	4 d	NOEC	1.0[a]		Slooff and Canton, 1983
Algae											
Chlorophyta											
Scenedesmus subspicatus	N	S	-	am	7.0	60	8 d	NOEC	0.8[b]		Schmidt and Schnabl, 1988
Scenedesmus pannonicus	N	S	-	am	-	54	4 d	NOEC	3.2[a]		Slooff and Canton, 1983
Macrophyta											
Lemna minor	N	S	-	am	-	268	7 d	NOEC	1.0[a]		Slooff and Canton, 1983
Crustaceans											
Daphnia magna, 1 d	N	R	-	am	8.2	200	21 d	NOEC	0.032[c]		Slooff and Canton, 1983
Daphnia magna, 1 d	N	R	-	am	8.2	200	21 d	NOEC	0.032[e]		Slooff and Canton, 1983
Daphnia magna, < 24 h	N	R	-	am	8.2	200	16 d	NOEC	0.015[a]		Deneer *et al.*, 1988
Insecta											
Culex pipiens, 1st instar	N	R	-	am	8.2	200	25 d	NOEC	10[c]		Slooff and Canton, 1983
Culex pipiens, 1st instar	N	R	-	am	8.2	200	25 d	NOEC	10[d]		Slooff and Canton, 1983
Coelenterata											
Hydra oligactis, budless	N	R	-	am	8.2	200	21 d	NOEC	3.2[a]		Slooff and Canton, 1983
Mollusca											
Lymnea stagnalis, 5 m	N	R	-	am	8.2	200	40 d	NOEC	3.2[c]		Slooff and Canton, 1983
Lymnea stagnalis, 5 m	N	R	-	am	8.2	200	40 d	NOEC	1.0[e]		Slooff and Canton, 1983
Lymnea stagnalis, eggs	N	R	-	am	8.2	200	7 d	NOEC	3.2[f]		Slooff and Canton, 1983
Amphibia											
Xenopus laevis, < 2 d	N	R	-	am	8.2	200	100 d	NOEC	1.0[a]		Sloof and Canton, 1983
Xenopus laevis, < 2 d	N	R	-	am	8.2	200	100 d	NOEC	1.0[c]		Sloof and Canton, 1983
Xenopus laevis, < 2 d	N	R	-	am	8.2	200	100 d	NOEC	0.32[d]		Sloof and Canton, 1983
Pisces											
Gasterosteus aculeatus, eggs	Y	R	≥99	-	-	-	28 d	NOEC	0.58[c]	α	Van den Dikkenberg *et al.*, 1989
Gasterosteus aculeatus, eggs	Y	R	≥99	-	-	-	28 d	NOEC	0.33[a]	α	Van den Dikkenberg *et al.*, 1989
Oryzias latipesI, eggs	N	R	-	am	8.2	200	40 d	NOEC	0.32[c]		Slooff and Canton, 1983
Oryzias latipes, eggs	N	R	-	am	8.2	200	40 d	NOEC	3.2[a]		Slooff and Canton, 1983
Poecilia reticulata, 3-4 w	N	R	-	am	8.2	200	28 d	NOEC	3.2[c]		Slooff and Canton, 1983
Poecilia reticulata, 3-4 w	N	R	-	am	8.2	200	28 d	NOEC	1.0[a]		Slooff and Canton, 1983

a growth
b growth, the reported EC10 is considered to be equal to the NOEC
c mortality
d development
e reproduction
f hatching

Appendix 2 continued. Chronic freshwater toxicity data.

2,6-dichloroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Pseudomonas putida	N	S	-	-	-	-	30 min	NOEC	158[a]	Knie *et al.*, 1983
Algae										
Chlorophyta										
Scenedesmus subspicatus	N	S	-	m	7.0	60	8 d	NOEC	2.2[b]	Schmidt and Schnabl, 1988
Haematococcus pluvialis	N	S	-	-	-	-	4 h	NOEC	65[a]	Knie *et al.*, 1983

a growth
b growth, the reported EC10 is considered to be equal to the NOEC

Appendix 2 continued. Chronic freshwater toxicity data.

3,4-chloroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l		Reference
Protozoa											
Tetrahymena pyriformis	N	S	anal.	am	-	-	48 h	NOEC	5.5[b]		Schäfer *et al.*, 1994
Tetrahymena pyriformis	N	S	anal.	am	-	-	96 h	NOEC	5.1[b]		Schäfer *et al.*, 1994
Rotatoria											
Brachionus calyciflorus	N	R	anal.	am	-	100	24 h	NOEC	2.5[a]		Janssen *et al.*, 1994
Brachionus calyciflorus	Y	R	anal.	am	-	80	96 h	NOEC	2.5[a]		Janssen *et al.*, 1994
Brachionus calyciflorus	N	S	anal.	am	-	-	72 h	NOEC	5.0[a]		Janssen *et al.*, 1994
Algae											
Chlorophyta											
Chlamydomonas reinhardi	N	S	anal.	am	-	-	72 h	NOEC	2.5[b]		Schäfer *et al.*, 1994
Chlamydomonas reinhardi	N	S	anal.	am	-	-	24 h	NOEC	3.0[c]		Schäfer *et al.*, 1994
Chlamydomonas reinhardi	Y	CF	anal.	am	-	-	4 d	NOEC	0.26[b]	α	Schäfer *et al.*, 1994
Chlamydomonas reinhardi	Y	CF	anal.	am	-	-	7 d	NOEC	0.33[b]	α	Schäfer *et al.*, 1994
Chlamydomonas reinhardi	Y	CF	anal.	am	-	-	10 d	NOEC	0.70[b]	α	Schäfer *et al.*, 1994
Scenedesmus subspicatus	N	S	anal.	am	-	-	72 h	NOEC	0.5[b]		Schäfer *et al.*, 1994
Scenedesmus subspicatus	N	S	anal.	am	-	-	24 h	NOEC	2.9[c]		Schäfer *et al.*, 1994
Crustaceans											
Daphnia magna	Y	R	-	am	8.0	-	21 d	NOEC	0.01[d]		Kühn *et al.*, 1989a
Daphnia magna, larvae, 1 mm	Y	R	pure	am	8.0	-	21 d	NOEC	0.0065[p]		Adema and Vink, 1981
Daphnia magna, larvae, 1 mm	Y	R	pure	am	8.0	-	21 d	NOEC	0.0065[f]		Adema and Vink, 1981
Daphnia magna, 1 instar	N	R	-	am	7.5	-	21 d	NOEC	0.010[h]		Baird *et al.*, 1991
Daphnia magna, 1 instar	N	R	-	am	7.5	-	21 d	NOEC	0.005[i]		Baird *et al.*, 1991
Daphnia magna, < 24 h	N	R	-	am	7.7	hard	19 d	NOEC	0.005[j]		Soares *et al.*, 1992
Daphnia magna, 10 d	Y	F	-	nw	8.1	198	55 d	NOEC	0.006[b]		Van der Hoeven, 1990
Daphnia magna, < 24 h	Y	R	-	am	7.7-8.4	162-250	21 d	NOEC	0.05[f]		Crossland and Hillaby, 1985
Daphnia magna, < 24 h	Y	R	-	am	7.7-8.4	162-250	21 d	NOEC	0.05[g]		Crossland and Hillaby, 1985
Daphnia magna, < 24 h	Y	R	-	am	7.7-8.4	162-250	21 d	NOEC	0.01[t]		Crossland and Hillaby, 1985
Daphnia magna, < 24 h	Y	R	-	am	7.7-8.4	162-250	21 d	NOEC	0.01[u]		Crossland and Hillaby, 1985
Gammarus pulex, < 2 w	Y	CF	-	am	8.6	229	25 d	NOEC	0.08[b]	α	Taylor *et al.*, 1994
Insecta											
Chironomus riparius, 3 instar	Y	CF	-	am	8.6	229	12 d	NOEC	0.76[b]	α	Taylor *et al.*, 1994
Chironomus riparius, 2 instar	Y	R	-	-	7.0	151	10 d	NOEC	0.17[b]	α	Taylor *et al.*, 1991
Mollusca											
Lymnea stagnalis, eggs	Y	F	pure	am	8.0	hard	16 d	NOEC	0.13[o]		Adema and Vink, 1981
Pisces											
Brachydanio rerio, ELS	Y	CF	99.5	tw	6.3-8.2	-	42 d	NOEC	0.020[e]		Nagel *et al.*, 1991

Appendix 2 continued. Chronic freshwater toxicity data.

3,4-chloroaniline (continued)

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Perca fluviatilis	Y	CF	99.5	tw	7.9	224	18 d	NOEC	0.002[e]	Schäfers and Nagel, 1993
Perca fluviatilis, eggs	Y	CF	99.5	tw	7.9	224	8 d	NOEC	0.002[v]	Schäfers and Nagel, 1993
Pimephales promelas, ELS	Y	CF	98	nw	7.6	44.4	28 d	NOEC	0.026[e]	Call *et al.*, 1987
Pimephales promelas, ELS	Y	CF	98	nw	7.6	44.4	28 d	NOEC	0.026[r]	Call *et al.*, 1987
Pimephales promelas, ELS	Y	CF	98	nw	7.6	44.4	28 d	NOEC	0.026[s]	Call *et al.*, 1987
Pimephales promelas, ELS	Y	CF	98	nw	7.6	44.4	28 d	NOEC	0.015[q]	Call *et al.*, 1987
Pimephales promelas, ELS	Y	CF	98	rw	7.2	50.7	28 d	NOEC	0.015[e]	Call *et al.*, 1987
Pimephales promelas, ELS	Y	CF	98	rw	7.2	50.7	28 d	NOEC	0.015[s]	Call *et al.*, 1987
Pimephales promelas, ELS	Y	CF	98	rw	7.2	50.7	28 d	NOEC	0.005[q]	Call *et al.*, 1987
Pimephales promelas, ELS	Y	CF	98	rw	7.2	50.7	28 d	NOEC	0.005[r]	Call *et al.*, 1987
Poecilia reticulata, 7 m	Y	CF	99.5	tw	8.2	246	CLC	NOEC	0.020[k]	Schäfers and Nagel, 1991
Poecilia reticulata, 7 m	Y	CF	99.5	tw	8.2	246	CLC	NOEC	0.020[w]	Schäfers and Nagel, 1991
Poecilia reticulata, ELS	Y	CF	99.5	tw	8.2	246	42 d	NOEC	0.020[n]	Schäfers and Nagel, 1991
Poecilia reticulata, 7 m	Y	CF	99.5	tw	8.2	246	CLC	NOEC	0.0007[l]	Schäfers and Nagel, 1991
Poecilia reticulata, 7 m	Y	CF	99.5	tw	8.2	246	CLC	NOEC	0.002[m]	Schäfers and Nagel, 1991

a intrinsic rate of natural increase
b growth
c effective photosynthesis rate
d reproduction rate
e survival
f mortaliteit
g length of surviving adults
h total egg production
i viable egg production
j fecundity; NOEC founf for 4 different clones (A, B, E, S-2, identified according to 1986 ring test (Baird *et al.*, 1991)
k % survival of F0 offspring
l % survival of F1 offspring; NOEC=LOEC/3
m weight of F1 females
n weight of F1 and F2 males and females
o hatchability
p reproduction
q length
r weight
s total biomass/chamber
t number of life and dead young
u first day producing young
v hatching rate
w weight of F0 females

3,5-dichloroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Pisces										
Brachydanio rerio, ELS test	Y	R	>97	rw	8.0-8.2	210	28 d	NOEC	0.32[a]	Van Leeuwen *et al.*, 1990

a survival, hatching and growth

Appendix 2 continued. Chronic freshwater toxicity data.

2,4,5-trichloroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Pisces										
Brachydanio rerio, ELS test	Y	R	>97	rw	8.0-8.2	210	28 d	NOEC	0.056[a]	Van Leeuwen *et al.*, 1990

a survival, hatching and growth

2,3,4,5-tetrachloroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Pisces										
Brachydanio rerio, ELS test	Y	R	>98	rw	8.0-8.2	210	28 d	NOEC	0.032[a]	Van Leeuwen *et al.*, 1990
Poecilia reticulata, 1 y	N	CF	>98	tw	7.8	-	14 d	NOEC	0.23[b]	De Wolf *et al.*, 1992a

a survival, hatching and growth
b survival

pentachloroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Pisces										
Brachydanio rerio, ELS test	Y	R	>98	rw	8.0-8.2	210	28 d	NOEC	0.01[a]	Van Leeuwen *et al.*, 1990

a survival, hatching and growth

Appendix 2 continued. Chronic freshwater toxicity data.

3-nitroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Selenastrum capricornutum	N	S	> 99	am	-	17	72 h	NOEC	5.3[a]	EAJ, 1991
Crustaceanse										
Daphnia magna, <24 h	N	R	> 99	rw	6.7-7.0	115	21 d	NOEC	0.5[b]	EAJ, 1991
Daphnia magna, <24 h	N	R	> 99	rw	6.7-7.0	115	21 d	NOEC	1.6[c]	EAJ, 1991

a growth rate; light regime: continuous illumination (4000 Lux)
b reproduction; light regime: 16h/8h light/dark; oxygen conc. >70%
c mortality; testcondition as b

4-nitroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Pseudomonas putida	N	S	-	am	7.0	77	16 h	NOEC	3.8[a]	Bringmann and Kühn, 1976
Protozoans										
Enthosiphon sulcatum	N	S	-	am	6.9	77	72 h	NOEC	6.9[a]	Bringmann and Kühn, 1980
Uronema parduczi	N	S	-	am	7.0	-	72 h	NOEC	3.1[a]	Bringmann and Kühn, 1981
Chilomonas paramecium	N	S	-	am	7.0	-	72 h	NOEC	5.0[a]	Bringmann and Kühn, 1981
Cyanophyta										
Microcystis aeruginosa	N	S	-	am	7.0	60	8 d	NOEC	0.4[a,b]	Bringmann and Kühn, 1978a
Algae										
Chlorophyta										
Scenedesmus quadricauda	N	S	-	am	7.0	60	8 d	NOEC	11[a,c]	Bringmann and Kühn, 1976

a cell multiplication inhibition, NOEC is expressed as the toxic treshold (TGK)
b same value as reported in Bringmann and Kühn (1978b, 1980) and in Bringmann (1975), in the latter value is expressed as LOEC
c same value as reported in Bringmann and Kühn (1978b)

Appendix 2 continued. Chronic freshwater toxicity data.

2,4-dinitroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Scenedesmus subspicatus	N	S	-	am	7.0	60	8 d	NOEC	0.1[a]	Schmidt and Schnabl, 1988

a growth, the reported EC10 is considered to be equal to the NOEC

2-methylaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Pseudomonas putida	N	S	-	am	7.0	77	16 h	NOEC	16[a]	Bringmann and Kühn, 1976
Protozoa										
Enthosiphon sulcatum	N	S	-	am	6.9	77	72 h	NOEC	76[a]	Bringmann and Kühn, 1980
Uronema parduczi	N	S	-	am	7.0	-	72 h	NOEC	21[a]	Bringmann and Kühn, 1981
Chilomonas paramecium	N	S	-	am	7.0	-	72 h	NOEC	237[a]	Bringmann and Kühn, 1981
Cyanophyta										
Microcystis aeruginosa	N	S	-	am	7.0	60	8 d	NOEC	0.3[a,b]	Bringmann and Kühn, 1978a
Algae										
Chlorophyta										
Scenedesmus quadricauda	N	-	-	am	7.0	60	8 d	NOEC	6.3[a,c]	Bringmann and Kühn, 1976

a cell multiplication inhibition; the reported toxic treshold (TGK) is considered the NOEC

b same value as in Bringmann and Kühn (1978b, 1980) and in Bringmann (1975), in the latter value is expressed as LOEC

c same value as in Bringmann and Kühn (1978b)

Appendix 2 continued. Chronic freshwater toxicity data.

3-methylaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l		Reference
Crustaceans											
Daphnia magna, < 24 h	N	R	-	am	8.2	200	16 d	NOEC	0.01[a]		Deneer *et al.*, 1988

a growth; solvent is ethanol (0.1 ml/l)

2,3-dimethylaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l		Reference
Crustaceans											
Daphnia magna, ≤ 24 h	Y	R	-	am	8.0	240	21 d	NOEC	0.16[a]	α	Kühn *et al.*, 1989a

a reproduction rate

2,4-dimethylaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Pseudomonas putida	N	S	-	am	7.0	77	16 h	NOEC	8.0[a]	Bringmann and Kühn, 1976
Protozoa										
Enthosiphon sulcatum	N	S	-	am	6.9	77	72 h	NOEC	9.8[a]	Bringmann and Kühn, 1980
Uronema parduczi	N	S	-	am	6.9	-	72 h	NOEC	12[a]	Bringmann and Kühn, 1981
Cyanophyta										
Microcystis aeruginosa	N	S	-	am	7.0	60	8 d	NOEC	0.4[a,b]	Bringmann and Kühn, 1978a
Algae										
Chlorophyta										
Scenedesmus quadricauda	N	S	-	am	7.0	60	8 d	NOEC	5.0[a,c]	Bringmann and Kühn, 1976
Scenedesmus subspicatus	N	S	-	am	7.0	60	8 d	NOEC	0.8[d]	Schmidt and Schnabl, 1988

a cell multiplication inhibition, the reported toxic treshold (TGK) is considered the NOEC
b same value as reported in Bringmann and Kühn (1978b, 1980) and in Bringmann (1975), in the latter value is expressed as LOEC
c same value as reported in Bringmann and Kühn (1978b)
d growth, NOEC=EC10

Appendix 2 continued. Chronic freshwater toxicity data.

3,4-dimethylaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l		Reference
Crustaceans											
Daphnia magna, ≤ 24 h	Y	R	-	am	8.0	240	21 d	NOEC	0.016[a]	α	Kühn *et al.*, 1989a

a reproduction rate

3-chloro-4-methylaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Scenedesmus subspicatus	N	S	-	am	7.0	60	8 d	NOEC	1.0[a]	Schmidt and Schnabl, 1988

a growth, NOEC=LOEC/2; LOEC is reprorted as the IC10

Appendix 2 continued. Acute freshwater toxicity data.

2-chloroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l		Reference
Bacteriophyta											
Escherischia coli	N	S	-	am	-	-	48 h	EC50	280[a]		Nendza and Seydel, 1990
Protozoa											
Tetrahymena pyriformis	N	S	-	-	-	-	24 h	EC50	200		Yoshioka *et al.*, 1985
Algae											
Chlorophyta											
Scenedesmus subspicatus	N	S	-	am	8.0	54	96 h	EC50	35[b]		Kühn and Pattard, 1990
Scenedesmus pannonicus	Y	S	> 99.9	am	8.2	200	-	EC50	32[b]	α	Canton *et al.*, 1985
Chlorella pyrenoidosa	N	-	≥ 99	am	8.7	90	96 h	EC50	32[d]		Maas-Diepeveen and Van Leeuwen, 1986
Crustaceans											
Daphnia magna	Y	S	> 99.9	am	8.2	200	48 h	EC50	0.46[c]	α	Canton *et al.*, 1985
Daphnia magna	Y	S	> 99.9	am	8.2	200	48 h	LC50	1.5	α	Canton *et al.*, 1985
Daphnia magna, < 24 h	N	R	≥ 99	nw	8.1	225	48 h	LC50	0.13		Maas-Diepeveen and Van Leeuwen, 1986
Pisces											
Brachydanio rerio, 3 m	Y	R	-	tw	8.6	-	96 h	LC50	5.2		Zok *et al.*, 1991
Pimephales promelas, 29 d	Y	S	98	nw	7.6	44.9	96 h	LC50	5.9	α	Geiger *et al.*, 1986

a EC50 is expressed as the concentration which inhibits the generation rate by 50% (I50), same value reported in Nendza and Seydel (1988a,b)
b growth
c immobility
d yield

Appendix 2 continued. Acute freshwater toxicity data.

3-chloroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Escherischia coli	N	S	-	am	-	-	48 h	EC50	340[a]	Nendza and Seydel, 1990
Protozoa										
Tetrahymena pyriformis	N	S	-	-	-	-	24 h	EC50	100[b]	Yoshioka *et al.*, 1985
Algae										
Chlorophyta										
Scenedesmus subspicatus	N	S	-	am	8.0	54	48 h	EC50	26[b]	Kühn and Pattard, 1990
Scenedesmus subspicatus	N	S	-	am	8.0	54	48 h	EC50	53[c]	Kühn and Pattard, 1990
Chlorella pyrenoidosa	N	-	≥ 99	am	8.7	90	96 h	EC50	21[e]	Maas-Diepeveen and Van Leeuwen, 1986
Crustaceans										
Daphnia magna, < 24 h	N	R	≥ 99	nw	8.1	225	48 h	LC50	0.1	Maas-Diepeveen and Van Leeuwen, 1986
Daphnia magna	N	S	-	am	8.0	-	48 h	EC50	0.35[d]	Kühn *et al.*, 1989a
Pisces										
Brachydanio rerio, 3 m	Y	R	-	tw	8.6	-	96 h	LC50	19	Zok *et al.*, 1991

a EC50 is expressed as the concentration which inhibits the generation rate by 50% (I50), same value reported in Nendza and Seydel (1988a,b)
b cell multiplication inhibition
c growth
d immobilisation
e yield

Appendix 2 continued. Acute freshwater toxicity data.

4-chloroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l		Reference
Bacteriophyta											
Escherischia coli	N	S	-	am	-	-	48 h	EC50	380[a]		Nendza and Seydel, 1990
Protozoa											
Tetrahymena pyriformis	N	S	-	-	-	-	24 h	EC50	10		Yoshioka *et al.*, 1985
Algae											
Chlorophyta											
Scenedesmus subspicatus	N	S	-	am	8.0	54	96 h	EC50	2.8[b]		Kühn and Pattard, 1990
Scenedesmus subspicatus	N	S	98	am	-	-	96 h	EC50	2.4[b]		Geyer *et al.*, 1985
Chlorella pyrenoidosa	N	-	> 99	am	8.7	90	96 h	EC50	4.0[c]		Maas-Diepeveen and Van Leeuwen, 1986
Crustaceans											
Daphnia magna, < 24 h	N	R	> 99	nw	8.1	225	48 h	LC50	0.05		Maas-Diepeveen and Van Leeuwen, 1986
Daphnia magna	N	S	98	-	-	-	48 h	EC50	0.11		Lee *et al.*, 1993
Pisces											
Pimephales promelas, juvenile	Y	CF	-	-	7.6	44	96 h	LC50	33	α	Veith and Broderius, 1987
Pimephales promelas, 34 d	Y	S	98	nw	7.7	44.3	96 h	LC50	31	α	Geiger *et al.*, 1988
Brachydanio rerio 3 m	Y	R	-	tw	8.6	-	96 h	LC50	35		Zok *et al.*, 1991
Brachydanio rerio	N	S	98	-	-	-	96 h	LC50	31		Lee *et al.*, 1993
Leuciscus idus melanotus	N	S	-	-	-	-	96 h	LC50	23		Knie *et al.*, 1983
Oryzias latipes, 28-43 d	Y	CF	99.9	nw	7.9	45.8	96 h	LC50	38	α	Holcombe *et al.*, 1995

a EC50 is expressed as the concentration which inhibits the generation rate by 50% (I50), same value reported in Nendza and Seydel (1988a,b)
b growth
c yield

Appendix 2 continued. Acute freshwater toxicity data.

2,4-dichloroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Escherichia coli	N	S	-	am	-	-	48 h	EC50	60[a]	Nendza and Seydel, 1990
Protozoa										
Tetrahymena pyriformis	N	S	-	-	-	-	24 h	EC50	31	Yoshioka *et al.*, 1985
Algae										
Chlorophyta										
Chlorella pyrenoidosa	N	-	≥ 99	am	8.7	90	96 h	EC50	10[b]	Maas-Diepeveen and Van Leeuwen, 1986
Crustaceans										
Daphnia magna, < 24 h	N	R	≥ 99	nw	8.1	225	48 h	LC50	0.5	Maas-Diepeveen and Van Leeuwen, 1986
Pisces										
Brachydanio rerio, 3 m	Y	R	-	tw	8.6	-	96 h	LC50	5.7	Zok *et al.*, 1991

a EC50 is expressed as the concentration which inhibits the generation rate by 50% (I50), same value reported in Nendza and Seydel (1988a,b)
b yield

2,5-dichloroaniline.

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Chlorella pyrenoidosa	N	-	> 90	am	8.7	90	96 h	EC50	10[a]	Maas-Diepeveen and Van Leeuwen, 1986
Crustaceans										
Daphnia magna, < 24 h	N	R	> 99	nw	8.1	225	48 h	LC50	2.9	Maas-Diepeveen and Van Leeuwen, 1986

a yield

Appendix 2 continued. Acute freshwater toxicity data.

2,6-dichloroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Escherischia coli	N	S	-	am	-	-	48 h	EC50	100[a]	Nendza and Seydel, 1990
Crustaceans										
Daphnia magna	N	S	-	-	-	-	48 h	EC50	6.0[b]	Knie *et al.*, 1983
Pisces										
Leuciscus idus melanotus	N	S	-	-	-	-	96 h	LC50	1.0	Knie *et al.*, 1983

a EC50 is expressed as the concentration which inhibits the generation rate by 50% (I50), same value reported in Nendza and Seydel (1988a,b)
b immobility

3,4-dichloroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Protozoa										
Tetrahymena pyriformis	N	S	anal.	am	-	-	48 h	EC50	9.2[a]	Schäfer *et al.*, 1994
Tetrahymena pyriformis	N	S	anal.	am	-	-	96 h	EC50	9.4[a]	Schäfer *et al.*, 1994
Algae										
Chlorophyta										
Chlamydomonas reinhardi	N	S	anal.	am	-	-	72 h	EC50	9.0[a]	Schäfer *et al.*, 1994
Chlorella pyrenoidosa	Y	S	pure	am	8.0	-	96 h	EC50	3.2[a]	Adema and Vink, 1981
Chlorella pyrenoidosa	N	-	> 90	am	8.7	90	96 h	EC50	4.2[b]	Maas-Diepeveen and Van Leeuwen, 1986
Scenedesmus subspicatus	N	S	anal.	am	-	-	72 h	EC50	15[a]	Schäfer *et al.*, 1994
Scenedesmus subspicatus	N	S	-	am	8.0	54	48 h	EC50	6.8[a]	Kühn and Pattard, 1990
Scenedesmus quadricauda	Y	S	pure	am	8.0	-	96 h	EC50	2.2[a]	Adema and Vink, 1981
Rotatoria										
Brachionus calyciflorus, cysts	N	S	-	am	7.6	90	24 h	LC50	62	Ferrando and Andreu-Moliner, 1991
Mollusca										
Dreissena polymorpha, adult, 1 cm	Y	S	pure	am	8.0	hard	96 h	LC50	22	Adema and Vink, 1981
Annelida										
Tubifex tubifex, 30-50 mm	-	-	-	-	-	-	48 h	LC50	11	Yoshioka *et al.*, 1986a
Pristina longiseta	N	S	99.5	tw	-	-	96 h	LC50	2.5	Schmitz and Nagel, 1995

a growth inhibition
b yield

Appendix 2 continued. Acute freshwater toxicity data.

3,4-dichloroaniline (continued)

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l		Reference
Crustaceans											
Daphnia magna, larvae, 1 mm	Y	S	pure	am	8.0	hard	96 h	LC50	0.16		Adema and Vink, 1981
Daphnia magna, adult, 3 mm	Y	S	pure	am	8.0	hard	96 h	LC50	1.0		Adema and Vink, 1981
Daphnia magna, < 24 h	N	S	-	tw	-	-	48 h	EC50	0.29		Crossland and Hillaby, 1985
Daphnia magna, < 24 h	N	R	> 90	nw	8.1	225	48 h	LC50	0.1		Maas-Diepeveen and Van Leeuwen, 1986
Daphnia longispina, < 24 h	N	S	-	tw	-	-	48 h	EC50	0.44		Crossland and Hillaby, 1985
Gammarus pulex, 3rd instar	Y	R	-	am	7.0	151	48 h	LC50	17	α	Taylor *et al.*, 1991
Gammarus pulex, 3rd instar	Y	R	-	am	7.0	151	240 h	LC50	5.0	α	Taylor *et al.*, 1991
Arachnida											
Hydrozetes lacustris	N	S	99.5	tw	-	-	96 h	LC50	4.7		Schmitz and Nagel, 1995
Insecta											
Chironomus riparius, 2nd instar	Y	R	-	am	7.0	151	48 h	LC50	15	α	Taylor *et al.*, 1991
Chironomus riparius, 2nd instar	Y	R	-	am	7.0	151	96 h	LC50	7.4	α	Taylor *et al.*, 1991
Chironomus riparius, 2nd instar	Y	R	-	am	7.0	151	120 h	LC50	5.5	α	Taylor *et al.*, 1991
Chironomus riparius, 2nd instar	Y	R	-	am	7.0	151	240 h	LC50	4.2	α	Taylor *et al.*, 1991
Pisces											
Brachydanio rerio, 200-350 mg	N	S	99.5	nw	7.6-8.2	204	96 h	LC50	9.8		Ensenbach and Nagel, 1995
Brachydanio rerio, 200-350 mg	N	S	99.5	tw	7.6-8.2	340-408	96 h	LC50	8.5		Ensenbach and Nagel, 1995
Oncorhynchus mykiss	N	S	>99	tw	7.8	-	96 h	LC50	1.9		Hodson, 1985
Perca fluviatilis, + 1 y	-	R	99.5	tw	8.2	-	96 h	LC50	3.1		Schäfers and Nagel, 1993
Perca fluviatilis, + 1 y	-	R	99.5	tw	8.2	-	120 h	LC50	2.3		Schäfers and Nagel, 1993
Perca fluviatilis, + 1 y	-	R	99.5	tw	8.2	-	240 h	LC50	1.5		Schäfers and Nagel, 1993
Pimephales promelas, juvenile	Y	CF	-	-	7.6	44	96 h	LC50	7.6	α	Veith and Broderius, 1987
Pimephales promelas, 30 d	Y	S	98	nw	7.2	50.3	96 h	LC50	7.7	α	Geiger *et al.*, 1988
Pimephales promelas, 28-34 d	Y	F	98	nw	7.6	43.5	96 h	LC50	7.5		Call *et al.*, 1987
Pimephales promelas, 28-34 d	Y	F	98	rw	7.2	50.2	96 h	LC50	7.7		Call *et al.*, 1987
Poecilia reticulata, young, bought	Y	S	pure	am	8.0	hard	96 h	LC50	9.0		Adema and Vink, 1981
Poecilia reticulata, young, lab.cult.	Y	S	pure	am	8.0	hard	96 h	LC50	8.7		Adema and Vink, 1981

Appendix 2 continued. Acute freshwater toxicity data.

3,5-dichloroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Chlorella pyrenoidosa	N	-	≥ 96	am	8.7	90	96 h	EC50	7.5[a]	Maas-Diepeveen and Van Leeuwen, 1986
Crustaceans										
Daphnia magna, < 24 h	N	R	≥ 96	nw	8.1	225	48 h	LC50	1.1	Maas-Diepeveen and Van Leeuwen, 1986
Pisces										
Brachydanio rerio, 3 m	Y	R	-	tw	8.6	-	96 h	LC50	8.6	Zok *et al.*, 1991

a yield

2,3,4-trichloroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Chlorella pyrenoidosa	N	-	> 97	am	8.7	90	96 h	EC50	1.3[a]	Maas-Diepeveen and Van Leeuwen, 1986
Crustaceans										
Daphnia magna, < 24 h	N	R	> 97	nw	8.1	225	48 h	LC50	0.73	Maas-Diepeveen and Van Leeuwen, 1986
Pisces										
Pimephales promelas, 28 d	Y	S	97	nw	7.5	53.0	96 h	LC50	3.6 α	Brooke *et al.*, 1984

a yield

Appendix 2 continued. Acute freshwater toxicity data.

2,4,5-trichloroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Chlorella pyrenoidosa	N	-	> 90	am	8.7	90	96 h	EC50	1.8[a]	Maas-Diepeveen and Van Leeuwen, 1986
Crustaceans										
Daphnia magna	N	S	95	am	8.1-8.3	-	48 h	EC50	1.9	Urresterazu Ramos and Vaes, 1996
Daphnia magna, < 24 h	N	R	> 90	nw	8.1	225	48 h	LC50	3.4	Maas-Diepeveen and Van Leeuwen, 1986
Pisces										
Poecilia reticulata, 1.6 cm, 48 mg	Y	-	95	-	7.4-8.0	-	96 h	LC50	2.4[b]	Urresterazu Ramos and Vaes, 1996

a yield
b solvent is isopropanol, amount unknown

2,4,6-trichloroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Crustaceans										
Daphnia magna	N	S	-	-	-	-	48 h	EC50	6.0	Knie *et al.*, 1983
Pisces										
Pimephales promelas, 28 d	Y	S	97	nw	7.5	53.0	96 h	LC50	3.6	α Brooke *et al.*, 1984
Leuciscus idus melanotus	N	S	-	-	-	-	96 h	LC50	2.3	Knie *et al.*, 1983

2,3,4,5-tetrachloroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Chlorella pyrenoidosa	N	-	> 90	am	8.7	90	96 h	EC50	0.7[a]	Maas-Diepeveen and Van Leeuwen, 1986
Crustaceans										
Daphnia magna, < 24 h	N	R	> 90	nw	8.1	225	48 h	LC50	0.64	Maas-Diepeveen and Van Leeuwen, 1986

a yield

Appendix 2 continued. Acute freshwater toxicity data.

2,3,5,6-tetrachloroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l		Reference
Pisces											
Pimephales promelas, 34 d	Y	S	97	nw	7.6	48.0	96 h	LC50	0.3	α	Brooke *et al.*, 1984

Appendix 2 continued. Acute freshwater toxicity data.

2-nitroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Escherichia coli	N	S	-	am	-	-	48 h	EC50	250[a]	Nendza and Seydel, 1990
Pisces										
Brachydanio rerio, 3 m, 200-350 mg	Y	R	-	tw	8.6	-	96 h	LC50	19	Zok *et al.*, 1991

a EC50 is expressed as the concentration which inhibits the generation rate by 50% (I50), same value reported in Nendza and Seydel (1988a,b)

3-nitroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Crustaceans										
Daphnia magna	Y	S	> 98	am	8.0-8.3	200	48 h	EC50	1.0[a]	Urresterazu Ramos and Vaes, 1996
Pisces										
Oryzias latipes	N	S	> 99	tw	7.4-7.9	-	96 h	LC50	67[b]	EAJ, 1991
Brachydanio rerio, 3 m, 200-350 mg	Y	R	-	tw	8.6	-	96 h	LC50	82	Zok *et al.*, 1991
Poecilia reticulata, 1.97 cm, 74 mg	Y	-	> 98	am	7.1-7.8	-	96 h	LC50	79	Urresterazu Ramos and Vaes, 1996

a immobility
b control plus solvent control; solvent is DMSO (concentration ≤ 211 mg/l, no mortality recorded at this concentration).

4-nitroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Escherischia coli	N	S	-	am	-	-	48 h	EC50	430[a]	Nendza and Seydel, 1990
Pisces										
Pimephales promelas	Y	S	-	rw	7.2-7.9	40-48	96 h	LC50	106[b]	Curtis and Ward, 1981
Pimephales promelas, 28-34 d	Y	CF	-	-	7.6	44	96 h	LC50	125	α Veith and Broderius, 1987
Brachydanio rerio, 3 m, 200-350 mg	Y	R	-	rw	8.6	-	96 h	LC50	125	Zok *et al.*, 1991
Brachydanio rerio	N	S	anal.	-	7.5	-	96 h	LC50	88	Wellens, 1982

a EC50 is expressed as the concentration which inhibits the generation rate by 50% (I50), same value reported in Nendza and Seydel (1988a,b)
b same value as reported in Curtis *et al.*, 1982

Appendix 2 continued. Acute freshwater toxicity data.

2,4-dinitroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l		Reference
Bacteriophyta											
Escherischia coli	N	S	-	am	-	-	48 h	EC50	75[a]		Nendza and Seydel, 1990
Crustaceans											
Daphnia magna, < 24 h	N	S	-	am	8.0	240	48 h	EC50	9.6[b]		Kühn *et al.*, 1989b
Pisces											
Pimephales promelas, 33 d	Y	S	96	nw	7.5	43	96 h	LC50	16	α	Brooke *et al.*, 1984
Pimephales promelas, 30 d	Y	S	96	nw	7.3	49	96 h	LC50	14	α	Geiger *et al.*, 1986

a EC50 is expressed as the concentration which inhibits the generation rate by 50% (I50), same value reported in Nendza and Seydel (1988a,b)
b immobility

2-chloro-4-nitroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l		Reference
Pisces											
Pimephales promelas, 32 d	Y	S	99	nw	7.4	43	96 h	LC50	22	α	Brooke *et al.*, 1984
Pimephales promelas, 35 d	Y	S	99	nw	7.6	46	96 h	LC50	19	α	Brooke *et al.*, 1984
Pimephales promelas, 28-34 d	Y	CF	-	-	7.6	44	96 h	LC50	20	α	Veith and Broderius, 1987

4-chloro-2-nitroaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Crustaceans										
Daphnia magna, < 24 h	N	S	-	am	8.0	240	48 h	EC50	3.2[a]	Kühn *et al.*, 1989b

a immobility

Appendix 2 continued. Acute freshwater toxicity data.

2,4-dichloro-6-nitroaniline.

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l		Reference
Crustaceans											
Daphnia magna, < 24 h	N	S	> 90	rw	8.2-8.4	173	48 h	EC50	2.1[a]	α	RIVM/CSR-archive, 1993

a EC50 calculated according to the trimmed Spearman-Karber method (1977/78)

Appendix 2 continued. Acute freshwater toxicity data.

2-methylaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Chlorella pyrenoidosa	N	-	≥ 99.5	am	8.7	90	96 h	EC50	55[a]	Maas-Diepeveen and Van Leeuwen, 1986
Crustaceans										
Daphnia magna, < 24 h	N	R	≥ 99.5	nw	8.1	225	48 h	LC50	0.52	Maas-Diepeveen and Van Leeuwen, 1986

a yield

3-methylaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Chlorella pyrenoidosa	N	-	≥ 99	am	-	-	96 h	EC50	44[a]	Maas-Diepeveen and Van Leeuwen, 1986
Crustaceans										
Daphnia magna, < 24 h	N	R	≥ 99	nw	8.1	225	48 h	LC50	0.15	Maas-Diepeveen and Van Leeuwen, 1986

a yield

Appendix 2 continued. Acute freshwater toxicity data.

4-methylaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l		Reference
Bacteriophyta											
Escherischia coli	N	S	-	am	-	-	16 h	EC50	1300[a]		Nendza and Seydel, 1990
Algae											
Chlorophyta											
Chlorella pyrenoidosa	N-	-	> 97	am	-	-	96 h	EC50	138[b]		Maas-Diepeveen and Van Leeuwen, 1986
Annelida											
Tubifex tubifex, 30-50 mm	-	-	-	-	-	-	48 h	LC50	25		Yoshioka *et al.*, 1986a
Crustaceans											
Daphnia magna, < 24 h	N	R	> 97	nw	8.1	225	48 h	LC50	0.2		Maas-Diepeveen and Van Leeuwen, 1986
Pisces											
Pimephales promelas, 31 d	Y	S	99	nw	7.6	48	96 h	LC50	149	α	Geiger *et al.*, 1986
Pimephales promelas, juvenile	Y	CF	-	-	7.6	44	96 h	LC50	149	α	Veith and Broderius, 1987

a EC50 is expressed as the concentration which inhibits the generation rate by 50% (I50), same value reported in Nendza and Seydel (1988a,b)
b yield

N-methylaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Pisces										
Brachydanio rerio, embryos	-	-	reag.	rw	8.0	200	96 h	LC50	0.076	Groth *et al.*, 1993

Appendix 2 continued. Acute freshwater toxicity data.

N,N-dimethylaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l		Reference
Crustaceans											
Daphnia magna	Y	S	-	am	8.1-8.3	200	48 h	EC50	14[a]		Urresterazu Ramos and Vaes, 1996
Pisces											
Pimephales promelas, juvenile, 0.12 g	Y	CF	-	-	7.6	44	96 h	LC50	66	α	Broderius and Kahl, 1985
Pimephales promelas, 32 d	Y	S	raeg.	nw	7.4	44	96 h	LC50	78	α	Brooke *et al.*, 1984
Pimephales promelas, 35 d	Y	S	reag.	nw	7.6	44	96 h	LC50	53	α	Brooke *et al.*, 1984
Poecilia reticulata, 2.0 cm, 95 mg	Y	-	-	-	7.3-8.2	-	96 h	LC50	57		Urresterazu Ramos and Vaes, 1996
Brachydanio rerio, embryos	-	-	reag.	nw	8.0	200	96 h	LC50	0.18		Groth *et al.*, 1993

a immobility

2,3-dimethylaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Algae										
Chlorophyta										
Scenedesmus subspicatus	N	S	-	am	8.0	-	48 h	EC50	44[a]	Kühn and Pattard, 1990

a growth inhibition

2,4-dimethylaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Escherichia coli	N	S	-	am	-	-	16 h	EC50	350[a]	Nendza and Seydel, 1990
Crustaceans										
Daphnia magna, < 24 h	N	S	-	am	8.0	240	48 h	EC50	9.9[b]	Kühn *et al.*, 1989b

a EC50 is expressed as the concentration which inhibits the generation rate by 50% (I50), same value reported in Nendza and Seydel (1988a,b)
b immobility

Appendix 2 continued. Acute freshwater toxicity data.

3,4-dimethylaniline.

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l		Reference
Algae											
Chlorophyta											
Scenedesmus subspicatus	N	S	-	am	8.0	-	48 h	EC50	24[a]		Kühn and Pattard, 1990

a growth inhibition

N,N,3-trimethylaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l		Reference
Pisces											
Pimephales promelas, 28-34 d	Y	CF	-	-	7.6	44	96 h	LC50	53	α	Broderius and Kahl, 1985
Pimephales promelas, 31 d	Y	S	99	nw	7.6	39	96 h	LC50	52	α	Geiger *et al.*, 1986
Pimephales promelas, 32 d	Y	S	99	nw	7.4	40	96 h	LC50	46	α	Geiger *et al.*, 1986

2-chloro-4-methylaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l		Reference
Pisces											
Pimephales promelas, 30 d	Y	S	98	nw	7.4	45	96 h	LC50	36	α	Brooke *et al.*, 1984

Appendix 2 continued. Acute freshwater toxicity data.

3-chloro-4-methylaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Escherichia coli	N	S	-	am	-	-	16 h	EC50	135[a]	Nendza and Seydel, 1990
Crustaceans										
Daphnia magna, < 24 h	N	S	-	am	8.0	240	48 h	EC50	0.6[b]	Kühn *et al.*, 1989b
Procambarus acutus acutus, juvenile	N	S	≥ 96	rw	-	-	96 h	LC50	8.8	Marking and Chandler, 1981
Insecta										
Isonychia sp., nymph	N	S	≥ 96	rw	-	24	96 h	LC50	3.8[c,e]	Marking and Chandler, 1981
Hydropsyche sp., larvae	N	S	≥ 96	rw	-	24	96 h	LC50	7.5[c,e]	Marking and Chandler, 1981
Mollusca										
Oxytrema catenaria, adult	N	S	≥ 96	rw	-	24	96 h	LC50	16[c]	Marking and Chandler, 1981
Corbicula manilensis, adult	N	S	≥ 96	rw	-	24	96 h	LC50	62[c]	Marking and Chandler, 1981
Amphibia										
Rana sphenocephala, larvae	N	S	≥ 96	rw	-	24	96 h	LC50	32[d]	Marking and Chandler, 1981

a EC50 is expressed as the concentration which inhibits the generation rate by 50% (I50), same value reported in Nendza and Seydel (1988a,b)
b immobility
c animals taken from the field, acclimatisation for 3 d prior to the experiment
d egg clusters taken from the field and divided into approximately equal clusters; survival hatchlings was recorded
e species not specified in reference

Appendix 3. Chronic marine water toxicity data

3,4-dichloroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Salinity ‰	Exposure time	Crite-rion	Result mg/l	Reference
Crustaceans										
Artemia salina, 3 d larvae	Y	F	pure	am	8.0	-	28 d	NOEC	0.032[a]	Adema and Vink, 1981
Annelida										
Ophryotrocha diadema, larvae, 2-3 d	Y	R	pure	am	8.0	33	38 d	NOEC	0.008[b]	Hooftman and Vink, 1980
Ophryotrocha diadema, larvae, 2-3 d	Y	R	pure	am	8.0	33	38 d	NOEC	0.003[c]	Hooftman and Vink, 1980
Pisces										
Pleuronectus platessa, eggs	Y	R	pure	am	8.0	-	3 m	NOEC	0.032[d]	Adema and Vink, 1981

a reproduction and mortality
b parent mortality
c mean number of larvae per egg mass, mortality in egg masses, and reproductive potential
d mortality and growth

3-chloro-4-methylaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Salinity ‰	Exposure-time	Crite-rion	Result mg/l	Reference
Crustaceanse										
Trigriopus brevicornis, females	-	-	-	nw	-	30	12 d	NOEC	0.4[a]	Lassus *et al.*, 1984
Trigriopus brevicornis, eggs	-	-	-	nw	-	30	7 d	NOEC	3.0[b]	Lassus *et al.*, 1984

a larvae production; NOEC=EC10, calculated by linear regression from EC0=0, EC32=1, EC73=3 mg/l
b hatching success

Appendix 3 continued. Acute marine water toxicity data.

3,4-dichloroaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Salinity ‰	Exposure time	Crite-rion	Result mg/l	Reference
Algae										
Phaeodactylum tricornutum	Y	S	-	am	-	20	72 h	EC50	1.1[a]	Kusk and Nyholm, 1992
Phaeodactylum tricornutum	Y	S	pure	am	8.0	-	96 h	EC50	0.45[a]	Adema and Vink, 1981
Rotatoria										
Brachionus plicatilis, cyst	N	S	-	am	7.7	15	24 h	LC50	57	Ferrando and Anreu-Moliner, 1991
Crustaceans										
Artemia salina, larvae, 1 mm	Y	S	pure	am	8.0	-	96 h	LC50	5.5	Adema and Vink, 1981
Artemia salina, adult, 1cm	Y	S	pure	am	8.0	-	96 h	LC50	14	Adema and Vink, 1981
Chaetogammarus marinus, larvae, 4 mm	Y	S	pure	am	8.0	-	96 h	LC50	3.2	Adema and Vink, 1981
Chaetogammarus marinus, adult, 1 cm	Y	S	pure	am	8.0	-	96 h	LC50	4.0	Adema and Vink, 1981
Crangon crangon, adult, 4 cm	Y	S	pure	am	8.0	-	96 h	LC50	2.3	Adema and Vink, 1981
Palaemonetes varians, adult, 4 cm	Y	S	pure	am	8.0	-	96 h	LC50	2.5	Adema and Vink, 1981
Mollusca										
Mytilus edulis, adult, 3 cm	Y	S	pure	am	8.0	-	96 h	LC50	9.5	Adema and Vink, 1981
Annelida										
Ophryotrocha diadema (larvae)	Y	S	-	am	8.0	33	96 h	LC50	4.0[c]	Hooftman and Vink, 1980
Ophryotrocha diadema (adult)	Y	S	-	am	8.0	33	96 h	LC50	15	Hooftman and Vink, 1980
Pisces										
Poecilia reticulata, young, bought	Y	S	pure	am	8.0	-	96 h	LC50	5.0	Adema and Vink, 1981
Poecilia reticulata, young, lab.cult.	Y	S	pure	am	8.0	-	96 h	LC50	3.5	Adema and Vink, 1981
Gobius microps, adult, 10 cm	Y	S	pure	am	8.0	-	96 h	LC50	4.6	Adema and Vink, 1981

a growth
b photosynthesis inhibition
c 24, 48, and 72 h LC50-values are 25, 8, and 4 mg/l, respectively

2-nitro-N-phenylaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Salinity ‰	Exposure time	Crite-rion	Result mg/l	Reference
Vibrio fischeri	N	S	h.p.	-	-	-	30 min	EC50	7.7[a]	Drzyzga *et al.*, 1995
Vibrio fischeri	N	S	h.p.	-	-	-	60 min	EC50	9.8[a]	Drzyzga *et al.*, 1995

a luminescence

Appendix 3 continued. Acute marine water toxicity data.

4-nitro-N-phenylaniline

Organism	A	Test-type	Test sub. purity	Test water	pH	Salinity ‰	Exposure time	Crite-rion	Result mg/l	Reference
Bacteriophyta										
Vibrio fischeri	N	S	h.p.	-	-	-	30 min	EC50	1.0[a]	Drzyzga *et al.*, 1995
Vibrio fischeri	N	S	h.p.	-	-	-	60 min	EC50	1.6[a]	Drzyzga *et al.*, 1995
Vibrio fischeri	N	S	h.p.	-	-	-	90 min	EC50	1.9[a]	Drzyzga *et al.*, 1995

a luminescence

3-chloro-4-methylaniline

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Salinity ‰	Exposure-time	Crite-rion	Result mg/l	Reference
Crustaceans										
Palaemonetes kadiakensis, juvenile	N	S	≥ 96	rw	-	-	96 h	LC50	4.5	Marking and Chandler, 1981

Appendix 4. Chronic toxicity data on soil organisms.

2-chloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
Bacteriophyta										
Pseudomonas putida	loamy sand	6.5	4.8	2.6	25	24 h	NOEC	50[a]	104	Rashid and Mayaudon, 1974
Macrophyta										
Lactuca sativa	OECD	7.8	1.4	12	20	14 d	NOEC	3.2[b]	16	Denneman and Van Gestel, 1990

a growth, NOEC=LOEC/2 (effect 15%)
b growth

4-chloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
Bacteria										
Pseudomonas putida	loamy sand	6.5	4.8	2.6	25	24 h	NOEC	50[a]	104	Rashid and Mayaudon, 1974

a growth, NOEC=LOEC/2 (effect 15%)

Appendix 4 continued. Chronic toxicity data soil organisms.

2,4-dichloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
Macrophyta										
Avena sativa	humic sand	5.1	3.7	-	25	14 d	NOEC	32[a]	86	Adema and Henzen, 1989
Avena sativa	loam	7.5	1.4	-	25	14 d	NOEC	10[a]	50	Adema and Henzen, 1989
Lycopersicon esculentum	humic sand	5.1	3.7	-	25	14 d	NOEC	32[a]	86	Adema and Henzen, 1989
Lycopersicon esculentum	loam	7.5	1.4	-	25	14 d	NOEC	10[a]	50	Adema and Henzen, 1989
Lactuca sativa	humic sand	5.1	3.7	-	25	14 d	NOEC	32[a]	86	Adema and Henzen, 1989
Lactuca sativa	loam	7.5	1.4	-	25	14 d	NOEC	10[a]	50	Adema and Henzen, 1989
Annelida										
Eisenia andrei	artificial	6.0	8.1	8.1	20	3 w	NOEC	56[b]	69	Van Gestel *et al.*, 1989

a growth
b cocoon production

3,4-dichloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
Bacteria										
Pseudomonas putida	loamy sand	6.5	4.8	2.6	25	24 h	NOEC	10[a]	21	Rashid and Mayaudon, 1974
Macrophyta										
Lactuca sativa	OECD	7.8	1.4	12	20	14 d	NOEC	1[b]	5	Denneman and Van Gestel, 1990

a growth, NOEC=LOEC/2 (effect 52%)
b growth

Appendix 4 continued. Chronic toxicity data soil organisms.

3,5-dichloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
Macrophyta										
Lactuca sativa	OECD	7.8	1.4	12	20	14 d	NOEC	3.2[a]	16	Denneman and Van Gestel, 1990

a growth

2,4,6-trichloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
Macrophyta										
Lactuca sativa	OECD	7.8	1.4	12	20	14 d	NOEC	10[a]	50	Denneman and Van Gestel, 1990

a growth

2,3,4,5-tetrachloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
Macrophyta										
Lactuca sativa	OECD	7.8	1.4	12	20	14 d	NOEC	10[a]	50	Denneman and Van Gestel, 1990

a growth

Appendix 4 continued. Chronic toxicity data soil organisms.

2,3,5,6-tetrachloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
Macrophyta										
Lactuca sativa	OECD	7.8	1.4	12	20	14 d	NOEC	3.2[a]	16	Denneman and Van Gestel, 1990

a growth

pentachloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
Macrophyta										
Lactuca sativa	OECD	7.8	1.4	12	20	14 d	NOEC	10[a]	50	Denneman and Van Gestel, 1990

a growth

Appendix 4 continued. Acute toxicity data soil organisms.

3-chloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	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	17	85	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	1.4	12	21	7 d	EC50	15	75	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	2.0	15	22	7 d	EC50	28[a]	140	Van Gestel *et al.*, 1996
Lactuca sativa	loam	7.5	2.0	15	22	14 d	EC50	23[a]	115	Van Gestel *et al.*, 1996
Lactuca sativa	OECD	6.2	8.1	8.1	22	7 d	EC50	126[a]	156	Van Gestel *et al.*, 1996
Lactuca sativa	OECD	6.2	8.1	8.1	22	14 d	EC50	60[a]	74	Van Gestel *et al.*, 1996
Annelida										
Eisenia andrei	sand	4.8	3.7	1.4	23	14 d	LC50	220	595	Van Gestel and Ma, 1993
Eisenia andrei	artificial	5.9	8.1	8.1	23	14 d	LC50	448	553	Van Gestel and Ma, 1993
Lumbricus rubellus	sand	4.8	3.7	1.4	23	14 d	LC50	195	527	Van Gestel and Ma, 1993
Lumbricus rubellus	artificial	5.9	8.1	8.1	23	14 d	LC50	332	410	Van Gestel and Ma, 1993

a growth; substance purity is ≥ 98 %

Appendix 4 continued. Acute toxicity data soil organisms

2,4-dicloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	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	32[a]	160	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	1.4	12	21	14 d	EC50	39[a]	145	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	1.8	14	21	7 d	EC50	24[a]	120	Hulzebos *et al.*, 1993
Lactuca sativa	humic sand	5.1	3.7	-	25	14 d	EC50	136[a]	368	Adema and Henzen, 1989
Lactuca sativa	loam	7.5	1.4	-	25	14 d	EC50	18[a]	90	Adema and Henzen, 1989
Avena sativa	humic sand	5.1	3.7	-	25	14 d	EC50	107[a]	289	Adema and Henzen, 1989
Avena sativa	loam	7.5	1.4	-	25	14 d	EC50	28[a]	140	Adema and Henzen, 1989
Lycopersicum esculentum	humic sand	5.1	3.7	-	25	14 d	EC50	68[a]	184	Adema and Henzen, 1989
Lycopersicum esculentum	loam	7.5	1.4	-	25	14 d	EC50	18[a]	90	Adema and Henzen, 1989
Annelida										
Eisenia andrei	artificial	6.0	8.1	8.1	20	3 w	EC50	176[b]	217	Van Gestel *et al.*, 1989
Eisenia andrei	sand	5.8	3.7	1.4	23	14 d	LC50	142	384	Van Gestel *et al.*, 1989
Eisenia andrei	sand	6.2	6.1	2.4	23	14 d	LC50	285	467	Van Gestel *et al.*, 1989
Eisenia andrei	artificial	6.2	8.1	8.1	23	14 d	LC50	319	394	Van Gestel *et al.*, 1989
Eisenia andrei	loamy sand	4.3	15.6	9.0	23	14 d	LC50	824	528	Van Gestel *et al.*, 1989
Lumbricus rubellus	sand	5.8	3.7	1.4	23	14 d	LC50	201	543	Van Gestel *et al.*, 1989
Lumbricus rubellus	sand	6.2	6.1	2.4	23	14 d	LC50	304	498	Van Gestel *et al.*, 1989
Lumbricus rubellus	artificial	6.2	8.1	8.1	23	14 d	LC50	190	235	Van Gestel *et al.*, 1989
Lumbricus rubellus	loamy sand	4.3	15.6	9.0	23	14 d	LC50	580	372	Van Gestel *et al.*, 1989

a growth
b cocoon production

Appendix 4 continued. Acute toxicity data soil organisms.

3,4-dicloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
Annelida										
Eisenia andrei	artificial	7.0	7.7	20	23	14 d	LC50	250	325	Denneman and Van Gestel, 1990
Eisenia andrei	sand	7.0	1.7	4.3	23	14 d	LC50	140	700	Denneman and Van Gestel, 1990
Eisenia andrei	sand	4.1	1.7	4.3	23	14 d	LC50	140	700	Denneman and Van Gestel, 1990

3,5-dichloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	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	16	80	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	1.4	12	21	14 d	EC50	13	65	Hulzebos *et al.*, 1993

Appendix 4 continued. Acute toxicity data soil organisms.

2,4,5-trichloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	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	25	125	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	1.4	12	21	14 d	EC50	17	85	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	2.0	15	22	7 d	EC50	35[a]	165	Van Gestel *et al.*, 1996
Lactuca sativa	loam	7.5	2.0	15	22	14 d	EC50	23[a]	115	Van Gestel *et al.*, 1996
Lactuca sativa	OECD	6.2	8.1	8.1	22	7 d	EC50	223[a]	275	Van Gestel *et al.*, 1996
Lactuca sativa	OECD	6.2	8.1	8.1	22	14 d	EC50	149[a]	184	Van Gestel *et al.*, 1996
Annelida										
Eisenia andrei	sand	4.8	3.7	1.4	23	14 d	LC50	134	362	Van Gestel and Ma, 1993
Eisenia andrei	artificial	5.9	8.1	8.1	23	14 d	LC50	233	288	Van Gestel and Ma, 1993
Lumbricus rubellus	sand	4.8	3.7	1.4	23	14 d	LC50	174	420	Van Gestel and Ma, 1993
Lumbricus rubellus	artificial	5.9	8.1	8.1	23	14 d	LC50	213	263	Van Gestel and Ma, 1993

a growth, substance purity is ≥ 98 %

2,4,6-trichloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	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	27	135	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	1.4	12	21	14 d	EC50	23	115	Hulzebos *et al.*, 1993

Appendix 4 continued. Acute toxicity data soil organisms.

2,3,4,5-tetrachloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	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	47	235	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	1.4	12	21	14 d	EC50	24	120	Hulzebos *et al.*, 1993

2,3,5,6-tetrachloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	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	64	320	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	1.4	12	21	14 d	EC50	16	80	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	2.0	15	22	7 d	EC50	50[a]	250	Van Gestel *et al.*, 1996
Lactuca sativa	loam	7.5	2.0	15	22	14 d	EC50	17[a]	85	Van Gestel *et al.*, 1996
Lactuca sativa	OECD	6.2	8.1	8.1	22	7 d	EC50	549[a]	678	Van Gestel *et al.*, 1996
Lactuca sativa	OECD	6.2	8.1	8.1	22	14 d	EC50	106[a]	131	Van Gestel *et al.*, 1996
Annelida										
Eisenia andrei	sand	4.8	3.7	1.4	23	14 d	LC50	116	314	Van Gestel and Ma, 1993
Eisenia andrei	artificial	5.9	8.1	8.1	23	14 d	LC50	133	164	Van Gestel and Ma, 1993
Lumbricus rubellus	sand	4.8	3.7	1.4	23	14 d	LC50	159	430	Van Gestel and Ma, 1993
Lumbricus rubellus	artificial	5.9	8.1	8.1	23	14 d	LC50	179	221	Van Gestel and Ma, 1993

a growth; substance purity is ≥ 98 %

Appendix 4 continued. Acute toxicity data soil organisms.

pentachloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	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	647	3200	Hulzebos *et al.*, 1993
Lactuca sativa	loam	7.5	1.4	12	21	14 d	EC50	471	2400	Hulzebos *et al.*, 1993
Annelida										
Eisenia andrei	sand	4.8	3.7	1.4	23	14 d	LC50	1014	2700	Van Gestel and Ma, 1993
Lumbricus rubellus	sand	4.8	3.7	1.4	23	14 d	LC50	825	2200	Van Gestel and Ma, 1993
Lumbricus rubellus	artificial	5.9	8.1	8.1	23	14 d	LC50	825	1000	Van Gestel and Ma, 1993

Appendix 5. Chronic toxicity data on microbial and enzymatic processes.

3-chloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
respiration	sandy loam	7.5	1.5	10.0	5	18 h	NOEC	50[a]	250	Rashid and Mayaudon, 1974
nitrification	loam	7.2	3	-	-	> 10 d	NOEC	5[b]	17	Denneman and Van Gestel, 1990

a inhibition, NOEC=LOEC/2 (effect 15%)
b duration of complete nitrification, difference of 3 days considered relevant

4-chloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
respiration	sandy loam	7.5	1.5	10.0	5	18 h	NOEC	50[a]	250	Rashid and Mayaudon, 1974
O_2-consumption	loamy sand	7.3	7.9	-	-	4 h	NOEC	100	127	Denneman and Van Gestel, 1990
CO_2-production	loamy sand	7.3	7.9	-	-	4 h	NOEC	10	13	Denneman and Van Gestel, 1990
ATP content	clay loam	6.4	3.2	33.6	20	48 d	NOEC	20	63	Zelles *et al.*, 1985

a inhibition, NOEC=LOEC/2 (effect 15%)

Appendix 5 continued. Chronic toxicity data on microbial and enzymatic processes.

3,4-dichloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
respiration	sandy loam	7.5	1.5	10.0	5	18 h	NOEC	33[a]	165	Rashid and Mayaudon, 1974
CO_2-production	loamy sand	7.3	7.9	-	-	48 h	NOEC	300	380	Denneman and Van Gestel, 1990
nitrification	loam	7.2	3	-	-	>10 d	NOEC	5[b]	17	Denneman and Van Gestel, 1990
acetate mineralization	sand	4.4	1.02	0.4	10	2 d	NOEC	260[c]	1300	Van Beelen and Fleuren-Kemilä, 1993
acetate mineralization	sand	4.4	1.02	0.4	10	2 d	NOEC	48[d]	240	Van Beelen and Fleuren-Kemilä, 1993

a inhibition, NOEC=LOEC/2 (effect 15%)
b difference in time in comparison to control
c decrease in final percentage mineralized after the incubation time; the reported EC_{10} is considered to be the NOEC
d inhibition of initial mineralization rate; the reported EC_{10} is considered to be the NOEC

Appendix 5 continued. Acute toxicity data on microbial and enzymatic processes.

3,4-dichloroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
acetate mineralization	sand	4.4	1.02	0.4	10	2 d	EC50	480[a]	2400	Van Beelen and Fleuren-Kemilä, 1993
acetate mineralization	sand	4.4	1.02	0.4	10	2 d	EC50	130[b]	650	Van Beelen and Fleuren-Kemilä., 1993
O_2-consumption	loamy sand	7.3	7.9	-	-	4 h	EC20	10	13	Denneman and Van Gestel, 1990

a decrease in final percentage mineralized after the incubation time
b inhibition of initial mineralization rate

Appendix 6. Chronic toxicity data from deviating freshwater tests.

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
3,4-dichloroaniline										
Crustaceans										
Daphnia magna	-	R	-	am	-	-	21 d	NOEC	0.02[a]	Morgado and Soares, 1995
Daphnia magna	N	R	99	am	-	-	?	NOEC	0.006[b]	Elendt, 1990
Daphnia magna	N	R	99	am	-	-	?	NOEC	0.024[c]	Elendt, 1990
Daphnia magna	N	R	99	am	-	-	?	NOEC	0.012[d]	Elendt, 1990
2,4-dimethylaniline										
Protozoa										
Chilomonas paramecium	N	S	-	am	6.9	-	72 h	NOEC	≥40[e]	Bringmann and Kühn, 1981

a fecundity; four concentrations tested
b life young per adult
c parent mortality
d total reproduction
e cell multiplication inhibition, NOEC expressed as the toxicity treshold (TGK)

Appendix 6 continued. Acute data from deviating freshwater tests.

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
2-chloroaniline										
Pisces										
Oryzias latipes	N	S	-	-	-	-	48 h	LC50	6.3	Yoshioka *et al.*, 1986b
Oryzias latipes, 28 d	N	R	-	nw	-	-	48 h	LC50	6.3	MITI, 1992
Poecilia reticulata, 2-3 m	N	R	≥99	-	-	25	14 d	LC50	6.3[a]	Hermens *et al.*, 1984
3-chloroaniline										
Pisces										
Poecilia reticulata, 2-3 m	N	R	≥ 99	-	-	25	14 d	LC50	13[a]	Hermens *et al.*, 1984
4-chloroaniline										
Pisces										
Oryzias latipes, 2 cm, 0.2 g	N	S	anal.	-	-	-	48 h	LC50	28[b]	Tonogai *et al.*, 1982
Poecilia reticulata, 2-3 m	N	R	> 99	-	-	25	14 d	LC50	26[a]	Hermens *et al.*, 1984
2,4-dichloroaniline										
Algae										
Chlorophyta										
Chlorella vulgaris	N	S	-	-	-	-	6-9 h	EC50	24[c]	Kramer, 1989
Pisces										
Poecilia reticulata, 2-3 m	N	R	-	-	-	25	14 d	LC50	12	Könemann, 1981
Poecilia reticulata, 2-3 m	N	R	≥ 99	-	-	25	14 d	LC50	6.3[a]	Hermens *et al.*, 1984
Oryzias latipes, 28 d	N	R	-	nw	-	-	48 h	LC50	13	MITI, 1992
2,5-dichloroaniline										
Pisces										
Oryzias latipes, 28 d	N	R	-	nw	-	-	48 h	LC50	11	MITI, 1992
Poecilia reticulata	N	R	> 90	-	-	25	14 d	LC50	1.7[a]	Hermens *et al.*, 1984

a solvent is 2-propanol, amount unknown
b LC50 expressed as the Median Tolerance Limit (Tl_m)
c growth inhibition; extinctions measured at 680 nm

Appendix 6 continued. Acute data from deviating freshwater tests.

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
3,4-dichloroaniline										
Rotatoria										
Brachionus calyciflorus (cysts)	N	S	-	am	7.8	90	3 h	EC50	41.2[b]	Ferrando *et al.*, 1993
Pisces										
Oryzias latipes, 28 d	N	R	-	nw	-	-	48 h	LC50	13	MITI, 1992
Poecilia reticulata	N	R	> 90	-	-	25	14 d	LC50	6.3[a]	Hermens *et al.*, 1984
3,5-dichloroaniline										
Pisces										
Poecilia reticulata	N	R	≥ 96	-	-	25	14 d	LC50	3.9[a]	Hermens *et al.*, 1984
2,3,4-trichloroaniline										
Pisces										
Poecilia reticulata, 2-3 m	N	R	> 97	-	-	25	14 d	LC50	1.4	Maas-Diepeveen and Van Leeuwen, 1986
2,4,5-trichloroaniline										
Algae										
Chlorophyta										
Chlorella vulgaris	N	S	-	-	-	-	6-9 h	EC50	9.0[b]	Kramer, 1989
Pisces										
Poecilia reticulata, 2-3 m	N	R	> 90	-	-	25	14 d	LC50	2.0	Maas-Diepeveen and Van Leeuwen, 1986
2,4,6-trichloroaniline										
Pisces										
Oryzias latipes, 28 d	N	R	-	nw	-	-	48 h	LC50	8.0	MITI, 1992
2,3,4,5-tetrachloroaniline										
Pisces										
Poecilia reticulata, 2-3 m	N	R	> 90	-	-	25	14 d	LC50	0.4	Maas-Diepeveen and Van Leeuwen, 1986
2-nitroaniline										
Algae										
Chlorophyta										
Chlorella vulgaris	N	S	-	-	-	-	6-9 h	EC50	91	Kramer, 1989
Protozoa										
Tetrahymena pyriformis	N	S	-	am	-	-	60 h	EC50	115[c]	Schultz and Applehans, 1985
Pisces										
Oryzias latipes, 28 d	N	R	-	nw	-	-	48 h	LC50	17	MITI, 1992
Poecilia reticulata, 2-3 m	Y	R	> 99	-	6.8-7.2	25	14 d	LC50	9.8[d]	Deneer *et al.*, 1987

a solvent is 2-propanol, amount unknown
b growth inhibition; extinctions measured at 680 nm
c population growth, EC50 expressed as concentration that inhibits 50 % growth (IGC50)
d recovery of the compound was at least 80%

Appendix 6 continued. Acute data from deviating freshwater tests.

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
3-nitroaniline										
Algae										
Chlorophyta										
Chlorella vulgaris	N	S	-	-	-	-	6-9 h	EC50	100[a]	Kramer, 1989
Pisces										
Oryzias latipes, 28 d	N	R	-	nw	-	-	48 h	LC50	96	MITI, 1992
Poecilia reticulata, 2-3 m	Y	R	> 98	-	6.8-7.2	25	14 d	LC50	51[b]	Deneer *et al.*, 1987
4-nitroaniline										
Algae										
Chlorophyta										
Chlorella vulgaris	N	S	-	-	-	-	6-9 h	EC50	138[a]	Kramer, 1989
Protozoa										
Tetrahymena pyriformis	N	S	-	am	-	-	60 h	EC50	10[c]	Schultz and Applehans, 1985
Crustaceans										
Daphnia magna, < 24 h	N	S	-	tw	7.6-7.7	270	24 h	LC50	24	Bringmann and Kühn, 1977
Daphnia magna, < 24 h	N	S	-	am	8.0	230	24 h	EC50	2.5[d]	Bringmann and Kühn, 1982
Daphnia magna, < 72 h	N	S	> 95	rw	7.8-8.2	200	24 h	EC50	9.9[d]	Devillers *et al.*, 1987
Pisces										
Leuciscus idus melanotus	N	S	-	-	-	-	48 h	LC50	35	Juhnke and Lüdemann, 1978
Oryzias latipes, 2 cm, 0.2 g	N	S	anal.	-	-	-	48 h	LC50	50[e]	Tonogai *et al.*, 1982
Oryzias latipes, 28 d	N	R	-	nw	-	-	48 h	LC50	84	MITI, 1992
Poecilia reticulata, 2-3 m	Y	R	> 98	-	6.8-7.2	25	14 d	LC50	54[b]	Deneer *et al.*, 1987
2-nitro-4-chloroaniline										
Pisces										
Oryzias latipes, 28 d	N	R	-	nw	-	-	48 h	LC50	17	MITI, 1992
2,6-dichloro-4-nitroaniline										
Pisces										
Oncorhynchus mykiss, 1.11g, 4,9 cm	N	S	-	-	-	-	96 h	LC50	1.6[f]	RIVM/CSR-archive, 1993
Carrassius auratus	N	S	-	-	-	-	96 h	LC50	> 32[f]	RIVM/CSR-archive, 1993
Lepomis macrochirus	N	S	-	-	-	-	96 h	LC50	37[f]	RIVM/CSR-archive, 1993

a growth inhibition; extinctions measured at 680 nm
b recovery of the compound was at least 80%;
c population growth, EC50 expressed as concentration that inhibits 50 % growth (IGC50), same value reported in Schultz *et al.* (1982)
d immobility
e LC50 expressed as the Median Tolerance Limit (Tl_m)
f 3 concentrations tested

Appendix 6 continued. Acute data from deviating freshwater tests.

Organism	A	Test-type	Test-sub. purity	Test-water	pH	Hardness mg $CaCO_3$/l	Exposure-time	Crite-rion	Result mg/l	Reference
4-nitro-N-phenylaniline										
Algae										
Chlorophyta			-							
Selenastrum capricornutum	-	-	-	-	-	-	96 h	EC50	27[a]	SIDS, 1995
Selenastrum capricornutum	-	-	-	-	-	-	96 h	EC50	36[b]	SIDS, 1995
Crustaceans										
Daphnia magna	-	-	-	-	-	-	48 h	LC50	1.0	SIDS, 1995
Pisces										
Pimephales promelas	-	-	-	-	-	-	96 h	LC50	2.4	SIDS, 1995
Lepomus macrochirus	-	-	-	-	-	-	96 h	LC50	17	SIDS, 1995
Oncorhynchus mykiss	-	-	-	-	-	-	96 h	LC50	16	SIDS, 1995

a cell growth
b chlorophyl a content

Appendix 6 continued. Acute data from deviating freshwater tests.

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
N-methylaniline										
Pisces										
Oryzias latipes, 2 cm, 0.2 g	N	S	anal.	tw	-	-	48 h	LC50	38[a]	Tonogai *et al.*, 1982
Oryzias latipes, *28* d	N	R	-	nw	-	-	48 h	LC50	98	MITI, 1992
Oryzias latipes	N	CF	-	-	-	-	48 h	LC50	86	Tonogai *et al.*, 1983
Crassius auratus	N	CF	-	-	-	-	48 h	LC50	88	Tonogai *et al.*, 1983
Cyprinus carpio	N	CF	-	-	-	-	48 h	LC50	55	Tonogai *et al.*, 1983
2-methylaniline										
Protozoa										
Tetrahymena pyriformis	N	S	-	am	-	-	24 h	EC50	520[b]	Yoshioka *et al.*, 1985
Tetrahymena pyriformis	N	-	-	am	-	-	24 h	LC100	29	Schultz *et al.*, 1978
Pisces										
Leuciscus idus melanotus	N	S	-	-	-	-	48 h	LC50	117	Juhnke and Lüdemann, 1978
Poecilia reticulata, 2-3 m	N	R	≥ 99.5	-	-	25	14 d	LC50	81	Maas-Diepeveen and Van Leeuwen, 1986
3-methylaniline										
Protozoa										
Tetrahymena pyriformis	N	S	-	am	-	-	60 h	EC50	280[c]	Schultz *et al.*, 1982
Tetrahymena pyriformis	N	S	-	am	-	-	24 h	EC50	370[b]	Yoshioka *et al.*, 1985
Pisces										
Poecilia reticulata, 2-3 m	N	R	≥ 99	-	-	25	14 d	LC50	36	Maas-Diepeveen and Van Leeuwen, 1986
4-methylaniline										
Protozoa										
Tetrahymena pyriformis	N	S	-	am	-	-	24 h	EC50	150[b]	Yoshioka *et al.*, 1985
Pisces										
Oryzias latipes, 2 cm, 0.2 g	N	S	anal.	-	-	-	48 h	LC50	42[a]	Tonogai *et al.*, 1982
Oryzias latipes	-	CF	-	-	-	-	48 h	LC50	100	Tonogai *et al.*, 1983
Poecilia reticulata, 2-3 m	N	R	> 97	-	-	25	14 d	LC50	11	Maas-Diepeveen and Van Leeuwen, 1986
Crassius auratus	-	CF	-	-	-	-	48 h	LC50	124	Tonogai *et al.*, 1983
Cyprinus carpio	-	CF	-	-	-	-	48 h	LC50	79	Tonogai *et al.*, 1983

a LC50 expressed as the Median Tolerance Limit (TL_m)
b growth rate
c population growth, EC50 expressed as the concentration that inhibits 50% growth (IGC50); solvent DMSO (concentration ≤ 0.0075 ml/l)

Appendix 6 continued. Acute data from deviating freshwater tests.

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
N,N-dimethylaniline										
Pisces										
Oryzias latipes, 2 cm, 0.2 g	N	S	anal.	tw	-	-	48 h	LC50	33[a]	Tonogai *et al.*, 1982
Oryzias latipes, *28* d	N	R	-	nw	-	-	48 h	LC50	102	MITI, 1992
Oryzias latipes	-	CF	-	-	-	-	48 h	LC50	78	Tonogai *et al.*, 1983
Crassius auratus	-	CF	-	-	-	-	48 h	LC50	69	Tonogai *et al.*, 1983
Cyprinus carpio	-	CF	-	-	-	-	48 h	LC50	69	Tonogai *et al.*, 1983
N,2-dimethylaniline										
Pisces										
Oryzias latipes, 28 d	N	R	-	nw	-	-	48 h	LC50	135	MITI, 1992
N,3-dimethylaniline										
Pisces										
Oryzias latipes, *28* d	N	R	-	nw	-	-	48 h	LC50	50	MITI, 1992
2,3-dimethylaniline										
Algae										
Chlorophyta										
Chlorella vulgaris	N	S	-	-	-	-	6-9 h	EC50	35[b]	Kramer, 1989
2,4-dimethylaniline										
Crustaceans										
Daphnia magna, < 24 h	N	S	-	tw	7.6-7.7	270	24 h	LC50	25	Bringmann and Kühn, 1977
Pisces										
Leuciscus idus melanotus	N	S	-	-	-	-	48 h	LC50	196	Juhnke and Lüdemann, 1978
2,5-dimethylaniline										
Pisces										
Oryzias latipes, *28* d	N	S	anal.	-	-	-	48 h	LC50	239	MITI, 1992
2,6-dimethylaniline										
Protozoa										
Tetrahymena pyriformis	N	-	-	am	-	-	24h	LC100	10	Schultz *et al.*, 1978
Pisces										
Oryzias latipes	-	CF	-	-	-	-	48 h	LC50	125	Tonogai *et al.*, 1983
Crassius auratus	-	CF	-	-	-	-	48 h	LC50	130	Tonogai *et al.*, 1983
Cyprinus carpio	-	CF	-	-	-	-	48 h	LC50	112	Tonogai *et al.*, 1983

a LC50 expressed as the Median Tolerance Limit (TL_m)
b growth inhibition; extinctions measured at 680 nm

Appendix 6 continued. Acute data from deviating freshwater tests.

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
3,4-dimethylaniline										
Algae										
Chlorophyta										
Chlorella vulgaris	N	S	-	-	-	-	6-9 h	EC50	25[a]	Kramer, 1989
Protozoa										
Tetrahymena pyriformis	N	S	-	am	-	-	60 h	EC50	235[b]	Schultz *et al.*, 1982
Tetrahymena pyriformis	N	S	-	am	-	-	24 h	EC50	9.0[c]	Yoshioka *et al.*, 1985
Pisces										
Oryzias latipes, *28* d	N	S	anal.	-	-	-	48 h	LC50	121	MITI, 1992
3,5-dimethylaniline										
Pisces										
Oryzias latipes, 2 cm, 0.2 g	N	S	anal.	tw	-	-	48 h	LC50	17[d]	Tonogai *et al.*, 1982
2,4,6-trimethylaniline										
Algae										
Chlorophyta										
Chlorella vulgaris	N	S	-	-	-	-	6-9 h	EC50	29	Kramer, 1989
N,N,3-trimethylaniline										
Pisces										
Oryzias latipes, 2 cm, 0.2 g	N	S	anal.	tw	-	-	48 h	LC50	20[d]	Tonogai *et al.*, 1982
4-chloro-2-methylaniline										
Pisces										
Oryzias latipes, *28* d	N	S	anal.	-	-	-	48 h	LC50	34	MITI, 1992

a growth inhibition; extinctions measured at 680 nm

b population growth, EC50 expressed as the concentration that inhibits 50% growth (IGC50); solvent DMSO (concentration ≤ 0.0075 ml/l)

c growth rate

d LC50 expressed as the Median Tolerance Limit (TL_m)

Appendix 6 continued. Chronic data from deviating marine water tests.

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l	Reference
3,4-dichloroaniline										
Palaemonetes varians	N	R	-	am	-	33	12-30	NOEC	0.49[a]	Van der Meer *et al.*, 1988

a mortality and larval development

Appendix 6 continued. Acute data from deviating marine water tests.

Organism	A	Test-type	Test sub. purity	Test water	pH	Hardness mg $CaCO_3$/l	Exposure time	Crite-rion	Result mg/l		Reference
3,4-dichloroaniline											
Algae											
Chlorophyta											
Dunaliella bioculata	N	S	-	am	-	20-28	6 h	EC50	5.8[c]		Kusk and Nyholm, 1992
Crustaceans											
Daphnia magna	N	S	98	am	EEC	EEC	24 h	LC50	0.2		Ferrando *et al.*, 1992
2-nitro-N-phenylaniline											
Bacteriophyta											
Vibrio fischeri	N	S	h.p.	-	-	-	90 min	EC50	> 11[b]		Drzyzga *et al.*, 1995
2,6-dichloro-4-nitroaniline											
Crustaceans											
Palaemonetes pugio, <20mm, juveniles	Y	S	-	nw	7.8	10	48 h	LC50	1.9[f]	α	Burton and Fisher, 1990
Fundulus heteroclitus, < 23 d	Y	S	-	nw	7.8	10	48 h	LC50	> 2.7[f]	α	Burton and Fisher, 1990
Mollusca											
Crassostrea sp.	N	-	-	-	-	-	96 h	EC50	2.3[g]		RIVM/CSR-archive, 1993
2-methylaniline											
Crustaceans											
Elasmopus pectenicrus, adult	N	-	-	-	-	30	7 d	LC50	> 40[d]		Lee and Nicol, 1978
3-chloro-4-methylaniline											
Crustaceans											
Trigriopus brevicornis, females	-	-	-	nw	-	30	96 h	LC50	16[e]		Lassus *et al.*, 1984

b luminescence
c photosynthesis inhibition
d animals taken from field populations and acclimated for 7 days prior to the experiment
e calculated accorrding to the method of Spearman and Karber (Hamilton *et al.*, 1977/78); four concentrations tested
f mortality; less than five concentrations tested; control and solvent control (0.0005ml/l); animals from field population
g growth; three concentrations tested

Appendix 6 continued. Chronic data from deviating soil tests.

2,6-dichloro-4-nitroaniline

Organism	Soil-type	pH	% O.m.	% Clay	Temp. °C	Exposure time	Crite-rion	Result test soil mg/kg d.w.	Result stand. soil mg/kg d.w.	Reference
Microbial processes										
S-oxidation	agr. soil	7.6	4.3	-	25	7 d	NOEC	100[a]	230	Wainwright, 1979
S-oxidation	agr. soil	7.6	4.3	-	25	14 d	NOEC	1.0[a]	2.3	Wainwright, 1979
S-oxidation	agr. soil	7.6	4.3	-	25	21 d	NOEC	0.1[a,b]	0.2	Wainwright, 1979

a compound purity unknown; pH in the treatments was consistently higher than in the control, for concentrations tested.
b NOEC=LOEC/10; similar results at higher concentrations

Appendix 7. Experimental log K_{oc} values.

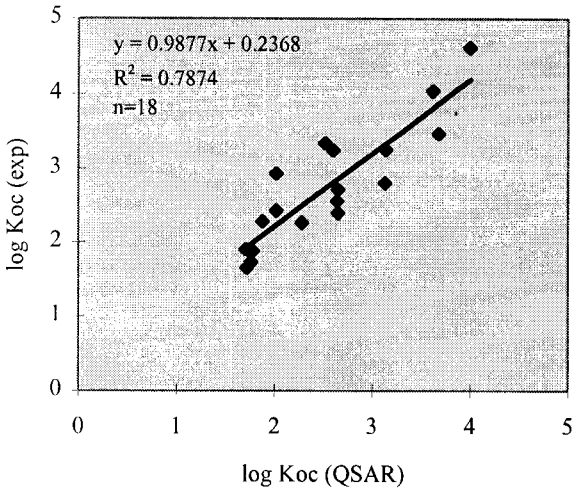
testsubstance	soil type	% oc	pH	CEC mmol/kg	solid/water g/l	mass balance	equil. time	log K_{oc}	reference
3-CA	sand	2.17	4.8	-	-	N	-	2.84	Van Gestel and Ma, 1993
	artificial	4.76	5.9	-	-	N	-	3.03	Van Gestel and Ma, 1993
4-CA	Speyer 2.1	0.69	7.0	50	200	N	24 h	3.13	Rippen *et al.*, 1982
	Speyer 2.2	2.24	5.8	95	200	N	24 h	2.05	Rippen *et al.*, 1982
	silt loam	0.76	7.5	-	200	N	24 h	3.10	Rippen *et al.*, 1982
	loamy sand	3.56	3.9	-	200	N	24 h	1.98	Rippen *et al.*, 1982
	silt loam	1.11	7.9	-	200	N	24 h	3.19	Rippen *et al.*, 1982
	silt loam	0.82	-	-	200	Y	3 h	1.97	Dao *et al*, 1986
2,4-DCA	loamy sand	9.15	4.3	-	-	N	-	2.84	Van Gestel and Ma, 1990
	artificial	4.76	6.2	-	-	N	-	2.47	Van Gestel and Ma, 1990
	sand	3.59	6.2	-	-	N	-	2.68	Van Gestel and Ma, 1990
	sand	2.18	5.8	-	-	N	-	2.87	Van Gestel and Ma, 1990
3,4-DCA	loam	3.00	-	-	170	Y	53 h	3.69	Beyerle-Pfnür and Lay, 1990
	silt loam	1.50	-	-	170	Y	53 h	3.70	Beyerle-Pfnür and Lay, 1990
	sand	1.20	-	-	170	Y	53 h	4.02	Beyerle-Pfnür and Lay, 1990
3,5-DCA	silt loam	1.94	-	-	10-800	N	24 h	2.11	Fu et *al.*, 1986
	silt loam	0.82	-	-	200	Y	3 h	2.50	Dao *et al*, 1986
2,3,4-TCA	silt loam	0.82	-	-	200	Y	3 h	2.61	Dao *et al.*, 1986
2,4,5-TCA	sand	2.17	4.8	-	-	N	-	3.30	Van Gestel and Ma, 1993
	artificial	4.76	5.9	-	-	N	-	3.23	Van Gestel and Ma, 1993
3,4,5-TCA	sand A1	6.34	4.5	-	200	N	10-64 h	3.53	Paya-Perez and Pelusio, 1992
	sand A2	1.87	4.9	-	200	N	10-64 h	3.62	Paya-Perez and Pelusio, 1992
	sand A3	0.50	5.0	-	200	N	10-64 h	3.60	Paya-Perez and Pelusio, 1992
	sand C1	0.17	5.1	-	200	N	10-64 h	3.88	Paya-Perez and Pelusio, 1992
	sand C2	0.03	5.2	-	200	N	10-64 h	4.49	Paya-Perez and Pelusio, 1992
	sand C3	0.12	5.0	-	200	N	10-64 h	4.00	Paya-Perez and Pelusio, 1992
	sand C4	0.16	4.8	-	200	N	10-64 h	4.00	Paya-Perez and Pelusio, 1992
2,3,4,5-TeCA	silt loam	0.82	-	-	200	Y	3 h	3.04	Dao *et al.*, 1986
2,3,5,6 TeCA	sand	2.17	4.8	-	-	N	-	4.05	Van Gestel and Ma, 1993
	artificial	4.76	5.9	-	-	N	-	4.13	Van Gestel and Ma, 1993

Appendix 7 continued. Calculated log K_{oc} values.

Substance	log K_{ow}	log[a] K_{oc}	log[d] K_{oc} (stdev; n)		Substance	log K_{ow}	log[b] K_{oc}	log[d] K_{oc}	Substance	log K_{ow}	log[c] K_{oc}	log[d] K_{oc}
2-CA	1.90	**2.03**			2-NA	1.85	**2.07**		2,4-DNA	1.72	**2.57**	
3-CA	1.88	**2.02**	2.93	(0.13; 2)	3-NA	1.37	**1.76**	1.73	2,6-DNA	1.79	**2.60**	
4-CA	1.88	**2.02**	2.42	(0.62; 7)	4-NA	1.39	**1.78**	1.88	3,5-DNA	1.89	**2.64**	2.55
2,3-DCA	2.86	**2.62**			2-C-4-NA	2.17	**2.27**		2,6-DN-4-CA	2.63	**2.92**	
2,4-DCA	2.91	**2.65**	2.71	(0.18; 4)	2-C-5-NA	2.17	**2.27**		2,4,6-TNA	2.63	**2.92**	
2,5-DCA	2.92	**2.66**			2-N-4-CA	2.72	**2.61**		TeNA	1.52	**2.50**	
2,6-DCA	2.82	**2.60**	3.25		3-N-4-CA	2.06	**2.20**					
3,4-DCA	2.69	**2.52**	3.35	(0.77; 4)	2,4-DC-6-NA	3.33	**3.00**					
3,5-DCA	2.90	**2.65**	2.39	(0.17; 5)	2,5-DC-4-NA	2.68	**2.59**					
2,3,4-TCA	3.68	**3.13**	2.80	(0.47; 5)	2,6-DC-4-NA	2.79	**2.66**					
2,4,5-TCA	3.69	**3.14**	3.26	(0.05; 2)	4-N-NPA	3.74	**3.26**					
2,4,6-TCA	3.69	**3.14**			2-N-NA	4.48	**3.72**					
3,4,5-TCA	-	-	3.86	(0.33; 7)								
2,3,4,5-TeCA	4.57	**3.68**	3.48	(0.66; 2)								
2,3,5,6-TeCA	4.46	**3.62**	4.04	(0.10; 3)								
PCA	5.08	**4.00**	4.62									
2-MA	1.32	**1.67**										
3-MA	1.40	**1.72**	1.65									
4-MA	1.39	**1.71**	1.90									
N-MA	1.66	**1.88**	2.28									
N,N-DMA	2.31	**2.28**	2.26									
N,2-DMA	2.16	**2.19**										
N,3-DMA	2.14	**2.18**										
N,4-DMA	2.15	**2.18**										
2,3-DMA	1.81	**1.97**										
2,4-DMA	1.68	**1.89**										
2,5-DMA	1.83	**1.98**										
2,6-DMA	1.84	**1.99**										
3,4-DMA	1.86	**2.00**										
3,5-DMA	1.91	**2.03**										
N,N,2-TMA	2.85	**2.62**										
N,N,3-TMA	2.80	**2.59**										
N,N,4-TMA	2.81	**2.59**										
2,4,6-TMA	2.31	**2.28**										
3,4,5-TMA	2.31	**2.28**										
2-C-4-MA	2.58	**2.45**										
2-C-6-MA	2.58	**2.45**										
3-C-2-MA	2.58	**2.45**										
3-C-4-MA	2.41	**2.34**										
3-C-6-MA	2.58	**2.45**										
4-C-N-MA	2.66	**2.50**										
4-C-2-MA	2.58	**2.45**										
3-C-N,N-DMA	3.22	**2.85**										
2,6-DC-3-MA	3.44	**2.98**										

a calculated according to Sabljic *et al.*(1995): eq. 10
b calculated according to Sabljic *et al.*(1995): eq. 4
c calculated according to Sabljic *et al.*(1995): eq. 12
d experimental data

Appendix 7 continued.



Comparison of log K_{oc} derived with QSARs (Sabljic *et al.*, 1995) with experimental log K_{oc}s.

Appendix 8. Derivation of individual MPCs.

Chloroanilines

Monochloroanilines

All $MPC_{freshwater}$ are calculated by using the preliminary effect assessment method (modified EPA-method). A factor 10 is applied on the lowest NOEC for these three compounds, resulting in a value of 0.003 mg/l, 0.001 mg/l and 0.001 mg/l for 2-CA, 3-CA and 4-CA, respectively. For the latter 5 NOECs are available and statistical extrapolation is applied resulting in a $MPC_{freshwater}$ of 0.0008 mg/l, which is a factor 12.5 lower than the lowest NOEC of the data set.

Dichloroanilines

The MPC_{water}s for the individual DCAs are presented in Appendix 9. The $MPC_{freshwater}$ for 2,4- and 3,4-DCA are calculated by applying statistical extrapolation. According to this method the $MPC_{freshwater}$ for 2,4-DCA and 3,4-DCA are 0.05 and 0.0009 mg/l, respectively. Applying the EPA-method a MPC of 0.003 mg/l is calculated for 2,5-DCA and 0.001 mg/l for 2,6-DCA, respectively, by applying a factor 1000 on the lowest $L(E)C_{50}$. It should be mentioned here that the $MPC_{freshwater}$ for 2,5-DCA is based only on two acute toxicity values. The $MPC_{freshwater}$ for 3,5-DCA is obtained by applying a factor 100 on the lowest $L(E)C_{50}$ for alage, crustaceans and pisces. This results in MPC of 0.01 mg/l.

Only for 3,4-DCA sufficient data are available to derive a $MPC_{saltwater}$. Applying the EPA-method result in a MPC of 0.0003 mg/l, which is a factor 3 lower than the $MPC_{freshwater}$. Freshwater and marine water data are combined to derive a MPC_{water}. Applying statistical extrapolation results in a MPC_{water} of 0.0008 mg/l, which is a factor 2.5 lower than the lowest NOEC found for the combined data set of 3,4-DCA.

Trichloroanilines

As mentioned before no data at all are found for 2,3,5- and 3,4,5-TCA. A factor 10 is applied on the lowest NOEC for 2,4,5-TCA, which revealed a $MPC_{freshwater}$ of 0.0056 mg/l. A factor 100 is applied on the lowest $L(E)C_{50}$ for 2,3,4-TCA and since acute values for representatives of the taxonomic groups algae, crustaceans and pisces are available, resulting in $MPC_{freshwater}$ of 0.007 mg/l. Applying a factor 1000 on the lowest $L(E)C_{50}$ for 2,4,6-TCA results in a $MPC_{freshwater}$ of 0.002 mg/l.

Tetrachloroanilines

Toxicity data on these compounds are even more limited. Two chronic and two acute data are found for 2,3,4,5-TeCA and one acute data for 2,3,5,6-TeCA. As a consequence the $MPC_{freshwater}$s found are very low since a factor 1000 is applied on the lowest $L(E)C_{50}$. The resulting MPC are 0.0006 and 0.0003 mg/l for 2,3,4,5-TeCA and 2,3,5,6-TeCA, respectively.

(Chloro)nitroanilines

Nitroanilines

The individual $MPC_{freshwater}$ for NAs are listed in Appendix 9. No chronic data on 2-NA are available, therefore, a factor 1000 is applied on the lowest $L(E)C_{50}$, resulting in a value of 0.02 mg/l. The same factor is applied to the lowest acute data on 3-NA. The resulting value of 0.001 mg/l is a factor 500 lower than the lowest NOEC. For 4-NA statistical extrapolation is applied, since 6 NOECs for 4 taxonomic groups are available. The resulting

$MPC_{freshwater}$ is 0.43 which is the same as the lowest NOEC. Since no marine water data are available, the MPC_{water}s for these compounds are considered to be the same as the $MPC_{freshwater}$s.
In the case of 2-N-NPA and 4-N-NPA only acute marine water data are available. Both $MPC_{saltwater}$s are derived by applying a factor 1000 on the lowest $L(EC)_{50}$, resulting in a value of 0.009 mg/l for the former and 0.001 mg/l for the latter. Both $MPC_{saltwater}$ are considered the MPC_{water} (Appendix 9).

Chloronitroanilines
2-C-4-NA, 4-C-2-NA and 2,4-DC-4-NA are the only compounds out of the group of chloro-substituted nitroanilines for which (acute) toxicity data are found. The $MPC_{freshwater}$ for all compounds is derived by the EPA-method. A factor 1000 is applied on the lowest $L(E)C_{50}$, which results in a value of 0.02, 0.003 and 0.002 mg/l, respectively. Since no marine water data are available for these compounds the MPC_{water} is considered to be the same as the $MPC_{freshwater}$ (Appendix 9).

(Chloro)methylanilines
Monomethylanilines
For 2-MA sufficient data are available to apply statistical extrapolation. The resulting value of 0.23 mg/l is factor 1.3 lower than the lowest NOEC. The $MPC_{freshwater}$ for 3-MA is calculated based on the lowest $L(E)C_{50}$. A factor 100 is applied in stead of a factor 1000, because the lowest $L(E)C_{50}$ for *Daphnia*, is much lower than acute $L(E)C_{50}$ values found for other species. Therefore, a factor 100 seems justified. For 4-MA data on representatives of algae, crustaceans and pisces are available. Therefore, a factor 100 is applied on the lowest $L(E)_{50}$, resulting in a $MPC_{freshwater}$ of 0.002 mg/l. For N-MA the $MPC_{freshwater}$ is derived by applying a factor 1000 on the lowest $L(E)C_{50}$ resulting in a value of 0.0001 mg/l. It should be noticed that this MPC is based solely on one acute value. Moreover, this value is derived from a study which is conducted with eggs of *B. rerio*. Eggs are considered to be a very sensitive stage.
For these compounds no marine water data are found. Therefore, the MPC_{water} is considered to be the same as the $MPC_{freshwater}$ (Appendix 9).

Dimethylanilines
A factor 10 is applied on the lowest NOEC for 2,3-DMA, resulting in a $MPC_{freshwater}$ of 0.02 mg/l. That value is a factor 10 lower than the lowest NOEC found for this compound. Since 6 NOECs for representatives of four taxonomic groups are available statistical extrapolation is applied to calculate the $MPC_{freshwater}$ for 2,4-DMA. The resulting value is 0.25 mg/l, which is a factor 1.6 lower than the lowest NOEC. The $MPC_{freshwater}$ for 3,4-DMA is calculated by applying a factor 10 on the lowest NOEC. The resulting MPC of 0.002 mg/l is a factor 10 lower than the lowest NOEC. The $MPC_{freshwater}$ for N,N-DMA is derived by applying a factor 100 on the lowest $L(E)C_{50}$, resulting in a value of 0.002 mg/l. Here, a factor 100 instead of a factor 1000 seems justified, since this $L(E)C_{50}$ found for *Brachydanio* is considerably lower than acute data found for other species.
For none of the compounds above marine water toxicity data are available. As a consequence the individual $MPC_{freshwater}$ is considered the individual MPC_{water} (Appendix 9).

Chloromethylanilines
The MPC_{water} for 2-C-4-MA and 3-C-4-MA are both based on the lowest $L(E)C_{50}$ found for these compounds. Applying a factor 1000 result in a $MPC_{freshwater}$ of 0.04 mg/l for the former and 0.001 mg/l for the latter

(Appendix 9). The $MPC_{freshwater}$ for 3-C-4-MA is a factor 2100 lower than the lowest chronic value found for that compound.

Applying a factor 1000 on the lowest $L(E)C_{50}$ for marine water result in a $MPC_{saltwater}$ of 0.005 mg/l for 3-C-4-MA (Appendix 9), which is a factor 220 lower than the lowest marine water NOEC.

Appendix 8 continued. Experimental data used for extrapolation of individual $MPC_{freshwater}$.

Substance	taxonomic group	A&S-method	EPA-method $L(E)C_{50}$ (mg/l)	EPA-method NOEC (mg/l)
Chloroanilines				
2-CA	Crustaceans			0.032
3-CA	Crustaceans			0.013
4-CA	Crustaceans	0.01		
	Algae	0.10[a]		
	Bacteriophyta	72		
	Pisces	0.05[b]		
	Pisces	0.75		
2,4-DCA	Bacteriophyta	1.0		
	Cyanophyta	10		
	Algae	0.8		
		3.2		
	Macrophyta	1.0		
	Coelenterata	3.2		
	Mollusca	1.8[c]		
	Crustaceans	0.015		
	Insecta	10		
	Pisces	0.33		
		0.32		
		1.0		
	Amphibia	0.32		
2,5-DCA	Crustaceans		2.9	
2,6-DCA	Pisces		1.0	
3,4-DCA	Protozoa	5.1		
	Algae	0.85[d]		
		1.2[e]		
	Rotatoria	2.5		
	Mollusca	0.13		
	Crustaceans	0.007[f]		
		0.08		
	Insecta	0.36[g]		
	Pisces	0.02		
		0.002		
		0.012[h]		
		0.004[i]		
3,5-DCA	Crustaceans		1.1	
2,3,4-TCA	Crustaceans		0.73	
2,4,5-TCA	Pisces			0.056
2,4,6-TCA	Pisces		2.3	
2,3,4,5-TeCA	Crustaceans		0.64	
2,3,5,6-TeCA	Pisces		0.3	
PCA	Pisces			0.01

a geometric mean of 2 NOECs growth *S. subspicatus* 0.03; 0.4 mg/l
b geometric mean of 2 NOECs reproducion *B. rerio* 0.2; 0.013 mg/l
c geometric mean 2 NOECs reproduction *L.stagnalis* 1.0; 3.2 mg/l
d geometric mean 5 NOECs growth *C. reinhardi* 2.5; 3.0; 0.26; 0.33; 0.70 mg/l
e geometric mean 2 NOECs growth *S. subspicatus* 0.5; 2.9 mg/l
f geometric mean 6 NOECs reproduction *D. magna* 0.01; 0.0065; 0.01; 0.005; 0.005; 0.01 mg/l
g geometric mean 2 NOECs growth *C. riparius* 0.76; 0.17 mg/l
h geometric mean 6 NOECs growth *P. promelas* 0.026; 0.026; 0.015; 0.015; 0.005; 0.005 mg/l
i geometric mean 2 NOECs mortality *P. reticulata* 0.02; 0.0007 mg/l

Appendix 8 continued. Experimental data used for extrapolation of individual $MPC_{freshwater}$.

Substance	taxonomic group	A&S-method	EPA-method $L(E)C_{50}$ (mg/l)	EPA-method NOEC (mg/l)
(Chloro)nitroanilines				
2-NA	Pisces		19	
3-NA	Crustaceans		1.0	
4-NA	Bacteriophyta	3.8		
	Protozoans	6.9		
		3.1		
		5.0		
	Cyanophyta	0.4		
	Algae	11		
2,4-DNA	Crustaceans		9.6	
2-C-4-NA	Pisces		20[a]	
4-C-2-NA	Crustaceans		3.2	
2,6-DC-4-NA	Crustaceans		2.1	
(Chloro)methylanilines				
2-MA	Bacteriophyta	16		
	Protozoa	76		
		21		
		237		
	Cyanophyta	0.3		
	Algae	6.3		
3-MA	Crustaceans		0.15	
4-MA	Crustaceans		0.2	
N-MA	Pisces		0.076	
2,3-DMA	Crustaceans			0.16
2,4-DMA	Bacteriophyta	8.0		
	Protozoa	9.8		
		12		
	Cyanophyta	0.4		
	Algae	5.0		
		0.8		
3,4-DMA	Crustaceans			0.016
N,N-DMA	Pisces		0.18	
N,N,3-TMA	Pisces		50[b]	
2-C-4-MA	Pisces		36	
3-C-4-MA	Crustaceans		0.6	

a geometric mean 3 LC50 *P. promelas* 22; 19; 20 mg/l
b geometric mean 3 LC50 *P. promelas* 53; 52; 46 mg/l

Appendix 8 continued. Experimental data used for extrapolation of individual $MPC_{saltwater}$.

Substance	taxonomic group	A&S-method	EPA-method $L(E)C_{50}$ (mg/l)	EPA-method NOEC (mg/l)
Chloroanilines				
3,4-DCA	Annelida			0.003
(Chloro)nitroanilines				
2-N-NPA	Bacteriophyta		8.7[a]	
4-N-NPA	Bacteriophyta		1.4[b]	
(Chloro)methylanilines				
3-C-4-MA	Crustaceans		4.5	

a geometric mean 2 EC_{50} bioluminescence *V. fischeri* 7.7; 9.8 mg/l
b geometric mean 3 EC_{50} bioluminescence *V. fischeri* 1.0; 1.6; 1.9 mg/l

Appendix 8 continued. Combined freshwater and marine water data used for extrapolation individual MPC_{water}.

Substance	taxonomic group	A&S-method	EPA-method $L(E)C_{50}$ (mg/l)	EPA-method NOEC (mg/l)
Chloroanilines				
3,4-DCA	Protozoa	5.1		
	Algae	0.85[a]		
		1.2[b]		
	Rotatoria	2.5		
	Mollusca	0.13		
	Annelida	0.003[g]		
	Crustaceans	0.007[c]		
		0.08		
		0.032[g]		
	Insecta	0.36[d]		
	Pisces	0.02		
		0.002		
		0.012[e]		
		0.004[f]		
		0.032[g]		
(Chloro)methylanilines				
3-C-4-MA	Crustaceans		0.6	

a geometric mean 5 NOECs growth *C. reinhardi* 2.5; 3.0; 0.26; 0.33; 0.70 mg/l
b geometric mean 2 NOECs growth *S. subspicatus* 0.03; 0.4 mg/l
c geometric mean 6 NOECs reproduction *D. magna* 0.01; 0.0065; 0.01; 0.005; 0.005; 0.01 mg/l
d geometric mean 2 NOECs growth *C. riparius* 0.76; 0.17 mg/l
e geometric mean 6 NOECs growth *P. promelas* 0.026; 0.026; 0.015; 0.015; 0.005; 0.005 mg/l
f geometric mean 2 NOECs mortality *P. reticulata* 0.02; 0.0007 mg/l
g marine water data

Appendix 9. Individual MPC_{water}.

Substance	$MPC_{freshwater}$ (mg/l)		$MPC_{saltwater}$ (mg/l)		MPC_{water} (mg/l)		Lowest NOEC (mg/l)	Lowest $L(E)C_{50}$ (mg/l)
Chloroanilines								
2-CA	0.003	EPA/10	-	-	0.0032	EPA/10	0.032	0.45[a]
3-CA	0.001	EPA/10	-	-	0.0013	EPA/10	0.013	0.1
4-CA	0.0008	A&S	-	-	0.0008	A&S	0.01	0.05
2,3-DCA	-	-	-	-	-	-	-	-
2,4-DCA	0.05	A&S	-	-	0.05	A&S	0.015	0.5
2,5-DCA	0.003	EPA/1000	-	-	0.003	EPA/1000	-	2.9
2,6-DCA	0.001	EPA/1000	-	-	0.001	EPA/1000	2.2	1.0
3,4-DCA	0.0009	A&S	0.0003	EPA/10	0.0008	A&S	0.002	0.25[b]
3,5-DCA	0.01	EPA/100	-	-	0.01	EPA/100	0.32	1.1
2,3,4-TCA	0.007	EPA/100	-	-	0.007	EPA/100	-	0.73
2,3,5-TCA	-		-	-	-		-	-
2,4,5-TCA	0.0056	EPA/10	-	-	0.0056	EPA/10	0.056	1.8
2,4,6-TCA	0.002	EPA/1000	-	-	0.002	EPA/1000	-	2.3
3,4,5-TCA	-		-	-	-		-	-
2,3,4,5-TeCA	0.0006	EPA/1000	-	-	0.0006	EPA/1000	0.032	0.64
2,3,5.6-TeCA	0.0003	EPA/1000	-	-	0.0003	EPA/1000	-	0.3
PCA	0.001	EPA/10	-	-	0.001	EPA/10	0.01	-
(Chloro)nitroanilines								
2-NA	0.02	EPA/1000	-		0.02	EPA/1000	-	19
3-NA	0.001	EPA/1000	-		0.001	EPA/1000	0.5	1.0
4-NA	0.43	A&S	-		0.43	A&S	0.4	105[c]
2-N-NPA	-	-	0.009	EPA/1000	0.009	EPA/1000	-	8.7[d]
4-N-NPA	-	-	0.001	EPA/1000	0.001	EPA/1000	-	1.4[e]
2,4-DNA	0.01	EPA/1000	-		0.01	EPA/1000	0.1	9.6
2-C-4-NA	0.02	EPA/1000	-		0.02	EPA/1000	-	20[f]
4-C-2-NA	0.003	EPA/1000	-		0.003	EPA/1000	-	3.2
2,4-DC-6-NA	0.002	EPA/1000	-		0.002	EPA/1000	-	2.1
(Chloro)methylanilines								
2-MA	0.23	A&S	-		0.23	A&S	0.3	0.52
3-MA	0.002	EPA/100	-		0.002	EPA/100	0.01	0.15
4-MA	0.002	EPA/100	-		0.002	EPA/100	-	0.2
N-MA	0.0001	EPA/1000	-		0.0001	EPA/1000	-	0.076
N,N-DMA	0.002	EPA/100	-		0.002	EPA/100	-	0.18
2,3-DMA	0.02	EPA/10	-		0.02	EPA/10	0.16	44
2,4-DMA	0.25	A&S	-		0.25	A&S	0.4	9.9
3,4-DMA	0.002	EPA/10	-		0.002	EPA/10	0.016	24
N,N,3-TMA	0.05	EPA/1000	-		0.05	EPA/1000	-	50[g]
2-C-4-MA	0.04	EPA/1000	-		0.04	EPA/1000	-	36
3-C-4-MA	0.001	EPA/1000	0.005	EPA/1000	0.001	EPA/1000	1.0	0.6

- no data available

a geometric mean 3 L(E)C50 *D. magna* 0.46; 1.5; 0.13 mg/l

b geometric mean 5 $L(E)C_{50}$ *D. magna* 0.2; 0.16; 1.0; 0.29; 0.1 mg/l

c geometric mean 2 LC50 *B. rerio* 125; 88 mg/l

d geometric mean 2 EC50 bioluminescence *V. fischeri* 7.7; 9.8 mg/l

e geometric mean 3 EC50 bioluminescence *V. fischeri* 1.0; 1.6; 1.9 mg/l

f geometric mean 3 LC50s *P. promelas* 22; 19; 20 mg/l

g geometric mean 3 LC50s *P. promelas* 53; 52; 46 mg/l

Appendix 10. Experimental data used for extrapolation of group $MPC_{freshwater}$.

Substance	taxonomic group	A&S-method	EPA-method $L(E)C_{50}$ (mg/l)	EPA-method NOEC (mg/l)
Chloroanilines				
MCA	Bacteriophyta	72		
	Algae	0.66[a]		
	Crustaceans	0.016[b]		
	Pisces	0.14[c]		
	Pisces	0.75		
DCA	Bacteriophyta	10		
		158		
	Protozoa	5.1		
	Algae	0.85[d]		
		1.26[e]		
		3.2		
		65		
		1.0		
	Macrophyta	1.0		
	Rotatoria	2.5		
	Coelenterata	3.2		
	Mollusca	0.75[f]		
	Crustaceans	0.007[g]		
		0.08		
	Insecta	0.36[h]		
		10		
	Pisces	0.08[i]		
		0.002		
		0.012[j]		
		0.03[k]		
		0.33		
		0.32		
	Amphibia	0.32		
TCA	Crustaceans			0.056
TeCA	Pisces		0.3	
PCA	Pisces			0.01

a geometric mean 4 NOECs growth *S. subspicatus* 3.9; 4.1; 0.03; 0.4 mg/l
b geometric mean 3 NOECs reproduction *D. magna* 0.01; 0.013; 0.032 mg/l
c geometric mean 3 NOECs reproduction *B. rerio* 1.0; 0.2; 0.013 mg/l
d geometric mean 5 NOECs growth *C. reinhardi* 2.5; 3.0; 0.26; 0.33; 0.70 mg/l
e geometric mean 4 NOECs growth *S. subspicatus* 0.5; 2.9; 0.8; 2.2 mg/l
f geometric mean 3 NOECs reproduction *L. stagnalis* 0.13; 1.0; 3.2 mg/l
g geometric mean 7 NOECs reproduction *D. magna* 0.01; 0.0065; 0.01; 0.005; 0.005; 0.01; 0.032 mg/l
h geometric mean 2 NOECs growth *C. riparius* 0.76; 0.17 mg/l
i geometric mean 2 NOECs mortality *B. rerio* 0.02; 0.32 mg/l
j geometric mean 6 NOECs growth *P. promelas* 0.026; 0.026; 0.015; 0.015; 0.005; 0.005 mg/l
k geometric mean 4 NOECs growth *P. reticulata* 0.02; 0.02; 0.002; 1.0 mg/l

Appendix 10 continued. Experimental data used for extrapolation of group $MPC_{freshwater}$.

Substance	taxonomic group	A&S-method	EPA-method $L(E)C_{50}$ (mg/l)	EPA-method NOEC (mg/l)
(Chloro)nitroanilines				
NA	Bacteriophyta	5.3		
	Protozoa	6.9		
		3.1		
		5.0		
	Algae	5.3		
		0.4		
		11		
	Crustaceans	0.5		
DNA	Crustaceans		9.6	
CNA	Crustaceans		3.2	
DCNA	Crustaceans		2.1	
(Chloro)methylanilines				
MA	Bacteriophyta	16		
	Protozoa	76		
		21		
		237		
	Cyanophyta	0.3		
	Algae	6.3		
	Crustaceans	0.01		
DMA	Bacteriophyta	8.0		
	Protozoa	9.8		
		12		
	Cyanophyta	0.4		
	Algae	5.0		
		0.8		
	Crustaceans	0.05[a]		
TMA	Pisces		50[b]	
CMA	Crustaceans		0.6	

a geometric mean 2 NOECs reproduction *D. magna* 0.016; 0.16 mg/l
b geometric mean 3 LC50s *P. promelas* 53; 52; 46 mg/l

Appendix 10 continued. Experimental data used for extrapolation of group $MPC_{saltwater}$.

Substance	taxonomic group	A&S-method	EPA-method $L(E)C_{50}$ (mg/l)	EPA-method NOEC (mg/l)
Chloroanilines				
DCA	Annelida			0.003
(Chloro) nitroanilines				
N-NPA	Bacteriophyta		2.96[a]	
(Chloro)methylanilines				
CMA	Crustaceans		4.5	

a geometric mean 5 EC_{50} luminescence 7.7; 9.8; 1.0; 1.6; 1.9 mg/l

Appendix 10 continued. Combined freshwater and marine water data used for extrapolation group MPC_{water}.

Substance	taxonomic group	A&S-method	EPA-method $L(E)C_{50}$ (mg/l)	EPA-method NOEC (mg/l)
Chloroanilines				
MCA	Bacteriophyta	72		
	Algae	1.18[a]		
	Crustaceans	0.016[b]		0.01
	Pisces	0.14[c]		
	Pisces	0.75		
DCA	Bacteriophyta	10		
		158		
	Protozoa	5.1		
	Algae	0.85[d]		
		1.26[e]		
		3.2		
		65		
		1.0		
	Macrophyta	1.0		
	Rotatoria	2.5		
	Coelenterata	3.2		
	Mollusca	0.75[f]		
	Annelida	0.003[l]		
	Crustaceans	0.007[g]		
		0.08		
		0.032[l]		
	Insecta	0.36[h]		
		10		
	Pisces	0.08[i]		
		0.002		
		0.012[j]		
		0.03[k]		
		0.33		
		0.32		
		0.032[l]		
	Amphibia	0.32		
TCA	Crustaceans			0.056
TeCA	Pisces		0.3	
PCA	Pisces			0.01

a geometric mean 4 NOECs growth *S. subspicatus* 3.9; 4.1; 0.3; 0.4 mg/l
b geometric mean 3 NOECs reproduction *D. magna* 0.01; 0.013; 0.032 mg/l
c geometric mean 3 NOECs reproduction *B. rerio* 1.0; 0.2; 0.013 mg/l
d geometric mean 5 NOECs growth *C. reinhardi* 2.5; 3.0; 0.26; 0.33; 0.70 mg/l
e geometric mean 4 NOECs growth *S. subspicatus* 0.5; 2.9; 0.8; 2.2 mg/l
f geometric mean 3 NOECs reproduction *L. stagnalis* 0.13; 1.0; 3.2 mg/l
g geometric mean 7 NOECs reproduction *D. magna* 0.01; 0.0065; 0.01; 0.005; 0.005; 0.01; 0.032 mg/l
h geometric mean 2 NOECs growth *C. riparius* 0.76; 0.17 mg/l
i geometric mean 2 NOECs mortality *B. rerio* 0.02; 0.32 mg/l
j geometric mean 6 NOECs growth *P. promelas* 0.026; 0.026; 0.015; 0.015; 0.005; 0.005 mg/l
k geometric mean 4 NOECs growth *P. reticulata* 0.02; 0.02; 0.002; 1.0 mg/l
l marine water data

Appendix 10 continued. Combined freshwater and marine water data used for extrapolation group MPC_{water}.

Substance	taxonomic group	A&S-method	EPA-method $L(E)C_{50}$ (mg/l)	EPA-method NOEC (mg/l)
(Chloro)nitroanilines				
NA	Bacteriophyta	5.3		
	Protozoa	6.9		
		3.1		
		5.0		
	Algae	5.3		
		0.4		
		11		
	Crustaceans	0.5		
DNA	Crustaceans		9.6	
CNA	Crustaceans		3.2	
DCNA	Crustaceans		2.1	
(Chloro)methylanilines				
MA	Bacteriophyta	16		
	Protozoa	76		
		21		
		237		
	Cyanophyta	0.3		
	Algae	6.3		
	Crustaceans	0.01		
DMA	Bacteriophyta	8.0		
	Protozoa	9.8		
		12		
	Cyanophyta	0.4		
	Algae	5.0		
		0.8		
	Crustaceans	0.05[a]		
TMA	Pisces		50[b]	
CMA	Crustaceans		0.6	

a geometric mean 2 NOECs reproduction *D. magna* 0.016; 0.16 mg/l
b geometric mean 3 LC50s *P. promelas* 53; 52; 46 mg/l

Appendix 11. Derivation of individual MPC_{soil} for chloroanilines.

Monochloroanilines

For 2-CA the MPC is derived by applying a factor 10 on the lowest NOEC (EPA-method). This results in a MPC_{soil} of 1.6 mg/kg. Since no chronic value is available for 3-CA, a factor 1000 is applied on the lowest $L(E)C_{50}$ resulting in a MPC_{soil} of 0.10 mg/kg. The MPC for 4-CA is extrapolated using the A&S-method, since 4 NOECs for different microbial/enzmymatic processes are available. This results in a MPC of 6.3 mg/kg, which is a factor 2 lower than the lowest NOEC.

Dichloroanilines

For 2,4- and 3,5-DCA the EPA-method is used for calculating the MPC. A factor 1000 is applied on the lowest $L(E)C_{50}$ which result in MPCs of 0.13 and 0.072 mg/kg, respectively. The former value is a factor 500 lower than the lowest NOEC and the latter a factor 230. The MPC for 3,4-DCA is derived by applying statistical extrapolation, resulting in a value of 7.8 mg/kg, which is a factor 1.6 larger than the lowest NOEC.

Trichloroanilines

For both of the TCAs the MPC_{soil} is calculated with the EPA-method. A factor 1000 is applied on the lowest $L(E)C_{50}$. This result in MPCs of 0.15 and 0.13 mg/kg for 2,4,5- and 2,4,6-TCA, respectively. The MPC for the latter is a factor 380 lower than the lowest NOEC found for this compound.

Tetrachloroanilines

A factor 1000 is applied on the lowest $L(E)C_{50}$, resulting in a MPC_{soil} of 0.17 and 0.19 for 2,3,4,5- and 2,3,5,6-TeCA, respectively. The former is a fator 290, the latter a factor 80 lower than the lowest NOEC.

Appendix 11 continued. Experimental data used for derivation individual MPC_{soil} for chloroanilines.

Substance	taxonomic group	A&S-method	EPA-method $L(E)C_{50}$ (mg/kg)	EPA-method NOEC (mg/kg)
Chloroanilines				
2-CA	Macrophyta			16
3-CA	Macrophyta		103[a]	
4-CA	respiration	250		
	O_2-consumption	127		
	CO_2-production	13		
	ATP-content	63		
2,4-DCA	Macrophyta		129[b]	
3,4-DCA	respiration	165		
	CO_2-production	380		
	nitrification	17		
	acetate mineralization	559		
3,5-DCA	Macrophyta		72[c]	
2,4,5-TCA	Macrophyta		147[d]	
2,4,6-TCA	Macrophyta		125[e]	
2,3,4,5-TeCA	Macrophyta		167[f]	
2,3,5,6-TeCA	Macrophyta		191[g]	
PCA	Annelida		1500[h]	

a geometric mean 6 EC_{50} growth *L. sativa* 85; 75; 140; 115; 156; 74 mg/kg
b geometric mean 2 EC_{50} growth *L. esculentum* 184; 90 mg/kg
c geometric mean 2 EC_{50} growth *L. sativa* 80; 65 mg/kg
d geometric mean 6 EC_{50} growth *L. sativa* 125; 85; 165; 115; 275; 184 mg/kg
e geometric mean 2 EC_{50} growth *L. sativa* 135; 115 mg/kg
f geometric mean 2 EC_{50} growth *L. sativa* 235; 120 mg/kg
g geometric mean 6 EC_{50} growth *L. sativa* 320; 80; 250; 85; 678; 131 mg/kg
h geometric mean 2 LC_{50} *L. rubellus* 2200; 1000 mg/kg

Appendix 12. Individual MPC_{soil} chloroanilines.

Substance	MPC_{soil} (mg/kg)		Lowest NOEC (mg/kg)	Lowest $L(E)C_{50}$ (mg/kg)
2-CA	1.60	EPA/10	16	-
3-CA	0.10	EPA/1000	-	103[a]
4-CA	6.30	A&S	13	-
2,4-DCA	0.13	EPA/1000	66[b]	129[c]
3,4-DCA	7.8	A&S	5.0	542[d]
3,5-DCA	0.072	EPA/1000	16	72[e]
2,4,5-TCA	0.15	EPA/1000	-	147[f]
2,4,6-TCA	0.13	EPA/1000	50	125[g]
2,3,4,5-TeCA	0.17	EPA/1000	50	167[h]
2,3,5,6-TeCA	0.19	EPA/1000	16	191[i]
PCA	1.50	EPA/1000	50	1500[j]

- no data available

a geometric mean 6 EC_{50} growth *L. sativa* 85; 75; 140; 115; 156; 74 mg/kg

b geometric mean 2 NOECs growth *A. sativa* 86; 50 mg/kg

c geometric mean 2 EC_{50} growth *L. esculentum* 184; 90 mg/kg

d geometric mean 3 LC_{50} *E. andrei* 325; 700; 700 mg/kg

e geometric mean 2 EC_{50} growth *L. sativa* 80; 65 mg/kg

f geometric mean 6 EC_{50} growth *L. sativa* 125; 85; 165; 115; 275; 184 mg/kg

g geometric mean 2 EC_{50} growth *L. sativa* 135; 115 mg/kg

h geometric mean 2 EC_{50} growth *L. sativa* 235; 120 mg/kg

i geometric mean 6 EC_{50} growth *L. sativa* 320; 80; 250; 85; 678; 131 mg/kg

j geometric mean 2 LC_{50} *L. rubellus* 2200; 1000 mg/kg

extrapolation method is placed behind MPCs

Appendix 13. Experimental data used for extrapolation of the group MPC_{soil} for chloroanilines.

Compound	taxonomic group	A&S-method	EPA-method $L(E)C_{50}$ (mg/kg)	EPA-method NOEC (mg/kg)
Chloroanilines				
MCA	respiration	250		
	nitrification	17		
	O_2-consumption	127		
	CO_2-production	13		
	ATP-content	63		
DCA	respiration	165		5.0
	CO_2-production	380		
	nitrification	17		
	acetate mineralization	559		
TCA	Macrophyta		125[b]	
TeCA	Macrophyta		167[c]	
PCA	Annelida		1500[d]	

a geometric mean 6 EC_{50} growth *L. sativa* 85; 75; 140; 115; 156; 74 mg/kg
b geometric mean 2 EC_{50} growth *L. sativa* 135; 115 mg/kg
c geometric mean 2 EC_{50} growth *L. sativa* 235; 120 mg/kg
d geometric mean 2 LC_{50} *L. rubellus* 2200; 1000 mg/kg

Appendix 14. Measured concentrations of the anilines in Dutch surface waters.

Chloroanilines (Venema, 1990).

	Location[a]					
Substance (µg/l)[b]	HARVS	IJMDN	LOBT	MAAS	SCHA	VROUW
2-CA	0.01-0.04	0.0-0.08	0.01-0.05	0.01-0.03	0.01-0.07	0.01-0.03
3-CA	0.0-0.03	0.0-0.04	0.0-0.06	0.0-0.04	0.0-0.03	0.0-0.03
4-CA	0.0-0.03	0.0-0.07	0.0-0.04	0.0-0.04	0.0-0.03	0.0-0.02
Σ[c]	0.01-0.08	0.01-0.09	0.0-0.09	0.01-0.09	0.01-0.10	0.01-0.06
2,3-DCA	0.0-0.02	0.0-0.01	0.0-0.05	0.0-0.05	0.0-0.02	0.0-0.01
2,4-DCA	0.0-0.02	0.0-0.05	0.0-0.04	0.0	0.01-0.09	0.0-0.02
2,5-DCA	0.0-0.02	0.0-0.01	0.0-0.05	0.0-0.03	0.0-0.01	0.0-0.01
3,4-DCA	0.0-0.01	0.0	0.0-0.02	0.0-0.01	0.0	0.0-0.01
3,5-DCA	0.0-0.03	0.0-0.01	0.0-0.07	0.0-0.04	0.0-0.02	0.0-0.02
Σ	0.01-0.08	0.01-0.06	0.03-0.19	0.01-0.12	0.01-0.10	0.01-0.04
2,4,5-TCA	0.0-0.02	0.0-0.01	0.01-0.08	0.0-0.04	0.0-0.01	0.0-0.01

a HARVS: Haringvlietsluis (Lake IJssel); IJMDN: Ijmuiden (North-Sea-Channel); LOBT: Lobith (Rhine); MAAS: Maassluis (Meuse); SCHA: Schaar van ouden Doel; VROUW: Vrouwenzand

b 0.0 = concentration below detection limit

c indicates the the concentration range for the sum of the found concentrations for different isomers detected at the same location and same time

Nitroanilines and methylanilines (Barreveld, 1991; Heymen, 1992).

Substance	n[a]	n < 0.1 µg/l[b]	max. concentration (µg/l)
2-NA	19	6	3.8
3-NA	34	33	0.3
2-MA	35	35	-
N-MA	35	35	-
2,4-DMA	35	35	-
2,6-DMA	35	31	0.2
N,N-DMA	35	33	0.2

a total number of measurements from 1988-1990

b number of measurements below 0.1 µg/l, which is considered as "worst case" since the detection limit is not determined individually