RIVM report 601501015/2002

Environmental Risk Limits for 2-propanol, formaldehyde and 4-chloromethylphenols - updated proposals

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This investigation has been performed by order and for the account of the Directorate-General for Environmental Protection, Directorate for Chemicals, Waste and Radiation, in the context of the project 'Setting Integrated Environmental Quality Standards', RIVM-project no. 601501.

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Abstract

In this report Environmental Risk Limits (ERLs) are derived for 2-propanol, formaldehyde, and the two 4-chloromethylphenols, PCOC (p-chloro-o-cresol; 4-chloro-2-methylphenol) and PCMC (4-chloro-m-cresol; 4-chloro-3-methylphenol), respectively.

Preface

Thanks are due to drs E.M. Maas, who was contact person at the Ministry of Housing, Spatial Planning and the Environment (VROM-DGM/SAS). We also want to acknowledge dr. M.P.M. Janssen and drs. T.P. Traas of the National Institute of Public Health and the Environment (RIVM) who are involved in the RIVM-project 601501 in which the work was performed.

The results as presented in this report have been discussed by the members of the 'Setting Integrated Environmental Quality Standards Advisory Group' (OZBG-eco), who are acknowledged for their contribution. The advisory group provides a non-binding scientific comment on the final draft of a report in order to advise the steering committee of the project Setting Integrated Environmental Quality Standards (INS) on the scientific merits of the report.

Contents

Samenvatting

In dit rapport zijn Maximaal Toelaatbare Risiconiveaus (MTR's), Verwaarloosbare Risiconiveaus (VR's) en 'Serious Risk Concentrations' voor ecosystemen (SRC_{eco}'s) afgeleid voor 2-propanol, formaldehyde en de twee 4-chloormethylfenolen, respectievelijk PCOC (p-chloor-o-cresol; 4-chloor-2-methylfenol) en PCMC (4-chloor-m-cresol; 4-chloor-3-methylfenol). Deze risiconiveaus zijn afgeleid voor de milieucompartimenten water (oppervlaktewater en grondwater), sediment en bodem. Hierbij wordt opgemerkt dat PCOC recentelijk is geëvalueerd in het kader van het EU Bestaande Stoffen-programma. De resultaten van de EU evaluatie, inclusief de afgeleide risiconiveaus, zijn overgenomen in dit RIVM-rapport (zie verder onderdeel 4.2.3).

De risiconiveaus zijn afgeleid met gebruik van ecotoxicologische en milieuchemische gegevens en geven een schatting van het potentiële risico van stoffen voor een ecosysteem. De risiconiveaus vormen de wetenschappelijke basis voor milieukwaliteitsnormen die worden vastgesteld door het ministerie van VROM.

Voor alle onderzochte verbindingen zijn voldoende toxiciteitsgegevens voor waterorganismen beschikbaar voor de afleiding van risicogrenzen voor water. Er zijn echter geen of nauwelijks toxiciteitsgegevens beschikbaar voor bodemorganismen en er zijn geen toxiciteitsgegevens voor sediment-organismen. De risiconiveaus voor standaard *NL* sediment/bodem (dat wil zeggen, bodem en sediment met 10% organische stof op drooggewicht basis) zijn daarom voor alle stoffen afgeleid met behulp van de evenwichts-partitie methode (EqP-methode).

Voor alle stoffen werden in eerdere RIVM-rapporten al SRC_{eco}'s afgeleid, maar geen MTR's en VR's. In dit rapport zijn de SRC_{eco}'s herzien op grond van de geactualiseerde gegevens betreffende ecotoxiciteit, partitiecoëfficiënten en (zo nodig) methodiek en zijn ook MTR's en VR's afgeleid op grond van de geactualiseerde gegevens. Tabel I en Tabel II geven een overzicht van alle nieuwe risiconiveaus die in dit rapport zijn afgeleid. Voor een overzicht van alle nieuwe én oude risiconiveaus wordt verwezen naar Tabel 6.1 en Tabel 6.2 in hoofdstuk 6.

Tabel I. SRC_{eco}'s, MTR's en VR's voor water (opgelost = totaal)

Compound	**SRC_{eco} (mg/l)**	**MTR (mg/l)**	**VR (mg/l)**
2-propanol	1000	98	0,98
formaldehyde	1,8	0,18	0,0018
PCOC	0,55	0,05	0,0005
PCMC	0,31	0,026	0,00026

Tabel II. SRC_{eco}'s, MTR's en VR's for standaard NL bodem/sediment

Compound	**SRC_{eco} (mg/kg dw)**	**MTR (mg/kg dw)**	**VR (mg/kg dw)**
2-propanol	200	20	0,2
formaldehyde	1,6	0,16	0,0016
PCOC	13	1,2	0,012
PCMC	7,4	0,62	0,0062

Summary

In this report Maximum Permissible Concentrations (MPCs), Negligible Concentrations (NCs) and Serious Risk Concentrations for the ecosystem ($SRCs_{eco}$) have been derived for 2-propanol, formaldehyde, and the two 4-chloromethylphenols, PCOC (p-chloro-o-cresol; 4-chloro-2-methylphenol) and PCMC (4-chloro-m-cresol; 4-chloro-3-methylphenol), respectively. These Environmental Risk Limits (ERLs) were derived for the compartments water (surface water and groundwater), sediment and soil. It is noted that PCOC has been evaluated recently in the framework of the EU-programme on existing substances. The results of the EU evaluation, including the derived ERLs, have been adopted in this RIVM report (see further section 4.2.3).

The ERLs have been derived using data on ecotoxicology and environmental chemistry, and represent the potential risk of the substances to the ecosystem. They are the scientific basis for Environmental Quality Standards (EQSs) set by the Ministry of VROM.

For all studied compounds there are sufficient toxicity data for water organisms to derive ERLs for water. However, toxicity data for soil organisms are lacking or very limited and toxicity data for sediment organisms are lacking. Hence, for all compounds the equilibrium partitioning method (EqP-method) was used to derive the ERLs for standard *NL* soil/sediment (i.e. soil or sediment containing 10% organic matter on a dry weight basis).

For all compounds, $SRCs_{eco}$ (but no MPCs and NCs) were derived in previous RIVM reports. In this report the $SRCs_{eco}$ were revised on the basis of the updated data on ecotoxicity, partition coefficients and (if necesssary) methodology and, in addition, MPC and NCs were derived from the updated data. Table I and Table II show an overview of all new ERLs that were derived in this report. For an overview of all new and old ERLs see Table 6.1 and Table 6.2 in chapter 6.

Table I. SRCs$_{eco}$, MPCs and NCs for water (dissolved = total)

Compound	**SRC$_{eco}$ (mg/l)**	**MPC (mg/l)**	**NC (mg/l)**
2-propanol	1000	98	0.98
formaldehyde	1.8	0.18	0.0018
PCOC	0.55	0.05	0.0005
PCMC	0.31	0.026	0.00026

Tabel II. SRCs$_{eco}$, MPCs and NCs for standard NL soil/sediment

Compound	**SRC$_{eco}$ (mg/kg dw)**	**MPC (mg/kg dw)**	**NC (mg/kg dw)**
2-propanol	200	20	0.2
formaldehyde	1.6	0.16	0.0016
PCOC	13	1.2	0.012
PCMC	7.4	0.62	0.0062

1. Introduction

This report is a result in the project 'Setting Integrated Environmental Quality Standards'. The aim of the project is to derive environmental risk limits (ERLs) for substances in the environment for the compartments air, (ground)water, sediment and soil. Environmental risk limits (ERLs) serve as advisory values to set environmental quality standards (EQSs) by the Ministry of VROM for various policy purposes. The term EQS is used to designate all statutory and non-statutory standards that are used in Dutch environmental policy and Table 1.1 shows the correspondence between ERLs and EQSs.

Table 1.1. Environmental Risk Limits (ERLs) and the related Environmental Quality Standards EQSs) that are set by the Dutch government in The Netherlands for the protection of ecosystems.

Description	ERL	EQS
The NC represents a concentration causing negligible effects to ecosystems. The NC is derived from the MPC by dividing it by 100. This factor is applied to take into account possible combined effects.	NC (for air, water, soil, groundwater and sediment)	Target Value (for air, water, soil, groundwater and sediment)
The MPC is a concentration of a substance in air, water, soil or sediment that should protect all species in ecosystems from adverse effects of that substance. A cut-off value is set at the fifth percentile if a species sensitivity distribution of NOECs is used. This is the Hazardous Concentration for 5% of the species, the HC_5^{NOEC} .	MPC (for air, water, soil, groundwater and sediment)	MPC (for air, water, sediment and air)
The SRC_{eco} is a concentration of a substance in the soil, sediment or groundwater at which functions in these compartments will be seriously affected or are threatened to be negatively affected. This is assumed to occur when 50% of the species and/or 50% of the microbial and enzymatic processes are possibly affected.	SRC_{eco} (for water, soil, groundwater and sediment)	Intervention Value (for soil, sediment and groundwater)

NC Negligible Concentration
MPC Maximum Permissible Concentration
SRC_{eco} Serious Risk Concentration for the ecosystem

The various ERLs are:

- the Negligible Concentration (NC) for water, soil, groundwater, sediment and air;
- the Maximum Permissible Concentration (MPC) for water, soil, groundwater, sediment and air;
- the Ecotoxicological Serious Risk Concentration (SRC_{eco}) for water, soil, groundwater and sediment.

The process of deriving integrated ERLs is shown schematically in Figure 1.1. ERLs for soil and sediment are calculated for a standardised soil. ERLs for water are reported for dissolved and total concentrations (including a standard amount of suspended matter) and if found significantly different, differentiated to freshwater and saltwater. Each of the ERLs and its corresponding EQS represents a different level of protection, with increasing numerical values in the order Target Value < MPC[1] < Intervention Value. The EQSs demand different actions when one of them is exceeded, see INS (1999) and VROM (1999).

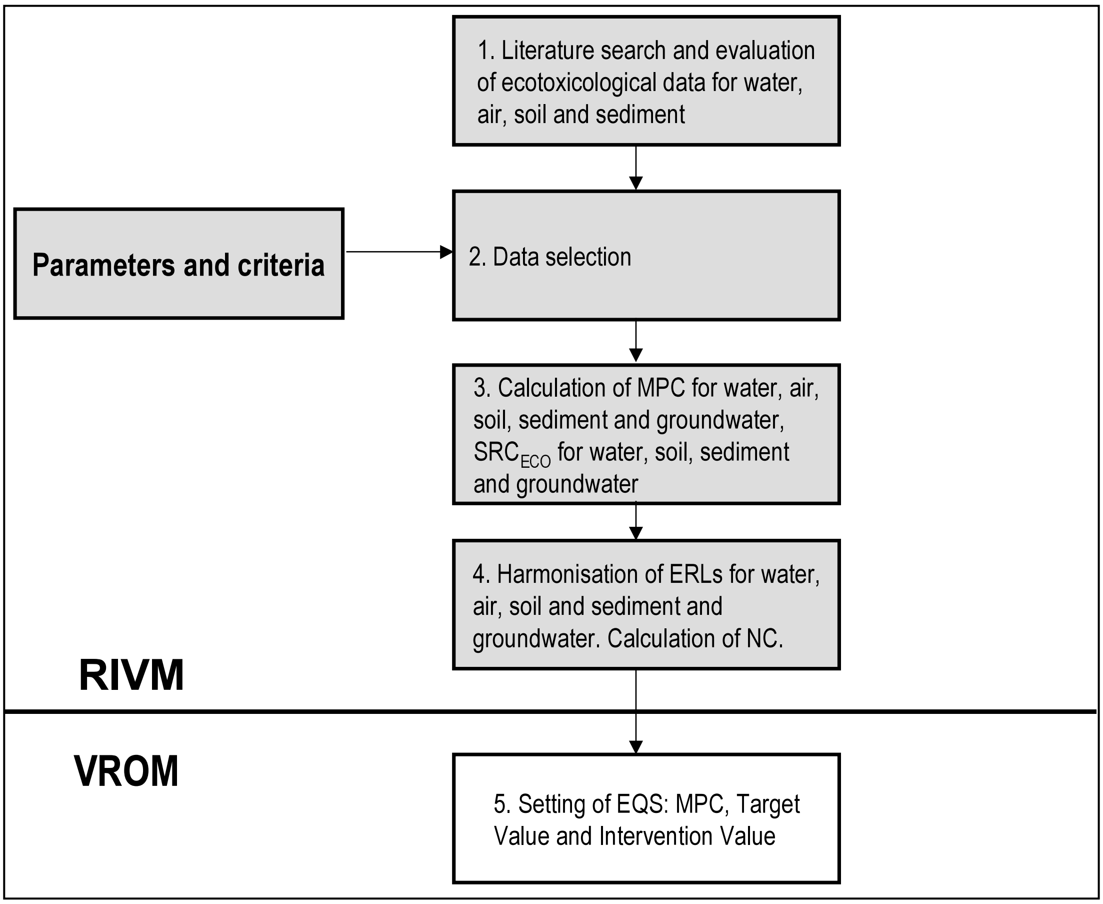


Figure 1.1. The process of deriving Integrated Environmental Risk Limits. Above the line the method to derive ERLs is indicated, i.e. MPC, NC and SRC$_{eco}$. Below the line the MPC, Target Value and Intervention Value is indicated, set by the Ministry of Housing, Spatial Planning and the Environment (VROM).

In this report ERLs have been derived for 4 substances (2-propanol, formaldehyde, PCOC and PCMC). It is noted that PCOC has been evaluated recently in the framework of the EU-

[1] A complicating factor is that the term MPC is used both as an ERL and as an EQS. For historical reasons, however, the same abbreviation is used.

programme on existing substances. The results of the EU evaluation, including the derived ERLs, have been adopted in this RIVM report (see further section 4.2.3).
The report is one of a series of RIVM reports that were published in the framework of the project 'Setting Integrated Environmental Quality Standards', in which ERLs and EQSs were derived for around 250 substances and groups of substances. For an overview of the EQSs set by the Ministry of VROM, see INS (1999) and VROM (1999).

2. Substance properties and use

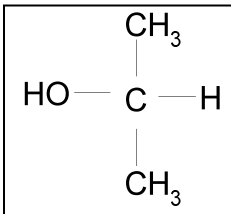
2.1 Physico-chemical properties

The data on physico-chemical properties of the substances, summarised in Tables 2.1 to 2.4, have been taken from several databases and reports. No evaluation of the validity of the reported properties was made, with the exception of the n-octanol/water partition coefficients (log K_{ow} values), because the log K_{ow} values have been used to calculate the soil/sediment sorption coefficients (log K_{oc} values); the resulting K_{oc} values have been used to calculate the partition coefficients for *standard* soil/sediment (K_p values, see section 2.2) which have been used for ERL derivation for soil/sediment, using the equilibrium partition method (see Chapter 3).

The selected log K_{ow} values have been taken from the MedChem database that comprises validated, measured log K_{ow} values (the so-called 'LogPstar' values), with the exception of the log K_{ow} for PCOC (DEPA, 1998) in which not the logPstar value but another (more recently derived) measured value was selected (see further section 2.2). If available, further measured log K_{ow} values are listed in Tables 2.1 to 2.4, as well as validated estimated log K_{ow} values which have been estimated with the ClogP programme; these estimated ClogP values are given for comparison with the measured (LogPstar) values. Both the LogPstar and ClogP values are available from Daylight Chemical Information System Inc., On-line (http://www.daylight.com/cgi-bin/contrib/pcmodels.cgi).
Note that attention was given especially to the log K_{ow} values for the two 4-chloromethyl-phenols (PCOC and PCMC), for the discussion whether or not these two substances are expected to show a similar environmental behaviour or not. In Posthumus et al. (1998), both the toxicity data and the physico-chemical data for PCOC and PCMC were combined, resulting in ERLs for the combined 4-chloromethylphenols.

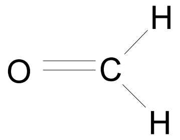
For the calculation of the log K_{oc} values from the log K_{ow} values, QSARs derived by Sabljic et al. (1995) have been used; these QSARs are the same as used in the EU Technical Guidance Documents (ECB, 1996; referring to Sabljic and Güsten, 1995).

Table 2.1. 2-Propanol



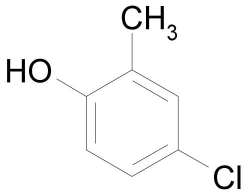
Properties	Value(s)	Reference
IUPAC name	2-propanol	
EINECS name	propan-2-ol	
Synonyms	isopropanol, isopropyl alcohol	
CAS number	67-63-0	
EINECS number	200-661-7	
Empirical formula	C3 H8 O1	
Molar mass	60.10	
Physical form at 1 atm. and 25 ^{0}C	liquid	
n-Octanol/water partition coefficient (log K_{ow})	0.05 (exp.): *logPstar value* 0.07 (est.): *ClogP value*	Daylight Chemical Information System Inc. On-line
Soil/sediment water sorption coefficient (log K_{oc})	0.52 (est.), *from QSAR for alcohols:* $\log K_{oc} = 0.39 \cdot \log K_{ow} + 0.50$	QSAR from Sabljic et al., 1995
Water solubility (mg/l)	infinite (miscible up to 100 vol. %)	WHO, 1990; OECD, 2000
Vapour pressure (Pa)	14000 at 25 deg. C (est.) 4300-7600 at 20-30 deg. C (exp. and est.)	EPIWIN MacKay et al., 2000
Henry's law constant (Pa. m^3. mol^{-1})	0.76 at 25 deg. C (est.; bond method) 1.15 at 25 deg. C (est.; group method)	EPIWIN
PKa (dissociation constant)	17.1 at 25 deg. C	Howard, 1990

Table 2.2. Formaldehyde



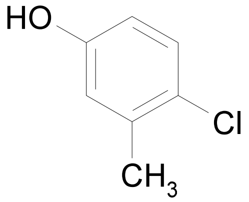
Properties	**Value(s)**	**Reference**
IUPAC and EINECS name	Formaldehyde	
Synonyms	methanal, methylene oxide	
CAS number	50-00-0	
EINECS number	200-001-8	
Empirical formula	C1 H2 O1	
Molar mass	30.03	
Physical form at 1 atm. and 25 ^{0}C	Gas	
n-Octanol/water partition coefficient (log K_{ow})	0.35 (exp.): *logPstar value* 0.35 (est): *ClogP value*	Daylight Chemical Information System Inc. On-line
Soil/sediment water sorption coefficient (log K_{oc})	1.20 (est.), *from QSAR for nonhydrophobics:* $log\ K_{oc} = 0.52*log\ K_{ow} + 1.02$	QSAR from Sabljic et al., 1995
Water solubility (mg/l)	very soluble, up to 55% (550,000 mg/l) (exp.)	Merck Index, 1983; MacKay et al., 2000; CHEMFINDER, On-line
Vapour pressure (Pa)	177,000 at 25 deg. C (est.) 518,000 at 25 deg. C (est.)	EPIWIN Howard, 1989; MacKay et al., 2000
Henry's law constant (Pa. m^3. mol^{-1})	9.4 at 25 deg. C (est.; bond method) 6.2 at 25 deg. C (est.; group method) 0.02 / 0.03 at 25 deg. C	EPIWIN WHO, 1989; MacKay et al., 2000
PKa (dissociation constant)		

Table 2.3. 4-Chloro-2-methylphenol (PCOC: p-chloro-o-cresol)



Properties	**Value(s)**	**Reference**
IUPAC name	4-chloro-2-methylphenol	
EINECS name	4-chloro-o-cresol	
Synomyms	p-chloro-o-cresol (PCOC) 4-chloro-6-methylphenol	
CAS number	1570-64-5	
EINECS number	216-381-3	
Empirical formula	C7 H7 Cl1 O1	
Molar mass	142.59	
Physical form at 1 atm. and 25 ^{0}C	Solid	
n-Octanol/water partition coefficient (log K_{ow})	2.78 (exp.): *logPstar value* 2.63 (exp.) 3.09 (exp.) 2.934 (est.): *ClogP value*	Daylight Chemical Information System Inc. On-line, and IUCLID 2000 *(from Hansch & Leo, 1985)* DEPA, 1998 (*from Hansch et al., 1995)* DEPA, 1998; IUCLID, 2000 *(from BASF, 1994, unpublished; based on OECD 107 test)* Daylight Chemical Information System Inc. On-line.
Soil/sediment water sorption coefficient (log K_{oc})	2.35 (est.), *from QSAR for predominantly nonhydrophobics:* *log K_{oc} = 0.81*log K_{ow} + 0.1* *(using log K_{ow} = 2.78)* 2.60 (est.), *from QSAR for predominantly nonhydrophobics:* *log K_{oc} = 0.81*log K_{ow} + 0.1* *(using log K_{ow} = 3.09)*	QSAR from Sabljic et al., 1995 DEPA, 1998; QSAR from Sabljic et al., 1995
Water solubility (mg/l)	7600 at 25 deg. C 2300 at 20 deg. C (exp.) 1800 at 25 deg. C (est.) <1000 at 15 deg. C 120 (est.)	IUCLID, 2000 DEPA, 1998 EPIWIN CHEMFINDER, On-line ECOSAR
Vapour pressure (Pa)	27 at 20 deg. C (exp.) 5.4 at 25 deg. C (est.)	DEPA, 1998 EPIWIN
Henry's law constant (Pa. m^3. mol^{-1})	0.046 at 25 deg. C (est.; bond method) 0.061 at 25 deg. C (est.; group method)	EPIWIN
PKa (dissociation constant)	9.7 at 25 deg. C	DEPA, 1998

Table 2.4. 4-Chloro-3- methylphenol (PCMC: p-chloro-m-cresol)



Properties	Value(s)	Reference
IUPAC name	4-chloro-3-methylphenol	
EINECS name	4-chloro-m-cresol	
Synomyms	p-chloro-m-cresol (PCMC) 4-chloro-5-methylphenol	
CAS number	59-50-7	
EINECS number	200-431-6	
Empirical formula	C7 H7 Cl1 O1	
Molar mass	142.59	
Physical form at 1 atm. and 25 ^{0}C	Solid	
n-Octanol/water partition coefficient (log K_{ow})	3.10 (exp.): *logPstar value* 3.02 (exp.) 3 (exp.) 2.984 (est.):*ClogP value*	Daylight Chemical Information System Inc. On-line; IUCLID *(from Hansch and Leo, 1985)* IUCLID, 2000 *(from Bayer, unpublished, based on OECD 107 test)* IUCLID, 2000 *(from Leo, 1991)* Daylight Chemical Information System Inc. On-line
Soil/sediment water sorption coefficient (log K_{oc})	2.61 (est.), *from QSAR for predominantly nonhydrophobics:* $log K_{oc} = 0.81*log K_{ow} + 0.1$ (using $log K_{ow} = 3.10$)	QSAR from Sabljic et al., 1995
Water solubility (mg/l)	3600-4000 at 20-25 deg.C 700 at 25 deg. C (est.) 120 (est)	MacKay, 2000; IUCLID, 2000 EPIWIN ECOSAR
Vapour pressure (Pa)	8.0 at 20 deg. C 6.7 5.4 at 25 deg. C (est.)	IUCLUD, 2000 MacKay et al., 2000 EPIWIN
Henry's law constant (Pa. m^3. mol^{-1})	0.046 at 25 deg. C (est.; bond method) 0.061 at 25 deg. C (est.; group method) 0.253 at 20 deg. C	EPIWIN
PKa (dissociation constant)	9.5 at 25 deg. C	HSDB, 2001

2.2 Partition coefficients (K_p values)

Table 2.5 shows for all substances the partition coefficients (K_p values) in standard *NL* soil/sediment, i.e. soil or sediment containing 10% organic matter on a dry weight basis, corresponding to 5.88% organic carbon (f_{oc} = 0.0588 g organic carbon / g dw soil). In addition, Table 2.5 shows the partition coefficients (K_p values) in standard *NL* suspended matter, i.e suspended matter containing 20% organic matter on a dry weight basis, corresponding to 11.76 % organic carbon (f_{oc} = 0.1176 g organic carbon / g dw soil).
The K_p values were calculated from the organic carbon-normalized partition coefficients (K_{oc} values, from Tables 2.1 to 2.4 in section 2.1) and the fraction organic carbon (f_{oc}), as follows: $K_p = K_{oc} * f_{oc}$.

Table 2.5. Partition coefficients for all substances in standard NL soil/sediment (f_{oc} = 0.0588) and suspended matter (f_{oc} = 0.1176)

Compound	**Log K_{oc} (l/kg)** [(a)]	**K_{oc} (l/kg)**	**$K_{p\ soil/sediment}$ (l/kg))** [(b)]	**$K_{p\ susp.\ matter}$ (l/kg)** [(b)]
2-propanol	0.52	3.3	0.2	0.4
formaldehyde	1.20	16	0.9	1.8
PCOC	2.60	400	24	48
PCMC	2.61	410	24	48

a: Log K_{oc} values: from Tables 2.1 to 2.4 in section 2.1. The log K_{oc} values were calculated from the n-octanol/water partition coefficients, log K_{ow} values, using the so-called 'logPstar' values, see section 2.1, except for PCOC. For PCOC the log K_{oc} was calculated from the log K_{ow} of 3.09 that was selected in the EU-RAR on PCOC (DEPA, 1998) instead of the logPstar value of 2.78.
b: K_p values: calculated from $K_p = K_{oc} * f_{oc}$ (see the text for further explanation).

Table 2.6 shows for PCOC the partition coefficients (Kp values) that were used in the EU-RAR on PCOC (DEPA, 1998) for standard *EU* soil, sediment and particulate matter.

Table 2.6. Partition coefficients for PCOC in standard EU soil (f_{oc} = 0.02), sediment (f_{oc} = 0.05) and suspended matter (f_{oc} = 0.1) (DEPA, 1998)

Compound	**Log K_{oc} (l/kg)** [(a)]	**K_{oc} (l/kg)**	**$K_{p\ soil}$ (l/kg))** [(b)]	**$K_{p\ sediment}$ (l/kg))** [(b)]	**$K_{p\ susp.\ matter}$ (l/kg))** [(b)]
PCOC	2.60	400	8	20	40

a: Log K_{oc}: from Table 2.3 in section 2.1. The log K_{oc} was calculated from the log K_{ow} of 3.09 that was selected in the EU RAR on PCOC (DEPA, 1998).
b: K_p values: calculated from $K_p = K_{oc} * f_{oc}$ (see the text for further explanation).

2.3 Use

This section merely summarises data on the use of the studied substances, without an effort to be comprehensive or to quantify the use in different applications. Likewise, no effort has been made to quantify the contribution of the different applications to the environmental concentrations, neither for the Netherlands, nor for other regions.

2-Propanol
2-Propanol is used in a large number of industrial and non-industrial applications and products (including consumer products, pharmaceuticals and food). The main uses are as solvent and chemical intermediate for the production of other solvents such as acetone. Further applications include the use as disinfectant (WHO, 1990; OECD, 2000).
2-Propanol is also present in the environment as a result of natural processes, being a metabolic product of a variety of microorganisms and a flavour volatile in foodstuffs, primarily plant products (WHO, 1990).

Formaldehyde
Formaldehyde is used in a large number of industrial and non-industrial applications and products (including building materials, consumer products, and food and feed). Especially the use as biocide (e.g. as disinfectant and preservative) in a variety of applications can result in emissions to soil (e.g. by use in agriculture) or water (e.g. by use in fish farming) (WHO, 1989; IUCLID, 2000; Mensink, 2000). With respect to the latter, formaldehyde is one of the most widely and frequently used chemicals applied in fish farming for profylactic and therapeutic treatment of fungal infections and ectoparasities of fish and fish eggs, often resulting into discharges to surface water. Use concentrations in fish farming are around 150-250 mg/l for 1-h treatments in tanks or raceways and 15-25 mg/l for indefenite periods in ponds (Bills et al., 1977; Reardon and Harrell, 1990).
Formaldehyde is also present in the environment as a result of natural processes. The major natural source is the formation of formaldehyde from methane which occurs in the trophosphere (WHO, 1989).

PCOC
PCOC is solely used as a chemical intermediate in the production of the phenoxy herbicides MCPA, MCPB and MCPP/MCPP-P; the formulated products contain up to 0.5% PCOC as impurity (DEPA, 1998). Phenoxy herbicides are used in agricultural and non-agricultural applications, resulting in environmental exposure (soil, water) to PCOC present as impurity or formed as degradation product (BUA, 1993, DEPA, 1998; Janus et al., 2000).

PCMC

PCMC (sodium salt) is used as biocide in several applications, including disinfectants used in the clinical sector, germicides, fungicides, and preservatives in consumer products, especially in leather and textile products (HSDB, 1989; BUA, 1995; Mensink, 2000).

3. Methods

3.1 Data search and selection

The majority of the selected toxicity data for all four compounds are from previous RIVM reports in which ecotoxicological ‘Serious Risk Concentrations’ ($SRCs_{eco}$, formerly denoted as ECOTOX-SCCs) were derived for these compounds in the framework of the project ‘Risks in relation to soil quality’. These RIVM reports are Crommentuijn et al., 1995 (includes data on formaldehyde) and Posthumus et al., 1998 (includes data on 2-propanol and 4-chloro-methylphenols). Additional data were retrieved from recent evaluations in the framework of international risk assessment programmes, being the ‘Screening Information Data Set’ on 2-propanol (OECD, 2000) and the EU ‘Risk Assessment Report’ on 4-chloro-2-methylphenol (DEPA, 1998). Furthermore, for all compounds an on-line literature search in TOXLINE PLUS (which includes BIOSYS) was performed for the period from 1995 and onwards and data were retrieved from the IUCLID 2000 CD-ROM ‘Public Data on High Production Volume Chemicals’ (ECB, 2000).

Both the chronic and acute data were divided in two categories: values ‘useful for ERL derivation’ and values ‘not useful for ERL derivation’. The useful toxicity values are chronic NOEC values from long-term studies and acute LC50 or EC50 values from short-term studies, all derived from reliable studies. The NOEC values are either ‘real’ NOEC values or ‘estimated’ NOEC values, see section 3.2 for general information on NOEC derivation and Appendix 2 for study-specific information on ‘estimated’ NOEC values. The majority of the useful toxicity values, especially the chronic NOEC values, have been derived from primary publications that were available for evaluation. Some additional toxicity values from secondary publications (reviews) were used, including the WHO Environmental Health Critera Documents for formaldehyde and 2-propanol (WHO, 1989; 1990; data from these reviews were already used in Crommentuijn et al., 1995 and in Posthumus et al., 1998), the EU Risk Assessment Report on 4-chloro-2-methylphenol (DEPA, 1998) and a recent evaluation of the aquatic toxicity of formaldehyde (Hohreiter and Rigg, 2001). Selected data from these reviews were considered useful for ERL derivation because these reviews have been thoroughly reviewed by independent experts. Toxicity values that were only available from the IUCLID (2000) files are not considered useful for ERL derivation, since the data in these files may not have undergone proper evaluation by independent reviewers. It it emphasised that the use of chronic NOEC values is preferred for ERL derivation and that especially for 2-propanol and formaldehyde there are sufficient chronic NOEC values for this purpose. For this reason the literature search and data selection were aimed primarily on chronic data and no effort has been made to retreive all acute data.
From the above it will be clear that classification in the category ‘not useful for ERL derivation’ does not necessarily means that the quality of the study or the toxicity value

derived from that study do not meet the criteria used in this report, but that classification in that category may be solely due to the fact that the primary literature source was not available.

With respect to acute *versus* chronic data is noted that acute LC50 and EC50 values usually are derived from short-term tests with a duration of four days or less (fish: up to around 14 days) and that chronic NOEC values usually are derived from long-term tests, the latter normally considerably longer than four days. However, whether a toxicity value can be regarded as chronic or acute is not determined solely by the duration of the test but also by the generation time of the species tested. For unicellular algae and other unicellular species (bacteria, cyanobacteria, protozoans), an exposure time of four days or even considerably less already covers one or more generations (multigeneration test) and thus for unicellular species, chronic NOEC values can be derived from tests with an exposure time of less than four days. On the other hand, for multicellular species that have a much longer generation time, for example fish, an exposure time of just over four days is much too short to derive a chronic NOEC.
With respect to the results of multigeneration tests with unicellular species, both NOEC and EC50 values have been reported in some studies; in those cases the NOEC values are reported in the chronic toxicity tables and the EC50 values in the acute toxicity tables in this report. This because EC50 values from multigeneration (but short-term) tests with unicellular species are treated as short-term EC50 values, to be added to the data base of acute L(E)50 values for multicellular species such as daphnids and fish.

A toxicity study is considered reliable if the design of the experiment is in agreement with international accepted guidelines, e.g. OECD guidelines. To judge studies that have not been performed according to these guidelines criteria have been developed for this project, as documented in Traas (2001). Effects on growth, reproduction or survival are used in the derivation of ERLs, as they are related to population dynamics. If for one species several chronic NOEC values based on the same toxicological endpoint are available, these values are averaged by calculating the geometric mean, resulting in the 'species mean' NOEC. With respect to this it is noted that the NOEC values should be from equivalent tests, for example from tests with similar exposure times. If for one species several (geometric mean) NOEC values based on different toxicological endpoints are available, the lowest value is selected. Likewise, 'species mean' L(E)C50 values have been calculated from the acute data.

3.2 Derivation of L(E)C50 and NOEC values

L(E)C50 values
As a rule, the L(E)C50 value as reported by the authors of the studies are accepted. thus without recalculation on the basis of the underlying data.

NOEC values

The following procedure is used to derive No Observed Effect Concentrations (Traas, 2001):

I. The highest reported concentration, not statistically different from the control at $p < 0.05$, is regarded as the NOEC, provided it is not the highest test concentration (thus, unbounded NOEC values are not used).

II. The highest concentration showing 10% effect or less is considered to be the NOEC if no statistical evaluation was applied.

III. If a 'real' NOEC cannot be derived from the data reported, the following procedure is used to derive the NOEC. In order of preference:

1) The NOEC is set at the EC10 level which is calculated from the effect concentrations, using a log-logistic concentration-response curve (at least two effect concentrations are needed.

2) The NOEC is derived from the LOEC (Lowest Observed Effect Concentration):

NOEC = LOEC/2, in case inhibition at the LOEC is >10% but ≤20%

NOEC = LOEC/3, in case inhibition at the LOEC is >20% but ≤50%.

NOEC = LOEC/10, in case inhibition at the LOEC is >50%.

3.3 Derivation of ERLs

The ecotoxicological Serious Risk Concentration(SRC_{eco}), Maximum Permissible Concentration (MPC) and Negligible Concentration (NC) for each compound are derived according to the methods generally applied within the project 'Setting Integrated Environmental Quality Standards' (Traas, 2001).

In short, chronic and acute toxicity studies for aquatic species (including sediment-dwelling species) and terrestrial species and terrestrial processes (such as mineralization) of a compound are searched for. The studies are evaluated for reliability and usefulness with respect to the toxicity data (chronic NOEC values or acute L(E)C50 values) that are reported in the publication or can be derived from the reported data. The SRC_{eco} and the MPC are derived using either the refined effect assessment method (statistical extrapolation, in case there are sufficient chronic NOEC values) as described by Aldenberg and Jaworska (2000) or using the preliminary effect assessment method (applying assessment factors) as laid down in Traas (2001). The ERLs are harmonised according to the equilibrium partition theory. In this way it is prevented that the concentration on a certain ERL level in one compartment leads to exceeding the corresponding ERL in another compartment.

The NC is derived directly from the MPC, by dividing it by 100, thus NC = MPC/100. The factor of 100 is supposed to function as protection against mixture toxicity, since species are always exposed in the environment to mixtures of chemicals and the effects of complex mixtures of chemicals are generally best described by concentration-addition (Van Leeuwen et al., 1996; Deneer, 2000).

3.3.1 Preliminary effect assessment

If chronic NOEC values are available for less than four taxonomic groups, assessment factors as described in Traas (2001) are used. The assessment factors that are applied for MPC derivation are in according with those for PNEC (Predicted No Effect Concentration) derivation as described in the EU Technical Guidance Documents, developed in the framework of EU Regulations on the risk assessment of new and existing substances (ECB, 1996)[2]. However, in the case that there is no complete base-set (i.e. acute (L(E)C50 values for algae, daphnids and fish), the assessment factors of the 'modified EPA method' are used, but never less strict than those according to the EU-TGD. For MPC derivation, the assessment factors are applied on the lowest acute L(E)C50 and (if available) on the lowest chronic NOEC; the lowest result is selected as MPC. For SRC_{eco} derivation, a default assessment factor of 10 is applied on the geometric mean value of acute L(E)C50 values (equivalent to the $HC50^{L(E)C50}$) and the result is compared to the geometric mean value of chronic NOEC values (equivalent to the $HC50^{NOEC}$); the lowest result is selected as SRC_{eco}. If possible the default assessment factor of 10, being the default acute-to-chronic ratio (ACR), is replaced by the compound-specific ACR.

3.3.2 Refined effect assessment

Chronic data

If chronic NOEC values are available for at least four different species, which must be of different taxonomic groups, statistical extrapolation is used. The aim of environmental quality standards as derived in the project 'Setting Integrated Environmental Quality Standards' is to protect all species in the ecosystem. For statistical considerations the MPC derived from chronic NOEC values is set equal to the concentration at which 95% of the species is protected, i.e. the HC5, assuming thereby to protect the whole ecosystem (VROM, 1989; Van Leeuwen et al., 1992). The HC50 is the median of the distribution and is used as a trigger value for serious soil or sediment contamination (cf. Chapter 1). A detailed description of the statistical background of the refined effect assessment method, in which different species sensitivity distributions can be used, is given in Posthuma et al., 2002.

In this report the statistical extrapolation method according to Aldenberg and Jaworska (2000) has been used. In this method it is assumed that the log of sensitivities of species in an ecosystem can be described by a normal probability distribution (other methods assume a log-logistic distribution or a triangular distribution, see Posthuma et al., 2002). The goodness of fit of the normal distribution is tested with the Anderson-Darling test (Aldenberg et al., 2001). This test highlights the differences between the tails of the fitted distribution and the data. The

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2 The EU Technical Guidance Documents have been updated in 2002.

average, the standard deviation, and the number of the underlying data define this distribution. Extrapolation factors as derived by Aldenberg and Jaworska (2000) are used to estimate the HC5 and HC50, respectively, and their upper (95%) and lower (5%) estimate, constituting a 90% two-sided confidence interval.

Acute data
Statistical extrapolation can also be used on acute L(E)C50 values. It will be clear, however, that the $HC5^{L(E)C50}$ and $HC50^{L(E)C50}$ derived from acute L(E)C50 values cannot be regarded as equivalent of the HC5 and HC50 derived from chronic NOEC values. Derived from the acute L(E)C50 values, the $HC5^{L(E)C50}$ and $HC50^{L(E)C50}$ are equivalent to the concentrations that *are expected to severely affect 5% and 50%*, respectively, of the species in the ecosystem at short-term exposure to that concentration. To derive an MPC and SRC_{eco} from the $HC5^{L(E)C50}$ and $HC50^{L(E)C50}$, respectively, requires an *additional assessment factor* (acute-to-chronic ratio, ACR) for extrapolation from acute L(E)C50 values to chronic NOEC values. If no compound-specific information is available, a default ACR of 10 is used.

3.3.3 Equilibrium partitioning and harmonisation between the compartments

By applying the equilibrium-partitioning concept (DiToro et al., 1991), it is assumed that there is equilibrium between the concentration in organic carbon and (pore) water. In addition, it is assumed that toxicity is related to pore water concentrations, and that the sensitivity of aquatic organisms is comparable to that of organisms living in soil or sediment. The partition coefficient between organic carbon in the soil/sediment and water (K_{oc}) is used to derive an MPC for soil/sediment when no data on terrestrial or sediment-dwelling organisms are available. By applying equilibrium partitioning, the K_{oc} is used to harmonise the ERLs for soil and sediment.

4. Toxicity data and derivation of ERLs

4.1 Aquatic toxicity data

The available aquatic toxicity data have been summarised in Appendix 2. For each compound the following data, are presented:
a) Chronic toxicity to freshwater species: NOEC values useful for ERL derivation.
b) Acute toxicity to freshwater species: LC50 and EC50 values useful for ERL derivation.
c) Acute toxicity to saltwater species: LC50 and EC50 values useful for ERL derivation.
d) Additional aquatic toxicity data freshwater and saltwater species: not useful for ERL derivation).
It is noted that useful chronic toxicity data for saltwater species are lacking for all four compounds.

The chronic NOEC values and the acute L(E)C50 values that are considered to be useful for ERL derivation are also presented in this chapter:
Table 4.1. 2-Propanol – selected data freshwater species
Table 4.2. 2-Propanol – selected data saltwater species
Table 4.3. Formaldehyde – selected data freshwater species
Table 4.4. Formaldhyde – selected data saltwater species
Table 4.5. 4-Chloro-2-methylphenol (PCOC): selected data freshwater species
Table 4.6. 4-Chloro-2-methylphenol (PCOC): additional data freshwater species
Table 4.7. 4-Chloro-3-methylphenol (PCMC): selected data freshwater species
Table 4.8. 4-Chloro-3-methylphenol (PCMC): selected data saltwater species

4.2 Derivation of ERLs for water

For 2-propanol and formaldehyde there are sufficient chronic NOEC values for species of different taxonomic groups to use the refined effect assesssment method (statistical extrapolation). For each of the two 4-chloromethylphenols, PCOC and PCMC, there are insufficient chronic NOEC values to apply stastistical extrapolation. Thus, ERL values for PCOC and PCMC were derived with the preliminary effect assessment method (assessment factors).
As noted earlier, PCOC has been evaluated recently in the framework of the EU-programme on existing substances. The results of the EU evaluation, including the derived ERLs, have been adopted in this RIVM report (see further section 4.2.3).

Below the results of the ERL derivation for water are presented for 2-propanol, formaldehyde and the 4-chloromethylphenols (PCOC and PCMC), respectively. For an overview of the derived ERLs for water see Table 4.8.

4.2.1 2-Propanol

For 2-propanol, useful (species mean) acute L(E)C50 values are available for 8 freshwater species (Table 4.1, from Table A2-1b in Appendix 2) and 4 saltwater species (Table 4.2, from Table A2-1c in Appendix 2). These acute L(E)C50 have not been used for ERL derivation, since there sufficient chronic NOEC values.

Useful chronic NOEC values are available for freshwater bacteria, cyanobacteria, protozoans, algae, and crustaceans (Table 4.1, from Table A2-1a in Appendix 2), with a total of 7 (species mean) values ranging from 100 to 4900 mg/l; there are no chronic NOEC values for saltwater species. The freshwater NOEC values have been used for ERL derivation; the species sensitivity distribution of these values is shown in Figure 4.1. A log-normal distribution of these values is accepted by the Anderson-Darling test. Using statistical extrapolation on the freshwater NOEC values results in an **MPC** (HC5) of **98 mg/l** *(90% CI: 10-290 mg/l)* and an **SRC_{eco}** (HC50) of **1000 mg/l** *(90% CI: 380-2700 mg/l).* The MPC of 98 mg/l results in an **NC** of **0.98 mg/l.**

Table 4.1. 2-Propanol – selected data freshwater species

Taxonomic groups and species	**Chronic NOEC (mg/l)**	**Taxonomic groups and species**	**Acute L(E)C50 (mg/l)**
Bacteria		**Protozoa**	
Pseudomonas. putida	1100	*Tetrahymena pyriformis*	4600
Cyanobacteria		**Crustacea**	
Microcystus aeruginosa	1000	*Daphnia magna*	5900 (b)
Protozoa		*Daphnia pulex*	10000
Chilomonas paramecium	100	**Insecta**	
Entosiphon sulcatum	4900	*Aedes aegypti*	25000
Uronema parduczi	3400	***Pisces***	
Algae		*Leuciscus id. melanotus*	9000 (c)
Scenedesmus quadricauda	1800	*Pimephales promelas*	9800 (d)
Crustacea		*Poecilia reticulata*	7900 (e)
Daphnia magna	330 (a)	*Rasbora heteromorpha*	4200

a: Geometric mean of 770 and 140 mg/l for *Daphnia magna* (endpoint growth).
b: Geometric mean of 7800, 9700, 2300 and 6900 mg/l for *Daphnia magna*.
c: Geometric mean of 9000, 9300 and 8900 mg/l for *Leuciscus idus melanotus*.
d: Geometric mean of 8700, 10000, 9600, 11000 and 9700 mg/l for *Pimephales promelas*.
e: Geometric mean of 7100 and 8700 mg/l for *Poecilia reticulata*.

Table 4.2. 2-Propanol – selected data saltwater species

Taxonomic groups and species	**Chronic NOEC (mg/l)**	**Taxonomic groups and species**	**Acute L(E)C50 (mg/l)**
	No data		
		Bacteria	
		Vibrio fisheri	32000 (a)
		Vibrio harveyi	3200
		Escherichia coli *	790
		Crustacea	
		Crangon crangon	1200

*: Test performed in brackish water (salinity 8 $^0/_{00}$).
a: Geometric mean of 35000, 42000 and 22000 mg/l for *Vibrio fisheri*.

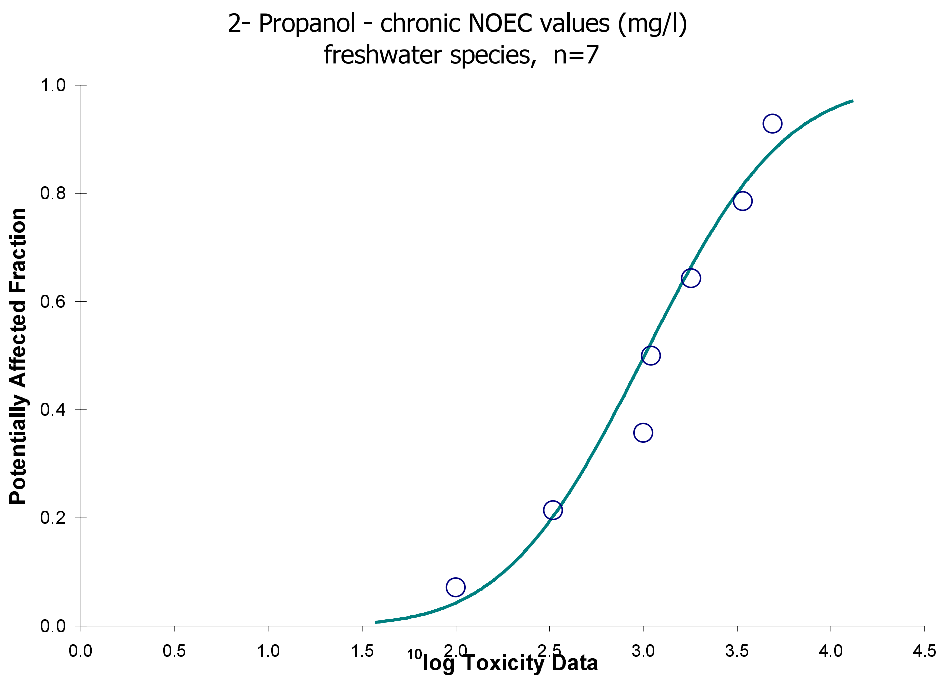

Figure 4.1. 2-Propanol - freshwater species sensitivity distribution of chronic NOEC values

4.2.2 Formaldehyde

For formaldehyde, useful (species mean) L(E)C50 values are available for 31 freshwater species (Table 4.3, from Table A2-2b in Appendix 2) and 3 saltwater species (Table 4.4, from Table A2-2c in Appendix 2). These acute L(E)C50 have not been used for ERL derivation, since there sufficient chronic NOEC values.
Useful chronic NOEC values are available for freshwater bacteria, cyanobacteria, protozoans, algae and crustaceans (Table 4.3, from Table A2-2a in Appendix 2), with a total of 11 (species mean) values ranging from 0.14 to 19 mg/l; there are no chronic NOEC values for saltwater species. The freshwater NOEC values have been used for ERL derivation; the species sensitivity distribution of these values is shown in Figure 4.2. A log-normal distribution of these values is accepted by the Anderson-Darling test. Using statistical extrapolation on the freshwater NOEC values results in an **MPC** (HC5) of **0.18 mg/l** *(90% CI: 0.04-0.44 mg/l)* and an **SRC_{eco}** (HC50) of **1.8 mg/l** *(90% CI: 0.85-3.7 mg/l)*. The MPC of 0.18 mg/l results in an **NC** of **0.0018 mg/l**.

Table 4.3. Formaldehyde - selected data freshwater species

Taxonomic groups and species	**Chronic NOEC (mg/l)**	**Taxonomic groups and species**	**Acute L(E)C50 (mg/l)**
Bacteria		**Protozoa**	
Escherischia coli	1	*Colpoda aspera*	2
Pseudomonas fluorescens	2 (a)	**Algae**	
Pseudomonas putida	4.9	*Scenedesmus quadricauda*	15
Cyanobacteria		**Mollusca**	
Microcystus aeruginosa	0.14	*Corbicula leana*	50
Protozoa		*Corbicula manilensis*	41 (d)
Chilomonas paramecium	1.6	*Helisoma sp.*	37
Colpoda aspera	0.78	**Crustacea**	
Entosiphon sulcatum	7.7	*Bosmina sp.*	20
Uronema parduczi	2.3	*Ceriodaphnia dubia*	11
Algae		*Cyclops sp.*	20
Scenedesmus quadricauda	0.51 (b)	*Cypridopsis vidua*	63
Crustacea		*Daphnia magna*	20 (e)
Ceriodaphnia dubia	1.7 (c)	*Daphnia pulex*	8.7 (f)
Cypridopsis vidua	19	*Palaemonetes kadiakensis*	186
		Insecta	
		Chironomus sp.	450
		Notonecta sp.	330
		Pisces	
		Anguilla rostrata	31
		Ictalurus melas	25
		Ictalurus punctatus	24 (g)
		Lepomis cyanellus	69
		Lepomis macrochirus	39 (h)
		Leuciscus id. melanotus	22 (i)
		Micropterus dolomieui	54
		Micropterus salmoides	57
		Morone saxatilis	17 (j)
		Oncorhynchus mykiss	59 (k)
		Pimephales promelas	25 (l)
		Poecilia reticulata	27
		Salmo salar	69
		Salvelinus namaycush	40
		Amphibians	
		Bufo sp.	19
		Rana catesbeiana	10
		Rana pipiens	8.7

a: Most sensitive endpoint for *Pseudomonas putida* (endpoint glucose degradation).
b: Geometric mean of 0.3 and 0.88 mg/l for *Scenedesmus quadricauda* (endpoint biomass).
c: Geometric mean of 1.0 and 3.0 mg/l for *Ceriodaphnia dubia* (endpoints survival and mobility).
d: Geometric mean of 35 and 47 mg/l for *Corbicula manilensis*.
e: Geometric mean of 18, 15, 60, 29, 7.6 and 20 mg/l for *Daphnia magna*.
f: Geometric mean of 13 and 5.8 mg/l for *Daphnia pulex*.

g: Geometric mean of 28, 25, 26, 23, 20, 25, 28 and 17 mg/l for *Ictalurus punctatus*.
h: Geometric mean of 35, 50, 40, 29, 36, 34, 42 and 47 mg/l for *Lepomis macrochirus*.
i: Geometric mean of 15 and 32 mg/l for *Leuciscus idus melanotus*.
j: Geometric mean of 7.3, 10, 15, 28, 21, 18, 11, 16, 19, 24, 20, 22 and 24 mg/l for *Morone saxatilis*.
k: Geometric mean of 68, 47, 69 ,69, 68, 50, 60, 50 and 54 mg/l for *Oncorhynchus mykiss*.
l: Geometric mean of 27 and 24 mg/l for *Pimephales promelas*.

Table 4.4. Formaldehyde - selected data saltwater species

Taxonomic groups and species	**Chronic NOEC (mg/l)**	**Taxonomic groups and species**	**Acute L(E)C50 (mg/l)**
	No data		
		Bacteria	
		Vibrio fisheri	5.0 (a)
		Vibrio harveyi	0.78 (b)
		Pisces	
		Morone saxatilis	4.6 (c)

a: Geometric mean of 3 and 8.5 mg/l for *Vibrio fisheri*.
b: Geometric mean of 0.44 and 1.4 mg/l for *Vibrio harveyi*.
c: Geometric mean of 5.0, 5.7, 3.9 and 4.0 for *Morone saxatilis*.

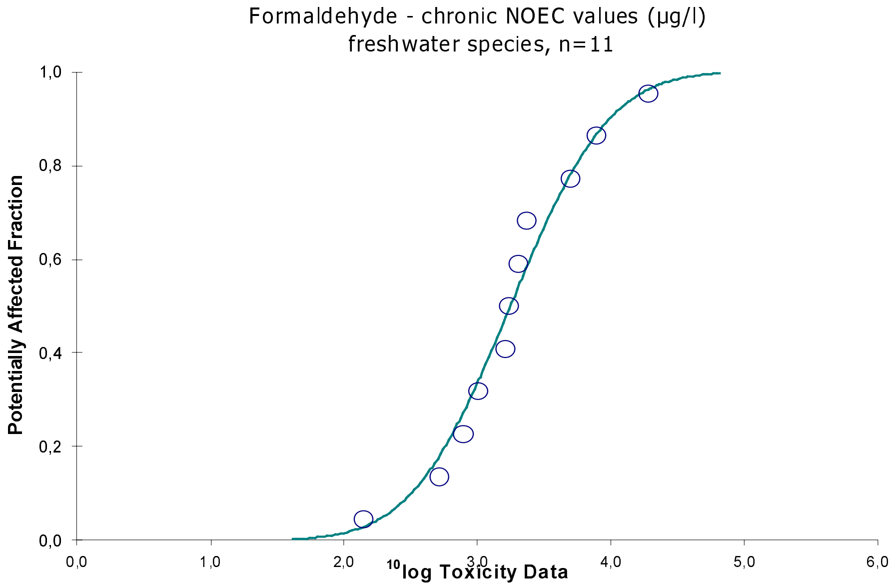

Figure 4.2. Formaldehyde - freshwater species sensitivity distribution of chronic NOEC values

4.2.3 4-Chloromethylphenols

One of the two 4-chloromethylphenols, namely PCOC, has been evaluated recently in the framework of the EU-programme on existing substances, resulting in an EU Risk Assessment Report (EU-RAR: DEPA, 1998). The results of the EU evaluation, including the derived ERLs, have been adopted in this RIVM report. Only in case the EU-RAR does not include an equivalent of an ERL normally derived in the Netherlands, that ERL has been derived in this RIVM report, but only using the data selected in the EU-RAR, regardless whether additional data are available or not. In addition, different weight fractions of organic carbon (f_{oc}) in soil and sediment are used for standard *NL* soil and sediment compared to standard *EU* soil and sediment, thus the ERLs for soil and sediment were calculated for *NL* soil and sediment.

4-Chloro-2-methylphenol (PCOC: p-chloro-o-cresol)

For PCOC, based on the DEPA (1998) selection, there are useful (species mean) L(E)C50 values available for freshwater bacteria, algae, macrophytes, crustaceans, and fish (Table 4.5, from Table A2-3c in Appendix 2), with a total of 8 (species mean) values ranging from 0.63 to 110 mg/l. These acute L(E)C50 values, have not been used for MPC derivation, since there are sufficient chronic NOEC values. The acute L(E)C50 values have been used, however, for SRC_{eco} derivation (see further). There are no acute L(E)C50 values for saltwater organisms. Based on the DEPA (1998) selection, chronic NOEC values are available for freshwater algae, crustaceans and fish (Table 4.5, from Table A2-3a in appendix 2), with a total of 3 values ranging from 0.5 to 0.97 mg/l; there are no chronic NOEC values for saltwater species. Using an assessment factor of 10 on the lowest NOEC (0.5 mg/l, for fish *Salmo trutta*) resulted in a Predicted No Effect Concentration (PNEC) of 0.05 mg/l (DEPA, 1998). The PNEC is equivalent to the Maximum Permissible Concentration (MPC), thus the **MPC** is set at **0.05 mg/l**. The MPC of 0.05 mg/l results in an **NC** of **0.0005 mg/l**.

The geometric mean value of the 3 chronic NOEC values in Table 4.5 is 0.55 mg/l (being the NOEC for crustacean *Daphnia magna*); the geometric mean value of the 8 acute L(E)C50 values ($HC50^{L(E)C50}$) is 7.6 mg/l *(90% CI: 2.2-26 mg/l).* Applying an acute-to-chronic ratio of 10 on the geometric mean value of the acute L(E)C50 values results in a value of 0.76 mg/l, which is higher than the geometric mean value of the chronic NOEC values (0.55 mg/l). This results in an $\mathbf{SRC_{eco}}$ of **0.55 mg/l**.

In Table 4.6 some additional freshwater toxicity values for PCOC are given (from Table A2-3A and Table A2-3c in Appendix 2). The values in Table 4.6 are consided useful based on the criteria used in this report, but these data were not included in the EU-RAR on PCOC (DEPA, 1998) and thus not used in this RIVM report either.

Table 4.5. 4-Chloro-2-methylphenol (PCOC) – selected data freshwater species (DEPA, 1998)

Taxonomic groups and species	**Chronic NOEC (mg/l)**	**Taxonomic groups and species**	**Acute L(E)C50 (mg/l)**
Algae		**Bacteria**	
Scenedesmus subspicatus	0.97 (a)	*Pseudomonas putida*	110
Crustacea		**Algae**	
Daphnia magna	0.55 (b)	*Scenedesmus subspicatus*	15 (d)
Pisces		**Macrophyta**	
Salmo trutta	**0.5** (c)	*Lemna minor*	93
		Crustacea	
		Daphnia magna	0.63 (e)
		Pisces	
		Brachydanio rerio	3.9 (f)
		Lepomis macrochirus	2.3
		Oryzias latipes	6.3
		Salmo trutta	2.1

a: Most sensitive endpoint for *Scenedesmus subspicatus* (72-h NOEC: endpoint biomass).

b: The (21-d) NOEC of 0.55 mg/l was considered to be useful in the EU-RAR on PCOC. It is noted, however, that this value should have been rejected (according to the criteria used in the EU-RAR programme and this RIVM report), since this NOEC is <u>un</u>bounded (i.e. no effect was found at 0.55 mg/l, the highest concentration tested) and thus this NOEC is not valid.

c. The (21-28 d) NOEC of 0.5 mg/l for *Salmo trutta* was considered useful in the EU-RAR on PCOC and, being the lowest chronic NOEC, used as the key study for PNEC derivation ($PNEC_{aquatic\ organisms}$ is lowest NOEC/10 = 0.5/10 = 0.05 mg/l). It is noted, however, that the validity of this NOEC is questionable, since the NOEC is based on endpoint histopathology (liver, kidneys and gills) and histopathological effects are usually not taken into account in ecotoxicity tests (except for histopathological effects in the reproductive organs). The reported results of the two tests from which this NOEC was derived did not indicate an effect on survival; further endpoints were not studied.

d: *Scenedesmus subspicatus:* 72-h EC50, endpoint biomass.

e: Geometric mean of 0.29, 0.63 and 1 mg/l for *Daphnia magna*.

f: Geometric mean of 3.7 and 4.2 mg/l for *Brachydanio rerio.*

Table 4.6. 4-Chloro-2-methylphenol (PCOC) – additional data freshwater species (This report)

Taxonomic groups and species	Chronic NOEC (mg/l)	Taxonomic groups and species	Acute L(E)C50 (mg/l)
Bacteria		**Pisces**	
Pseudomonas sp.	38 (a)	*Leuciscus id. melanotus*	3.6
Amphibia			
Xenopus laevis	4		

a: Geometric mean of 37 mg/l for *Pseudomonas putida* and 40 mg/l for *Pseudomonas sp.* (NOEC). In the EU-RAR on PCOC, only the EC50 from the *Pseudomonas putida* study is included, not the NOEC of 37 mg/l derived from that study.

4-Chloro-3-methylphenol (PCMC: p-chloro-m--cresol)

For PCMC, acute L(E)C50 values are available for freshwater protozoans, crustaceans, and fish (Table 4.7, from Table A2-3d in Appendix 2), with a total of 6 (species mean) values ranging from 1.3 to 23 mg/l. In addition there is one acute EC50 for saltwater bacterium *Vibrio fisheri,* being 0.27 mg/l (Table 4.8, from Table A2-3e in Appendix 2). These acute L(E)C50 values have not been used for MPC derivation, since there are sufficient chronic NOEC values. The acute L(E)C50 values have been used, however, for SRC_{eco} derivation (see further).

Chronic NOEC values are available for freshwater bacteria, algae, and crustaceans (Table 4.7, from Table A2-3b in Appendix 2), with a total of 4 (species mean) values ranging from 1.3 to 35 mg/l; there are no chronic NOEC values for saltwater species. These chronic data are too limited to apply the refined effect assessment method, thus the preliminary effect assessment method is used for ERL derivation. Using an assessment factor of 50 on the lowest NOEC (1.3 mg/l, for crustacean *Daphnia magna*) results in an **MPC** of **0.026 mg/l**. An assessment factor of 50 (instead of a factor of 10 as used for the derivation of the MPC for PCOC, see earlier) is used because there is no chronic NOEC for fish. The MPC of 0.026 mg/l results in an **NC** of **0.00026 mg/l**.

The geometric mean value of the 4 chronic NOEC values ($HC50^{NOEC}$) is 6.7 mg/l *(90% CI: 1.3-34 mg/l);* the geometric mean value of the 7 acute L(E)C50 values ($HC50^{L(E)C50}$) is 3.1 mg/l *(90% CI: 1.1-8.6 mg/l*; freshwater L(E)C50 values and saltwater EC50 combined). Applying an acute-to-chronic ratio of 10 on the geometric mean value of the acute L(E)C50 values results in a value of 0.31 mg/l, which is lower than the geometric mean value of the chronic NOEC values (6.7 mg/l). This results in an $\mathbf{SRC_{eco}}$ of **0.31 mg/l**.

Table 4.7. 4-Chloro-3-methylphenol (PCMC) – selected data freshwater species

Taxonomic groups and species	**Chronic NOEC (mg/l)**	**Taxonomic groups and species**	**Acute L(E)C50 (mg/l)**
Bacteria		**Protozoa**	
Bacillus subtilis	9.3	*Tetrahymena pyriformis*	23
Pseudomonas sp.	35	**Crustacea**	
Algae		*Daphnia magna*	2.6 (b)
Scenedesmus subspicatus	4.7 (a)	*Daphnia pulex*	3.1
Crustacea		**Pisces**	
Daphnia magna	**1.3**	*Pimephales promelas*	6.0 (c)
		Poecilia reticulata	6.7
		Salmo trutta	1.3

a: Most sensitive endpoint for *Scenedesmus subspicatus* (72-h NOEC: endpoint biomass).
b: Geometric mean of 4.4 and 1.5 mg/l for *Daphnia magna*.
c: Geometric mean of 7.4, 4.1, 6.5, 5.4 and 7.3 for *Pimephales promelas*.

Table 4.8. 4-Chloro-3-methylphenol (PCMC) – selected data saltwater species

Taxonomic groups and species	**Chronic NOEC (mg/l)**	**Taxonomic groups and species**	**Acute L(E)C50 (mg/l)**
	No data		
		Bacteria	
		Vibrio fisheri	0.27

Conclusion ERLs for water

Table 4.9 gives an overview of the ERLs ($SRCs_{eco}$, MPCs and NCs) for water. The ERLs as derived above are considered to be dissolved concentrations, since these values were derived from the results of laboratory studies in mostly artificial (reconstituted) test waters that usually contain little suspended matter. For the studied compounds, however, the total concentration in *NL* standard water (i.e. water with a suspended matter content of 30 mg/l, the suspended matter having an organic matter content of 20%) is equal to the dissolved concentration, as can be calculated from the dissolved concentration, the suspended matter content and the partition coefficients for standard suspended matter (K_p values, which are very low for these substances, see section 2.2). For example, for PCMC which is the substance with the highest estimated $K_{p\text{- suspended matter}}$, the dissolved concentration is 99.85% of the total concentration.

Table 4.9. $SRCs_{eco}$, MPCs and NCs for water (dissolved = total)

Compound	**SRC_{eco} (mg/l)**	**MPC (mg/l)**	**NC (mg/l)**
2-propanol	1000	98	0.98
formaldehyde	1.8	0.18	0.0018
PCOC	0.55	0.05	0.0005
PCMC	0.31	0.026	0.00026

4.3 Derivation of ERLs for sediment

No sediment toxicity data have been found for the studied compounds, thus the equilibrium partitioning method (EqP-method) has been used to derive ERLs for sediment, as follows: $ERL_{sediment}$ (dw) = ERL_{water} (dissolved) * K_p.

The resulting MPCs and NCs for standard *NL* sediment are shown in Table 4.10; the resulting $SRCs_{eco}$ for standard *NL s*ediment are shown in Table 4.11. These tables also show the ERLs for water (from section 4.2) and the K_p values (from section 2.2) used to calculate the ERLs for sediment.

Table 4.10. MPCs and NCs for water (dissolved) and standard NL sediment (based on EqP-method)

Compound	**MPC_{water} (mg/l)**	**NC_{water} (mg/l)**	**$K_{p\ sediment}$ (l/kg)**	**$MPC_{sediment}$ (mg/kg dw)**	**$NC_{sediment}$ (mg/kg dw)**
2-propanol	98	0.98	0.2	20	0.2
formaldehyde	0.18	0.0018	0.9	0.16	0.0016
PCOC	0.05	0.0005	24	1.2	0.012
PCMC	0.026	0.00026	24	0.62	0.0062

Table 4.11. $SRCs_{eco}$ for water (dissolved) and standard NL sediment (based on EqP-method)

Compound	**SRC_{eco} water (mg/l)**	**$K_{p\ sediment}$ (l/kg)**	**SRC_{eco} Sediment (mg/kg dw)**
2-propanol	1000	0.2	200
formaldehyde	1.8	0.9	1.6
PCOC	0.55	24	13
PCMC	0.31	24	7.4

In the EU-RAR on PCOC (DEPA, 1998), no ERLs for sediment were derived.

4.4 Derivation of ERLs for soil

For 2-propanol, PCOC and PCMC, one useful terrestrial study is available, being a 14-d study with lettuce *Lactuca sativa,* resulting in 14-d EC50 values (endpoint growth) of >1000 mg/kg dw for 2-propanol, 66 mg/kg dw for PCOC and 66 mg dw for PCMC; these values are the results in the test soil (Hulzebos et al., 1993). Normalized to standard *NL* soil on the basis of the organic matter content, these values are >5,000, 330 and 330 mg/kg dw standard *NL* soil, respectively, see Appendix 3. Further terrestrial data are not available, neither for species nor for microbial processes. In addition to the preliminary effect assessment, which can be applied only for PCOC and PCMC (not for 2-propanol since the EC50 for 2-propanol is unbounded), the equilibrium partitioning method (EqP-method, see also section 4.3) has been used for all studied compounds.

I. Preliminary effect assessment (assessment factor method): PCOC and PCMC
Applying an assessment factor of 1000 on the EC50 of 330 mg/kg dw standard *NL* soil results for both compounds in an MPC of 0.33 mg/kg dw. Applying an assessment factor of 10 on the EC50 results in a SRC_{eco} of 33 mg/kg dw. The MPC of 0.33 mg/l results in an NC of 0.0033 mg/kg dw.

II. Equilibrium partitioning method (EqP-method): all compounds
For standard *NL* soil the use of the EqP-method results in the same ERLs as for standard *NL* sediment, see Table 4.10 (MPCs and NCs) and Table 4.11 ($SRCs_{eco}$), as for both compartments the same fraction organic carbon (f_{oc} = 0.0588) is used and thus for each compound the K_p is the same in both compartments.

In the EU-RAR on PCOC (DEPA, 1998), terrestrial toxicity data is not included and thus only the EqP method was used, resulting in a $PNEC_{soil}$ of 0.36 mg/kg wet standard *EU* soil containing 60% solids (density 2500 kg/m^3), 20% water (density 1000 kg/m^3) and 20% air, i.e. 88% solids by weight; this PNEC is equivalent to 0.41 mg/kg dry soil. Normalisation of this PNEC for standard *EU* soil (f_{oc} = 0.02) to standard *NL* soil (f_{oc} = 0.0588) results in an MPC of 1.2 mg/kg dry soil, equal to the corresponding EqP result in this RIVM report.

Conclusion ERLs for soil

Table 4.12 gives an overview of the ERLs ($SRCs_{eco}$, MPCs and NCs) for standard *NL* soil. For 1-propanol and formaldyde, only the EqP method could be applied for ERL derivation. For PCOC and PCMC both the preliminary effects assessment method and the EqP method could be applied, the former method resulting in lower MPCs and NCs compared to the EqP method, but resulting in higher $SRCs_{eco}$ compared to the EqP method. In the EU-RAR on PCOC only the EqP method was used for PNEC derivation. As the ERLs from the EU-RAR on PCOC are adopted in this RIVM report, the results of the EqP method were selected for ERL derivation (SRC_{eco}, MPC and NC) for PCOC. To be consistent with this, the results of the EqP method were also selected for ERL derivation for PCMC. Thus, all ERLs for soil (Table 4.12) are equal to the corresponding values in sediment (Table 4.10 and 4.11).

Table 4.12. SRCs$_{eco}$, MPCs and NCs for NL standard soil

Compound	**SRC$_{eco}$ (mg/kg dw)**	**MPC (mg/kg dw)**	**NC (mg/kg dw)**	**Method**
2-propanol	200	20	0.2	EqP
formaldehyde	1.6	0.16	0.0016	EqP
PCOC	13	1.2	0.012	EqP
PCMC	7.4	0.62	0.0062	EqP

5. Preliminary risk analysis

There are no data on measured environmental concentrations of the studied compounds, with the exception of data on PCMC and 2-propanol concentrations in groundwater (data available from the Dutch groundwater quality monitoring network, run by RIVM) and data on the PCMC concentrations in influent and effluent of sewage treatment plants (data available from RIVO, the Netherlands Institute for Fisheries Research). Because of the lack of data for surface water, sediment and soil, no preliminary risk analysis can be performed.

6. Conclusions and discussion

Table 6.1 and Table 6.2 show the new ERLs (from this report) and the old ERLs (from Crommentuijn et al., 1995 and Posthumus et al., 1998) for water and standard *NL* soil/sediment, respectively. Differences between new and old $SRCs_{eco}$ are explained in the text below. Note that no MPCs and NCs were derived in the earlier reports. Furthermore, a reliability score of the $SRCs_{eco}$ for soil/sediment is given, based on the three reliability classes ('high', 'medium' and 'low') as defined in Verbruggen et al. (2001).

Table 6.1. $SRCs_{eco}$, MPCs and NCs for water (dissolved = total)

Compound	new SRC_{eco} (mg/l)	*old SRC_{eco} (mg/l)*	new MPC (mg/l)	*old MPC (mg/l)*	New NC (mg/l)	old NC (mg/l)
2-propanol	1000	1100	98	-	0.98	-
Formaldehyde	1.8	2.3	0.18	-	0.0018	-
PCOC	0.55	3.6 (a)	0.05	-	0.0005	-
PCMC	0.31	3.6 (a)	0.026	-	0.00026	-

-: Not derived.
a: Based on combined data for PCOC and PCMC.

Table 6.2. $SRCs_{eco}$, MPCs and NCs for standard NL soil/sediment (based on EqP-method)

Compound	new SRC_{eco} (mg/kg dw)	*old SRC_{eco} (mg/kg dw)*	new MPC (mg/kg dw)	*old MPC (mg/kg dw)*	new NC (mg/kg dw)	old NC (mg/kg dw)
2-propanol	200 [m]	220	20	-	0.2	-
Formaldehyde	1.6 [m]	0.30 (b)	0.16	-	0.0016	-
PCOC	13 [m]	15 (a)	1.2	-	0.012	-
PCMC	7.4 [m]	15 (a)	0.62	-	0.0062	-

-: Not derived
a: Based on combined data for PCOC and PCMC.
b: Based on the formaldehyde concentration in the water fraction in soil, as a K_p of 0 l/kg was used.
[m]: Reliability score: 'medium'.

<u>2-Propanol</u>
The slight difference between the new and old SRC_{eco} for water is due to the revision of one of the chronic NOEC values used in the refined effect assessment method (*Daphnia magna*: new NOEC of 330 mg/l *versus* the old NOEC of 770 mg/l). Likewise, the new SRC_{eco} for soil/sediment is slightly lower than the old value (there was no revision of the K_p).

Although the new SRC_{eco} for soil was derived with the equilibrium partitioning method from the SRC_{eco} for water (terrestrial toxicity data not available), a 'medium' reliability score is assigned to this SRC_{eco} for soil/sediment, as the SRC_{eco} for water is based on the refined effect assessment method and furthermore there is a reliable $K_{p.}$

Formaldehyde

The slight difference between the new and old SRC_{eco} for water is due to a revision of the dataset of chronic NOEC values (as additional data are now available) and due to the current use of the refined effect assessment method instead of the preliminary effect assessment method that was applied earlier. The considerable difference between the new and old SRC_{eco} for soil/sediment are mainly due to the revision of the K_p for soil/sediment: new K_p of 0.9 l/kg *versus* the old K_p of 0 l/kg. Thus, the new SRC_{eco} for soil/sediment is 5-times higher than the old value, although the new SRC_{eco} for water is slightly lower than the old value. Although the new SRC_{eco} for soil was derived with the equilibrium partitioning method from the SRC_{eco} for water (terrestrial toxicity data not available), a 'medium' reliability score is assigned to this SRC_{eco} for soil/sediment, as the SRC_{eco} for water is based on the refined effect assessment method and furthermore there is a reliable $K_{p.}$

Recently, Hohreiter and Rigg (2001) derived a *'chronic aquatic life water quality criterion'* of 1.6 mg/l for formaldehyde, using the U.S. EPA guidelines described in Stephan et al. (1985). Just like the MPC for water, this criterion is a risk limit aiming at the protection of aquatic ecosystems. It is noted that the criterion derived by Hohreiter and Rigg (2001) is considerably higher than the MPC (0.18 mg/l) derived by RIVM. The difference between the two values is due to a different selection of toxicity data and to the use of a different extrapolation method. In this RIVM report, the MPC was derived from the chronic NOEC values (including that for unicellular bacteria, cyanobacteria, protozoans and algae, see Table 4.3), applying statistical extrapolation according to Aldenberg and Jaworska (2000). Based on the U.S. EPA guidelines, the NOEC values for unicellular species were rejected by Hohreiter and Rigg (2001). Thus there were insufficient chronic values remaining to apply statistical extrapolation and the *'chronic aquatic life water quality criterion'* was derived from the *'final acute value' (*FAV: derived by statistical extrapolation from acute L(E)50 values) and the acute-to-chronic ratio (ACR)[3].

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[3] *Final acute value (FAV):* 9.2 mg/l. The FAV, which is the estimated concentration assumed to protect 95% of aquatic organisms from acute effects, is calculated from the four lowest genus mean acute values (GMAVs). Note that the FAV is equivalent to the $HC5^{L(E)C50}$, see Chapter 3).
Chronic aquatic life water quality criterion: 1.6 mg/l (FAV/ACR). The acute-to-chronic ratio (ACR) was calculated as the geometric mean value of the ACRs for three different species (families), being two actual ACRs (4.5 for the daphnid *Ceriodaphnia dubia* and 2.1 for the seed shrimp *Cypridopsis vidua)* and one default value of 20 for fish, resulting in a final ACR of 5.7.

For formaldehyde, the 'estimated threshold concentration' (ETC) in water for flavour impairment of fish is 95 mg/l and the no effect concentration for this effect is 56 mg/l, based on 48-h exposure of rainbow trout. The no effect concentration is similar to the 'threshold odour concentration' (TOC) in water which is 50 mg/l (Persson, 1984). The MPC as well as the SRC_{eco} for water derived in this RIVM report (0.18 and 1.8 mg/l, respectively) are considerably lower than the ETC and TOC, thus no effects on the palatability of fish and the odour of water will occur at concentrations as high as the SRC_{eco} or even considerably higher.

4-Chloromethylphenols

For both PCOC and PCMC there is a considerable difference between the new and old $SRCs_{eco}$ for water, due to differences in extrapolation methodology and underlying toxicity data. The new $SRCs_{eco}$ (for PCOC and PCMC, respectively) were derived with the preliminary effect assessment method using the toxicity data for the individual substances, while the old SRC_{eco} (one value for both PCOC and PCMC) was derived with the refined effect assessment method using the combined toxicity data. The differences between the new and old $SRCs_{eco}$ for soil/sediment are considerably lower than those for water, due to the revision of the K_p soil/sediment: new K_p of 24 l/kg *versus* the old K_p of 4.3 l/kg. Thus, the new $SRCs_{eco}$ for soil/sediment are within a factor of 2 of the old value, although the new $SRCs_{eco}$ for water are 7- to 12-times lower than the old value.
Although the new $SRCs_{eco}$ for soil were derived with the equilibrium partitioning method from the $SRCs_{eco}$ for water that were derived with the preliminary effect assessment method, a 'medium' reliability score is assigned to these $SRCs_{eco}$ for soil/sediment, as there is a useful terrestrial EC50 for both substances that support the result of the EqP method and furthermore there is a reliable K_p.

With respect to the differences in ERLs for PCOC and PCMC it is noted that there appears to be no real difference in toxicity when all available data are taken into consideration (see also section 4.2). If the aquatic toxicity data of both substances would be combined, this would allow the application of the refined effect assessment method which would result in ERLs (SRC_{eco}, MPC and NC) for both water and soil that are higher than the currently derived values. Moreover, the validity of the lowest two aquatic NOEC values for PCOC that were selected in the EU-RAR on PCOC (DEPA, 1998), including the key study used for PNEC and thus for MPC and NC derivation, are questionable (see footnotes Table 4.5) and there are additional, higher aquatic NOEC values for PCOC that are not included in the EU-RAR. Thus, the currently derived ERLs for PCOC and PCMC (for PCOC based on the data selection in the EU-RAR) are considered to be conservative.

For PCOC, the 'estimated threshold concentration' (ETC) in water for flavour impairment of fish is 0.03-0.075 mg/l, with a geometric mean of 0.05 mg/l, based on 48-h exposure of rainbow trout (no effect concentration not reported). The 'threshold odour concentration' (TOC) in water is 1.8 mg/l (Persson, 1984). It is noted that the MPC for water derived in this

RIVM report (0.05 mg/l) is equal to the geometric mean ETC and that the SRC_{eco} (0.55 mg/l) is considerably higher, thus effects on the palatability of fish may occur at concentrations as high as the MPC and especially the SRC_{eco}.

Human-toxicological evaluation

In the framework of the project ‘Setting Integrated Environmental Quality Standards’, MPCs for volatile compounds are evaluated with respect to the risk to humans exposed by air, water, food and soil contact. In the human-toxicological evaluation, critical exposure concentrations derived from human-toxicological data are compared to the ecotoxicological risk limits for consistency. For 2-propanol and formaldehyde, both being highly volatile compounds, the results of the human-toxicological evaluation will be reported later.

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30. dr. B. van Hattum (IVM)
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33. prof. dr. N. van Straalen (VU)
34. drs. M. Scholten (TNO)
35. drs. C. Reuther (RWS, Directie Noordzee)
36. drs. F. Noppert (RWS, Directie Oost)
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76. Hoofd Laboratorium voor Milieumetingen (RIVM/LVM)
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94. SBD/ Communicatie
95. Bureau Rapportenregistratie
96. Bibliotheek RIVM

97 -110. Bureau Rapportenbeheer

111-120. Reserve-exemplaren

Appendix 2: Aquatic toxicity data

Legend

Species (and properties)	Organism used in the test, followed by species properties (age, size, weight or life stage) if available.
Analysis	Y = test substance analyzed in test water. N = test substance not analyzed in test water.
Test type	S = static, R = static with renewal, F = flow through.
Test water	Freshwater nw = natural water, tw = tap water, aw = artificial (reconstituted) water (e.g. DSW: Dutch Standard water), nm = nutrient medium (non-liquid, e.g. agar). Saltwater nsw = natural seawater, asw = artificial (reconstituted) seawater.
pH	Initial value in test water, thus prior to the addition of the test substance (unless stated otherwise).
Hardness	Total (calcium plus magnesium) hardness, expresses as mg $CaCO_3$/l.
Exposure time	d = day(s), h = hour(s), m = month(s), min = minute(s), w = week(s), yr: year(s).
Criterion	LC50: Median lethal concentration, i.e. the concentration which is calculated from a series of test concentrations to cause mortality in 50% of the number of organisms exposed to that concentration. EC50: Median effect concentration, i.e. the concentration which is calculated from a series of test concentrations to cause a particular response in 50% of the number of organisms exposed to that concentration. EC(..%): At the concentration indicated (usually the only concentration tested), the toxicological endpoint was inhibited by ..%. Example: EC (21%). NOEC: No observed effect concentration, i.e. the highest concentration (in a series of test concentrations) without effect. In some cases, NOEC values have been estimated from effect concentrations. See section 3.2 for general information on NOEC derivation and the tables in this Appendix for study-specific information on ‘estimated’ NOEC values.
Endpoint	Toxicological endpoint, usually survival, growth and/or reproduction.
Value	A value preceeded by ‘>’ is the highest concentration used in the test. When no effect is found at the highest test concentration, the ‘unbounded’ NOEC is not useful because the real NOEC may be higher. Likewise, ‘unbounded’ L(E)C50 values are not useful.
-	No data available.

Table A2-1a: Chronic toxicity of 2-propanol (isopropanol) to freshwater organisms: NOEC values useful for ERL derivation

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test Water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value * (mg/l)	Note	Reference
Bacteria													
Pseudomonas putida		N	S	-	aw	7.0	-	16 h	NOEC	growth (biomass)	**1100**	1	Bringmann & Kühn, 1976, 1977a, 1980b
Cyanobacteria													
Microcystus aeruginosa		N	S	-	aw	7.0	-	8 d	NOEC	growth (biomass)	**1000**	1	Bringmann & Kühn, ’75, ’76, 78a,b
Protozoa													
Chilomonas paramecium		N	S	-	aw	6.9	-	48 h	NOEC	growth (biomass)	**100**	1	Bringmann et al., 1980
Entosiphon sulcatum		N	S	-	aw	5.9	-	72 h	NOEC	growth (biomass)	**4900**	1	Bringmann, 1978; Bringmann & Kühn, 1980b
Uronema parduczi		N	S	-	aw	6.9	-	20 h	NOEC	growth (biomass)	**3400**		Bringmann & Kühn, 1980a
Algae (unicellular)													
Scenedesmus quadricauda		N	S	-	aw	7.0	-	8 d	NOEC	growth (biomass)	**1800**	1	Bringmann & Kühn, 1977a, 1978a,b, 1980b
Crustacea													
Daphnia magna	age < 24 h	Y	R	-	aw (DSW)	8.0-8.4	200	16 d	NOEC	growth reproduction	**770** 1400		De Wolf et al., 1988
Daphnia magna	age <24 h	Y	S	-	aw (DSW)	8.0-8.4	200	16 d	NOEC	growth	**140**		Hermens et al., 1985

* The NOEC values that have been printed **bold** were used for ERL derivation (after calculation of the geometric ‘species mean’ NOEC, where appropriate; see Chapter 4).

1. Bringmann & Kühn studies: NOEC = Toxic Threshold (TT), defined as the concentration at which 3%-5% inhibition occurs (the limit of 3% or 5% depends on the species tested).

Table A2-1b: Acute toxicity of 2-propanol (isopropanol) to freshwater organisms: LC50 and EC50 values useful for ERL derivation

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
Protozoa													
Tetrahymena pyriformis		N	S	-	aw	7.4	75	40 h	EC50	growth (biomass)	4600		Schultz, 1997
Crustacea													
Daphnia magna		-	-	-	-	-	-	48 h	EC50		7800		Genoni, 1997
Daphnia magna	age < 24 h	N	S	-	aw	8.0	250	24 h	EC50	mobility	9700		Bringmann & Kühn, 1982
Daphnia magna	age < 24 h	Y	S	-	aw (DSW)	8.0-8.4	200	48 h	EC50	mobility	2300		Hermens et al., 1984
Daphnia magna	age 24 h	N	S	-	aw	7.6	190	24 h	EC50		6900		Lilius et al., 1995
Daphnia pulex	age 24 h	N	S	-	aw	7.6	190	24 h	EC50		10000		Lilius et al., 1995
Insecta													
Aedes aegypti	3th instar larvae	-	S	-	-	-	-	4 h	LC50		25000		Kramer et al., 1983, cited in WHO, 1990
Pisces													
Leuciscus idus melanotus	weiight 1.5 g	N	S	-	tw	7.0	255	48 h	LC50		9000	1	Juhnke & Lüdemann, 1978
Leuciscus idus melanotus	weight 1.5 g	N	S	-	tw	7.0	255	48 h	LC50		9300	1	Juhnke & Lüdemann, 1978
Leuciscus idus melanotus	-	-	-	-	-	-	-	96 h	LC50		8900		Gunatilleka & Poole, 1999
Pimephales promelas	-	-	-	-	-	-	-	96 h	LC50		8700		Gunatilleka & Poole, 1999
Pimephales promelas	-	-	-	-	-	-	-	96 h	LC50		10000		Genoni, 1997
Pimephales promelas	-	Y	F	-	-	7.5	45	96 h	LC50		9600		Veith et al., 1983, cited in W HO, 1990 and IUCLID, 2000
Pimephales promelas	-	-	S	-	-	-	-	96 h	LC50		11000		Mattson et al., 1976, cited in WHO, 1990
Pimephales promelas	-	-	F	-	-	-	-	96 h	LC50		9700		U.S EPA, cited in Schullz, 1997
Poecilia reticulata	age 2-3 m	N	R	-	-	-	25	7 d	LC50		7100		Könemann, 1981
Poecilia reticulata	-	-	-	-	-	-	-	96 h	LC50		8700		Gunatilleka & Poole, 1999
Rasbora heteromorpha	length 1-3 cm	N	F	90%	-	8.1	20	96 h	LC50		4200	2	Tooby & Hursey, 1975

1. Results of tests performed in two different test laboratories (comparable test conditiions). Data on standardized test conditions in *Leuciscus idus* test: from Hamburger et al. (1977).
2. *Rasbora heteromorpha:* saltwater fish, but test assumed to be performed in freshwater (see low value for hardness).

Table A2-1c. Acute toxicity of 2-propanol (isopropanol) to saltwater organisms: LC50 and EC50 values useful for ERL derivation

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Salinity (^{0}/oo)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
Bacteria													
Vibrio fisheri		N	S	-	asw	-	20	5 min	EC50	biolumin.	35000	1,2	Cronin & Schultz, 1997
Vibrio fisheri		N	S	pure	asw	-	20	5 min	EC50	biolomin	42000	1,2	Bulich et al., 1981
Vibrio fisheri		-	S	-	-	-	20	15 min	EC50	biolumin.	22000	1,2,3	Bulich et al., 1990, cited in IUCLID, 2000
Vibrio harveyi		-	S	-	asw	7	25	5 h	EC50	biolumin.	3200	5	Thomulka et al., 1993
Escherichia coli		-	S	-	-	7.4	8	1 h	EC50	biolumin.	790	1,4	Lampinen et al., 1999
Crustacea													
Crangon crangon	-	N	R	-	nsw	-	-	96 h	LC50		1200		Blackman, 1974

1. Microtox test (standardized bacterial bioluminescence test with *Vibrio fisheri*).
2 Salinity (20 ^{0}/oo) is based on that in standard medium for *Vibrio fisheri* (reported in Lampinen et al., 1999).
3. Although the primary publication (Bulich et al., 1990) was not checked, the test is considered useful for ERL derivation since this is a standardized test.
4. Test species *Escherichia coli* cloned wtih bacterial *Vibrio harveyi* genes encoding luciferase.
5. Two different bacterial bioluminescence tests were performed with living *Vibrio harveyi* cells, one with growing cell suspensions (EC50: 3200 mg/l, this table) and one with non-growing cell suspensions (EC50: >10000, see Table A2-e1). These methods differ from the standardized Microtox test which uses rehydrated suspensions of lyophilized *Vibrio fisheri* cells.

Table A2-1d: Chronic and acute toxicity of 2-propanol (isopropanol) to freshwater organisms: additional data (not useful for ERL derivation)

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
CHRONIC TOXICITY													
Bacteria													
Pseudomonas putida		-	S	-	tw	-	-	3 h	TT	respiration rate	>1000	5	Gerike & Gode, 1990
Pseudomonas putida		-	-	-	-	-	-	18 h	NOEC (EC10)	growth (rate)	5200		Huels AG (not available: confidential), cited in IUCLID, 2000
Algae (unicellular)													
Scenedesmus subspicatus		-	-	-	-	-	-	96 h	NOEC	growth (rate)	1000		Knacker et al., 1989 (not available), cited in IUCLID, 2000
Crustacea													
Daphnia magna	-	-	-	-	-	-	-	21 d	NOEC	-	30	2	Huels AG (not available: confidential, cited in IUCLID, 2000
ACUTE TOXICITY													
Crustacea													
Daphnia magna	age ≤ 24 h	N	S	-	tw	7.6	270	24 h	EC50	mobilily	>10000		Bringmann & Kühn, 1977b
Daphnia magna	-	-	-	-	-	-	-	48 h	EC50	mobility	13000		McCauley (no futher bibliographic data), cited in Vaishnav & Korthals, 1990
Insecta													
Drosophila melanogaster.	eggs, larvae	-	S	-	nm	-	-	-	EC(74%)	viability	7900	4	Vilageliu, 1980, cited in WHO, 1990
Drosophila melanogaster and D. simulans	larvae	-	S	-	nm	-	-	48 h	LC50		11400	1,4	David & Bocquet, 1976, cited in WHO, 1990
Drosophila simulans	eggs, larvae	-	S	-	nm	-	-	-	EC(100%)	development	7900	4	Vilageliu, 1980, cited in WHO, 1990
Pisces													
Carassius auratus	-	Y	S	-	-	6.0-8.0	-	24 h	LC50		>5000		Bridie et al., 1979, cited in WHO, 1990 and IUCLID, 2000
Pimephales promelas	-	-	S	-	-	5.9	-	96 h	LC50		11000		Mattson et al., 1996, cited in IUCLID, 2000
Semolitus atromaculatus	-	-	S	-	-	8.3	98	24 h	NOEC	survival	900		Gillette et al., 1952, cited in IUCLID, 2000
Amphibia													
Rana pipiens	tadpoles	-	S	-	tw	-	-	acute	EC(100%)	narcosis	23000	3	Munch, 1972
-	tadpoles	-	-	-	-	-	-	-	EC(100%)	narcosis	7800	3	Overton, 1901, cited in Munch, 1972

Footnotes Table A2-1d

1. Geometric mean of 10000 and 13000 mg/l (the LC50 values for the two *Drosophila* species were reported to be between these concentrations).
2. Endpoint not reported.
3. Result reported as Threshold Narcotic Concentration, defined as the concentration at which touching the tadpoles failed to cause motion. This concentration is assumed to affect all animals exposed.
4. *Drosophila sp.* tests: in nutrient medium, assumed to be agar or comparable non-liquid medium.
5. Modified OECD 209 (Activated sludge respiration inhibition test): *Pseudomonas putida* used as bacterial inoculum instead of activated sludge. NOEC = Toxic Threshold, reported as inhibition limit (definition and method of derivation of this threshold concentration were not reported). Data on test conditions not reported, but based on OECD 209. The test is not useful for ERL derivation since the Toxic Threshold is unbounded and not defined. In addition, it is assumed that sludge, inoculated with *P. putida*, was present in the test water.

Table A2-1e: Acute toxicity of 2-propanol (isopropanol) to saltwater organisms: additional data (not useful for ERL derivation)

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Salinity (^{0}/oo)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
Bacteria													
Vibrio fisheri		-	S	-	-	7	-	2 min	TT	biolomin.	15000	1	Bulich, 1979, cited in WHO, 1990
Vbrio harveyi		-	S	asw	-	7	-	1 h	EC50	biolumin.	>10000	2	Thomulka et al., 1993
Tubificidae													
Tubifex tubifex	-	-	S	-	-	-	-	2 min	EC100	mobility	51000		Chvapil et al., 196, cited in WHO, 1990 and IUCLID, 2000
Crustacea													
Artemia salina	-	-	S	-	-	-	-	24 h	EC50	-	>10000		Price et al., 1974, cited in WHO, 1990 and IUCLID, 2000

1. Microtox test (standardized bacterial bioluminescence test with *vibrio fisheri*). TT = Toxic threshold. The test is not useful for ERL derivation since the definition and method of derivation of this hreshold concentration were not reported.
2. Two different bacterial bioluminescence tests were performed with living *Vibrio harveyi* cells, one with non-growing cell suspensions (EC50: >10000; this table) and one with growing cell suspensions (EC50: 3200 mg/l, see Table A2-1c). These methods differ from the standardized Microtox test which uses rehydrated suspensions of lyophilized *Vibrio fisheri* cells.

Table A2-2a. Chronic toxicity of formaldehyde to freshwater organisms: NOEC values useful for ERL derivation (NOEC values as formaldehyde, i.e 100 a.i.)

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value * (mg/l)	Note	Reference
Bacteria													
Escherischia coli		N	S	-	nw	7.5	200	> 6 h	NOEC	glucose deg.	**1**	3, 4	Bringmann & Kühn, 1959, 1960
Pseudomonas fluorescens		N	S	-	nw	7.5	200	> 16 h	NOEC	glucose deg.	**2**	3, 4	Bringmann & Kühn, 1960
Pseudomonas fluorescens		N	S	35%	aw	7.0	-	16 h	NOEC	growth (biomass)	4.9	3	Bringmann & Kühn, 1973
Pseudomonas putida		N	S	35%	aw	7.0	-	16 h	NOEC	growth (biomass)	**4.9**	1,3	Bringmann & Kühn, 1976, 1977a, 1980b
Cyanobacteria													
Microcystus aeruginosa		N	S	35%	aw	7.0	-	8 d	NOEC	growth (biomass)	**0.14**	1,3	Bringmann & Kühn, '75, 76, 78a,b
Protozoa													
Chilomonas paramaecium		N	S	35%	aw	6.9	-	48 h	NOEC	growth (biomass)	**1.6**	1,3	Bringmann et al.,1980
Colpoda aspera		N	*S*	37%	aw	6.9	-	24 h	NOEC (EC10)	growth (rate)	**0.78**	1	Kachiichi et al., 1995
Entosiphon sulcatum		N	S	35%	aw	5.9	-	72 h	NOEC	growth (biomass)	**7.7**	1,3	Bringmann, 1978, Bringmann & Kühn, 1980b
Uronema parduczi		N	S	35%	aw	6.9	-	20 h	NOEC	growth (biomass)	**2.3**	1,3	Bringmann & Kühn, 1980a
Algae (unicellular)													
Scenedesmus quadricauda		N	S	-	nw	7.5	200	96 h	NOEC	growth (biomass)	**0.3**	3,4	Bringmann & Kühn, 1959, 1960
Scenedesmus quadricauda		N	S	35%	aw	7.0	-	8 d	NOEC	growth (biomass)	**0.88**	1,3	Bringmann & Kühn, 1977a, 1978a,b, 1980b
Scenedesmus quadricauda		N	S	37%	nw	8.4	230	24 h	NOEC (EC10)	assimilation	3.6	5	Tisler & Zagorc-Koncan, 1997
Crustacea													
Ceriodaphnia dubia	age < 24 h	-	R	-	-	-	-	7 d	NOEC	survival and mobilty	**1.7**	2	Vasu, 1990), cited in Hohreiter & Rigg, 2001
Cypridopsis vidua	-	Y	-	-	-	-	-	5 w	NOEC	survival and reproduction	**19**	6	Cooney & Bourgoin, 2001, cited in Hohreiter & Rigg, 2001

Footnote Table A2-2a

* The NOEC values that have been printed bold were used for ERL derivation (after calculation of the geometric 'species mean' NOEC, where appropriate; see Chapter 4).

1. Value adjusted to formaldehyde-basis (100% a.i); test substance and results originally reported by the authors of the study as formalin (mg/l) e.g. as formalin (37%) which is a solution of 37% (w/w or v/v) of formaldehyde gas in water.
   (Note: According to the Merck Index and other publications, formalin 37% by weight is the "full strength" commercial grade formalin and also known as Formalin 100% or Formalin 40 which signifies that it contains 40 grams of formaldehyde within 100 ml of the solution; $D^{25}_{25} = 1.08$).
2. Geometric mean of 1.0 and 3.0 mg/l (results of two tests). Although the primary publication (Vasu, 1990) is not available, the study is accepted for ERL derivation since it concerns a standardized test: (7-d *Ceriodaphnia dubia* chronic toxicity test; life-cycle test) and the test was accepted by Hohreiter & Rigg (2001). Data on test method from Masters et al. (1991) in which the method is summarised. See Mount and Norberg (1984) for a full description of the 7-d *C. dubia* test.
3. Bringmann & Kühn studies: NOEC = Toxic Threshold (TT), defined as the concentration at which 3%-5% inhibition occurs (the limit of 3% or 5% depends on the oganism tested).
4. Test substance reported as formaldehyd; results (reported in mg/l) assumed to be 100% a.i. In the *Escherischia coli* test and the *Pseudomonas fluorescens* tests, the inhibition of glucose degradation in the test water was studied by pH measurements: glucose degradation results in a decrease in pH value.
5. Test substance reported as formaldehyd; results (reported in mg/l) assumed to be 100% a.i. The net accumulation was studied by measuring the oxygen production and consumption rates.
6. NOEC based on actual formaldehyde concentrations; the nominal NOEC was 25 mg/l. Although the primary publication (Cooney & Bourgoin, 2001; in preparation) is not available, the study is accepted for ERL derivation since the test was accepted by Hohreiter & Rigg (2001) and reported to be performed using currently accepted U.S. EPA method and QA/QC procedures.

Table A2-2b: Acute toxicity of formaldehyde to freshwater organisms: LC50 and EC50 values useful for ERL derivation (LC50 and EC50 values as formaldehyde, i.e 100% a.i.)

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
Algae (unicellular)													
Scenedesmus quadricauda		N	S	37%	nw	8.4	230	24 h	EC50	assimilation	15	10	Tisler & Zagorc-Koncan, 1997
Protozoa													
Colpoda aspera		N	*S*	37%	aw	6.9	-	24 h	EC50	growth (rate)	2.0	2	Kachiichi et al., 1995
Mollusca													
Corbicula leana	-	N	S	37%	aw	7.5	"soft"	96 h	EC50		50	2,3	Bills et al., 1977
Corbicula manilensis	-	N	F	-	-	-	-	96 h	L(E)C50	-	35	16	Chandler & Marking, 1979, cited in Hohreiter & Rigg, 2001
Corbicula manilensis	-	N	S	-	-	-	-	96 h	L(E)C50	-	47	16	Chandler & Marking, 1979, cited in Hohreiter & Rigg, 2001
Helisoma sp.	-	N		37%	aw	6.5	20	96 h	EC50		37	2,4	Bills et al., 1977
Crustacea													
Bosmina sp.	-	N	-	-	-	-	-	96 h	EC50	-	20	16	Prasad, 1980, cited in Hohreiter & Rigg, 2001
Ceriodaphnia dubia	-	N	S	-	-	-	-	48 h	EC50	mobility	13	2	Warne & Schifko, 1999
Ceridaphnia dubia	-	Y	S	-	-	-	-	48 h	L(E)C50	survival and behaviour	9.5	11,14, 16	Cooney & Bourgoin, 2001, cited in Hohreiter & Rigg, 2001
Ceriodaphnia dubia	≤ 24 h	N	S	-	-	-	-	48 h	L(E)C50	-	12	16, 23	Vasu, 1990, cited in Hohreiter & Rigg, 2001
Cyclops sp.	-	N	-	-	-	-	-	96 h	EC50	-	20	16	Prasad, 1980, cited in Hohreiter & Rigg, 2001
Cypridopsis vidua	>300 µm	Y	R	-	-	-	-	96 h	LC50 EC50	survival behaviour	104 63	11,12 11,13, 16	Cooney & Bourgoin, 2001, cited in Hohretier & Rigg, 2001

Table A2-2b: Acute toxicity of formaldehyde to freshwater organisms: LC50 and EC50 values useful for ERL derivation (continued) (LC50 and EC50 values as formaldehyde, i.e 100% a.i.)

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
Crustacea (continued)													
Daphnia magna	≤ 24 h	N	S	35%	tw	7.6	270	24 h	EC50	mobility	18	2	Bringmann & Kühn, 1977b
Daphnia magna	≤ 24 h	N	S	35%	aw	8.0	250	24 h	EC50	mobility	15	2	Bringmann & Kühn, 1982
Daphnia magna	-	-	-	-	-	-	-	24 h	EC50		60		Todeschini et al., 1996
Daphnia magna	-	N	S	-	-	-	-	48 h	EC50	-	29	16	Janssen & Persoone, 1993, cited in Hohreiter & Rigg, 2001
Dapnia magna	-	N	R	-	-	-	-	48 h	EC50	-	7.6	16	Nazarenko, 1960, cited in Hohreiter & Rigg, 2001
Daphnia magna		N	-	-	-	-	-	96 h	EC50	-	20	16	Prasad, 1980, cited in Hohreiter & Rigg, 2001
Daphnia pulex	-	Y	S	-	-	-	-	48 h	L(E)C50	survival and behaviour	13	11,15, 16	Cooney & Bourgoin, 2001, cited in Hohreiter & Rigg, 2001
Daphnia pulex	< 24 h	N	S	37%	nw	8.4	230	48 h	EC50	mobility	5.8	10	Tisler & Zagorc-Koncan, 1997
Palaemonetes kadiakensis	-	N	S	37%	nw	6.5	20	96 h	EC50	mobility	186	2	Bills et al., 1977
Insecta													
Chironomus sp.	-	N	-	-	-	-	-	96	L(E)C50	-	450		Prasad, 1980, cited in Hohreiter & Riggs, 2001
Notonecta sp.	-	N	S	37%	aw	6.5	20	96 h	EC50		330	2,4	Bills et al., 1977
Pisces													
Anguilla rostrata	glass eels	N	S	37%	-	-	-	96 h	LC50		31	2,16, 20,22	Hinton & Eversole, 1978, cited in Hohreiter & Rigg, 2001
Ictalurus (Ameiuruas) melas	0.8 g	N	F	37%	aw	7.5	"soft"	96 h	LC50		25	1,2	Bills et al., 1977
Ictalurus punctatus	0.4 g	N	F	37%	aw	6.6	"very soft"	96 h	LC50		28	1,2	Bills et al., 1977
Ictalurus punctatus	0.4 g	N	F	37%	aw	6.5	"soft"	96 h	LC50		25	1,2	Bills et al., 1977
Ictalurus punctatus	0.4 g	N	F	37%	aw	7.5	"soft"	96 h	LC50		26	1,2,6,7 11	Bills et al., 1977
Ictalurus punctatus	0.4 g	N	F	37%	aw	8.5	"soft"	96 h	LC50		23	1,2	Bills et al., 1977
Ictalurus punctatus	0.4 g	N	F	37%	aw	7.8	"hard"	96 h	LC50		20	1,2	Bills et al., 1977
Ictalurus punctatus	0.4 g	N	F	37%	aw	8.2	"very hard"	96 h	LC50		25	1,2	Bills et al., 1977
Ictalurus punctatus	finger-lings	N	S	37%	-	-	-	96 h	LC50		28	2,16	Clemens & Sneed, 1958m, cited in Hohreiter & Rigg, 2001
Ictalurus punctatus	fry	N	S	37%	-	-	-	96 h	LC50		17	2,16, 21	Howe et al., 1995, cited in Hohreiter & Rigg, 2001

Table A2-2b: Acute toxicity of formaldehyde to freshwater organisms: LC50 and EC50 values useful for ERL derivation (continued) (LC50 and EC50 values as formaldehyde, i.e 100% a.i.)

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
Pisces (continued)													
Lepomis cyanellus	0.7 g	N	F	37%	aw	7.5	"soft"	96 h	LC50		69	1,2	Bills et al., 1977
Lepomis macrochirus	0.5 g	N	F	37%	aw	6.6	"very soft"	96 h	LC50		35	1,2	Bills et al., 1977
Lepomis macrochirus	0.5 g	N	F	37%	aw	6.5	"soft"	96 h	LC50		50	1,2	Bills et al., 1977
Lepomis macrochirus	0.5 g	N	F	37%	aw	7.5	"soft"	96 h	LC50		40	1,2, 6	Bills et al., 1977
Lepomis macrochirus	0.5 g	N	F	37%	aw	7.5	"soft"	96 h	LC50		29	1,2, 7	Bills et al., 1977
Lepomis macrochirus	0.5 g	N	F	37%	aw	7.5	"soft"	96 h	LC50		36	1,2, 8	Bills et al., 1977
Lepomis macrochirus	0.5 g	N	F	37%	aw	8.5	"soft"	96 h	LC50		34	1,2	Bills et al., 1977
Lepomis macrochirus	0.5 g	N	F	37%	aw	7.8	"hard"	96 h	LC50		42	1,2	Bills et al., 1977
Lepomis macrochirus	0.5 g	N	F	37%	aw	8.2	"very hard"	96 h	LC50		47	1,2	Bills et al., 1977
Leuciscus idus melanotus	1.5 g	N	S	30%	tw	7.0	255	48 h	LC50		15	2,9	Juhnke & Lüdemann, 1978
Leuciscus idus melanotus	1.5 g	N	S	30%	tw	7.0	255	48 h	LC50		32	2,9	Juhnke & Lüdemann, 1978
Micropterus dolomieui	0.7 g	N	F	37%	aw	7.5	"soft"	96 h	LC50		54	1,2	Bills et al., 1977
Micropterus salmoides	1 g	N	F	37%	aw	7.5	"soft"	96 h	LC50		57	1,2	Bills et al., 1977
Morone saxatilis	finger-lings	N	S	37%	-	-	-	96 h	LC50		7.3	2,16	Wellborn, 1969; cited in Hohreiter & Rigg, 2001
Morone saxatilis	fry	N	S	-	-	-	-	96 h	LC50		10	2,16	Hughes, 1973, cited in Hohreiter & Rigg, 2001
Morone saxatilis	finger-lings	N	S	-	-	-	-	96 h	LC50		15	2,16	Hughes, 1973, cited in Hohreiter & Rigg, 2001
Morone saxatilis	-	N	S	37%	-	-	-	96 h	LC50		28	2,16, 17	Bills et al., 1993, cited in Hohreiter & Rigg, 2001
Morone saxatilis	-	N	S	37%	-	-	-	96 h	LC50		21	2,16, 17	Bills et al., 1993, cited in Hohreiter & Rigg, 2001
Morone saxatilis	-	N	S	37%	-	-	-	96 h	LC50		18	2,16, 17	Bills et al., 1993, cited in Hohreiter & Rigg, 2001
Morone saxatilis	-	N	S	37%	-	-	-	96 h	LC50		11	2,16, 17	Bills et al., 1993, cited in Hohreiter & Rigg, 2001
Morone saxatilis	-	N	S	37%	-	-	-	96 h	LC50		16	2,16, 17	Bills et al., 1993, cited in Hohreiter & Rigg, 2001

Table A2-2b: Acute toxicity of formaldehyde to freshwater organisms: LC50 and EC50 values useful for ERL derivation (continued) (LC50 and EC50 values as formaldehyde, i.e 100% a.i.)

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
Pisces (continued)													
Morone saxatilis (continued)	-	N	S	37%	-	-	-	96 h	LC50		19	2,16, 17	Bills et al., 1993, cited in Hohreiter & Rigg, 2001
Morone saxatilis	-	N	S	37%	-	-	-	96 h	LC50		24	2,16, 17	Bills et al., 1993, cited in Hohreiter & Rigg, 2001
Morone saxatilis	-	N	S	37%	-	-	-	96 h	LC50		20	2,16, 17	Bills et al., 1993, cited in Hohreiter & Rigg, 2001
Morone saxatilis	-	N	S	37%	-	-	-	96 h	LC50		22	2,16, 17	Bills et al., 1993, cited in Hohreiter & Rigg, 2001
Morone saxatilis	-	N	S	37%	-	-	-	96 h	LC50		24	2,16, 17	Bills et al., 1993, cited in Hohreiter & Rigg, 2001
Oncorhynchus mykiss	0.6 g	N	F	37%	aw	6.5	“soft”	96 h	LC50		68	1,2	Bills et al., 1977
Oncorhynchus mykiss	0.6 g	N	F	37%	aw	7.5	“soft”	96 h	LC50		47	1,2	Bills et al., 1977
Oncorhynchus mykiss	0.6 g	N	F	37%	aw	8.5	“soft”	96 h	LC50		69	1,2	Bills et al., 1977
Oncorhynchus mykiss	0.6 g	N	F	37%	aw	7.8	“hard”	96 h	LC50		69	1,2	Bills et al., 1977
Oncorhynchus mykiss	0.6 g	N	F	37%	aw	8.2	“very hard”	96 h	LC50		68	1,2	Bills et al., 1977
Oncorhynchus mykiss	10 cm	N	S	37%	nw	8.4	230	48 h	LC50		50	10	Tišler & Zagorc-Končan, 1997
Oncorhynchus mykiss	-	N	F	37%	-	-	-	96 h	LC50		60	2,16	Bills et al., 1981, cited in Hohreiter & Rigg, 2001
Oncorhynchus mykiss	fry	N	S	37%	-	-	-	96 h	LC50		50	2,16, 18,20	Howe et al., 1995, cited in Hohreiter & Rigg, 2001
Oncorhynchus mykiss	finger-lings	N	S	37%	-	-	-	96 h	L(E)C50		54	2,16, 19,20	Bills, 1974, cited in Hohreiter & Rigg, 2001
Pimephales promelas	age 7 d	Y	R	-	-	-	-	96 h	L(E)C50	survival and behaviour	27	11,16	Cooney & Bourgoin, 2001, cited in Hohretier & Rigg, 2001
Pimephales promelas	juveniles	Y	R	37%		-	-	96 h	LC50		24	16	Geiger et al., 1990, cited in Hohreiter & Rigg, 2001
Poecilia reticulata	9-13 w	-	R	-	aw	6.5-7.5	20	14 d	LC50		27	5	Deneer et al., 1988
Salmo salar	0.6 g	N	F	37%	aw	7.5	“soft”	96 h	LC50		69	2	Bills et al., 1977
Salvelinus namaycush	0.5 g	N	F	37%	aw	7.5	“soft”	96 h	LC50		40	2	Bills et al., 1977

Table A2-2b: Acute toxicity of formaldehyde to freshwater organisms: LC50 and EC50 values useful for ERL derivation (continued) (LC50 and EC50 values as formaldehyde, i.e 100% a.i.)

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
Amphibians													
Bufo sp.	tadpoles	N	S	-	-	-	-	72 h	LC50		19	16	Helms, 1967, cited in Hohreiter & Rigg, 2001
Rana catesbeiana	tadpoles (1-2 inches)	N	S	-	-	-	-	72 h	LC50		10	16,20, 23	Helms, 1967, cited in Hohreiter & Rigg, 2001
Rana pipiens	tadpoles	N	S	-	-	-	-	72 h	LC50		8.7	16	Helms, 1967, cited in Hohreiter & Rigg, 2001

Footnotes Table A2-2b

1. Bills et al. (1977): All fish tests performed at T = 12 ^{0}C, unless stated otherwise. Tested life stage: fingerlings. Both flow-through tests and static tests were performed, it was not indicated which species were tested in which test system. It is assumed that the fish species were tested in a flow-through system and the invertebrates in a static system.
2. Value adjusted to formaldehyd-basis (100% a.i); test substance and results originally reported by the authors of the study as formalin (in mg/l or µl/l), e.g. as formalin (37%) which is a solution of 37% (w/w or v/v) of formaldehyde gas in water.
(Note: According to the Merck Index and other publications, formalin 37% by weight is the "full strength" commercial grade formalin and also known as Formalin 100% or Formalin 40 which signifies that it contains 40 grams of formaldehyde within 100 ml of the solution; D^{25}_{25} = 1.08).
3. Ability to resist attempts to open valves and respond to tactile stimulus.
4. Ability to respond to tactile stimulus.
5. Value corrected for loss of the compound during the 24-h period between renewal of the solutions.
6. LC50 at 12 deg. C.
7. LC50 at 17 deg. C.
8. LC50 at 22 deg. C
9. Results of tests performed in two different test laboratories (comparable conditions). Data on standardized test conditions in *Leuciscus idus* test: from Hamburger et al. (1977).
10. Test substance reported as formaldehyd; results (reported in mg/l) assumed to be 100% a.i.
11. Results based on actual formaldehyde concentrations.
12. Geometric mean of 98 mg/l (test 1, temperature not reported), 99 mg/l (test 2, at 25 ^{0}C) and 114 mg/l (test 3, at 16 ^{0}C).
13. Geometric mean of 68 mg/l (test 1, temperature not reported), 69 mg/l (test 2, at 25 ^{0}C) and 54 mg/l (test 3, at 16 ^{0}C).
14. Geometric mean of 9.5 and 9.6 mg/l.
15 Geometric mean of 12 and 15 mg/l.
16. Although the primary publications have not been evaluated in this report, the studies are considered useful for ERL derivation since these studies were accepted by Hohreiter & Rigg (2001) on the basis of current U.S. EPA criteria. All values reported in Hohreiter & Rigg (20001) are reported as formaldehyde (100% a.i), thus adjusted from formalin when appropriate.
17. Bills et al. (1993) used test waters with various water characteristics (no further details given in Hohreiter & Rigg, 2001).
18. Geometric mean of 50, 50, 50 and 49 mg/l (four tests, with combinations of formalin and paraformalin, i.e polymerized formalin). Green eggs were found to be less sensitive than fry. See also footnote 20.
19. Geometric mean of 58, 54 and 50 mg/l. Green eggs, eyed eggs and sac fry were found to be less sensitive than fingerlings (sensitivity increased with age). See also footnote 20.
20. According to U.S. EPA guidelines, the L(E)C50 values for less sensitive life stages were not used by Hohreiter & Rigg (2001) for the derivation of water quality criteria, provided the difference in sensitivity is at least a fastor of two. Hence, only the data for the most sensitive life stage were reported in Hohreiter & Rigg (2001).
21. Geometric mean of 22, 14, 14 and 19 mg/l (four tests, with combinations of formalin and paraformalin, i.e polymerized formalin).
22. Black eel and adult eel were found to be less sensitive than glass eel. See also footnote 20.
23. Larger tadpoles were found to be less sensitive than the smallest (1-2 inches) tadpoles.

Table A2-2c: Acute toxicity of formaldehyde to saltwater organisms: LC50 and EC50 values useful for ERL derivation (LC50 and EC50 values as formaldehyde, i.e 100% a.i.)

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Salinity (^{o}/oo)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
Bacteria													
Vibrio fisheri		N	S	-	asw	-	20	5 min	EC50	biolumin.	3	3	Bulich et al., 1981
Vibrio fisheri		-	S	-	asw	-	20	30 min	EC50	biolumin.	8.5	3	McKinnon & Kaiser, 1993
Vibrio harveyi		-	S	-	asw	7	25	1 h	EC50	biolumin.	0.44	1,4	Thomulka et al., 1993
Vibrio harveyi		-	S	-	asw	7	25	5 h	EC50	biolumin.	1.4	1,4	Thomulka et al., 1993
Pisces													
Morone saxatilis	1.8 g	N	S	37%	asw (I)	8.4	5 (H = 620)	96 h	LC50		5.0	1,2	Reardon & Harrell, 1990
Morone saxatilis	1.8 g	N	S	37%	asw (I)	8.2	10 (H = 1600)	96 h	LC50		5.7	1,2	Reardon & Harrell, 1990
Morone saxatilis	1.8 g	N	S	37%	asw (II)	7.6	10 (H = 1800)	96 h	LC50		3.9	1,2	Reardon & Harrell, 1990
Morone saxatilis	1.8 g	N	S	37%	asw (I)	8.3	15 (H = 2400)	96 h	LC50		4.0	1,2	Reardon & Harrell, 1990

1. Value adjusted to formaldehyde-basis (100% a.i.); test substance and results originally reported by the authors of the study as formalin (purity of 37%) in Reardon & Harrell (1990) and unspecified purity in Thomulka et al. (1993), the latter also assumed to be formalin 37% (w/w/).
(Note: According to the Merck Index and other publications, formalin 37% by weight is the "full strength" commercial grade formalin and also known as Formalin 100% or Formalin 40 which signifies that it contains 40 grams of formaldehyde within 100 ml of the solution; D^{25}_{25} = 1.08).
2. Test water I = ground water plus synthetic sea salt; salinity 5, 10 or 15 ^{0}/oo. Test water II = river water plus synthetic sea salt; salinity 10 ^{0}/oo. All test fish were acclimated to the 10 ^{0}/oo saliniity (the salinity which is isosmotic to *M. saxatilis)* river water prior to testing. The LC50 values at the different salinities were not significantly different from each other, but were significantly higher than the LC50 of 1.8 mg/l from a test performed in groundwater without sea salt added, see Table A2-2d. H = hardness.
3. Microtox test (standardized bacterial bioluminescence test with *Vibrio fisheri*). The salinity (20 ^{0}/oo) is based on that in standard medium for *Vibrio fisheri* (reported in Lampinen et al., 1999).
4. Two different bacterial bioluminescence tests were performed with living *Vibrio harveyi* cells, one with non-growing cell suspensions (EC50: 0.44 mg/l) and one with growing cell suspensions (EC50: 1.4 mg/l). These methods differ from the standardized Microtox test which uses rehydrated suspensions of lyophilized *Vibrio fisheri* cells.

Table A2-2d: Chronic and acute toxicity of formaldehyde to freshwater organisms: additional data (<u>not</u> useful for ERL derivation)
(Toxicity values as values as formaldehyde, i.e 100% a.i.)

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
CHRONIC TOXICITY													
Bacteria													
Alcaligenes faecalis		N	S	37%	aw	6.9	-	24 h	TT	growth	19	2,5	Kachiichi et al., 1995
Municipal wastewater bacteria (mixed culture)		N	S	37%	nw	8.4	230	120 h	EC50 EC10	peptone deg.	34 15	6	Tisler & Zagorc-Koncan, 1997
Pseudomonas putida		-	S	-	tw	-	-	3 h	TT	respiration rate	30	7	Gerike & Gode, 1990
Algae (unicellular)													
Ankistoderma falcatus	-	-	-	-	-	-	-	46 d	EC	growth	5		Nazarenko, 1960 (not available), cited in Hohreiter & Rigg, 20001
Aphanothece sp., Oscillatoria sp, Rhizoclonium sp.	-	-	-	-	-	-	-	7 d	NOEC	survival ?	>40	2,4	Helms, 1964 (not available), cited in Hohreiter & Rigg, 2001
Scenedusmus sp., Sirogonium sp., Spirogyra sp., Stigeocloneum sp.	-	-	-	-	-	-	-	7 d	EC	survival	6-20	2,4	Helms, 1964m (not available), cited in Hohreiter & Rigg, 2001
Algae (multi-cellular)													
Ceratopyllum demersum	-	-	-	-	-	-	-	27 d	EC	growth	5		Nazarenko, 1960 (not available), cited in Hohreiter & Rigg, 2001
Crustaceans													
Daphnia magna	-	-	-	-	-	-	-	23 d	NOEC NOEC	survival reproduction	0.5 1	3	Nazarenko, 1960 (not available), cited in Hohreiter & Rigg, 2001

Table A2-2d: Chronic and acute toxicity of formaldehyde to freshwater organisms: additional data (not useful for ERL derivation) (continued) (Toxicity values as values as formaldehyde, i.e 100% a.i.)

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
ACUTE TOXICITY													
Crustacea													
Cypridopsis sp.	-	N	S	37%	nw	6.5	20	96 h	EC50	mobility	0.42	1,2,9	Bills et al., 1977
Pisces													
Ictalurus punctatus	0.4 g	N	F	37%	aw	9.5	"soft"	96 h	LC50		17	1,2	Bills et al., 1977
Lepomis macrochirus	0.5 g	N	F	37%	aw	9.5	"soft"	96 h	LC50		40	1,2	Bills et al., 1977
Morone saxatilis	1.8 g	N	S	37%	nw	8.5	44	96 h	LC50		1.8	2, 8	Reardon & Harrell, 1990
Oncorhynchus mykiss	0.6 g	N	F	37%	aw	9.5.	"soft"	96 h	LC50		40	1,2	Bills et al., 1977
Oncorhynchus mykiss	0.6 g	N	F	37%	aw	7.5	"soft"	96 h	LC50 at 7 ^{0}C		98	1,2	Bills et al., 1977

1: Bills et al. (1977): All fish tests performed at T = 12 ^{0}C, unless stated otherwise. Not useful for ERL derivation: pH of test water or temperature during the test are outside the recommendations for tests with the indicated species (see OECD Guidelines).
2: Value adjusted to formaldehyde-basis (100% a.i.); test substance and results originally reported by the authors of the study as formalin, e.g. as formalin (37%) which is a solution of 37% (w/w or v/v/) of formaldehyde gas in water.
(Note: According to the Merck Index and other publications, formalin 37% by weight is the "full strength" commercial grade formalin and also known as Formalin 100% or Formalin 40 which signifies that it contains 40 grams of formaldehyde within 100 ml of the solution; D^{25}_{25} = 1.08).
3. According to the data reported in Hohreiter & Riggs (2001), formaldehyde concentrations of 0.5 and 1 mg/l had little effect on reproduction, and concentrations of 5 and 50 mg/l inhibited reproduction. The mortality observed at both 1 and 5 mg/l was equal. The test was rejected by Hohreiter & Riggs (2001) for the derivation of water quality criteria; the reason for rejecting this test is unclear.
4. Single-species tests. The tests with *Scenedusmus sp., Sirogonium sp., Spirogyra sp. and Stigeocloneum sp*. resulted in effect concentrations ranging from 6 to 20 mg/l (no species-specific values were reported by Hohreiter & Rigg (2001).
5. TT = Toxic Threshold, reported as minimum inhibitory concentration; the test is not useful for ERL derivation since the definition and method of derivation of this hreshold concentration were not reported.
6. Test substance reported as formaldehyd; results (reported in mg/l) assumed to be 100% a.i. The peptone degradation in the test water was measured by the oxygen consumption rate. The test is not useful for ERL derivation since it is not a single-species test.
7. Modified OECD 209 (Activated sludge respiration inhibition test): *Pseudomonas putida* used as bacterial inoculum instead of activated sludge. TT = Toxic Threshold, reported as inhibition limit. Data on test conditions not reported, but based on OECD 209. The test is not useful for ERL derivation since the definition and method of derivation of this hreshold concentration were not reported. In addition, it is assumed that sludge, inoculated with *P. putida*, was present in the test water.
8. Test water: ground water. The test is not useful for ERL derivation since the test fish were acclimated to 10 ^{0}/oo saliniity (the salinity which is isosmotic to *M. saxiilis*) prior to testing and since the LC50 from this test (1.8 mg/l) is significantly lower than the LC50 values found in this study at salinities of 5 to 15 mg/l (3.9 to 5.7 mg/l, see Table A2-2b). The low LC50 in ground water found in this test appears to be related to osmotic dysfunction (due to testing at a salinity of "0" ^{0}/oo after accclimation to a salinity of 10 ^{0}/oo). Furthermore, the LC50 of 1.8 mg/l is considerably lower than the LC50 values found in other freshwater tests with *M. saxatilis*, see Table A2-2b.
9. This test is not useful for ERL derivation since the 96-h EC50 from this test (0.42 mg/l for *Cypridopsis sp.*, from Bills et al., 1977) is two orders of magnitude lower than the 96-h EC50 values (54-69 mg/l) and 96-h LC50 values (98-114 mg/l) derived in three recent and high quality tests with *Cypridopsis vidua* (see Table A2-2b, from Cooney & Bourgoin, 2001, cited in Hohretier & Rigg, 2001).

Table A2-2e: Chronic and acute toxicity of formaldehyde to saltwater organisms: additional data (not useful for ERL derivation) (Toxicity values as formaldehyde, i.e 100% a.i.)

Species	Species prop.	Ana-lysis	Test type	Subst. purity	Test water	pH	Salinity (⁰/oo)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
CHRONIC TOXICITY													
Macroalgae													
Phyllospora comosa	4-d old embryos	N	R	37%	nw	8.0	34	28 d	LOEC NOEC	growth survival	0.1 1	1	Burridge et al., 1995a
Phyllospora comosa	12–h old zygotes	N	S	37%	nw	8.0	34	48 h	LOEC	germinatiion	0.1	1	Burridge et al., 1995a
Phyllospora comosa	24-h old zygotes	N	S	37%	nw	8.0	34	96 h	LOEC	survival	0.1	1	Burridge et al., 1995b
Phyllospora comosa	7-d old embryos	N	S	37%	nw	8.0	34	96 h	NOEC	survival	1	1	Burridge et al., 1995b
ACUTE TOXICTY													
Pisces													
Chanos chanos	6 g	N	S	-	-	8.0	32	96 h	LC50		86	2	Cruz & Pitogo, 1989

1. In the tests with macroalga *Phyllospora comosa,* germination and survival (starting with ≤ 24 h zygotes) and growth (starting with 4-d embryos) were statistically significant inhibited at 0.1 mg/l, the lowest concentration tested. The effect on growth was observed only during the first two weeks of the 4-w exposure period. Test substance reported as formaldehyd (37%); results reported for formaldehyde, in mg/l, assumed to be 100% a.i.
2. Value adjusted to formaldehyde-basis (100% a.i.); test substance and results originally reported by the authors of the study as formalin (purity not specified), assumed to be formalin 37% (w/w). The test is not useful for ERL derivation, since the test water was aerated during the test and no actual concentrations were measured during the test. Hence, the nominal LC50 of 86 mg/l, which is the highest of all available LC50 values for fish, is considered unreliable. Test substance and result (232 mg/l) originally reported by the authors of the study as formalin (purity unspecified), assumed to be formalin 37% (w/w/)).

Table A2-3a: Chronic toxicity of 4-chloro-2-methylphenol (p-chloro-o-cresol, PCOC) to freshwater organisms: NOEC values useful for ERL derivation

Species	Species prop.	Ana-lysis	Test type	Test. subst.	Subst. Purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value * (mg/l)	Note	Reference
Part 1. Data selected in EU-RAR on PCOC (DEPA, 1998): used for ERL derivation														
Algae (unicellular) *Scenedesmus subspicatus*		-	S	PCOC	-	-	-	-	72 h 72 h 96 h	NOEC (EC10) NOEC (EC10) NOEC (EC10)	growth (biomass) growth (rate) growth (biomass)	**0.97** >10 0.89	3	BASF AG, not available (confidential), cited in EU-RAR (DEPA, 1998)
Crustacea *Daphnia magna*	-	Y	R	PCOC	-	-	-	-	21 d	NOEC	survival, reproduction and growth	>**0.55**	1	PCOC Task Force, 1997, cited in EU-RAR (DEPA, 1998)
Pisces *Salmo trutta*	5 g	N	R	PCOC	>99%	-	-	-	21-28 d 21-d	NOEC *NOEC*	histo-pathology survival	**0.5** >1.5	2	Hattula et al, 1979
Part 2. Additional data (this report): not used for ERL derivation														
Bacteria *Peseudomonas putida*		N	S	PCOC	-	-	-	-	17 h	NOEC (EC10)	growth (biomass)	37	4	BASF AG, not available (confidential), cited in EU-RAR (DEPA, 1998) and AIDA, 1991
Pseudomonas sp		-	-	PCOC	-	-	-	-	-	NOEC (TT/2)	growth (biomass)	40	5	Rübelt et al., 1982
Amphibia *Xenopus laeviss*	eggs	N	S	PCOC	-	aw	-	101	5 d	NOEC (LOEC/10)	survival	4	6	Vismara et al., 1995

Footnotes Table A2-3a

* The NOEC values that have been printed **bold** were used for ERL derivation (see Chapter 4).

1. Test according to OECD 202-II (*Daphnia sp.* reproduction test). The 21-d chronic NOEC of 0.55 mg/l was considered to be useful in DEPA (1998), although this result seems to be inconsistent with the results of the acute toxicity tests (especially that by LeBlanc (1980) resulting in an 48 h EC50 of 0.29 mg/l (nominal concentration, see Table A2-3c), which is lower than the chronic NOEC of 0.55 mg/l). However. regardless of this, the NOEC of 0.55 mg/l should have been rejected (according to the criteria used in the EU-RAR programme and this RIVM report), since this NOEC is unbounded (i.e. no effect was found at 0.55 mg/l, the highest concentration tested) and thus this NOEC is not valid.
2. Aquaria covered by glass plates.Two tests were performed: one 28-d test at 0.5 and 1.0 mg/l and one 21-d test at 0.5, 1.0 and 1.5 mg/l. The tests were aimed at histopathological effects in liver, kidneys and gills; the reported data don't indicate an effect on survival; further endpoints were not studied. The (21-28 d) NOEC of 0.5 mg/l, for endpoint histopathology, was considered useful in DEPA (1998) and, being the lowest chronic NOEC, used as the key study for PNEC derivation ($PNEC_{aquatic\ organisms}$ is lowest NOEC/10 = 0.5/10 = 0.05 mg/l, see also Chapter 4. It is noted, however, that the validity of this NOEC is questionable, since the NOEC is based on endpoint histopathology (liver, kidneys and gills) and histopathological effects are usually not taken into account in ecotoxicity tests (except for histopathological effects in the reproductive organs).
3. Based on OECD 201 (Alga growth inhibition test).; the 72-h value is prefered and thus used for ERL derivation.
4. Standardized test method, referring to DIN 38412 – Teil 8. In DEPA (1998) only the 17-h EC50 (110 mg/l) is reported; the EC10 is reported only in the IUCLID (2000) file, together with the EC50 and EC90. It is noted that in the framework of the EU-programme bacterial data are not used for the derivation of a PNEC for surface water ($PNEC_{aquatic\ organisms}$) but only used for the derivation of a PNEC for STP effluent ($PNEC_{microorganisms}$), to protect microorganisms in biological sewage treatment plants.
5. Standardized test method, referring to Testverfahren Deutscher Bundestag (1974). Test species: Pseudomonas (Stam Berlin 33/2). NOEC = TT/2. The Toxic Threshold (80 mg/l for PCOC) is the concentration at which the growth inhibition exceeded two times the standard deviation of the control growth.
6. NOEC = LOEC/10 (63% embryonal mortality at 40 mg/l).

Table A2-3b: Chronic toxicity of 4-chloro-3-methylphenol (p-chloro-m-cresol, PCMC) to freshwater organisms: NOEC values useful for ERL derivation

Species	Species prop.	Ana-lysis	Test type	Test. subst.	Subst. Purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value * (mg/l)	Note	Reference
Bacteria														
Bacillus subtilis		-	S	PCMC	-	aw	-	-	24 h	NOEC (EC25/3)	growth (biomass)	**9.3**		Voets et al., 1976
Pseudomonas sp.		-	-	PCMC	-	-	-	-	-	NOEC (TT/2)	growth (biomass)	**35**	1	Rübelt et al., 1982
Algae (unicellular)														
Scenedesmus subspicatus		-	S	PCMC	-	aw	7-8	-	72 h	NOEC (EC10)	growth (biomass)	**4.7**	2	Kühn & Pattard, 1990
									72 h	NOEC (EC10)	growth (rate)	>10		
									96 h	NOEC (EC10)	growth (biomass)	5.2		
Crustacea														
Daphnia magna	$\leq$ 24 h	Y	R	PCMC	-	aw	8.0	250	21 d	NOEC	reproduction rate	**1.3**	3	Kühn et al., 1989

* The NOEC values that have been printed **bold** were used for ERL derivation (see Chapter 4).

1. Standardized test method, referring to Testverfahren Deutscher Bundestag (1974). Test species: Pseudomonas (Stam Berlin 33/2). NOEC = TT/2. The Toxic Threshold (70 mg/l for PCMC) is the concentration at which the growth inhibition exceeded two times the standard deviation of the control growth.
2. Based on OECD 201 (Alga growth inhibition test); the 72-h value is prefered and thus used for ERL derivation.
3. Reproduction rate most sensitive (the appearance of the first offspring and survival of the parent animals were less sensitive endpoints).

Table A2-3c. Acute toxicity of 4-chloro-2-methylphenol (p-chloro-o-cresol, PCOC) to freshwater organisms: LC50 and EC50 values useful for ERL derivation

Species	Species prop.	Ana-lysis	Test type	Test subst.	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. Time	criterion	Endpoint	Value * (mg/l)	Note	Reference
Part 1. Data selected in EU-RAR on PCOC (DEPA, 1998): used for ERL derivation														
Bacteria														
Pseudomonas putida		N	S	PCOC	-	-	-	-	17 h	EC50	growth (biomass)	**110**	1	BASF AG, not available (confidential), cited in EU-RAR (DEPA, 1998) and AIDA, 1991
Algae (unicellular)														
Scenedesmus subspicatus		-	S	PCOC	-	-	-	-	72 h	EC50	growth (biomass)	**15**	2	BASF AG, not available (confidential), cited in EU-RAR (DEPA, 1998)
									72 h	EC50	growth (rate)	>10		
									96 h	EC50	growth (biomass)	8.2		
Macrophyta														
Lemna minor	-	N	S	PCOC	-	-	5.1	-	48 h	EC50	chlorosis	**93**		Blackman et al., 1955, cited in EU-RAR (DEPA, 1998)
Crustacea														
Daphnia magna	<24 h	N	S	PCOC	>80%	aw	8.3	173	48 h	LC50		**0.29**		LeBlanc, 1980
Daphnia magna	-	N	S	PCOC	97%	-	-	-	48 h	EC50		**0.63**		VKI, 1983, cited in EU-RAR (DEPA, 1998)
Daphnia magna	-	-	-	PCOC	-	-	-	-	48 h	EC50		**1.0**		BASF, cited in EU-RAR (DEPA, 1998) and AIDA, 1991
Pisces														
Brachydanio rerio	-	-	-	PCOC	-	-	-	-	96 h	LC50		**3.7**	3	Bayer, cited in EU-RAR (DEPA, 12998) and AIDA, 1991
Brachydanio rerio	-	-	S	PCOC	-	-	-	-	96 h	LC50		**4.2**	4	VKI, 1983, cited in EU-RAR (DEPA, 1998)
Lepomis macrochirus	juveniles	N	S	PCOC	≥80%	nw	7.1	28-44	96 h	LC50		**2.3**		Buccafusco et al., 1981
Oryzias latipes		N	S	PCOC	-	-	-	-	48 h	LC50		**6.3**		MITI, 1992, cited in EU-RAR (DEPA, 1998)
Salmo trutta	2.5 g	N	S	PCOC	>99%	-	-	-	24 h	LC50		**2.1**		Hattula et al., 1979
Part 2. Additional data (this report): not used for ERL derivation														
Leuciscus idus melanotus	-	-	-	PCOC	-	-	-	255	48 h	LC50		3.6		Rübelt et al., 1982

Footnotes Table A2-3c

* The LC50 and EC50 values that have been printed **bold** were used for ERL derivation (after calculation of the ‘species mean’ L(E)C50, where appropriate, see Chapter 4).

1 Standardized test method, referring to DIN 38412 – Teil 8.
2. Based on OECD 201 (Alga growth inhibition test); the 72-h value is prefered and thus used for ERL derivation.
3. Geometric mean of 3.2 and 4.2 mg/l (reported data: LC0 = 3.2 mg/l; LC80 = 4.2 mg/l).
4. Geometric mean of 3 and 6 mg/l (LC50 reported as 3 to 6 mg/l).

Table A2-3d. Acute toxicity of 4-chloro-3 -methylphenol (p-chloro-m-cresol, PCMC) to freshwater organisms: LC50 and EC50 values useful for ERL derivation

Species	Species prop.	Ana-lysis	Test type	Test subst.	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. Time	criterion	Endpoint	Value * (mg/l)	Note	Reference
Protozoa														
Tetrahymena pyriformis		N	S	PCMC	-	aw	7.4	75	40 h	EC50	growth (biomass)	**23**		Schulz, 1997
Crustacea														
Daphnia magna	≤ 24 h	Y	S	PCMC	-	aw	8.0	250	24 h	EC50		**4.4**		Kühn et al., 1989
Daphnia magna	-	-	-	PCMC		-	-	-	24 h	EC50		**1.5**		Gunatilleka & Poole, 1999
Daphnia pulex	-	N	S	PCMC	-	-	-	-	96 h	LC50		**3.1**		Trabalka, 1980
Pisces														
Pimephales promelas	31-d old, 0.11 g	Y	S	PCMC	99%	aw	7.2	46	96 h	LC50		**7.4**		Geiger et al., 1985
Pimephales promelas	30-d old, 0.1 g	Y	S	PCMC		aw	7.7	-	96 h	LC50		**4.1**		Geiger et al., 1985
Pimephales promelas	-	N	S	PCMC	-	-	-	-	96 h	LC50		**6.5**		Verhaar et al., 1996
Pimephales promelas	-	-	-	PCMC	-	-	-	-	96 h	LC50		**5.4**		Gunatilleka & Poole, 1999
Pimephales promelas	-	-	F	PCMC	-	-	-	-	96 h	LC50		**7.3**		U.S. EPA, cited in Schulz, 1997
Poecilia reticulata	-	-	-	PCMC	-	-	-	-	96 h	LC50		**6.7**		Gunatilleka & Poole, 1999
Salmo trutta	4.5 g	N	S	PCMC	>97%	-	-	-	24 h	LC50		**1.3**		Hattula et al.,1981

* Combined with the saltwater EC50 from Table A2-3e, all LC50 and EC50 values (printed **bold**) from this table were used for ERL derivation (after calculation of the 'species mean' L(E)C50, where appropriate, see Chapter 4).

Table A2-3e. Acute toxicity of 4-chloro-3-methylphenol (p-chloro-m-cresol, PCMC) to saltwater organisms: EC50 value useful for ERL derivation

Species	Species prop.	Ana-lysis	Test type	Test. subst.	Subst. purity	Test water	pH	Salinity (^{0}/oo)	Exp. time	Criterion	Endpoint	Value * (mg/l)	Note	Reference
Bacteria														
Vibrio fisheri		N	S	PCMC	-		-	20	5 min	EC50	biolumin.	**0.27**	1	Cronin & Schulz, 1997

* Combined with the freshwater L(E)C50 values from Table A2-3d, this saltwater EC50 (printed **bold**) was used for ERL derivation (see Chapter 4).

1. Microtox test (standardized bacterial bioluminescence test with *Vibrio fisheri*). The salinity (20 ^{0}/oo) is based on that in standard medium for *Vibrio fisheri* (reported in Lampinen et al., 1999).

Table A2-3f. Toxicity of 4-chloro-2-methylphenol (p-chloro-o-cresol, PCOC) to freshwater organisms: additional data (not useful for ERL derivation)

Species	Species prop.	Ana-lysis	Test type	Test. subst.	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
Protozoa														
Tetrahymna pyriformis		-	-	PCOC	-	-	-	-	48 h	EC50	growth (biomass)	14		IUCLID, 1997
Crustacea														
Daphnia magna	-	-	S	PCOC	-	-	-	-	-	EC50 EC100		>0.56 <1.8	1	PCOC Task Force, 1997, cited in EU-RAR (DEPA, 1998)

1. Range-finding study for the reproduction test, see Table A2-3a.

Table A2-3g. Chronic and acute toxicity of 4-chloro-3-methylphenol (p-chloro-m-cresol, PCMC) to freshwater organisms: additional data (not useful for ERL derivation)

Species	Species prop.	Ana-lysis	Test type	Test. subst.	Subst. purity	Test water	pH	Hardness (mg/l, as $CaCO_3$)	Exp. time	Criterion	Endpoint	Value (mg/l)	Note	Reference
CHRONIC TOXICITY														
Bacteria														
Pseudomonas putida		-	S	PCMC	-	tw	-	-	3 h	TT	respiration rate	32	1	Gerike & Gode, 1990
Algae														
Scenedesmus subspicatus		N	S	PCMC	99.9	-	-	-	72 h	NOEC (EC10)	growth (biomass)	1.9		Bayer AG, unpublished, cited in IUCLID, 2000
Pisces														
Brachydanio rerio	-	Y	F	PCMC	99.97 %	aw	7.1-7.8	255	14 d	NOEC	survival	1	2	Bayer AG, unpublished, cited in IUCLID 2000
ACUTE TOXICITY														
Algae														
Scenedesmus subspicatus		N	S	PCMC	99.9	-	-	-	72 h	EC50	growth (biomass)	4.2		Bayer AG, unpublished, cited in IUCLID, 2000
Scenedesmus subspicatus		-	S	PCMC	-	aw	7-8	-	72 h & 96 h	EC50	growth (biomass)	>10	3	Kühn & Pattard, 1990
									72 h	EC50	growth (rate)	>10		
Crustacea														
Daphnia magna	-	-	S	PCMC	>99%	-	7.5-8.0	-	48 h	EC50	mobility	2		IUCLID 2000
Pisces														
Brachydanio rerio	-	Y	F	PCMC	99.97 %	aw	7.1-7.8	255	5 d	LC100		3.2	2	Bayer AG, unpublished, cited in IUCLID 2000
Brachydanio rerio	-	-	S	PCMC	-	-	-	-	24 h	LC50		1 – 3.5		IUCLID, 2000
Leuciscus idus melanotus	-	N	S	PCMC	99.9%	-	-	-	48 h	LC50		1.2		IUCLID, 2000
Leuciscus idus melanotus	-	-	S	PCMC	-	-	7-8	255	48 h	LC50		2.4		IUCLID, 2000
Oncorhynchus mykiss	-	Y	R	PCMC	99.9%	-	7.1-7.6	-	96 h	LC50		0.92	4	IUCLID, 2000
Oryzias latipes	-	-	-	PCMC	-	-	-	-	48 h	LC50		4.6		IUCLID, 2000
Pimephales promelas	-	-	F	PCMC	99%	-	6.9-7.7	44	96 h	LC50		7.6		IUCLID, 2000
Poecilia reticulata	-	-	S	PCMC	-	tw	7.7	320	24 h	LC50		2.2		IUCLID, 2000
Salmo trutta	-	-	S	PCMC	-	-	-	-	24 h	LC50		50		IUCLID, 2000

Footnotes Table A2-3g

1. Modified OECD 209 (Activated sludge respiration inhibition test): *Pseudomonas putida* used as bacterial inoculum instead of activated sludge. NOEC = Toxic Threshold, reported as inhibition limit (definition and method of derivation of this threshold concentration were not reported). Data on test conditions not reported, but based on OECD 209. The test is not useful for ERL derivation since the Toxic Threshold is not defined. In addition, it is assumed that sludge, inoculated with *P. putida*, was present in the test water.
2. A very steep concentration-effect curve for PCMC was found in this 14-d study with *Brachydanio rerio:* the 14-day NOEC was 1 mg/l, while all fish exposed to 3.2 mg/l died in 5 days. This is in conformity with other fish tests that also showed a very steep concentration-effect curve for PCMC, for example the two acute toxicity studies with *Leuciscus idus melanotus* that showed a factor of 1.5 and 4, respectively, between the LC0 (NOEC) and LC100.
3. Based on OECD 201 (Alga growth inhibition test).
4. Lowest acute LC50 of PCMC for fish. Appears to be a high quality test based on the data reported in IUCLID, 2000 (renewal test, analysis of test concentrations, very high purity of test compound, GLP statement, but primary publication not available.

Appendix 3: Terrestrial toxicity data

Legend

Species (and properties)	Organism used in the test, followed by species properties (age, size, weight or life stage) if available.
Analysis	Y = test substance analyzed in test soil. N = test substance not analyzed in test soil.
Soil type	Type of soil used in the test (natural soils, unless stated otherwise).
pH	Initial value of test soil, thus prior to the addition of the test substance (unless stated otherwise).
% OM	Percentage organic matter of test soil (based on dry weights).
% Clay	Percentage clay of test soil (based on dry weights).
Temp.	Temperature at which the test was performed.
Exposure time	d = day(s), h = hour(s), m = month(s), min = minute(s), w = week(s), yr: year(s).
Criterion	EC50: Median effect concentration, i.e. the concentration which is calculated from a series of test concentrations to cause a particular response in 50% of the number of organisms exposed to that concentration.
Endpoint	Toxicological endpoint, usually survival, growth and/or reproduction.
Value	A value preceeded by '>' is the highest concentration used in the test. When no effect is found at the highest test concentration, the 'unbounded' NOEC is not useful because the real NOEC may be higher. Likewise, 'unbounded' EC50 values are not useful.
Value in test soil	Actual result in test soil.
Value in standard *NL* soil	Result normalised for standard *NL* soil (i.e. soil containing 10% organic matter), calculated as follows: $Value_{standard\ soil} = Value_{test\ soil} \times (\%OM_{standard\ soil} / \%OM_{test\ soil})$. Note: When the actual %OM in test soil is <2%, a $\%OM_{test\ soil}$ of 2% is used in the calculation.

Toxicity of 2-propanol, PCMC and PCOC to terrestrial organisms

Species	Species prop.	Ana-lysis	Test subst.	Soil type	pH	% O.M..	% Clay	Temp ^{0}C	Exp. time	Criterion	Endpoint	Value in test soil (mg/kg d.w.)	Value in standard *NL* soil (mg/kg d.w.) *	Reference
Macrophytes														
Lactuca sativa	seeds	Y	2-pro-panol	loam	7.8	1.4	12	20	14 d	EC50	growth	>1,000	>5,000	Hulzebos et al., 1993 [1]
Lactuca sativa	seeds	Y	PCMC	loam	7.8	1.4	12	20	14 d	EC50	growth	66	**330**	Hulzebos et al., 1993 [1,2]
Lactuca sativa	seeds	Y	PCOC	loam	7.8	1.4	12	20	14 d	EC50	growth	66*	**330**	Hulzebos et al., 1993 [1,2]

* The EC50 values that have been printed **bold** were used for ERL derivation, see Chapter 4.

[1] Pot experiments; test trays covered with glass plates untill germination of seedlings. Purity test substances: $\geq$95%. Endpoint: fresh weight of shoots. Results are based on nominal concentrations.

[2] The EC50 of 66 mg/kg d.w. for PCMC and PCOC, reported by Hulzebos et al. (1993), is the arithmetic mean value of 32 and 100 mg/kg d.w. (32 mg/kg d.w. < EC50 < 100 mg/kg d.w.)

PCOC = p-chloro-o-cresol (4-chloro-2-methylphenol)
PCMC = p-chloro-m-cresol (4-chloro-3-methylphenol)