National Institute
for Public Health
and the Environment

Report 601782013/2009

R.H.L.J. Fleuren | P.J.C.M. Janssen | L.R.M. de Poorter

Environmental risk limits for twelve volatile aliphatic hydrocarbons

An update considering human-toxicological data

rivm

RIVM report 601782013/2009

Environmental risk limits for twelve volatile aliphatic hydrocarbons

An update considering human-toxicological data

R.H.L.J. Fleuren
P.J.C.M. Janssen
L.R.M. de Poorter

Contact:
Leon de Poorter
Expertise Centre for Substances
leon.de.poorter@rivm.nl

This investigation has been performed by order and for the account of Directorate-General for Environmental Protection, Directorate Environmental Safety and Risk Management, within the framework of project 'International and national Environmental Quality Standards for Substances in the Netherlands (INS)'.

rivm

Abstract

Environmental risk limits for twelve volatile aliphatic hydrocarbons
An update considering human-toxicological data

The National Institute for Public Health and the Environment (RIVM) has derived environmental risk limits for twelve volatile substances in water, groundwater, soil and air. The following substances were considered: 1,1,2-trichloroethane, hexachloroethane, chloroethylene (vinylchloride), 1,1-dichloroethylene, 3-chloropropene, 2-chlorobutadiene, 1,1,1-trichloroethane, 1,1,2,2-tetrachloroethane, 1,2-dichloropropane, 1,2-dichloroethylene, 1,3-dichloropropene, and 2,3-dichloropropene.

Environmental risk limits are the maximum allowable concentrations of a substance in the environment to protect humans and the environment for any adverse effect. Four different levels are distinguished: Negligible Concentration (NC), the concentration at which no harmful effects are to be expected (Maximum Permissible Concentration, MPC), the Maximum Acceptable Concentration for ecosystems specifically for short-term exposure in water (MAC_{eco}) and a concentration at which serious effects are to be expected (Serious Risk Concentrations, SRC_{eco}). For deriving the environmental risk limits RIVM used the most recent methodology, as required by the European Water Framework Directive (WFD) among others. Environmental risk limits are scientifically based proposals on which the Dutch Interdepartmental Steering Committee for Substances sets the environmental quality standards.

Human risk limits derived in this report were compared with ecosystem risk limits as previously reported in 2007. This resulted in the selection of final environmental risk limits for water, soil and air. No risk limits were derived for the sediment compartment, because sorption to sediment is below the trigger value to derive such risk limits (exposure of water organisms via the sediment is considered to be negligible).

For most substances the newly derived environmental risk limits are lower than the current environmental quality standards. Based on a limited set of monitoring data a preliminary risk assessment for freshwater was performed: this indicated that for some substances the Negligible Concentration (NC) is exceeded, but not the Maximum Permissible Concentration (MPC).

Key words:
environmental risk limits, maximum permissible concentration, volatile aliphatic hydrocarbons, WFD

rivm

Rapport in het kort

Milieurisicogrenzen voor twaalf vluchtige, alifatische koolwaterstoffen
Een herziening op basis van humaan-toxicologische informatie

Het RIVM heeft milieurisicogrenzen voor water, bodem en lucht afgeleid voor twaalf vluchtige koolwaterstoffen. Het gaat om de volgende stoffen: 1,1,2-trichloorethaan, hexachloorethaan, chloorethyleen (vinylchloride), 1,1-dichloorethyleen, 3-chloorpropeen, 2-chloorbutadieen, 1,1,1-trichloorethaan, 1,1,2,2-tetrachloorethaan, 1,2-dichloorpropaan, 1,2-dichloorethyleen, 1,3-dichloorpropeen en 2,3-dichloorpropeen.

Milieukwaliteitsnormen zijn concentraties van een stof in het milieu die mens en ecosysteem op verschillende niveaus beschermen tegen nadelige effecten. Het RIVM heeft de afleiding van de milieurisicogrenzen uitgevoerd volgens de methodiek die is voorgeschreven door de Europese Kaderrichtlijn Water (KRW). De milieurisicogrenzen worden gebruikt in het Nederlandse milieubeleid: ze dienen als advieswaarden voor de Nederlandse Interdepartementale Stuurgroep Stoffen, die de uiteindelijke milieukwaliteitsnormen beleidsmatig vaststelt. De milieurisicogrenzen zoals afgeleid in dit rapport zijn dus voorstellen zonder officiële status. Nederland onderscheidt vier milieurisicogrenzen: een niveau waarbij het risico verwaarloosbaar wordt geacht (VR), een niveau waarbij geen schadelijke effecten zijn te verwachten (MTR), het maximaal aanvaardbare niveau voor ecosystemen, specifiek voor kortdurende blootstelling in water (MAC_{eco}) en een niveau waarbij mogelijk ernstige effecten voor ecosystemen zijn te verwachten (ER_{eco}).

De grenzen voor risico's specifiek voor de mens uit dit rapport zijn vergeleken met grenzen voor risico's specifiek voor het ecosysteem, die in 2007 gepubliceerd zijn. De laagste waarde van de twee is vervolgens gekozen als definitieve milieurisicogrens voor de desbetreffende stof in water, bodem en lucht. Voor de waterbodem zijn geen milieurisicogrenzen afgeleid, want de binding van de koolwaterstoffen aan sediment blijft beneden het hiervoor vastgestelde criterium (minimale blootstelling van organismen aan de stoffen via sediment).

De nieuw afgeleide milieurisicogrenzen liggen voor de meeste stoffen lager dan de bestaande milieukwaliteitsnormen. Op basis van een beperkte evaluatie van monitoringsgegevens van oppervlaktewater zijn er aanwijzingen dat voor een aantal stoffen het Verwaarloosbaar Risiconiveau wordt overschreden, maar het Maximaal Toelaatbaar Risiconiveau niet.

Trefwoorden:
milieurisicogrenzen, maximaal toelaatbaar risiconiveau, vluchtige alifatische koolwaterstoffen, KRW

Preface

The goal of this report is to derive risk limits that protect both man and the environment. This is done in accordance with the methodology of the Water Framework Directive (WFD). This methodology is incorporated in the Guidance for the derivation of environmental risk limits within the framework of the project 'International and National environmental quality standards for Substances in the environment (INS)' (Van Vlaardingen and Verbruggen, 2007).

The results presented in this report have been discussed by the members of the scientific advisory group for the INS-project (WK-INS). This advisory group provides a non binding scientific advice on the final draft of a report in order to advise the Dutch Steering Committee for Substances on the scientific merits of the report.

Acknowledgements

Thanks are due to ing. Mario Adams and ir. Janine Killaars, contact persons at the Ministry of VROM, and to dr. Martien Janssen who is program coordinator for the derivation of environmental risk limits at the RIVM.

The results of the present report have been discussed in the scientific advisory group INS (WK-INS). The members of this group are acknowledged for their contribution.

rivm

Contents

Summary		**11**
Samenvatting		**15**
1	**Introduction**	**19**
1.1	Project framework and background of the report	19
1.2	Current environmental quality standards for the twelve substances	20
1.3	Production, use and discharge	20
1.4	Status of the results	20
2	**Methods**	**21**
2.1	Data collection	21
2.2	Derivation of ERLs	21
2.2.1	Drinking water	21
2.2.2	$MAC_{eco, marine}$	22
3	**Substance identification, physico-chemical properties, fate and human toxicology**	**23**
3.1	Identity	23
3.2	Physico-chemical properties	24
3.3	Bioconcentration and biomagnification	24
3.4	Derivation of human-toxicological threshold limits	25
3.4.1	Introductory comments	25
3.4.2	Classification	26
3.4.3	Human-toxicological threshold limits	27
3.4.4	Reliability evaluation	32
4	**Derivation of environmental risk limits**	**33**
4.1	Derivation of MPC_{water} and MPC_{marine}	33
4.1.1	$MPC_{eco, water}$ and $MPC_{eco, marine}$	33
4.1.2	$MPC_{sp, water}$ and $MPC_{sp, marine}$	33
4.1.3	$MPC_{hh\ food, water}$	33
4.1.4	Selection of the MPC_{water} and MPC_{marine}	35
4.2	Derivation of $MPC_{dw, water}$	35
4.2.2	Overview of derived (provisional) $MPC_{dw, water}$	37
4.3	Derivation of MAC_{eco}	37
4.3.1	1,1,2-Trichloroethane	37
4.3.2	Hexachloroethane	37
4.3.3	Chloroethylene	38
4.3.4	1,1-Dichloroethylene	38
4.3.5	3-Chloropropene	38
4.3.6	2-Chlorobutadiene	38
4.3.7	1,1,1-Trichloroethane	38
4.3.8	1,1,2,2-Tetrachloroethane	38
4.3.9	1,2-Dichloropropane	38
4.3.10	1,2-Dichloroethylene	39
4.3.11	1,3-Dichloropropene	39
4.3.12	2,3-Dichloropropene	39

4.3.13	Overview of derived $MAC_{eco, water}$ and $MAC_{eco, marine}$	39
4.4	Derivation of NC_{water}	39
4.5	Derivation of $SRC_{eco, water}$	40
4.6	Derivation of sediment ERLs	40
4.7	Derivation of MPC_{soil}	41
4.7.1	$MPC_{eco, soil}$	41
4.7.2	$MPC_{sp, soil}$	41
4.7.3	$MPC_{human, soil}$	41
4.7.4	Selection of MPC_{soil}	43
4.8	Derivation of NC_{soil}	44
4.9	Derivation of $SRC_{eco, soil}$	44
4.10	Derivation of MPC_{gw}	45
4.10.1	$MPC_{eco, gw}$	45
4.10.2	$MPC_{human, gw}$	46
4.10.3	Selection of the MPC_{gw}	46
4.11	Derivation of NC_{gw}	47
4.12	Derivation of $SRC_{eco, gw}$	47
4.13	Derivation of MPC_{air}	48
4.13.1	$MPC_{eco, air}$	48
4.13.2	$MPC_{human, air}$	48
4.13.3	Selection of MPC_{air}	49
4.14	Derivation of NC_{air}	49
5	**Preliminary risk analysis for freshwater**	**51**
6	**Conclusions**	**53**
References		**55**
Appendix 1. Current environmental quality standards		**59**
Appendix 2. Derivation of $MPC_{human,soil}$: input data and results		**61**

rivm

Summary

In the RIVM report 601782002 ‘Ecotoxicologically based environmental risk limits for several volatile aliphatic hydrocarbons’ (De Jong et al., 2007), environmental risk limits (ERLs) for a number of volatile substances were derived, based on ecotoxicological data. Since then, the guidance for deriving ERLs within the framework of the project ‘International and National Environmental Quality Standards for Substances in the Netherlands (INS)’ was revised, implementing the methodology as required by the Water Framework Directive (WFD) (Van Vlaardingen and Verbruggen, 2007). The WFD requires that risks for humans due to the consumption of fish or fishery products are considered when deriving ERLs for water. In addition, human-toxicological information is also required for derivation of ERLs for soil, ground water, drinking water and air.

In the present report, human-toxicologically based ERLs are therefore derived for twelve of these substances.These twelve substances were selected because they are included in the draft version of the Dutch ‘Besluit Kwaliteitseisen en monitoring water’. This decree sets the environmental quality standards for compounds that are specifically relevant for the Netherlands within the context of the WFD. The compounds are listed below:

1	1,1,2-trichloroethane	7	1,1,1-trichloroethane
2	hexachloroethane	8	1,1,2,2-tetrachloroethane
3	chloroethylene (vinylchloride)	9	1,2-dichloropropane
4	1,1-dichloroethylene	10	1,2-dichloroethylene
5	3-chloropropene	11	1,3-dichloropropene
6	2-chlorobutadiene	12	2,3-dichloropropene

Subsequently, the ERLs based on direct ecotoxicity and human-toxicology were compared and final ERLs were selected for the environmental compartments water, sediment (when appropriate), soil and air. Secondary poisoning was also taken into account when applicable. It should be noted that these ERLs are scientifically derived values. They serve as advisory values for the Dutch Steering Committee for Substances, which is appointed to set the Environmental Quality Standards (EQSs) from these ERLs. ERLs should thus be considered as preliminary values that do not have an official status.

When human-toxicological threshold limits had already been established by RIVM or other recognised agencies or regulatory bodies (e.g. US-EPA, WHO), these limits were adopted for derivation of ERLs. Where needed, limit values were updated using scientific literature published since existing risk limits were established. When no existing human toxicological threshold limits were available for a substance, publicly available literature was evaluated and new risk limits were based on the available information.

Human-toxicologically based ERLs are derived according to the INS-guidance (Van Vlaardingen and Verbruggen, 2007). Selection of the final ERLs, taking all possible routes into account, is also based on this guidance. An overview of the final ERLs is given in Table 1.

Table 1. Derived MPC, NC, MAC_{eco}, and SRC_{eco} values (in $\mu g.L^{-1}$ for water and groundwater, in $mg.kg_{dw}^{-1}$ for soil, in $\mu g.m^{-3}$ for air). n.d. = not derived.

	1,1,2-trichloroethane	hexachloroethane	chloroethylene	1,1-dichloroethylene	3-chloropropene	2-chlorobutadiene
Freshwater						
MPC	22	0.44	9.1×10^{-2} [b]	9.0	0.34	0.19
NC	0.22	4.4×10^{-3}	9.1×10^{-4} [b]	9.0×10^{-2}	3.4×10^{-3}	1.9×10^{-3}
MAC_{eco}	3.0×10^{2}	1.4	n.d.	90	3.4	n.d.
SRC_{eco}	1.6×10^{4}	1.1×10^{2}	n.d.	1.1×10^{4}	1.9×10^{3}	1.9×10^{3}
Drinking water						
MPC	14 [a]	3.5 [a]	0.50 [a]	1.8×10^{2} [a]	19 [a]	0.14 [a]
Marine water						
MPC	22	6.7×10^{-2}	9.1×10^{-2} [b]	0.9	3.4×10^{-2}	0.19
NC	0.22	6.7×10^{-4}	9.1×10^{-4} [b]	9.0×10^{-3}	3.4×10^{-4}	1.9×10^{-3}
MAC_{eco}	1.9×10^{2}	0.28	n.d.	9.0	0.34	n.d.
SRC_{eco}	1.6×10^{4}	1.1×10^{2}	n.d.	1.1×10^{4}	1.9×10^{3}	1.9×10^{3}
Soil						
MPC	0.16	1.4×10^{-2}	1.6×10^{-4} [b]	4.4×10^{-2}	6.5×10^{-4}	1.4×10^{-3}
NC	1.6×10^{-3}	1.4×10^{-4}	1.6×10^{-6} [b]	4.4×10^{-4}	6.5×10^{-6}	1.4×10^{-5}
SRC_{eco}	91	16	n.d.	53	3.6	10
Groundwater						
MPC	14	0.67	0.50	9.0	0.34	0.14
NC	0.14	6.7×10^{-3}	5.0×10^{-3}	9.0×10^{-2}	3.4×10^{-3}	1.4×10^{-3}
SRC_{eco}	1.6×10^{4}	1.1×10^{2}	n.d.	1.1×10^{4}	1.9×10^{3}	1.9×10^{3}
Air						
MPC [d]	17	87	3.6×10^{-2}	2.0×10^{2}	7.4	0.02
NC [d]	0.17	0.87	3.6×10^{-4}	2.0	7.4×10^{-2}	2×10^{-4}

Table 1 (continued). Derived MPC, NC, MAC_{eco}, and SRC_{eco} values (in $\mu g.L^{-1}$ for water and groundwater, in $mg.kg_{dw}^{-1}$ for soil, in $\mu g.m^{-3}$ for air). n.d. = not derived.

	1,1,1-trichloroethane	1,1,2,2-tetrachloroethane	1,2-dichloropropane	1,2-dichloroethylene	1,3-dichloropropene	2,3-dichloropropene
Freshwater						
MPC	21	8.0	2.8×10^{2}	6.8	0.18	n.d.
NC	0.21	8.0×10^{-2}	2.8	6.8×10^{-2}	1.8×10^{-3}	n.d.
MAC_{eco}	54	84	1.3×10^{3}	n.d.	51	n.d.
SRC_{eco}	1.5×10^{3}	1.7×10^{3}	2.0×10^{4}	1.1×10^{4}	28	n.d.
Drinking water						
MPC	7.0×10^{3} [a]	1.8×10^{2} [a]	2.5×10^{2} [a]	1.1×10^{2} [a]	3.5×10^{-2} [a]	3.5×10^{-2} [a]
Marine water						
MPC	2.1	0.8	28	0.68	1.8×10^{-2}	n.d.
NC	2.1×10^{-2}	8.0×10^{-3}	0.28	6.8×10^{-3}	1.8×10^{-4}	n.d.
MAC_{eco}	5.4	8.4	1.3×10^{2}	n.d.	5.1	n.d.
SRC_{eco}	1.5×10^{3}	1.7×10^{3}	2.0×10^{4}	1.1×10^{4}	28	n.d.
Soil						
MPC	0.15	7.0×10^{-2}	1.6	2.0×10^{-2}	3.0×10^{-4}	3.0×10^{-4} [b]
NC	1.5×10^{-3}	7.0×10^{-4}	1.6×10^{-2}	2.0×10^{-4}	3.0×10^{-6}	3.0×10^{-6} [b]
SRC_{eco}	11	14	59	32	8.7×10^{-2}	n.d.
Groundwater						
MPC	21	8.0	2.5×10^{2}	6.8	3.5×10^{-2}	3.5×10^{-2} [c]
NC	0.21	8.0×10^{-2}	2.5	6.8×10^{-2}	3.5×10^{-4}	3.5×10^{-4} [c]
SRC_{eco}	1.5×10^{3}	1.7×10^{3}	2.0×10^{4}	1.1×10^{4}	28	n.d.
Air						
MPC [d]	3.8×10^{2}	65 [d]	12	60	0.25	0.25
NC [d]	3.8	0.65 [d]	0.12	0.60	2.5×10^{-3}	2.5×10^{-3}

a: For all substances, except chloroethylene, the value represents a $MPC_{dw, water, provisional}$, *i.e.* not based on a established Drinking Water Standard (DWS) conform EU Directive 98/83/EC or an A1-value conform Directive 75/440/EEC.

b: Values are not based on MPC_{eco}-values (not available), but are considered sufficiently protective for both man and environment (see text in this report).

c: Values are not based on MPC_{eco}-values (not available), but are - based on the data for 1,3-dichloropropene - considered sufficiently protective for both man and environment (see text in this report).

d: All MPC- and NC-values for air are at least based on $MPC_{human, air}$-values, except for 1,1,2,2-tetrachloroethane where only a $MPC_{eco, air}$ value is available. Therefore the values for 1,1,2,2-tetrachloroethane should be regarded as preliminary, since future availability of reliable chronic inhalation toxicity data may lead to lower values.

rivm

Samenvatting

In RIVM-rapport 601782002 ‘Ecotoxicologically based environmental risk limits for several volatile aliphatic hydrocarbons’ (De Jong et al., 2007), zijn milieurisicogrenzen afgeleid voor een aantal vluchtige stoffen. Deze waarden waren gebaseerd op ecotoxicologische gegevens. Inmiddels is de methodiek voor het afleiden van milieurisicogrenzen binnen het project (Inter)nationale normstelling Stoffen (INS) aangepast en in lijn gebracht met de Kaderrichtlijn Water (KRW) (Van Vlaardingen en Verbruggen, 2007). De KRW vereist dat bij het afleiden van milieurisicogrenzen voor water ook de mogelijke risico’s voor de mens als gevolg van consumptie van vis en visserijproducten worden meegewogen. Daarnaast worden humane risico’s meegenomen bij de afleiding van milieurisicogrenzen voor bodem, grondwater, drinkwater en lucht.

In dit rapport worden daarom voor twaalf stoffen uit bovengenoemd rapport milieurisicogrenzen afgeleid die zijn gebaseerd zijn op humaan-toxicologische gegevens. Deze twaalf stoffen zijn geselecteerd omdat ze zijn opgenomen in het ontwerp-Besluit ‘Kwaliteitseisen en monitoring water’. De stoffen waar het om gaat zijn:

1	1,1,2-trichloorethaan	7	1,1,1-trichloorethaan
2	hexachloorethaan	8	1,1,2,2-tetrachloorethaan
3	chloorethyleen (vinylchloride)	9	1,2-dichloorpropaan
4	1,1-dichloorethyleen	10	1,2-dichloorethyleen
5	3-chloorpropeen	11	1,3-dichloorpropeen
6	2-chloor(-1,3-)butadieen	12	2,3-dichloorpropeen

Vervolgens zijn de ecotoxicologische en humaan-toxicologische milieurisicogrenzen vergeleken en zijn de uiteindelijke milieurisicogrenzen afgeleid voor de compartimenten water, sediment (indien relevant), bodem en lucht. Waar relevant is doorvergiftiging ook in ogenschouw genomen.

Opgemerkt moet worden dat de hier bepaalde milieurisicogrenzen wetenschappelijk afgeleide waarden zijn. Ze dienen als advieswaarden voor de Nederlandse Interdepartementale Stuurgroep Stoffen, die de uiteindelijke milieukwaliteitsnormen beleidsmatig vaststelt. De milieurisicogrenzen zoals afgeleid in dit rapport zijn dus voorstellen zonder officiële status.

Wanneer er al humaan-toxicologische grenswaarden waren vastgesteld door het RIVM of andere instellingen (zoals US-EPA, WHO), dan zijn deze waarden overgenomen. Indien noodzakelijk zijn ze herzien op basis van wetenschappelijke publicaties die sindsdien beschikbaar gekomen zijn. Als er geen bestaande humaan-toxicologische grenswaarden beschikbaar waren voor een stof, dan zijn nieuwe risicogrenzen afgeleid op basis van evaluatie van de openbare literatuur.

Op basis van de humaan-toxicologische grenswaarden zijn vervolgens milieurisicogrenzen afgeleid volgens de handleiding voor het project ‘(Inter)nationale Normen Stoffen’ (Van Vlaardingen en Verbruggen, 2007). De selectie van de uiteindelijke milieurisicogrenzen, waarbij zowel de ecotoxicologische als humaan-toxicologische route wordt meegenomen, is ook uitgevoerd volgens deze handleiding. Een overzicht van deze milieurisicogrenzen is gegeven in Tabel 2.

Tabel 2. Afgeleide MTR-, VR-, MAC_{eco}- en ER_{eco}-waarden (in $\mu g.L^{-1}$ voor water and grondwater, in $mg.kg_{dw}^{-1}$ voor bodem, in $\mu g.m^{-3}$ voor lucht). n.a. = niet afgeleid.

	1,1,2-trichloorethaan	hexachloorethaan	chloorethyleen (vinylchloride)	1,1-dichlooretheen (1,1-dichloorethyleen)	3-chloorpropeen	2-chloor-1,3-butadieen (chloropreen)
Zoet water						
MTR	22	0,44	$9{,}1 \times 10^{-2}$ [b]	9,0	0,34	0,19
VR	0,22	$4{,}4 \times 10^{-3}$	$9{,}1 \times 10^{-4}$ [b]	$9{,}0 \times 10^{-2}$	$3{,}4 \times 10^{-3}$	$1{,}9 \times 10^{-3}$
MAC_{eco}	$3{,}0 \times 10^{2}$	1,4	n.a.	90	3,4	n.a.
ER_{eco}	$1{,}6 \times 10^{4}$	$1{,}1 \times 10^{2}$	n.a.	$1{,}1 \times 10^{4}$	$1{,}9 \times 10^{3}$	$1{,}9 \times 10^{3}$
Drinkwater						
MTR	14 [a]	3,5 [a]	0,50 [a]	$1{,}8 \times 10^{2}$ [a]	19 [a]	0,14 [a]
Marien water						
MTR	22	$6{,}7 \times 10^{-2}$	$9{,}1 \times 10^{-2}$ [b]	0,9	$3{,}4 \times 10^{-2}$	0,19
VR	0,22	$6{,}7 \times 10^{-4}$	$9{,}1 \times 10^{-4}$ [b]	$9{,}0 \times 10^{-3}$	$3{,}4 \times 10^{-4}$	$1{,}9 \times 10^{-3}$
MAC_{eco}	$1{,}9 \times 10^{2}$	0,28	n.a.	9,0	0,34	n.a.
ER_{eco}	$1{,}6 \times 10^{4}$	$1{,}1 \times 10^{2}$	n.a.	$1{,}1 \times 10^{4}$	$1{,}9 \times 10^{3}$	$1{,}9 \times 10^{3}$
Bodem						
MTR	0,16	$1{,}4 \times 10^{-2}$	$1{,}6 \times 10^{-4}$ [b]	$4{,}4 \times 10^{-2}$	$6{,}5 \times 10^{-4}$	$1{,}4 \times 10^{-3}$
VR	$1{,}6 \times 10^{-3}$	$1{,}4 \times 10^{-4}$	$1{,}6 \times 10^{-6}$ [b]	$4{,}4 \times 10^{-4}$	$6{,}5 \times 10^{-6}$	$1{,}4 \times 10^{-5}$
ER_{eco}	91	16	n.a.	53	3,6	10
Grondwater						
MTR	14	0,67	0,50	9,0	0,34	0,14
VR	0,14	$6{,}7 \times 10^{-3}$	$5{,}0 \times 10^{-3}$	$9{,}0 \times 10^{-2}$	$3{,}4 \times 10^{-3}$	$1{,}4 \times 10^{-3}$
ER_{eco}	$1{,}6 \times 10^{4}$	$1{,}1 \times 10^{2}$	n.a.	$1{,}1 \times 10^{4}$	$1{,}9 \times 10^{3}$	$1{,}9 \times 10^{3}$
Lucht						
MTR [d]	17	87	$3{,}6 \times 10^{-2}$	$2{,}0 \times 10^{2}$	7,4	0,02
VR [d]	0,17	0,87	$3{,}6 \times 10^{-4}$	2,0	$7{,}4 \times 10^{-2}$	2×10^{-4}

Tabel 2 (vervolg). Afgeleide MTR-, VR-, MAC_{eco}- en ER_{eco}-waarden (in $\mu g.L^{-1}$ voor water and grondwater, in $mg.kg_{dw}^{-1}$ voor bodem, in $\mu g.m^{-3}$ voor lucht). n.a. = niet afgeleid.

	1,1,1-trichloorethaan	1,1,2,2-tetrachloorethaan	1,2-dichloorpropaan	1,2-dichlooretheen (1,2-dichloorethyleen)	1,3-dichloorpropeen	2,3-dichloorpropeen
Zoet water						
MTR	21	8,0	$2,8 \times 10^{2}$	6,8	0,18	n.a.
VR	0,21	$8,0 \times 10^{-2}$	2,8	$6,8 \times 10^{-2}$	$1,8 \times 10^{-3}$	n.a.
MAC_{eco}	54	84	$1,3 \times 10^{3}$	n.a.	51	n.a.
ER_{eco}	$1,5 \times 10^{3}$	$1,7 \times 10^{3}$	$2,0 \times 10^{4}$	$1,1 \times 10^{4}$	28	n.a.
Drinkwater						
MTR	$7,0 \times 10^{3}$ [a]	$1,8 \times 10^{2}$ [a]	$2,5 \times 10^{2}$ [a]	$1,1 \times 10^{2}$ [a]	$3,5 \times 10^{-2}$ [a]	$3,5 \times 10^{-2}$ [a]
Marien water						
MTR	2,1	0,8	28	0,68	$1,8 \times 10^{-2}$	n.a.
VR	$2,1 \times 10^{-2}$	$8,0 \times 10^{-3}$	0,28	$6,8 \times 10^{-3}$	$1,8 \times 10^{-4}$	n.a.
MAC_{eco}	5,4	8,4	$1,3 \times 10^{2}$	n.a.	5,1	n.a.
ER_{eco}	$1,5 \times 10^{3}$	$1,7 \times 10^{3}$	$2,0 \times 10^{4}$	$1,1 \times 10^{4}$	28	n.a.
Bodem						
MTR	0,15	$7,0 \times 10^{-2}$	1,6	$2,0 \times 10^{-2}$	$3,0 \times 10^{-4}$	$3,0 \times 10^{-4}$ [b]
VR	$1,5 \times 10^{-3}$	$7,0 \times 10^{-4}$	$1,6 \times 10^{-2}$	$2,0 \times 10^{-4}$	$3,0 \times 10^{-6}$	$3,0 \times 10^{-6}$ [b]
ER_{eco}	11	14	59	32	$8,7 \times 10^{-2}$	n.a.
Grondwater						
MTR	21	8,0	$2,5 \times 10^{2}$	6,8	$3,5 \times 10^{-2}$	$3,5 \times 10^{-2}$ [c]
VR	0,21	$8,0 \times 10^{-2}$	2,5	$6,8 \times 10^{-2}$	$3,5 \times 10^{-4}$	$3,5 \times 10^{-4}$ [c]
ER_{eco}	$1,5 \times 10^{3}$	$1,7 \times 10^{3}$	$2,0 \times 10^{4}$	$1,1 \times 10^{4}$	28	n.a.
Lucht						
MTR [d]	$3,8 \times 10^{2}$	65 [d]	12	60	0,25	0,25
VR [d]	3,8	0,65 [d]	0,12	0,60	$2,5 \times 10^{-3}$	$2,5 \times 10^{-3}$

a: Voor alle stoffen, uitgezonderd chlooretheeen, is de weergegeven waarde een $MTR_{dw,\ water,\ provisional,}$. D.w.z. de waarde is niet gebaseerd op een vastgestelde Drinkwaternorm (DWS) volgens EU Directive 98/83/EC of een A1-waarde volgens Directive 75/440/EEC.

b: Waarden zijn niet gebaseerd op MTR_{eco}-waarden (niet beschikbaar), maar worden voldoende beschermend geacht voor zowel mens als milieu (zie rapporttekst).

c: Waarden zijn niet gebaseerd op MTR_{eco}-waarden (niet beschikbaar), maar worden – op basis van de gegevens voor 1,3-dichloorpropeen - voldoende beschermend geacht voor zowel mens als milieu (zie rapporttekst).

d: Alle MTR- and VR-waarden voor lucht zijn tenminste gebaseerd op $MTR_{humaan,\ lucht}$-waarden, uitgezonderd voor 1,1,2,2-tetrachlooroethaan waarvoor alleen een $MTR_{eco,\ lucht}$ waarde beschikbaar is. De waarden voor 1,1,2,2-tetrachloorethaan dienen als voorlopige waarden beschouwd te worden, omdat toekomstige beschikbaarheid van betrouwbare gegevens over chronische inhalatoire toxiciteit kunnen leiden tot lagere waarden.

rivm

1 Introduction

1.1 Project framework and background of the report

In this report environmental risk limits (ERLs) for surface water (freshwater and marine), soil and air are derived for twelve volatile aliphatic hydrocarbons. The following compounds are included:

1	1,1,2-trichloroethane	7	1,1,1-trichloroethane
2	hexachloroethane	8	1,1,2,2-tetrachloroethane
3	chloroethylene (vinylchloride)	9	1,2-dichloropropane
4	1,1-dichloroethylene	10	1,2-dichloroethylene
5	3-chloropropene	11	1,3-dichloropropene
6	2-chlorobutadiene (2-chlorobuta-1,3-diene)	12	2,3-dichloropropene

These twelve substances are selected because they are included in the Dutch draft 'Besluit Kwaliteitseisen en monitoring water' (draft Decree on Quality demands and monitoring water), which sets the environmental quality standards for compounds that are specifically relevant for the Netherlands within the context of the WFD.

The present report further elaborates on RIVM report 601782002 'Ecotoxicologically based environmental risk limits for several volatile aliphatic hydrocarbons' (De Jong et al., 2007). In that report ERLs for a number of volatile substances were derived, based on ecotoxicological data. The Water Framework Directive (WFD), however, requires that the potential risks for humans due to consumption of fish or shellfish are also considered when deriving ERLs. In addition, according to the updated guidance for deriving ERLs in the context of the project 'International and National Environmental Quality Standards for Substances in the Netherlands (INS)' by (Van Vlaardingen and Verbruggen, 2007), human-toxicological data should also be used for derivation of ERLs for soil, ground- and drinking water and air.

Therefore, human-toxicological threshold limits and ERLs based on human toxicology are derived in this report. Subsequently, the ecotoxicologically based ERLs from De Jong et al. (2007) and the newly derived human-toxicologically based ERLs are compared to derive final ERLs for each environmental compartment.

The following ERLs are derived (VROM, 2004):

- Negligible Concentration (NC) – concentration at which effects to ecosystems are expected to be negligible and functional properties of ecosystems must be safeguarded fully. It defines a safety margin which should exclude combination toxicity. The NC is derived by dividing the MPC (see next bullet) by a factor of 100.
- Maximum Permissible Concentration (MPC) – concentration in an environmental compartment at which:
  1. no effect to be rated as negative is to be expected for ecosystems;
  2a no effect to be rated as negative is to be expected for humans (for non-carcinogenic substances);

2b for humans no more than a probability of 10^{-6} per year of death can be calculated (for genotoxic carcinogenic substances). Within the scope of the WFD, a probability of 10^{-6} on a life-time basis is used.

Within the scope of the Water Framework Directive the MPC is specifically referring to long-term exposure.

- Maximum Acceptable Concentration (MAC_{eco}) – concentration protecting aquatic freshwater ecosystems for effects due to short-term exposure or concentration peaks.
- Serious Risk Concentration (SRC_{eco}) – concentration at which 50% of the species potentially present in an ecosystem may experience negative effects.

The results presented in this report have been discussed by the members of the scientific advisory group for the INS-project (WK-INS). It should be noted that the Environmental Risk Limits (ERLs) in this report are scientifically derived values, based on (eco)toxicological, fate and physico-chemical data. They serve as advisory values for the Dutch Steering Committee for Substances, which is appointed to set the Environmental Quality Standards (EQSs). ERLs should thus be considered as preliminary values that do not have an official status.

1.2 Current environmental quality standards for the twelve substances

Current environmental quality standards for the twelve substances are presented in Appendix 1. For most substances the underlying ERLs were derived by Van de Plassche and Bockting (1993). EQS-values are available for fresh water (MPC and NC), soil (NC), groundwater (NC) for most of the twelve substances. In some cases, (*ad hoc*) EQS-values for air (MPC and NC) are available.

1.3 Production, use and discharge

Data on production, use and discharge for the twelve hydrocarbons were reported in RIVM report 601782002 (De Jong et al., 2007).

1.4 Status of the results

The results presented in this report have been discussed by the members of the scientific advisory group for the INS-project (WK-INS). It should be noted that the ERLs in this report are scientifically derived values, based on (eco)toxicological, fate and physico-chemical data. They serve as advisory values for the Dutch Steering Committee for Substances, which is appointed to set the Environmental Quality Standards (EQSs). ERLs should thus be considered as proposed values that do not have an official status.

2 Methods

The methodology used is described in detail in Van Vlaardingen and Verbruggen (2007), further referred to as the 'INS-Guidance'. This guidance is in accordance with the guidance of the Fraunhofer Institute (FHI; Lepper, 2005) and prepared within the context of the WFD.

The process of ERL-derivation contains the following steps: data collection, data evaluation and selection, and derivation of the ERLs on the basis of the selected data. Specific items will be discussed below.

2.1 Data collection

When available, existing human-toxicological threshold limits (e.g. Tolerable Daily Intake, TDI; Tolerable Concentration in Air, TCA) as derived by RIVM or other recognised scientific institutes or agencies were adopted. In these cases, publicly available scientific literature that was published after the establishment of these risk limits was also evaluated in order to make sure the risk limits are up-to-date. This approach has previously been described by Janssen and Speijers (1997).

When no reliable human-toxicological threshold limits were available for a substance, the published scientific literature was evaluated and new threshold limits were derived from the available information.

Ecotoxicologically based ERLs were taken from RIVM report 601782002 (De Jong et al., 2007).

2.2 Derivation of ERLs

For a detailed description of the procedure for derivation of the ERLs, reference is made to the INS-Guidance. With respect to the selection of the final MPC_{water}, some additional comments should be made.

2.2.1 Drinking water

The INS-Guidance includes the MPC for surface waters intended for the abstraction of drinking water ($MPC_{dw, water}$) as one of the MPCs from which the lowest value should be selected as the general MPC_{water} (see INS-Guidance, section 3.1.6 and 3.1.7). According to the proposal for the daughter directive Priority Substances, however, the derivation of the AA-EQS (= MPC) should be based on direct exposure, secondary poisoning, and human exposure due to the consumption of fish. Drinking water was not included in the proposal and is thus not guiding for the general MPC_{water} value. The $MPC_{dw, water}$ is therefore presented as a separate value in this report.

The $MPC_{dw, water}$ is also used to derive the MPC_{gw}. For the derivation of the $MPC_{dw, water}$, a substance specific removal efficiency related to simple water treatment may be needed. Because there is no agreement as yet on how the removal fraction should be calculated, water treatment is not taken into account.

2.2.2 $MAC_{eco, marine}$

In this report, a MAC_{eco} is also derived for the marine environment. The assessment factor for the $MAC_{eco, marine}$ value is based on:

- the assessment factor for the $MAC_{eco, water}$ value when acute toxicity data for at least two specific marine taxa are available, or
- using an additional assessment factor of 5 when acute toxicity data for only one specific marine taxon are available (analogous to the derivation of the MPC according to Van Vlaardingen and Verbruggen, 2007), or
- using an additional assessment factor of 10 when no acute toxicity data are available for specific marine taxa.

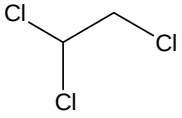
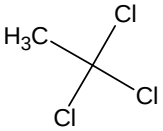
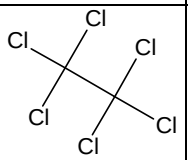
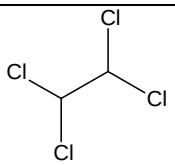
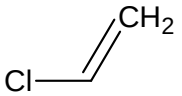
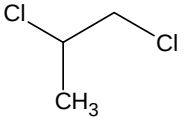
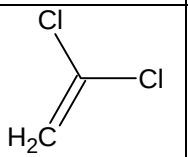
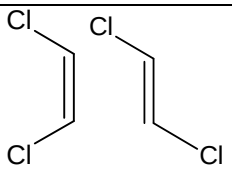
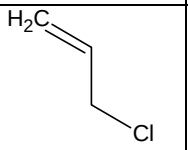
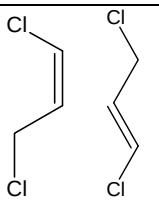
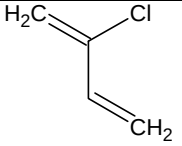
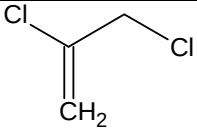
If freshwater and marine data sets are not combined the $MAC_{eco, marine}$ is derived on the marine toxicity data using the same additional assessment factors as mentioned above. It has to be noted that this procedure is currently not agreed upon. Therefore, the $MAC_{eco, marine}$ value needs to be re-evaluated once an agreed procedure is available.

3 Substance identification, physico-chemical properties, fate and human toxicology

3.1 Identity

All information in this section is taken from RIVM report 601782002 (De Jong et al., 2007). Structural formulas and CAS numbers of the compounds are presented below.

Table 3. Structural formulas and CAS numbers of the selected substances.

1,1,2-trichloroethane CAS 79-00-5		1,1,1-trichloroethane CAS NO. 71-55-6	
hexachloroethane CAS 67-72-1		1,1,2,2-tetrachloroethane CAS 79-34-5	
chloroethylene (vinylchloride) CAS 75-01-4		1,2-dichloropropane CAS 78-87-5	
1,1-dichloroethylene CAS 75-35-4		1,2-dichloroethylene CAS 540-59-0 156-59-2 (*cis*) 156-60-5 (*trans*)	 *cis* *trans*
3-chloropropene CAS 107-05-1		1,3-dichloropropene CAS 542-75-6 10061-01-5 (*cis*) 10061-02-6 (*trans*)	 *cis* *trans*
2-chlorobutadiene CAS 126-99-8		2,3-dichloropropene CAS 78-88-6	

3.2 Physico-chemical properties

All information in this section is taken from RIVM report 601782002 (De Jong et al., 2007).

Table 4. Physico-chemical properties for the selected substances.

Substance	Molecular weight [g.mol^{-1}]	Solubility [mg.L^{-1}]$^{\Phi}$	log $K_{ow}$$^{\$}$ [-]	log K_{oc}* [-]	Henry's law constant [Pa.m^3.mol^{-1}]*
1,1,2-trichloroethane	133.41	4580	2.07	1.95	88.5
hexachloroethane	236.74	27.2	4.14	3.40	162.1
chloroethylene	62.50	2700	1.52[a]	1.33	2564.6
1,1-dichloro-ethylene	96.94	2250	2.13	1.82	3797.7
3-chloro-propene	76.53	2940[d]	1.51[a]	1.32	1804.1
2-chloro-butadiene	88.54	856	2.15[a]	1.85	5684.0
1,1,1-trichloroethane	133.41	1300	2.49	2.02	1668.6
1,1,2,2-tetrachloroethane	167.85	2900	2.62	2.12	33.9
1,2-dichloropropane	112.99	3000	1.99	1.63	287.0
1,2-dichloroethylene	96.94	3810[e]	2.09/1.86[b]	1.61/1.78[b]	959.3[c]
1,3-dichloropropene	110.97	1080 [f]	1.82	1.64	899.9
2,3-dichloropropene	110.97	1000[d]	2.34	2.00	2482.0

Φ: all data from section 2.1 in De Jong et al. (2007).
$: taken from Table 4.1 from De Jong et al. (2007).
*: taken from Table 3.1 from De Jong et al. (2007).
a: derived from ClogP calculations (BioByte, 2004).
b: for the *cis*- and *trans*-isomer, respectively.
c: measured value of the *trans*-isomer is taken.
d: geomean of 2 reported estimated values.
e geomean of all reported values for both *cis*- and *trans*-isomer.
f: geomean of 2 values for *cis*- and *trans*-isomer (1071 and 1088 mg.L^{-1}).

3.3 Bioconcentration and biomagnification

Information on bioaccumulation is taken from Table 4.1 of RIVM report 601782002 (De Jong et al., 2007). An overview of the bioaccumulation data for the selected substances is given in Table 5. Where experimental data are available, these are used for ERL derivation, otherwise ERL derivation is based on calculated BCF values.

Table 5. Calculated or measured biocentration factors (BCF) [L.kg^{-1}] and default biomagnification factors (BMF) [kg.kg^{-1}].

Substance	BCF (fish)[a]	$BMF_{1,2}$[b]
1,1,2-trichloroethane	11	1
hexachloroethane	659	1
	139 (exp.)[c]	1
chloroethylene	4	1
1,1-dichloroethylene	13	1
3-chloropropene	4	1
2-chlorobutadiene	13	1
1,1,1-trichloroethane	26	1
1,1,2,2-tetrachloroethane	34	1
1,2-dichloropropane	10	1
1,2-dichloroethylene	12/8[d]	1
1,3-dichloropropene	7	1
2,3-dichloropropene	19	1

a: calculated using the QSAR for BCF from the TGD (European Commission, 2003) for substances with log K_{ow} < 6: log BCF = 0.85 × log K_{ow} - 0.70.

b: BMF_1 for biomagnification in prey of freshwater predators and BMF_2 for biomagnification in prey of marine top-predators

c: Barrows et al. (1980) as cited in De Jong et al. (2007). MPC calculations are based on the experimentally determined BCF value (when BCF is needed as input), because De Jong et al. (2007) considered the experimental value to be reliable. Reliable experimental data are preferred over QSAR-based calculated data.

d: for the *cis*- and *trans*-isomer, respectively.

3.4 Derivation of human-toxicological threshold limits

3.4.1 Introductory comments

In this paragraph, the derivation of human-toxicological threshold limits is described. Following the usual approach taken in human regulatory toxicology, a TDI (Tolerable Daily Intake) is derived. The TDI is the estimated dose to which humans may be exposed throughout their entire lifetime without any health effects occurring. The TDI is based on the notion that a threshold exists in the toxic action by the compound in question, *i.e.* a dose level below which the normal physiological and biochemical capacity of the organism is able to deal with the compound, preventing any harmful effects from occurring. For genotoxic carcinogens such a threshold is not assumed to exist and for these compounds TDI-derivation is not appropriate. Any dose, however low, is assumed to present increased risk on cancer. The size of this risk is dose dependent. Regulatory bodies derive so-called risk-specific doses for these compounds, intake levels associated with pre-determined acceptable cancer risk levels. Which risk specific dose is to be used in regulatory contexts is a risk management decision. As indicated by Van Vlaardingen and Verbruggen (2007) within the scope of ERL-derivations in the context of the WFD and INS, an additional cancer risk level of one in million per lifetime is used. For the inhalation route, a TCA (Tolerable Concentration in Air) is derived in the same way as the TDI for the oral route. For inhalation of genotoxic carcinogens, the one in million per lifetime extra risk also applies (lifetime 10^{-6} risk specific concentration).

As already indicated, human-toxicological ERLs are derived alongside ecotoxicological ERLs and subsequently these values are compared aimed at selection of an appropriate overall ERL. To facilitate this final selection of the overall ERL, reliability of the respective risk limits is a factor to taken into account. For ecotoxicological ERLs, a baseset is defined and when derivation is possible the result can thus be seen as reliable. Human-toxicological TDIs or risk specific doses, however, regularly have to be derived from imperfect data (incomplete datasets). The alternative would be to not derive a value at all in such cases which, however, might lead to the undesirable situation of insufficient protection of human health for potentially toxic compounds. Hence TDIs or risk specific doses qualified as preliminary because of data gaps, may still be as the basis for overall ERLs. To facilitate the choice between ecotoxicologically based and human-toxicologically based ERLs, all TDIs and risk specific doses derived are scored as either Low, Medium or High in reliability. Use of values scored as Low is unwanted in principle. For compounds with a high toxic or carcinogenic potential (also based on presumed structure activity relations) use of values of low reliability might nevertheless be defensible. Expert judgement is used to make the final choice.

3.4.2 Classification

An overview of the classification phrases for the selected substances is given in Table 6.

Table 6. Classification of the selected substances.

Substance	Classification
1,1,2-trichloroethane	R20/21/22: Harmful by inhalation, in contact with skin and if swallowed. R40: Limited evidence of a carcinogenic effect. R66: Repeated exposure may cause skin dryness or cracking.
hexachloroethane	not classified
chloroethylene	R12: Extremely flammable. R45: May cause cancer.
1,1-dichloroethylene	R12: Extremely flammable. R20: Harmful by inhalation. R40: Limited evidence of a carcinogenic effect.
3-chloropropene	R11: Highly flammable. R20/21/22: Harmful by inhalation, in contact with skin and if swallowed. R36/37/38: Irritating to eyes, respiratory system and skin. R40: Limited evidence of a carcinogenic effect. R48/20: Harmful: danger of serious damage to health by prolonged exposure through inhalation. R50: Very toxic to aquatic organism. R68: Possible risk of irreversible effects.
2-chlorobutadiene	R11: Highly flammable. R20/22: Harmful by inhalation and if swallowed. R36/37/38: Irritating to eyes, respiratory system and skin. R45: May cause cancer. R48/20: Harmful: danger of serious damage to health by prolonged exposure through inhalation.
1,1,1-trichloroethane	R20: Harmful by inhalation. R59: Dangerous for the ozone layer
1,1,2,2-tetrachloroethane	R26/27: Very toxic by inhalation and in contact with skin. R51/53: Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
1,2-dichloropropane	R11: Highly flammable. R20/22: Harmful by inhalation and if swallowed.

Table 6 (continued).

Substance	Classification
1,2-dichloroethylene	R11: Highly flammable. R20: Harmful by inhalation. R52/53: Harmful to aquatic organisms, may cause adverse effects in the aquatic environment.
1,3-dichloropropene	R10: Flammable. R20/21: Harmful by inhalation and in contact with skin. R25: Toxic if swallowed R36/37/38: Irritating to eyes, respiratory system and skin. R43: May cause sensitisation by skin contact. R50/53: Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
2,3-dichloropropene	R11: Highly flammable. R20/21/22: Harmful by inhalation, in contact with skin and if swallowed. R37/38: Irritating to respiratory system and skin R41: Risk of serious damage to eyes. R52/53: Harmful to aquatic organisms, may cause adverse effects in the aquatic environment. R68: Possible risk of irreversible effects.

3.4.3 Human-toxicological threshold limits

In the following sections, the important information on human toxicology is presented for each compound and the derivation of the threshold limits is outlined. An overview is presented in section 3.4.3.13.

3.4.3.1 1,1,2-Trichloroethane

In RIVM report 711701004 (Janssen et al., 1998), a preliminary TDI of 4 $\mu g.kg_{bw}^{-1}.d^{-1}$ and TCA of 17 $\mu g.m^{-3}$ were derived. These values were considered preliminary because of inconclusive data on carcinogenicity and mutagenicity. Additional search of the scientific literature from 1997 until October 2007 was performed. However, this yielded no additional information that provided crucial new insights. Therefore, the preliminary TDI and TCA are used for MPC derivation and are set to 4 $\mu g.kg_{bw}^{-1}.d^{-1}$ and 17 $\mu g.m^{-3}$, respectively (both with Reliability score: medium).

3.4.3.2 Hexachloroethane

The US-EPA (1991) derived a RfD (reference dose) of 1 $\mu g.kg_{bw}^{-1}.d^{-1}$. This value is adopted as TDI within the present scope. Additionally, a search in scientific literature from 2003 until October 2007 was performed. However, this yielded no usable additional information. Therefore, the TDI for hexachloroethane is set to 1 $\mu g.kg_{bw}^{-1}.d^{-1}$ (Reliability score: medium).
RIVM derived a preliminary TCA of 87 $\mu g.m^{-3}$ (Janssen, 1995). This was based on an inhalatory limit value (Minimal Risk Level, MRL) of 870 $\mu g.m^{-3}$ derived by ATSDR (1994) from a 6-week rat study (administration 6 $h.d^{-1}$, 5 $d.week^{-1}$). The NOAEL was 48 ppm, which was corrected for exposure to 9 ppm. Using an assessment factor of 100 and a conversion factor from ppm to $mg.m^{-3}$ (1 ppm = 9.68 $mg.m^{-3}$), this resulted in the MRL of 870 $\mu g.m^{-3}$. Applying an additional assessment factor of 10 for extrapolation from intermediate to chronic exposure resulted in a preliminary TCA of 87 $\mu g.m^{-3}$.
Additional literature search did not yield relevant new information for this compound. Therefore, a preliminary TCA of 87 $\mu g.m^{-3}$ (Reliability score: medium) will be used in this report.

3.4.3.3 Chloroethylene

In RIVM report 711701025 (Baars et al., 2001), a risk specific dose of 0.6 $\mu g.kg_{bw}^{-1}.d^{-1}$ and a risk specific concentration of 3.6 $\mu g.m^{-3}$ were derived, both based on an additional cancer risk of 10^{-4}/life. This was based on an extensive data set which did not change in recent years. Recalculation to a probability of 10^{-6} results in an oral risk-specific dose for 10^{-6}/life of 6×10^{-3} $\mu g.kg_{bw}^{-1}.d^{-1}$ and a risk-specific concentration in air for 10^{-6}/life of 0.036 $\mu g.m^{-3}$, respectively (both with Reliability score: high)

3.4.3.4 1,1-Dichloroethylene

In RIVM report 711701004 (Janssen et al., 1998), a preliminary TDI of 3 $\mu g.kg_{bw}^{-1}.d^{-1}$ and a preliminary TCA of 14 $\mu g.m^{-3}$ were derived. Additionally, a search in scientific literature was performed from 1997 until October 2007. This search did not yield new toxicity studies for this substance. However, new evaluations from IARC, US-EPA en WHO were found. In Janssen et al. (1998), 1,1-dichloroethylene was considered to be a genotoxic carcinogen. However, as was pointed out in the 1998 evaluation, the evidence was limited: only one mouse study showed kidney tumours after inhalation. IARC (1999) classified the substance in group 3 (not classifiable based on insufficient evidence of carcinogenicity in humans and limited evidence of carcinogenicity in test animals). In their evaluations, US-EPA (2002) and the WHO (2003) point out that the available carcinogenicity studies were limited, including the only positive test in mice. Although uncertainty remains concerning the carcinogenic and genotoxic potential of the compound, the approaches of US-EPA and WHO are considered sufficiently reliable and safe and will be adopted accordingly here. In order to derive human risk limits, both US-EPA and WHO used the threshold approach, based on BMDLs (Benchmark Dose Limits), for both the oral and inhalatory route with fatty degeneration of the liver as critical effect.
Based on a $BMDL_{10}$ of 4.6 $mg.kg_{bw}^{-1}.d^{-1}$ (chronic drinking water study with rats) and using an assessment factor of 100 (10 for interspecies extrapolation and 10 for intraspecies extrapolation, this yielded a TDI of 50 $\mu g.kg_{bw}^{-1}.d^{-1}$ (Reliability score: medium; rounded value as reported by US-EPA, 2002; WHO, 2003).
Based on a $BMDL_{10}$ (human equivalent concentration) of 6.9 $mg.m^{-3}$ (chronic inhalation study with rats) and using an assessment factor of 30 (3 for interspecies extrapolation and 10 for intraspecies extrapolation), this yielded a TCA of $2x10^{2}$ $\mu g.m^{-3}$ (Reliability score: medium; rounded value as reported by US-EPA, 2002; WHO, 2003).

3.4.3.5 3-Chloropropene

No human-toxicological threshold limits are currently available for 3-chloropropene. Therefore, a search in scientific literature from 1985 until October 2007 was performed. Evaluation of the data thus obtained showed that no adequate oral no-observed-adverse-effect levels (NOAELs) are available. In oral studies, observed toxic effects were too severe (mortality, tumours) for derivation of an adequate lowest-observed-adverse-effect level (LOAEL). However, since the alternative would be to derive no limit value at all for this potent toxicant, the TDI calculation is nevertheless based on the lowest observed effect level from the oral studies. This LOAEL is 55 $mg.kg_{bw}^{-1}.d^{-1}$ in female rats. The effects at this level were: increased mortality, growth retardation, clinical symptoms (NCI, 1978). Using an assessment factor of 10000 (10 intraspecies, 10 interspecies, 10 for using a LOAEL, 10 for the severity of the effects) yields a preliminary TDI of 5.5 $\mu g.kg_{bw}^{-1}.d^{-1}$ (Reliability score: low).
A preliminary TCA of 7.4 $\mu g.m^{-3}$ (Reliability score: low) is derived, based on a semichronic NOAEL of 31 $mg.m^{-3}$ (corrected for exposure duration: 7.38 $mg.m^{-3}$) taken from Nagano et al. (1991, as cited in OECD SIDS, 1996) and using an assessment factor of 1000 (10 for extrapolation from animal to human, 10 for protection of sensitive individuals and 10 for the lack of a chronic NOAEL and carcinogenicity data).

The low reliability of both TDI and TCA is due to data gaps, specifically the lack of adequate *in vivo* genotoxicity and carcinogenicity data for this structural analogue of vinylchloride.

3.4.3.6 2-Chlorobutadiene

No human-toxicological threshold limits are currently available for 2-chlorobutadiene. Since oral toxicity data are missing, the TDI is based on inhalatory toxicity data. For the oral route, lung tumours as observed in a mouse inhalation study are considered to be less relevant due to the route specific metabolism by inhalation (toxicokinetics deviate from those via the oral route). In this mouse inhalation study (NTP, 1998), in which animals were exposed to 46 $mg.m^{-3}$ for 6 $hours.d^{-1}$, 5 $d.week^{-1}$ for 2 years, a 20% tumour increase was observed in hemangiomas, hemangiosarcomas and liver carcinomas. Recalculated to continuous exposure the tested concentration equals 8.2 $mg.m^{-3}$. Assuming a respiratory volume of 0.04 $m^3.d^{-1}$ and a body weight of a mouse of 40 g, this results in a body dose of 8.2 $mg.kg_{bw}^{-1}.d^{-1}$ (assuming 100% absorption). Linear extrapolation based on the observed tumour incidence of 20% to 1 in 10^{-6} results in a preliminary oral risk-specific dose for 10^{-6}/life of 0.041 $\mu g.kg_{bw}^{-1}.d^{-1}$ (Reliability score: low).
The TCA is based on this same mouse study. At the lowest tumorigenic test concentration the lung tumour incidence was 39%. Based on linear extrapolation, the concentration in air can be calculated at which the extra risk for developing cancer equals $1:10^6$ per life. This leads to preliminary risk-specific concentration for 10^{-6}/life of 0.02 $\mu g.m^{-3}$ (Reliability score: medium).

3.4.3.7 1,1,1-Trichloroethane

In RIVM report 715810009, (Janssen et al,. 1995) derived a preliminary TDI of 80 $\mu g.kg_{bw}^{-1}.d^{-1}$ (extrapolated route-to-route from the TCA, which was 380 $\mu g.m^{-3}$). For the current report, an additional search in scientific literature from 1994 until August 2008 was performed. This yielded a new rat study where the substance was administered orally (NTP, 2000). Information on this route of exposure was missing in the report of Janssen et al. (1995).
US-EPA (2007) derived a Reference Dose (equivalent to a TDI) of 2 $mg.kg_{bw}^{-1}.d^{-1}$ based on the new oral data (Reliability score: high). This was based on a $BMDL_{10}$ (Benchmark Dose for 10% effect, lower confidence limit) of 2155 $mg.kg_{bw}^{-1}.d^{-1}$ and using an assessment factor of 1000 (10 for extrapolation for test species to humans, 10 for sensitive groups in the population and 10 because adequate information on sensitive neurological parameters is missing).
Additional literature research did not yield new relevant information for the TCA. Therefore, the TCA for 1,1,1-trichloroethane is set to 380 $\mu g.m^{-3}$ (Reliability score : high) as derived by Janssen et al. (1995).

3.4.3.8 1,1,2,2-Tetrachloroethane

Currently, no established human-toxicological threshold limits are available. Therefore, for the current report, a literature search was performed.
Based on the available literature, 1,1,2,2-tetrachloroethane is not considered to be genotoxic. Minor effects on the liver were observed in a 14-week oral study with male rats (LOAEL = 20 $mg.kg_{bw}^{-1}.d^{-1}$ as stated by the Dutch Health Council (Gezondheidsraad, 2007). In view of the minor effects, an assessment factor of 2 was considered sufficient by the Dutch Health Council to extrapolate from LOAEL to NOAEL. An additional factor of 2 (extrapolation to chronic exposure, factor according to new REACH guidance), a factor of 10 (extrapolation from test species to humans) and another factor of 10 (for sensitive groups in the population) results in a total assessment factor of 400. This results in a TDI of 50 $\mu g.kg_{bw}^{-1}.d^{-1}$ (Reliability score: medium).
Literature search yielded insufficient data for inhalatory toxicity to determine a TCA. Therefore, the TCA was determined by route-to-route extrapolation from the oral TDI (50 $\mu g.kg_{bw}^{-1}.d^{-1}$). This resulted in a preliminary TCA of 175 $\mu g.m^{-3}$ (Reliability score: low), based on a body weight of 70 kg, a

respiratory volume of 20 $m^3.d^{-1}$ and assuming total absorption for both routes. It has to be noted that this extrapolation is uncertain, since after oral exposure the liver is the target organ and 'site of first contact', whereas for inhalatory exposure neurological effects might be critical. The available inhalation studies were inconclusive on the latter point. The low reliability of the TCA is due to uncertainty in extrapolation from oral data in which liver effects were critical.

3.4.3.9 1,2-Dichloropropane

In RIVM report 711701004 (Janssen et al., 1998), a TDI of 70 $\mu g.kg_{bw}^{-1}.d^{-1}$ and a TCA of 12 $\mu g.m^{-3}$ were derived. Additionally, a search in scientific literature from 1997 until August 2008 was performed. However, this yielded no additional information that provided crucial new insights. Therefore, the TDI for 1,2-dichloropropane is set to 70 $\mu g.kg_{bw}^{-1}.d^{-1}$ and the TCA to 12 $\mu g.m^{-3}$ (both with Reliability score: high).

3.4.3.10 1,2-Dichloroethylene

There are different TDIs available for the *cis*- and *trans*-isomer in RIVM report 711701025 (Baars et al., 2001), 6 and 17 $\mu g.kg_{bw}^{-1}.d^{-1}$, respectively.
For the current report, an additional search in scientific literature from 2001 until August 2008 was performed. This yielded one new relevant study (performed within the scope of the American NTP, 2002), a 13-week dietary rat and mouse study with *trans*-1,2-dichloroethylene. This resulted in NOAELs of 190 and 915 $mg.kg_{bw}^{-1}.d^{-1}$ for rat and mouse, respectively. Results of the genotoxicity studies newly performed by NTP with each isomer and with the mixture of both isomers contradicted a similar study that was previously evaluated by Baars et al. (2001). In the new NTP study, no effects were observed *in vivo* for *cis*-1,2-dichloroethene in the bone marrow of mice after intraperitoneal injection. The quality of the new study is considered to be higher than that of the similar study evaluated by Baars et al. (2001).
Based on this new study, the assessment factor of 5 that was used by Baars et al. (2001) for possible non-threshold genotoxicity can be omitted. Furthermore, based on the evaluation of all available information (including the new studies) possible differences in toxicity between the two isomers appear are considered less likely than previously estimated. In view of the new data, an overall NOAEL for *cis*- and *trans*-1,2-dichloroethylene of 32 $mg.kg_{bw}^{-1}.d^{-1}$ is selected (from the study by McCauley et al., 1995 as cited in Baars et al., 2001). The NOAELs from the NTP study were not used, due to the observed deviations in immunotoxicological parameters at lower levels in the study from McCauley et al. Using an assessment factor of 1000 (10 for interspecies variability, 10 for intraspecies variability and 10 for the limited duration of the test and an incomplete dataset) results in a TDI of 30 $\mu g.kg_{bw}^{-1}.d^{-1}$ (Reliability score: medium).
The additional literature search from 2001 until August 2008 did not yield new relevant inhalatory toxicity studies. Since it was concluded from the new genotoxicity studies that there is no clear evidence for differences in toxicity between the *cis* and the *trans*-isomer, the TCA for *trans*-1,2-dichloroethylene of 60 $\mu g.m^{-3}$ (Reliability score: medium) is also considered applicable to *cis*-1,2-dichloroethylene.

3.4.3.11 1,3-Dichloropropene

No established human-toxicological threshold limits are currently available. For the current report, a search in scientific literature from 2000 until August 2008 was performed.
This compound was previously used in the Netherlands as soil fumigant and nematicide. This use has been discontinued due to the genotoxic and carcinogenic properties as observed in the relevant animal assays. In an evaluation for both of these endpoints, Feron and Kroese (1996) concluded that 1,3-dichloropropeen should be considered as a genotoxic carcinogen. However, more recently an EU-evaluation for classification has accepted the presence of epichlorohydrin as an explanation for the

positive results in genotoxicity assays. Accordingly, only classification as R68 was considered necessary for this compound. Before this evaluation, EFSA (2006) had stated that the *in vivo* genotoxicity and carcinogenicity was uncertain and therefore only a preliminary ADI could be derived, *i.e.* of 12.5 $\mu g.kg_{bw}^{-1}.d^{-1}$. US-EPA (2000) has published a review concluding that a genotoxic mechanism of tumour formation *in vivo* cannot be ruled out based on existing evidence. In view of this information non-threshold extrapolation is chosen as a conservative approach for deriving human-toxicological limit values within the present scope. The unit risks as developed by US-EPA (2000) can be used in this non-threshold evaluation.
For the oral route US-EPA (2000) calculated a cancer unit of 0.1 per $mg.kg_{bw}^{-1}.d^{-1}$ risk based on bladder carcinomas in mice. Recalculated to an extra cancer risk of 10^{-6} for lifetime exposure (one additional cancer incident in 10^6 persons taking up the substance daily for 70 years), this results in a risk specific dose for 10^{-6}/life of 0.01 $\mu g.kg_{bw}^{-1}.d^{-1}$ (Reliability score: high).
For the inhalation route US-EPA (2000) calculated a unit risk of 4×10^{-6} per $\mu g.m^{-3}$ based on increased long tumours in mice. Recalculated to an extra cancer risk of 10^{-6} for lifetime exposure (one additional cancer incident in 10^6 persons exposed to the substance continuously for 70 years), this results in a risk specific concentration for 10^{-6}/life of 0.25 $\mu g.m^{-3}$ (Reliability score: high).

3.4.3.12 2,3-Dichloropropene

No established human-toxicological threshold limits are currently available. For the current report, a search in scientific literature from as far back as possible until August 2008 was performed. This yielded no studies usable for limit value derivation. The limited data indicated similar action as 1,3-dichloropropene. Therefore read across with 1,3-dichloropropene (see above) is chosen. Thus the risk specific dose for 10^{-6}/life and risk specific concentration for 10^{-6}/life for 1,3-dichloropropene (0.01 $\mu g.kg_{bw}^{-1}.d^{-1}$ and 0.25 $\mu g.m^{-3}$, respectively) were adopted for 2,3-dichloropropene (both with Reliability score: low). These ‘low’ scores were given because very few data were available for this potentially toxic compound.

3.4.3.13 Overview of derived human-toxicological threshold limits

An overview of the human-toxicological threshold limits as derived in the previous sections is presented in Table 7.

Table 7. Overview of derived human-toxicological threshold limits for the selected substances: Tolerable Daily Intake (TDI) or risk specific dose [$\mu g.kg_{bw}^{-1}.d^{-1}$] and Tolerable Concentration in Air (TCA) or risk specific concentration [$\mu g.m^{-3}$].

Substance	TDI or risk specific dose [$\mu g.kg_{bw}^{-1}.d^{-1}$]	Reliability score	TCA or risk specific concentration [$\mu g.m^{-3}$]	Reliability score
1,1,2-trichloroethane	4	medium	17	medium
hexachloroethane	1	medium	87	medium
chloroethylene	6×10^{-3}	high	3.6×10^{-2}	high
1,1-dichloroethylene	50	medium	2×10^{2}	medium
3-chloropropene	5.5	low	7.4	low
2-chlorobutadiene	4.1×10^{-2}	low	0.02	medium
1,1,1-trichloroethane	2×10^{3}	high	3.8×10^{2}	high
1,1,2,2-tetrachloroethane	50	medium	$(1.8 \times 10^{2})^{a}$	low
1,2-dichloropropane	70	high	12	high
1,2-dichloroethylene	30	medium	60	medium
1,3-dichloropropene	0.01	high	0.25	high
2,3-dichloropropene	0.01	low	0.25	low

a: Value with low reliability and not to be used for further calculation (see explanation below)

3.4.4 Reliability evaluation

From Table 7 it appears that for 4 substances a reliability score 'low' was given. As discussed above in section 3.4.1, a decision should be made as to whether human-toxicological threshold limits with a reliability score 'low' should be used for ERL-derivation.

- For 3-chloropropene data indicate a possible genotoxic action. For such compounds, risk-specific doses for accepted cancer risk levels tend to be low to very low. Given this fact, the low-reliability values for this compound are retained for calculation of ERLs.
- The same applies to 2-chlorobutadiene. This compound is suspected of a genotoxic carcinogenic action and the oral risk-specific dose is retained despite its low reliability.
- The TCA for 1,1,2,2-tetrachloroethane is of low reliability and is not used for further calculation of ERLs. This TCA was derived by route-to-route-extrapolation from an oral value based on liver toxicity. The outcome of this extrapolation in this case is even more uncertain than in general for this kind of cross-route extrapolation.
- For 2,3-dichloropropene only very limited data were available. These limited data suggest similar action as 1,3-dichloropropene, for which a low risk-specific dose/concentration was derived. Based on this suggested similar action the risk-specific dose/concentration for 1,3-dichloropropene are retained for calculation of human-toxicological ERLs for 2,3-dichloropropene despite their low reliability.

4 Derivation of environmental risk limits

4.1 Derivation of MPC_{water} and MPC_{marine}

4.1.1 $MPC_{eco, water}$ and $MPC_{eco, marine}$

All information in this section is taken from RIVM report 601782002 (De Jong et al., 2007). An overview of the $MPC_{eco, water}$ and $MPC_{eco, marine}$ for the selected substances is given in Table 8.

Table 8. $MPC_{eco, water}$ and $MPC_{eco, marine}$ for the selected substances.

Substance	$MPC_{eco, water}$ [$\mu g.L^{-1}$]	$MPC_{eco, marine}$ [$\mu g.L^{-1}$]
1,1,2-trichloroethane	3.0×10^{2}	30
hexachloroethane	0.67	6.7×10^{-2}
chloroethylene[a]	n.d.	n.d.
1,1-dichloroethylene	9	0.9
3-chloropropene	0.34	3.4×10^{-2}
2-chlorobutadiene	19	1.9
1,1,1-trichloroethane	21	2.1
1,1,2,2-tetrachloroethane	8	0.8
1,2-dichloropropane	2.8×10^{2}	28
1,2-dichloroethylene	6.8	0.68
1,3-dichloropropene	0.18	1.8×10^{-2}
2,3-dichloropropene[b]	n.d.	n.d.

a: n.d. = not derived. Only few ecotoxicity data were available. Since data for algae and daphnids are lacking, a reliable MPC could not be derived.

b: n.d. = not derived. Insufficient data for MPC derivation.

4.1.2 $MPC_{sp, water}$ and $MPC_{sp, marine}$

Secondary poisoning is only triggered for hexachloroethane (BCF ≥ 100 L/kg and/or log K_{ow} ≥ 3). The $MPC_{sp, water}$ and $MPC_{sp, marine}$ for freshwater and marine waters as derived by De Jong et al. (2007) is 4.79 $\mu g.L^{-1}$.

4.1.3 $MPC_{hh\ food, water}$

In this section, MPCs based on the uptake of compounds via human consumption of fishery products are derived for those compounds that meet the triggers as defined in the INS-Guidance. For 1,1,1-trichloroethane; 1,1,2,2-tetrachloroethane; 1,2-dichloropropane; 1,2-dichloroethylene; 1,3-dichloropropene and 2,3-dichloropropene the derivation of MPCs for human consumption of fishery products is not triggered based on their R-phrase classification or bioaccumulation potential. The $MPC_{hh\ food, water}$ for the other compounds is derived below. It is assumed that consumption of fish(products) may contribute at most for 10% to the threshold, and that the daily intake for a 70 kg person is 115 g fish.

4.1.3.1 1,1,2-Trichloroethane

A preliminary TDI of 4 $\mu g.kg_{bw}^{-1}.d^{-1}$ is derived for 1,1,2-trichloroethane (see section 3.4), resulting in an $MPC_{hh\ food}$ of $(0.1 \times 4 \times 70)/0.115 = 243\ \mu g.kg_{food}^{-1}$. This results in an $MPC_{hh\ food, water}$ of

243/ (11 × 1) = 22 µg.L^{-1}.

4.1.3.2 Hexachloroethane

A TDI of 1 µg.kg_{bw}^{-1}.d^{-1} is derived for hexachloroethane (see section 3.4), resulting in an $MPC_{hh\ food}$ of (0.1 × 1 × 70)/0.115 = 61 µg.kg_{food}^{-1}, which results in an $MPC_{hh\ food,\ water}$ of 61/(139 × 1) = 0.44 µg.L^{-1}.

4.1.3.3 Chloroethylene

A 10^{-6} per lifetime risk-specific oral dose of 6 × 10^{-3} µg.kg_{bw}^{-1}.d^{-1} is derived for chloroethylene (see section 3.4), resulting in an $MPC_{hh\ food}$ of (0.1 × 6 × 10^{-3} × 70)/0.115 = 0.37 µg.kg_{food}^{-1}, which results in an $MPC_{hh\ food,\ water}$ of 0.37/(4 × 1) = 0.091 µg.L^{-1}.

4.1.3.4 1,1-Dichloroethylene

A TDI of 50 µg.kg bw^{-1}.d^{-1} is derived for 1,1-dichloroethylene (see section 3.4), resulting in an $MPC_{hh\ food}$ of (0.1 × 50 × 70)/0.115 = 3043 µg.kg_{food}^{-1}, which results in an $MPC_{hh\ food,\ water}$ of 3043/(13 × 1) = 234 µg.L^{-1}.

4.1.3.5 3-Chloropropene

A preliminary TDI of 5.5 µg.kg bw^{-1}.d^{-1} is derived for 3-chloropropene (see section 3.4), resulting in an $MPC_{hh\ food}$ of (0.1 × 5.5 × 70)/0.115 = 335 µg.kg_{food}^{-1}, which results in an $MPC_{hh\ food,\ water}$ of 335/(4 × 1) = 84 µg.L^{-1}.

4.1.3.6 2-Chlorobutadiene

A preliminary 10^{-6} per lifetime risk-specific oral dose of 0.041 µg.kg bw^{-1}.d^{-1} is derived for 2-chlorobutadiene (see section 3.4), resulting in an $MPC_{hh\ food}$ of (0.1 × 0.041 × 70)/0.115 = 2.50 µg.kg_{food}^{-1}, which results in an $MPC_{hh\ food,\ water}$ of 2.50/(13 × 1) = 0.19 µg.L^{-1}.

4.1.3.7 Overview of derived $MPC_{hh\ food,\ water}$

An overview of the derived $MPC_{hh\ food,\ water}$, which are valid for both fresh and marine waters, is shown in Table 9.

Table 9. $MPC_{hh\ food,\ water}$ for the selected substances.

Substance	$MPC_{hh\ food,\ water}$ [µg.L^{-1}]
1,1,2-trichloroethane	22
hexachloroethane	0.44
chloroethylene	9.1 × 10^{-2}
1,1-dichloroethylene	2.3 × 10^{2}
3-chloropropene	84
2-chlorobutadiene	0.19
1,1,1-trichloroethane	not triggered
1,1,2,2-tetrachloroethane	not triggered
1,2-dichloropropane	not triggered
1,2-dichloroethylene	not triggered
1,3-dichloropropene	not triggered
2,3-dichloropropene	not triggered

4.1.4 Selection of the MPC_{water} and MPC_{marine}

The lowest value for the aquatic compartment from sections 4.1.1 to 4.1.3 is chosen as the final MPC_{water} or MPC_{marine}. An overview is given in Table 10.

Table 10. MPC_{water} and MPC_{marine} for the selected substances.

Substance	MPC_{water} [µg.L^{-1}]	MPC_{marine} [µg.L^{-1}]
1,1,2-trichloroethane	22	22
hexachloroethane	0.44	6.7×10^{-2}
chloroethylene	9.1×10^{-2a}	9.1×10^{-2a}
1,1-dichloroethylene	9	0.9
3-chloropropene	0.34	3.4×10^{-2}
2-chlorobutadiene	0.19	0.19
1,1,1-trichloroethane	21	2.1
1,1,2,2-tetrachloroethane	8	0.8
1,2-dichloropropane	2.8×10^{2}	28
1,2-dichloroethylene	6.8	0.68
1,3-dichloropropene	0.18	1.8×10^{-2}
2,3-dichloropropene	n.d. [a]	n.d. [a]

n.d.: not derived

a: see text below

For chloroethylene, an MPC_{eco} is not available due to insufficient data (data on algae and daphnids are not available). Normally, this would mean that an overall MPC_{water} cannot be determined. However, the available ecotoxicity data ($E(L)C_{50}$ values for protozoans of 405 mg.L^{-1} and for fishes of 1100 and 1200 mg.L^{-1} are a factor of 4.5×10^{6} – 1.3×10^{7} above the MPC_{water} based on human toxicological data (9.1×10^{-2} µg.L^{-1}). This value is based on the carcinogenic properties of the substance. Furthermore, it is a volatile substance (Henry's law constant is 2564.6 Pa.m.mol^{-1}). Therefore, it can be assumed that the $MPC_{hh\ food,\ water}$ will also be protective enough for ecosystems.

For 2,3-dichloropropene, an $MPC_{eco,\ water}$ is not available due to insufficient data (data on algae and daphnids are not available). $MPC_{hh\ food,\ water}$ is not triggered. Therefore, an MPC_{water} and an MPC_{marine} cannot be derived.

4.2 Derivation of $MPC_{dw,\ water}$

In this paragraph MPCs based on the uptake of compounds via human consumption of drinking water are derived. When an established Drinking Water Standard (DWS) conform EU Directive 98/83/EC or A1-value conform Directive 75/440/EEC is available, this is used to derive the $MPC_{dw,\ water}$. Otherwise, a $MPC_{dw,\ water,\ provisional}$ is calculated using the human-toxicological threshold limits as derived in section 3.4. It is assumed that drinking water may contribute at most for 10 % to the threshold, and that the daily intake for a 70 kg person is 2 L. See section 2.2.1. for remarks about the derivation of $MPC_{dw,\ water}$.

4.2.1.1 1,1,2-Trichloroethane

No A1-value or DWS is available. Therefore an $MPC_{dw,\ water}$ is calculated based on the preliminary TDI of 4 µg.kg$_{bw}^{-1}$.d^{-1} . This results in a $MPC_{dw,\ water,\ provisional}$ of $0.1 \times 4 \times 70/2 = 14$ µg.L^{-1}.

4.2.1.2 Hexachloroethane

No A1-value or DWS is available. Therefore a provisional $MPC_{dw, water}$ is calculated based on the TDI of 1 $\mu g.kg_{bw}^{-1}.d^{-1}$. This results in an $MPC_{dw, water, provisional}$ of $0.1 \times 1 \times 70/2 = 3.5$ $\mu g.L^{-1}$.

4.2.1.3 Chloroethylene

For chloroethylene a Drinking Water Standard (DWS) of 0.50 $\mu g.L^{-1}$ is available in Council Directive 98/83/EC (European Commission, 1998). This value is a parametric value that refers to the residual monomer concentration in the water as calculated according to specifications of the maximum release from the corresponding polymer in contact with water (as stated in a footnote of a table, taken from part B of Council Directive 98/83/EC (EC, 1998)). This results in an $MPC_{dw, water}$ of 0.50 $\mu g.L^{-1}$.

4.2.1.4 1,1-Dichloroethylene

No A1-value or DWS is available. Therefore a provisional $MPC_{dw, water}$ is calculated based on the TDI of 50 $\mu g.kg_{bw}^{-1}.d^{-1}$. This results in an $MPC_{dw, water, provisional}$ of $0.1 \times 50 \times 70/2 = 175$ $\mu g.L^{-1}$.

4.2.1.5 3-Chloropropene

No A1-value or DWS is available. Therefore a provisional $MPC_{dw, water}$ is calculated based on the preliminary TDI of 5.5 $\mu g.kg_{bw}^{-1}.d^{-1}$. This results in an $MPC_{dw, water, provisional}$ of $0.1 \times 5.5 \times 70/2 = 19$ $\mu g.L^{-1}$

4.2.1.6 2-Chlorobutadiene

No A1-value or DWS is available. Therefore a provisional $MPC_{dw, water}$ is calculated based on the preliminary 10^{-6} per lifetime risk-specific oral dose of 0.041 $\mu g.kg_{bw}^{-1}.d^{-1}$. This results in an $MPC_{dw, water, provisional}$ of $0.1 \times 0.041 \times 70/2 = 0.14$ $\mu g.L^{-1}$.

4.2.1.7 1,1,1-Trichloroethane

No A1-value or DWS is available. Therefore a provisional $MPC_{dw, water}$ is calculated based on the TDI of 2000 $\mu g.kg_{bw}^{-1}.d^{-1}$. This results in an $MPC_{dw, water, provisional}$ of $0.1 \times 2000 \times 70/2 = 7000$ $\mu g.L^{-1}$.

4.2.1.8 1,1,2,2-Tetrachloroethane

No A1-value or DWS is available. Therefore a provisional $MPC_{dw, water}$ is calculated based on the TDI of 50 $\mu g.kg_{bw}^{-1}.d^{-1}$. This results in an $MPC_{dw, water, provisional}$ of $0.1 \times 50 \times 70/2 = 175$ $\mu g.L^{-1}$.

4.2.1.9 1,2-Dichloropropane

No A1-value or DWS is available. Therefore a provisional $MPC_{dw, water}$ is calculated based on the TDI of 70 $\mu g.kg_{bw}^{-1}.d^{-1}$. This results in an $MPC_{dw, water, provisional}$ of $0.1 \times 70 \times 70/2 = 245$ $\mu g.L^{-1}$.

4.2.1.10 1,2-Dichloroethylene

No A1-value or DWS is available. Therefore a provisional $MPC_{dw, water}$ is calculated based on the preliminary TDI of 30 $\mu g.kg_{bw}^{-1}.d^{-1}$. This results in an $MPC_{dw, water, provisional}$ of $0.1 \times 30 \times 70/2 = 105$ $\mu g.L^{-1}$.

4.2.1.11 1,3-Dichloropropene

No A1-value or DWS is available. Therefore a provisional $MPC_{dw, water}$ is calculated based on the 10^{-6} per lifetime risk-specific oral dose of 0.01 $\mu g.kg_{bw}^{-1}.d^{-1}$. This results in an $MPC_{dw, water, provisional}$ of $0.1 \times 0.01 \times 70/2 = 0.035$ $\mu g.L^{-1}$.

4.2.1.12 2,3-Dichloropropene

No A1-value or DWS is available. Therefore a provisional $MPC_{dw, water}$ is calculated based on the preliminary 10^{-6} per lifetime risk-specific oral dose of 0.01 $\mu g.kg_{bw}^{-1}.d^{-1}$. This results in an $MPC_{dw, water, provisional}$ of $0.1 \times 0.01 \times 70/2 = 0.035$ $\mu g.L^{-1}$.

4.2.2 Overview of derived (provisional) $MPC_{dw, water}$

An overview of the derived values for $MPC_{dw, water}$ is shown in Table 11.

Table 11. $MPC_{dw, water, provisional}$ (unless stated otherwise) for the selected substances.

Substance	$MPC_{dw, water, provisional}$ [$\mu g.L^{-1}$]
1,1,2-trichloroethane	14
hexachloroethane	3.5
chloroethylene	0.50[a]
1,1-dichloroethylene	1.8×10^2
3-chloropropene	19
2-chlorobutadiene	0.14
1,1,1-trichloroethane	7.0×10^3
1,1,2,2-tetrachloroethane	1.8×10^2
1,2-dichloropropane	2.5×10^2
1,2-dichloroethylene	1.1×10^2
1,3-dichloropropene	3.5×10^{-2}
2,3-dichloropropene	3.5×10^{-2}

a: $MPC_{dw, water}$ value: equal to Drinking Water Standard from Council Directive 98/83/EC

4.3 Derivation of MAC_{eco}

MAC_{eco} values were not derived in De Jong et al. (2007). Therefore, MAC_{eco} values are be derived in this report, based on the ecotoxicological data available in De Jong et al. (2007). In all cases, a t-test confirmed that the acute fresh- and saltwater toxicity data for these substances can be combined. See section 2.2.2 for further comments on the derivation of the $MAC_{eco, marine}$.

4.3.1 1,1,2-Trichloroethane

Based on the lowest $L(E)C_{50}$ of 1.9×10^3 $\mu g.L^{-1}$ (*Nitrosomonas sp.*) and an assessment factor of 10 (mode of action is likely to be narcosis and fish are amongst the most sensitive species in the dataset), a $MAC_{eco, water}$ of 190 $\mu g.L^{-1}$ is derived. However, since this value is lower than the MPC_{eco} (300 $\mu g.L^{-1}$), the $MAC_{eco, water}$ is set to 300 $\mu g.L^{-1}$.
The lowest $L(E)C_{50}$ is 1.9×10^3 $\mu g.L^{-1}$ for *Nitrosomonas sp.*. An assessment factor of 10 is applied, because the mode of action is known and data for molluscs, annelids and a marine crustacean (e.g. *Crangon crangon)* are available next to data for bacteria, algae and fish. The $MAC_{eco, marine}$ is 190 $\mu g.L^{-1}$.

4.3.2 Hexachloroethane

Based on the lowest $L(E)C_{50}$ of 140 $\mu g.L^{-1}$ (*Vibrio fischeri*) and an assessment factor of 100 (bioaccumulating potential, mode of action is likely to be narcosis and fish are amongst the most sensitive species in the dataset), a $MAC_{eco ,water}$ of 1.4 $\mu g.L^{-1}$ is derived.

Based on the lowest L(E)C_{50} of 140 µg.L^{-1} (*V. fischeri*) and an assessment factor of 500 (due to the bioaccumulating potential, known mode of action and one marine taxon is available), a $MAC_{eco, marine}$ of 0.28 µg.L^{-1} is derived.

4.3.3 Chloroethylene

Since the base set is not complete, a $MAC_{eco, water}$ cannot be derived.

4.3.4 1,1-Dichloroethylene

Based on the lowest L(E)C_{50} of 9×10^3 µg.L^{-1} (*Chlamydomonas reinhardtii*) and an assessment factor of 100, a $MAC_{eco, water}$ of 90 µg.L^{-1} is derived.
Based on the lowest L(E)C_{50} of 9×10^3 µg.L^{-1} (*C. reinhardtii*) and an assessment factor of 1000, a $MAC_{eco, marine}$ of 9 µg.L^{-1} is derived.

4.3.5 3-Chloropropene

It has to be noted that the acute freshwater toxicity base set is not complete (algae are missing), but a chronic algae value is available, which is not lower than the lowest L(E)C_{50}. Therefore, a $MAC_{eco, water}$ can be derived. Based on the lowest L(E)C_{50} of 340 µg.L^{-1} (*Xenopus laevis*) and an assessment factor of 100, a $MAC_{eco ,water}$ of 3.4 µg.L^{-1} is derived.
Based on the lowest L(E)C_{50} of 340 µg.L^{-1} (*X. laevis*) and an assessment factor of 1000, a $MAC_{eco, marine}$ of 0.340 µg.L^{-1} is derived.

4.3.6 2-Chlorobutadiene

The acute freshwater toxicity base set is not complete (data for crustacea are missing). There is a chronic toxicity value for crustacea available, but this value is far lower (1.9 mg.L^{-1}) than the acute toxicity data for fish and algae (245 and 380 mg.L^{-1}). Therefore, a $MAC_{eco, water}$ cannot be derived. Furthermore, saltwater data are not available. Therefore, no $MAC_{eco, marine}$ can be derived.

4.3.7 1,1,1-Trichloroethane

Based on the lowest L(E)C_{50} of 536 µg.L^{-1} (*Chlamydomonas reinhardtii*) and an assessment factor of 10 (mode of action is likely to be narcosis and fish are amongst the most sensitive species in the dataset), a $MAC_{eco, water}$ of 53.6 µg.L^{-1} is derived.
Based on the lowest L(E)C_{50} of 536 µg.L^{-1} (*C. reinhardtii*) and an assessment factor of 100, a $MAC_{eco, marine}$ of 5.36 µg.L^{-1} is derived.

4.3.8 1,1,2,2-Tetrachloroethane

Based on the lowest L(E)C50 of 840 µg.L^{-1} (*Artemia salina*) and an assessment factor of 10 (mode of action is likely to be narcosis and fish are amongst the most sensitive species in the dataset), a $MAC_{eco, water}$ of 84 µg.L^{-1} is derived.
Based on the lowest L(E)C_{50} of 840 µg.L^{-1} (*A. salina*) and an assessment factor of 100, a $MAC_{eco, marine}$ of 8.4 µg.L^{-1} is derived.

4.3.9 1,2-Dichloropropane

Based on the lowest L(E)C_{50} of 13×10^3 µg.L^{-1} (*Ceriodaphnia reticulata*) and an assessment factor of 10 (mode of action is likely to be narcosis and fish are amongst the most sensitive species in the dataset), a $MAC_{eco, water}$ of 1300 µg.L^{-1} is derived.
Based on the lowest L(E)C_{50} of 13×10^3 µg.L^{-1} (*C. reticulata*) and an assessment factor of 100, a $MAC_{eco, marine}$ of 130 µg.L^{-1} is derived.

4.3.10 1,2-Dichloroethylene

The acute freshwater toxicity base set is not complete (data for crustacea and algae are missing). When data for 1,2-dichloroethylene are combined with data for *trans*-1,2-dichloroethylene and *cis*-dichloroethylene, daphnid data are included but data for algae are still missing. Saltwater data are only available for crustacea. There are also no chronic algal ecotoxicity data available that could be used as supportive. Therefore, a $MAC_{eco,\ water}$ and a $MAC_{eco,\ marine}$ cannot be derived.

4.3.11 1,3-Dichloropropene

Based on the lowest $L(E)C_{50}$ of 510 $\mu g.L^{-1}$ (*Poecilia reticulata*) and an assessment factor of 10 (little variation in ecotoxicity data, mode of action is likely to be narcosis and fish are amongst the most sensitive species in the dataset), a $MAC_{eco,\ water}$ of 51 $\mu g.L^{-1}$ is derived.
Based on the lowest $L(E)C_{50}$ of 510 $\mu g.L^{-1}$ (*P. reticulata*) and an assessment factor of 100, a $MAC_{eco,\ marine}$ of 5.1 $\mu g.L^{-1}$ is derived.

4.3.12 2,3-Dichloropropene

The acute freshwater toxicity base set is not complete (data for crustacea and algae are missing). There are also no chronic ecotoxicity data available that could be used as supportive data. Furthermore, saltwater data are not available. Therefore, a $MAC_{eco,\ water}$ and $MAC_{eco,marine}$ cannot be derived.

4.3.13 Overview of derived $MAC_{eco,\ water}$ and $MAC_{eco,\ marine}$

An overview of the derived $MAC_{eco,\ water}$ and $MAC_{eco,\ marine}$ values is given in Table 12.

Table 12. MAC_{eco} values for the selected substances.

Substance	$MAC_{eco,water}$ [$\mu g.L^{-1}$]	$MAC_{eco,\ marine}$ [$\mu g.L^{-1}$]
1,1,2-trichloroethane	3.0×10^2	1.9×10^2
hexachloroethane	1.4	0.28
chloroethylene	n.d.	n.d.
1,1-dichloroethylene	90	9
3-chloropropene	3.4	0.34
2-chlorobutadiene	n.d.	n.d.
1,1,1-trichloroethane	54	5.4
1,1,2,2-tetrachloroethane	84	8.4
1,2-dichloropropane	1.3×10^3	1.3×10^2
1,2-dichloroethylene	n.d.	n.d.
1,3-dichloropropene	51	5.1
2,3-dichloropropene	n.d.	n.d.

n.d.: not derived. Base set was not complete, therefore a MAC_{eco} could not be derived.

4.4 Derivation of NC_{water}

The NC_{water} is set a factor 100 lower than the MPC_{water}. An overview of the NC_{water} for the selected substances is given in Table 13.

Table 13. NC_{water} for the selected substances.

Substance	NC_{water} [µg.L^{-1}]	NC_{marine} [µg.L^{-1}]
1,1,2-trichloroethane	0.22	0.22
hexachloroethane	4.4×10^{-3}	6.7×10^{-4}
chloroethylene	9.1×10^{-4}	9.1×10^{-4}
1,1-dichloroethylene	9.0×10^{-2}	9.0×10^{-3}
3-chloropropene	3.4×10^{-3}	3.4×10^{-4}
2-chlorobutadiene	1.9×10^{-3}	1.9×10^{-3}
1,1,1-trichloroethane	0.21	2.1×10^{-2}
1,1,2,2-tetrachloroethane	8.0×10^{-2}	8.0×10^{-3}
1,2-dichloropropane	2.8	0.28
1,2-dichloroethylene	6.8×10^{-2}	6.8×10^{-3}
1,3-dichloropropene	1.8×10^{-3}	1.8×10^{-4}
2,3-dichloropropene	n.d.	n.d.

n.d.: not derived. Insufficient data to derive MPC values.

4.5 Derivation of $SRC_{eco, water}$

$SRC_{eco, water}$ and $SRC_{eco, marine}$ values are taken from RIVM report 601782002 (De Jong et al., 2007). An overview of the $SRC_{eco, water}$ and $SRC_{eco, marine}$ for the selected substances is given in Table 14

Table 14. $SRC_{eco, water}$ and $SRC_{eco, marine}$ for the selected substances.

Substance	$SRC_{eco, water}$ [µg.L^{-1}]	$SRC_{eco, marine}$ [µg.L^{-1}]
1,1,2-trichloroethane	1.6×10^{4}	1.6×10^{4}
hexachloroethane	1.1×10^{2}	1.1×10^{2}
chloroethylene	n.d.	n.d.
1,1-dichloroethylene	1.1×10^{4}	1.1×10^{4}
3-chloropropene	1.9×10^{3}	1.9×10^{3}
2-chlorobutadiene	1.9×10^{3}	1.9×10^{3}
1,1,1-trichloroethane	1.5×10^{3}	1.5×10^{3}
1,1,2,2-tetrachloroethane	1.7×10^{3}	1.7×10^{3}
1,2-dichloropropane	2.0×10^{4}	2.0×10^{4}
1,2-dichloroethylene	1.1×10^{4}	1.1×10^{4}
1,3-dichloropropene	28	28
2,3-dichloropropene	n.d.	n.d.

n.d.: not derived. Insufficient data available to derive an ERL.

4.6 Derivation of sediment ERLs

De Jong et al. (2007) derived sediment ERLs in their report. Trigger values for derivation of sediment ERLs were not established at that time yet. Now trigger values are available, it is concluded that derivation of sediment ERLs is not triggered for any of the 12 substances (all log $K_{p, susp-water}$ values < 3). Therefore sediment ERLs from De Jong et al. (2007) are not included in the current report.

4.7 Derivation of MPC_{soil}

4.7.1 $MPC_{eco, soil}$

$MPC_{eco, soil}$ values are taken from RIVM report 601782002 (De Jong et al., 2007). An overview of the $MPC_{eco, soil}$ for the selected substances is given in Table 15.

Table 15. $MPC_{eco, soil}$ for the selected substances.

Substance	$MPC_{eco, soil}$ [$mg.kg_{dwt}^{-1}$]
1,1,2-trichloroethane	1.7
hexachloroethane	0.10
chloroethylene[a]	n.d.
1,1-dichloroethylene	4.4×10^{-2}
3-chloropropene	6.5×10^{-4}
2-chlorobutadiene	0.10
1,1,1-trichloroethane	0.15
1,1,2,2-tetrachloroethane	7.0×10^{-2}
1,2-dichloropropane	3.9
1,2-dichloroethylene	2.0×10^{-2}
1,3-dichloropropene	5.6×10^{-4}
2,3-dichloropropene	n.d.

n.d.: not derived: insufficient data available.

4.7.2 $MPC_{sp, soil}$

Secondary poisoning is only triggered for hexachloroethane (BCF ≥ 100 L/kg and/or log K_{ow} ≥ 3). An $MPC_{sp, soil}$ of 0.22 $mg.kg_{dwt}^{-1}$ is derived in De Jong et al. (2007).

4.7.3 $MPC_{human, soil}$

In this paragraph, MPCs are derived based on the uptake of compounds via human consumption of leafy crops, root crops, milk and meat. Calculations are performed in accordance with Van Vlaardingen and Verbruggen (2007). Physico-chemical input was taken from section 3.2. The input and results of the calculations are given in Appendix 2. Derivation of the mentioned TDIs (or risk specific doses) can be found in section 3.4.

4.7.3.1 1,1,2-Trichloroethane

A preliminary TDI of 4 $\mu g.kg_{bw}^{-1}.d^{-1}$ is derived for 1,1,2-trichloroethane, resulting in a $MPC_{human, soil}$ of 0.16 $mg.kg_{dwt}^{-1}$ (critical route is consumption of root crops).

4.7.3.2 Hexachloroethane

A TDI of 1 $\mu g.kg_{bw}^{-1}.d^{-1}$ is derived for hexachloroethane, resulting in an $MPC_{human, soil}$ of 0.014 $mg.kg_{dwt}^{-1}$ (critical route is consumption of root crops).

4.7.3.3 Chloroethylene

A 10^{-6} per lifetime risk-specific oral dose of $6x10^{-3}$ $\mu g.kg_{bw}^{-1}.d^{-1}$ is derived for chloroethylene, resulting in an $MPC_{human, soil}$ of $1.6x10^{-4}$ $mg.kg_{dwt}^{-1}$ (critical route is consumption of root crops).

4.7.3.4 1,1-Dichloroethylene

A TDI of 50 $\mu g.kg_{bw}^{-1}.d^{-1}$ is derived for 1,1-dichloroethylene, resulting in an $MPC_{human, soil}$ of 1.6 $mg.kg_{dwt}^{-1}$ (critical route is consumption of root crops).
It has to be noted that the soil pore water concentration (calculated from the concentration in the leaves) exceeded the aqueous solubility. Therefore, calculations were performed using the aqueous solubility.

4.7.3.5 3-Chloropropene

A preliminary TDI of 5.5 $\mu g.kg_{bw}^{-1}.d^{-1}$ is derived for 3-chloropropene, resulting in a $MPC_{human, soil}$ of 0.14 $mg.kg_{dwt}^{-1}$ (critical route is consumption of root crops). It has to be noted that the soil pore water concentration (calculated from the concentration in the leaves) exceeded the aqueous solubility. Therefore, calculations were performed using the aqueous solubility.

4.7.3.6 2-Chlorobutadiene

A preliminary 10^{-6} per lifetime risk-specific oral dose of 0.041 $\mu g.kg_{bw}^{-1}.d^{-1}$ is derived for 2-chlorobutadiene, resulting in a $MPC_{human, soil}$ of 1.4×10^{-3} $mg.kg_{dwt}^{-1}$ (critical route is consumption of root crops). It has to be noted that the soil pore water concentration (calculated from the concentration in the leaves) exceeded the aqueous solubility. Therefore, calculations were performed using the aqueous solubility.

4.7.3.7 1,1,1-Trichloroethane

A TDI of 2000 $\mu g.kg_{bw}^{-1}.d^{-1}$ was derived for 1,1,1-trichloroethane, resulting in an $MPC_{human, soil}$ of 47 $mg.kg_{dwt}^{-1}$ (critical route is consumption of root crops).
It has to be noted that the soil pore water concentration (calculated from the concentration in the leaves) exceeded the aqueous solubility. Therefore, calculations were performed using the aqueous solubility.

4.7.3.8 1,1,2,2-Tetrachloroethane

A TDI of 50 $\mu g.kg_{bw}^{-1}.d^{-1}$ is derived for 1,1,2,2-tetrachloroethane, resulting in an $MPC_{human, soil}$ of 1.1 $mg.kg_{dwt}^{-1}$ (critical route is consumption of root crops).

4.7.3.9 1,2-Dichloropropane

A TDI of 70 $\mu g.kg_{bw}^{-1}.d^{-1}$ is derived for 1,2-dichloropropane, resulting in an $MPC_{human, soil}$ of 1.6 $mg.kg_{dwt}^{-1}$ (critical route is consumption of root crops).
It has to be noted that the soil pore water concentration (calculated from the concentration in the leaves) exceeded the aqueous solubility. Therefore, calculations were performed using the aqueous solubility.

4.7.3.10 1,2-Dichloroethylene

A TDI of 30 $\mu g.kg_{bw}^{-1}.d^{-1}$ is derived for 1,2-dichloroethylene. Using the geometric mean for water solubility and K_{ow} for the *cis*- and *trans*-isomer, this results in an $MPC_{human, soil}$ of 0.71 $mg.kg_{dwt}^{-1}$ (critical route is consumption of root crops).
It has to be noted that the soil pore water concentration (calculated from the concentration in the leaves) exceeded the aqueous solubility. Therefore, calculations were performed using the aqueous solubility.

4.7.3.11 1,3-Dichloropropene

A 10^{-6} per lifetime risk-specific oral dose of 0.01 $\mu g.kg_{bw}^{-1}.d^{-1}$ is derived for 1,3-dichloropropene, resulting in an $MCP_{human, soil}$ of 3.0×10^{-4} $mg.kg_{dwt}^{-1}$ (critical route is consumption of root crops).

4.7.3.12 2,3-Dichloropropene

A preliminary 10^{-6} per lifetime risk-specific oral dose of 0.01 $\mu g.kg_{bw}^{-1}.d^{-1}$ is derived for 2,3-dichloropropene, resulting in an $MCP_{human, soil}$ of 3.0×10^{-4} $mg.kg_{dwt}^{-1}$ (critical route is consumption of root crops).

4.7.3.13 Overview of derived $MPC_{human, soil}$

An overview of the derived $MPC_{human, soil}$ values is shown in Table 16.

Table 16. $MPC_{human, soil}$ for the selected substances.

Substance	$MPC_{human, soil}$ $[mg.kg_{dwt}^{-1}]$
1,1,2-trichloroethane	0.16
hexachloroethane	1.4×10^{-2}
chloroethylene	1.6×10^{-4}
1,1-dichloroethylene	1.6
3-chloropropene	0.14
2-chlorobutadiene	1.4×10^{-3}
1,1,1-trichloroethane	47
1,1,2,2-tetrachloroethane	1.1
1,2-dichloropropane	1.6
1,2-dichloroethylene	0.71
1,3-dichloropropene	3.0×10^{-4}
2,3-dichloropropene	3.0×10^{-4}

4.7.4 Selection of MPC_{soil}

Based on the previous sections, the final MPC_{soil} values are shown in Table 17.

Table 17. MPC_{soil} for the selected substances.

Substance	MPC_{soil} $[mg.kg_{dwt}^{-1}]$
1,1,2-trichloroethane	0.16
hexachloroethane	1.4×10^{-2}
chloroethylene[a]	1.6×10^{-4} [a]
1,1-dichloroethylene	4.4×10^{-2}
3-chloropropene	6.5×10^{-4}
2-chlorobutadiene	1.4×10^{-3}
1,1,1-trichloroethane	0.15
1,1,2,2-tetrachloroethane	7.0×10^{-2}
1,2-dichloropropane	1.6
1,2-dichloroethylene	2.0×10^{-2}
1,3-dichloropropene	3.0×10^{-4}
2,3-dichloropropene	3.0×10^{-4} [a]

a: see text below

For chloroethylene, an $MPC_{eco, soil}$ is not available due to lack of data (no terrestrial data available). In the absence of an $MPC_{eco, water}$, equilibrium partitioning cannot be used to derive an $MPC_{eco, soil}$ either. Normally, this would mean that an overall MPC_{soil} cannot be determined. However, for the aquatic compartment, it was shown that the available aquatic ecotoxicity data are a factor of $4.5 \times 10^{6} – 1.3 \times 10^{7}$ above the MPC_{water} based on human toxicological data (9.1×10^{-2} µg.L^{-1}). This difference can be largely contributed to the carcinogenic properties of the substance. Furthermore, it is a volatile substance (Henry's law constant is 2564.6 Pa.m.mol^{-1}). Therefore, although there are no terrestrial ecotoxicity data available, it can be assumed that the MPC_{soil} based on human toxicological data will also be protective enough for ecosystems.
A similar reasoning applies to 2,3-dichloropropene. An $MPC_{eco, soil}$ is not available due to the lack of terrestrial data and equilibrium partitioning cannot be applied. The MPC_{soil} for 2,3-dichloropropene is therefore solely based on $MPC_{human, soil}$, of which the value was based on 1,3-dichloropropene. Since the determining value for MPC_{soil} for 1,3-dichloropropene is the $MPC_{human, soil}$, also the value for MPC_{soil}, for 2,3-dichloropropene is considered reliable.

4.8 Derivation of NC_{soil}

The NC_{soil} is set a factor 100 lower than the MPC_{soil}. An overview of the NC_{soil} for the selected substances is given in Table 18.

Table 18. $NC_{soil, eco}$ for the selected substances.

Substance	NC_{soil} [mg.kg$_{dwt}^{-1}$]
1,1,2-trichloroethane	1.6×10^{-3}
hexachloroethane	1.4×10^{-4}
chloroethylene	1.6×10^{-6}
1,1-dichloroethylene	4.4×10^{-4}
3-chloropropene	6.5×10^{-6}
2-chlorobutadiene	1.4×10^{-5}
1,1,1-trichloroethane	1.5×10^{-3}
1,1,2,2-tetrachloroethane	7.0×10^{-4}
1,2-dichloropropane	1.6×10^{-2}
1,2-dichloroethylene	2.0×10^{-4}
1,3-dichloropropene	3.0×10^{-6}
2,3-dichloropropene	3.0×10^{-6}

4.9 Derivation of $SRC_{eco, soil}$

$SRC_{eco, soil}$ values are taken from RIVM report 601782002 (De Jong et al., 2007). An overview of the $SRC_{eco, soil}$ for the selected substances is given in Table 19.

Table 19. $SRC_{eco, soil}$ for the selected substances.

Substance	$SRC_{eco, soil}$ [$mg.kg_{dwt}^{-1}$]
1,1,2-trichloroethane	91
hexachloroethane	16
chloroethylene[a]	n.d. [a]
1,1-dichloroethylene	53
3-chloropropene	3.6
2-chlorobutadiene	10
1,1,1-trichloroethane	11
1,1,2,2-tetrachloroethane	14
1,2-dichloropropane	59
1,2-dichloroethylene	32
1,3-dichloropropene	8.7×10^{-2}
2,3-dichloropropene[b]	n.d. [b]

a: Not derived. Only few ecotoxicity data were available. No reliable $SRC_{eco, soil}$ could not be derived.

b: Not derived. No terrestrial data available.

4.10 Derivation of MPC_{gw}

4.10.1 $MPC_{eco, gw}$

According to the guidance, in view of the absence of groundwater-specific ecotoxicological information, the $MPC_{eco, gw}$ is set to the $MPC_{eco, water}$. An overview of the $MPC_{eco, gw}$ for the selected substances is given in Table 20.

Table 20. $MPC_{eco, gw}$ for the selected substances.

Substance	$MPC_{eco, gw}$ [$\mu g.L^{-1}$]
1,1,2-trichloroethane	3.0×10^{2}
hexachloroethane	0.67
chloroethylene	n.d.
1,1-dichloroethylene	9
3-chloropropene	0.34
2-chlorobutadiene	19
1,1,1-trichloroethane	21
1,1,2,2-tetrachloroethane	8
1,2-dichloropropane	2.8×10^{2}
1,2-dichloroethylene	6.8
1,3-dichloropropene	0.18
2,3-dichloropropene	n.d.

n.d.: No $MPC_{eco, water}$ available due to insufficient data.

4.10.2 $MPC_{human, gw}$

According to the guidance, the $MPC_{human, gw}$ is set to the $MPC_{water, dw}$. As described in section 2.2.1 water treatment is currently not taken into account. An overview of the $MPC_{human, gw}$ for the selected substances is given in Table 21.

Table 21. $MPC_{human, gw}$ for the selected substances.

Substance	$MPC_{human, gw}$ [$\mu g.L^{-1}$]
1,1,2-trichloroethane	14
hexachloroethane	3.5
chloroethylene	0.50
1,1-dichloroethylene	1.8×10^{2}
3-chloropropene	19
2-chlorobutadiene	0.14
1,1,1-trichloroethane	7.0×10^{3}
1,1,2,2-tetrachloroethane	1.8×10^{2}
1,2-dichloropropane	2.5×10^{2}
1,2-dichloroethylene	1.1×10^{2}
1,3-dichloropropene	3.5×10^{-2}
2,3-dichloropropene	3.5×10^{-2}

4.10.3 Selection of the MPC_{gw}

The MPC_{gw} is set at the lowest derived value and are given in Table 22.

Table 22. MPC_{gw} for the selected substances.

Substance	MPC_{gw} [$\mu g.L^{-1}$]
1,1,2-trichloroethane	14
hexachloroethane	0.67
chloroethylene	0.50[a]
1,1-dichloroethylene	9
3-chloropropene	0.34
2-chlorobutadiene	0.14
1,1,1-trichloroethane	21
1,1,2,2-tetrachloroethane	8
1,2-dichloropropane	2.5×10^{2}
1,2-dichloroethylene	6.8
1,3-dichloropropene	3.5×10^{-2}
2,3-dichloropropene	3.5×10^{-2} [a]

a: Value is solely based on $MPC_{human, gw}$, since no $MPC_{eco, gw}$ is available (due to lack of data for derivation of $MPC_{eco, water}$): value is considered as reliable.

4.11 Derivation of NC_{gw}

The NC_{gw} is set a factor 100 lower than the MPC_{gw}. The resulting NC_{gw} are shown in Table 23.

Table 23. NC_{gw} for the selected substances.

Substance	NC_{gw} [µg.L^{-1}]
1,1,2-trichloroethane	0.14
hexachloroethane	6.7×10^{-3}
chloroethylene	5.0×10^{-3}
1,1-dichloroethylene	0.09
3-chloropropene	3.4×10^{-3}
2-chlorobutadiene	1.4×10^{-3}
1,1,1-trichloroethane	0.21
1,1,2,2-tetrachloroethane	8.0×10^{-2}
1,2-dichloropropane	2.5
1,2-dichloroethylene	6.8×10^{-2}
1,3-dichloropropene	3.5×10^{-4}
2,3-dichloropropene	3.5×10^{-4}

4.12 Derivation of $SRC_{eco,\ gw}$

The $SRC_{eco,\ gw}$ is set equal to $SRC_{eco,\ water}$. An overview of the $SRC_{eco,\ gw}$ for the selected substances is given in Table 24.

Table 24. $SRC_{eco,\ gw}$ for the selected substances.

Substance	$SRC_{eco,\ gw}$ [µg.L^{-1}]
1,1,2-trichloroethane	1.6×10^{4}
hexachloroethane	1.1×10^{2}
chloroethylene	n.d.
1,1-dichloroethylene	1.1×10^{4}
3-chloropropene	1.9×10^{3}
2-chlorobutadiene	1.9×10^{3}
1,1,1-trichloroethane	1.5×10^{3}
1,1,2,2-tetrachloroethane	1.7×10^{3}
1,2-dichloropropane	2.0×10^{4}
1,2-dichloroethylene	1.1×10^{4}
1,3-dichloropropene	28
2,3-dichloropropene	n.d.

n.d.: Not derived; derivation of $SRC_{eco,water}$ not possible.

4.13 Derivation of MPC_{air}

Due to the high-vapour pressure of the selected substances, the atmosphere is a major recipient. Therefore, ERLs for air are derived in the following sections.

4.13.1 $MPC_{eco, air}$

$MPC_{eco, air}$ values are taken from RIVM report 601782002 (De Jong et al., 2007). An overview of the $MPC_{eco, air}$ for the selected substances is given in Table 25.

Table 25. $MPC_{eco, air}$ for the selected substances.

Substance	$MPC_{air, eco}$ [µg.m^{-3}]
1,1,2-trichloroethane	n.d.
hexachloroethane	n.d.
chloroethylene	n.d.
1,1-dichloroethylene	n.d.
3-chloropropene	n.d.
2-chlorobutadiene	n.d.
1,1,1-trichloroethane	1.3×10^4
1,1,2,2-tetrachloroethane	65
1,2-dichloropropane	n.d.
1,2-dichloroethylene	7.8×10^4 [a]
1,3-dichloropropene	n.d.
2,3-dichloropropene	n.d.

n.d.: Not derived; no data available.

a: Value was calculated for the trans-isomer.

4.13.2 $MPC_{human, air}$

The $MPC_{human, air}$ values are set equal to the available Tolerable Concentrations in Air (TCA), or risk specific concentrations for genotoxic carcinogenic substances. Available TCAs and their references can be found in section 3.4 and in Table 7. An overview of $MPC_{human, air}$ values for the selected substances is given in Table 26.

Table 26. $MPC_{human, air}$ for the selected substances.

Substance	$MPC_{human, air}$ [µg.m^{-3}]
1,1,2-trichloroethane	17
hexachloroethane	87
chloroethylene	3.6×10^{-2}
1,1-dichloroethylene	2.0×10^2
3-chloropropene	7.4
2-chlorobutadiene	0.02
1,1,1-trichloroethane	3.8×10^2
1,1,2,2-tetrachloroethane	n.a.
1,2-dichloropropane	12
1,2-dichloroethylene	60
1,3-dichloropropene	0.25
2,3-dichloropropene	0.25

n.a.: Not available; TCA value is not considered reliable for ERL derivation.

4.13.3 Selection of MPC_{air}

An overview of MPC_{air} values as selected from $MPC_{eco, air}$ and $MPC_{human, air}$ for the selected substances is given in Table 27.

Table 27. MPC_{air} for the selected substances.

Substance	MPC_{air} [$\mu g.m^{-3}$]
1,1,2-trichloroethane	17
hexachloroethane	87
chloroethylene	3.6×10^{-2}
1,1-dichloroethylene	2.0×10^{2}
3-chloropropene	7.4
2-chlorobutadiene	0.02
1,1,1-trichloroethane	3.8×10^{2}
1,1,2,2-tetrachloroethane	65 *
1,2-dichloropropane	12
1,2-dichloroethylene	60
1,3-dichloropropene	0.25
2,3-dichloropropene	0.25

*: Preliminary value solely based on $MPC_{eco, air}$ (no $MPC_{human, air}$ available due to unreliable TCA value).

4.14 Derivation of NC_{air}

The NC_{air} is derived by dividing the overall MPC_{air} divided by a factor of 100. This results in the NC_{air} values given in Table 28.

Table 28. $NC_{, air}$ for the selected substances.

Substance	$NC_{, air}$ [$\mu g.m^{-3}$]
1,1,2-trichloroethane	0.17
hexachloroethane	0.87
chloroethylene	3.6×10^{-4}
1,1-dichloroethylene	2.0
3-chloropropene	8.0×10^{-2}
2-chlorobutadiene	2×10^{-4}
1,1,1-trichloroethane	3.8
1,1,2,2-tetrachloroethane	0.65 *
1,2-dichloropropane	0.12
1,2-dichloroethylene	0.60
1,3-dichloropropene	2.5×10^{-3}
2,3-dichloropropene	2.5×10^{-3}

*: Preliminary value solely based on $MPC_{eco, air}$ (no $MPC_{human, air}$ available due to unreliable TCA value).

5 Preliminary risk analysis for freshwater

The data on freshwater monitoring for the years 1999-2004 for several locations, as reported in RIVM report 601782002 (De Jong et al., 2007), are compared with the newly derived ERLs for water. A comparison is not possible for 2,3-dichloropropene, since no ERL was derived for this compound.

For all substances the maximum and average values per year are below the presently derived MPC values. For chloroethylene, measured values were always below the limit of detection (LOD) of 1 $\mu g.L^{-1}$. However, since the MPC_{water} (0.091 $\mu g.L^{-1}$) is lower than this LOD value, no conclusion can be drawn as to whether the MPC_{water} is exceeded.

Exceeding of $MAC_{eco, water}$ values by the maximum values is not found or is not likely for the eleven substances.

The average measured yearly concentrations for hexachloroethane (10% of n=68), for *trans*- and *cis*-1,2-dichloroethylene (3% of n= 63) and for *trans*- and *cis*-1,3-dichloropropene (7% of n=88) exceed the presently derived NC_{water}-values. For chloroethylene, 3-chloropropene and 2-chlorobutadiene, the measurements are all below the LOD. Because the NC value is also below the LOD, no conclusion can be drawn whether or not the NC values for these substances are exceeded.

6 Conclusions

In this report, the environmental risk limits Negligible Concentration (NC), Maximum Permissible Concentration (MPC), Maximum Acceptable Concentration for ecosystems (MAC_{eco}), and Serious Risk Concentration for ecosystems (SRC_{eco}) are derived for 12 volatile aliphatic hydrocarbons in water, sediment, groundwater, soil and air. No risk limits were derived for the sediment compartment because the trigger to derive such limits is not reached.

The derived ERLs are summarised in Table 29.

Table 29. Derived MPC, NC, MAC_{eco}, and SRC_{eco} values (in µg.L^{-1} for water and groundwater, in mg.kg$_{dw}^{-1}$ for soil, in µg.m^{-3} for air). n.d. = not derived.

	1,1,2-trichloroethane	hexachloroethane	chloroethylene	1,1-dichloroethylene	3-chloropropene	2-chlorobutadiene
Freshwater						
MPC	22	0.44	9.1×10^{-2} [b]	9.0	0.34	0.19
NC	0.22	4.4×10^{-3}	9.1×10^{-4} [b]	9.0×10^{-2}	3.4×10^{-3}	1.9×10^{-3}
MAC_{eco}	3.0×10^{2}	1.4	n.d.	90	3.4	n.d.
SRC_{eco}	1.6×10^{4}	1.1×10^{2}	n.d.	1.1×10^{4}	1.9×10^{3}	1.9×10^{3}
Drinking water						
MPC	14 [a]	3.5 [a]	0.50 [a]	1.8×10^{2} [a]	19 [a]	0.14 [a]
Marine water						
MPC	22	6.7×10^{-2}	9.1×10^{-2} [b]	0.9	3.4×10^{-2}	0.19
NC	0.22	6.7×10^{-4}	9.1×10^{-4} [b]	9.0×10^{-3}	3.4×10^{-4}	1.9×10^{-3}
MAC_{eco}	1.9×10^{2}	0.28	n.d.	9.0	0.34	n.d.
SRC_{eco}	1.6×10^{4}	1.1×10^{2}	n.d.	1.1×10^{4}	1.9×10^{3}	1.9×10^{3}
Soil						
MPC	0.16	1.4×10^{-2}	1.6×10^{-4} [b]	4.4×10^{-2}	6.5×10^{-4}	1.4×10^{-3}
NC	1.6×10^{-3}	1.4×10^{-4}	1.6×10^{-6} [b]	4.4×10^{-4}	6.5×10^{-6}	1.4×10^{-5}
SRC_{eco}	91	16	n.d.	53	3.6	10
Groundwater						
MPC	14	0.67	0.50	9.0	0.34	0.14
NC	0.14	6.7×10^{-3}	5.0×10^{-3}	9.0×10^{-2}	3.4×10^{-3}	1.4×10^{-3}
SRC_{eco}	1.6×10^{4}	1.1×10^{2}	n.d.	1.1×10^{4}	1.9×10^{3}	1.9×10^{3}
Air						
MPC [d]	17	87	3.6×10^{-2}	2.0×10^{2}	7.4	0.02
NC [d]	0.17	0.87	3.6×10^{-4}	2.0	7.4×10^{-2}	2×10^{-4}

Table 29 (continued). Derived MPC, NC, MAC_{eco}, and SRC_{eco} values (in $\mu g.L^{-1}$ for water and groundwater, in $mg.kg_{dw}^{-1}$ for soil, in $\mu g.m^{-3}$ for air). n.d. = not derived.

	1,1,1-trichloroethane	1,1,2,2-tetrachloroethane	1,2-dichloropropane	1,2-dichloroethylene	1,3-dichloropropene	2,3-dichloropropene
Freshwater						
MPC	21	8.0	2.8×10^{2}	6.8	0.18	n.d.
NC	0.21	8.0×10^{-2}	2.8	6.8×10^{-2}	1.8×10^{-3}	n.d.
MAC_{eco}	54	84	1.3×10^{3}	n.d.	51	n.d.
SRC_{eco}	1.5×10^{3}	1.7×10^{3}	2.0×10^{4}	1.1×10^{4}	28	n.d.
Drinking water						
MPC	7.0×10^{3} [a]	1.8×10^{2} [a]	2.5×10^{2} [a]	1.1×10^{2} [a]	3.5×10^{-2} [a]	3.5×10^{-2} [a]
Marine water						
MPC	2.1	0.8	28	0.68	1.8×10^{-2}	n.d.
NC	2.1×10^{-2}	8.0×10^{-3}	0.28	6.8×10^{-3}	1.8×10^{-4}	n.d.
MAC_{eco}	5.4	8.4	1.3×10^{2}	n.d.	5.1	n.d.
SRC_{eco}	1.5×10^{3}	1.7×10^{3}	2.0×10^{4}	1.1×10^{4}	28	n.d.
Soil						
MPC	0.15	7.0×10^{-2}	1.6	2.0×10^{-2}	3.0×10^{-4}	3.0×10^{-4} [b]
NC	1.5×10^{-3}	7.0×10^{-4}	1.6×10^{-2}	2.0×10^{-4}	3.0×10^{-6}	3.0×10^{-6} [b]
SRC_{eco}	11	14	59	32	8.7×10^{-2}	n.d.
Groundwater						
MPC	21	8.0	2.5×10^{2}	6.8	3.5×10^{-2}	3.5×10^{-2} [c]
NC	0.21	8.0×10^{-2}	2.5	6.8×10^{-2}	3.5×10^{-4}	3.5×10^{-4} [c]
SRC_{eco}	1.5×10^{3}	1.7×10^{3}	2.0×10^{4}	1.1×10^{4}	28	n.d.
Air						
MPC [d]	3.8×10^{2}	65 [d]	12	60	0.25	0.25
NC [d]	3.8	0.65 [d]	0.12	0.60	2.5×10^{-3}	2.5×10^{-3}

a: For all substances, except chloroethylene, the value represents a $MPC_{dw, water, provisional}$, *i.e.* not based on a established Drinking Water Standard (DWS) conform EU Directive 98/83/EC or an A1-value conform Directive 75/440/EEC.

b: Values are not based on MPC_{eco} values (not available), but are considered sufficiently protective for both man and environment (see text in this report).

c: Values are not based on MPC_{eco} values (not available), but are - based on the data for 1,3-dichloropropene - considered sufficiently protective for both man and environment (see text in this report).

d: All MPC and NC values for air are at least based on $MPC_{human, air}$ values, except for 1,1,2,2-tetrachloroethane where only a $MPC_{eco, air}$ value is available. Therefore the values for 1,1,2,2-tetrachloroethane should be regarded as preliminary, since future availability of reliable chronic inhalation toxicity data may lead to lower values.

rivm

References

ATSDR (1994). Toxicological Profile for Hexachloroethane (draft June 1994). Agency for Toxic Substances and Disease Registry. U.S. Department of Health and Human Services.

Baars AJ, Theelen RMC, Janssen PJCM, Hesse JM, Van Apeldoorn ME, Meijerink MCM, Verdam L, Zeilmaker MJ. (2001). Herevaluatie van humaan-toxicologische maximum toelaatbare risico-waarden. RIVM report 711701025, National Institute for Public Health and the Environment, Bilthoven, The Netherlands.

Barrows ME, Petrocelli SR, Macek KJ, Carroll JJ. (1980). Bioconcentration and elimination of selected water pollutants by bluegill sunfish (*Lepomis macrochirus*). Dynamics, Exposure and Hazard Assessment of Toxic Chemicals, p. 379-392, Ann Arbor Science Pub.

BioByte. (2004). BioLoom [computer program]. version 1.0 (ClogP 4.0). Claremont, CA, USA: BioByte Corporation.

De Jong, FMW, Posthuma-Doodeman, CJAM, Verbruggen, EMJ. (2007). Ecotoxicologically based environmental risk limits for several volatile aliphatic hydrocarbons. RIVM report 601782002, National Institute for Public Health and the Environment, Bilthoven, The Netherlands.

EFSA (2006). Conclusion regarding the peer review of the pesticide risk assessment of the active substance 1,3-dichloropropene, finalised: 12 May 2006 (version of 14 June 2006 with minor editorial changes marked yellow). EFSA Scientific Report (2006) 72, p.1-99. http://www.efsa.europe.eu/cs/BlobServer/PRAPER_Conclusion/praper_concl_sr72_13dichloropropene_rev1_en1.pdf?ssbinary=true (viewed August 2008)

European Commission (1998). Council Directive 98/83/EC of 3 November 1998 on the quality of water intended for human consumption. Brussels, Belgium: EC. L330. p.32-54

European Commission (2003). Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/8/EC of he European Parliament and of the Council concerning the placing of biocidal products on the market. Ispra, Italy: European Chemicals Bureau, Institute for Health and Consumer Protection.

Feron, VJ, Kroese, ED. (1996). Carcinogeniteit van Cis-1,2-Dichloropropeen. Op verzoek van het College voor de Toelating van Bestrijdingsmiddelen werd nagegaan of cis-1,2-dichloropropeen beschouwd moet worden als een genotoxisch of een niet-genotoxisch carcinogeen. RIVM/TNO-adbvies d.d. 25-01-1996.

Gezondheidsraad (2007). Tetrachloroethane – Health-based recommended occupational exposure limit. DECOS – Health Council of the Netherlands document no. 2006/09OSH.

IARC (1999) IARC monographs on the evaluation of the carcinogenic risk of chemicals to humans: Re-evaluation of some organic chemicals, hydrazine, and hydrogen peroxide (Part two). Lyon, France: Internation Agency for Research on Cancer, World Health Organisation 71, p.1163-1180.

Janssen PJCM (1995). Enige informatie over de humaantoxicologie van hexachloorethaan, CAS 67-72-1 (i.v.m. bodemverontreiniging?) (24 juli 1995). RIVM internal memorandum for J. Kliest (in Dutch), National Institute for Public Health and the Environment, Bilthoven, The Netherlands.

Janssen PJCM, Van Apeldoorn ME, Van Koten-Vermeulen, JEM, Mennes, WC. (1995). Human-Toxicological Criteria for Serious Soil Contamination: Compounds evaluated in 1993 & 1994. RIVM report 715810009, National Institute for Public Health and the Environment, Bilthoven, The Netherlands.

Janssen, PJCM, Speijers, GJA. (1997). Guidance on the Derivation of Maximum Permissible Risk Levels for Human Intake of Soil Contaminants. RIVM report 711701006, National Institute for Public Health and the Environment, Bilthoven, The Netherlands.

Janssen PJCM, Van Apeldoorn ME, Van Engelen JGM, Schielen PCJI, Wouters MFA. (1998). Maximum Permissible Risk Levels for Human Intake of Soil Contaminants: Fourth Series of Compounds. Maximum Toelaatbare Risico-Niveaus voor Inname van Bodemcontaminanten door de Mens: Vierde tranche van stoffen. RIVM report 711701004, National Institute for Public Health and the Environment, Bilthoven, The Netherlands.

Lepper P. (2005). Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC). Schmallenberg, Germany: Fraunhofer-Institute Molecular Biology and Applied Biology.

McCauley PT, Robinson M, Daniel FB, Olson GR. (1995). The effects of subacute and subchronic oral exposure to cis-1,2-dichloroethylene in Sprague-Dawley rats. Drug and Chemical Toxicology 18, p.171-184.

Nagano, M, Hotoschi, T, Fuatsuka, M. (1991). Neurotoxicity in rats. Dose-effect relationship following long-term exposure. Sangyo-Igaku, 33 (2), 73-80

NCI (National Cancer Institute) (1978). Bioassay of allyl chloride for possible carcinogenicity. CAS No. 107-05-1. NCI-CG-TR-73. DHEW Publ. No. (NIH) 78-1323.

NTP(1998). TR-467 Toxicology and Carcinogenesis Studies of Chloroprene (CAS No. 126-99-8) in F344/N Rats and B6C3F1 Mice (Inhalation Studies). http://ntp.niehs.nih.gov/index.cfm?objectid=070A80D0-96F2-115A-6354967089C17F9B (viewed October 2007).

NTP (2000). NTP Technical Report on the Toxicity Studies of 1,1,1-Trichlorethane (CAS No. 76-55-6). Administered in Microcapsules in Feed to F344/N Rats and B6C3F1 Mice. National Toxicology Program Toxicity Report Series Number 41. http://ntp.niehs.nih.gov/ntp/htdocs/ST_rpts/tox041.pdf (viewed July 2008).

NTP (2002). NTP Technical Report on the toxicity studies of trans-1,2-dichloroethylene (CAS no. 156-60-5) administered in microcapsules in feed to F344/N rats and B6C3F(1) mice. http://ntp.niehs.nih.gov/ntp/htdocs/ST_rpts/tox055.pdf (viewed August 2008)

OECD SIDS (1996). Chloropropene. CAS N^{o} 107-05-1. http://www.chem.unep.ch/irptc/sids/OECDSIDS/Chloropropene.pdf (viewed October 2007)

US-EPA (1991). Oral RfD Assessment (I.A.), 04-01-1991. http://www.epa.gov/ncea/iris/subst/0167.htm#revhis (October 2008)

US-EPA (2000). Toxicological review of 1,3-dichloropropene (CAS No. 542-75-6). In support of Summary Information on the Integrated Risk Information System (IRIS). http://www.epa.gov/ncea/iris/toxreviews/0224-tr.pdf (Viewed August 2008)

US-EPA (2002). Oral RfD Assessment (I.A.), Inhalation RfC Assessment (I.B.), Carcinogenicity Assessment (II.), 13-08-2002. http://www.epa.gov/ncea/iris/subst/0039.thm (Viewed August 2008)

US-EPA (2007). Toxicological review of 1,1,1-trichloroethane (CAS No. 71-55-6). In support of Summary Information on the Integrated Risk Information System (IRIS). http://www.epa.gov/ncea/iris/toxreviews/0197-tr.pdf (viewed July 2008)

Van de Plassche EJ, Bockting GJM. (1993). Towards integrated environmental quality objectives for several volatile compounds. RIVM report 679101011, National Institute for Public Health and the Environment, Bilthoven, The Netherlands.

Van Vlaardingen PLA, Verbruggen EMJ. (2007). Guidance for the derivation of environmental risk limits within the framework of 'International and national environmental quality standards for substances in the Netherlands (INS). RIVM report 601782001. National Institute for Public Health and the Environment, Bilthoven, The Netherlands.

VROM (2004). (Inter)nationale Normen Stoffen. Den Haag, The Netherlands: Ministerie van Volkshuisvesting, Ruimtelijke Ordening en Milieubeheer (in Dutch).
WHO (2003). Concise International Chemical Assessment Document (CICAD) no. 51 – Vinylidene chloride. Geneva, WHO/IPCS. http://www.who.int/ipcs/publications/cicad/en/cicad51.pdrf (viewed August 2008).

rivm

Appendix 1. Current environmental quality standards

Source: website www.rivm.nl/rvs, subpage on Environmental quality standards (in Dutch): http://www.rivm.nl/rvs/normen/mil/ (consulted on 2-7-2009).

Units: $\mu g.L^{-1}$ for fresh water and groundwater, $mg.kg_{dw}^{-1}$ for soil, $\mu g.m^{-3}$ for air.

See also further explanations below the second table.

	1,1,2-trichloroethane	hexachloroethane	Chloroethylene	1,1-dichloroethylene	3-chloropropene	2-chlorobutadiene
Fresh water						
MPC	7900	83	820	3400	3	10
NC	79	0.8	8	34	0.03	
Soil						
NC	0.4	0.2	0.01	0.1	$5x10^{-5}$	
Groundwater						
NC	0.01 (=DL)	0.8	0.01 (=DL)	- (<DL)	0.03	
Air						
MPC				200	7	
NC				2	0.07	

	1,1,1-trichloroethane	1,1,2,2-tetrachloroethane	1,2-dichloropropane	1,2-dichloroethylene	1,3-dichloropropene	2,3-dichloropropene
Fresh water						
MPC	2100	3300	76	6100	8	8
NC	21	33	0.8	61	0.08	0.08
Soil						
NC	0.07	0.1	0.002	0.2	0.0002	0.0004
Groundwater						
NC	0.01 (=DL)	33	0.8	- (<DL)	0.08	0.08
Air						
MPC	4800	(94.2) [a]	12		40	
NC	48		0.1		0.4	

DL: Detection limit

=DL: Value was set at DL level

a: Present *ad hoc* standard for MPC_{air}. However, a later derived *ad hoc* environmental risk limit is available, but was not yet set as the new *ad hoc* standard for MPC_{air} (*ad hoc* MTR_{air} = 74.2 µg.m^{-3}; Source : Hansler et al. (2008). Indicative environmental quality standards 2004. RIVM report 601782012. National Institute for Public Health and the Environment, Bilthoven, The Netherlands (in Dutch)).

rivm

Appendix 2. Derivation of $MPC_{human,soil}$: input data and results

1,1,2-trichloroethane

Calculation of MPChuman_comp values based on EUSES 2.0.3 equations for "indirect exposure of humans via the environment".
Four human consumption routes are incorporated: leaf crops, root crops, milk and meat.
Each route contributes to 10% of the TDI (by definition); the lowest of the calculated soil and groundwater concentrations is selected and presented under Output.
Note that pore water concentrations are set equal to the aqueous solubility if the pore water concentration exceeds the aqueous solubility in the model calculations. A warning will display when this is the case.
Note that some bioconcentrations factors are Kow determined. When the Kow is outside of the range of applicability of the respective QSAR (TSCF, BAFmeat and BAFmilk), model calculations are performed with the upper or lower limit of the Kow range for the respective QSAR. A warning will display when this is the case.

User input		**Mind the units in which the parameters should be entered:**	
TDI	4,00E-03	[$mg.kg_{bw}^{-1}.d^{-1}$]	
HENRY	8,85E+01	[$Pa.m^3.mol^{-1}$]	**!Delete cell content if no Henry constant is available.**
K_{oc}	89,13	[$L.kg^{-1}$]	
K_{ow}	117,49	[-]	
SOL	4,58E+03	[$mg.L^{-1}$]	aqueous solubility
T_{SOL}	3,13E+01	[°C]	temperature at which aqueous solubility is determined

Output			
$MPC_{human\ soil}$	1,580E-01	[$mg.kg_{dwt}^{-1}$]	Expressed in Dutch standard soil

The critical route is: consumption of root crops (MPChuman, soil root)

Warnings

log Kow is below the range for BAFmilk calculation, log Kow = 3 is used in calculations

hexachloroethane

Calculation of MPChuman_comp values based on EUSES 2.0.3 equations for "indirect exposure of humans via the environment".
Four human consumption routes are incorporated: leaf crops, root crops, milk and meat.
Each route contributes to 10% of the TDI (by definition); the lowest of the calculated soil and groundwater concentrations is selected and presented under Output.
Note that pore water concentrations are set equal to the aqueous solubility if the pore water concentration exceeds the aqueous solubility in the model calculations. A warning will display when this is the case.
Note that some bioconcentrations factors are Kow determined. When the Kow is outside of the range of applicability of the respective QSAR (TSCF, BAFmeat and BAFmilk), model calculations are performed with the upper or lower limit of the Kow range for the respective QSAR. A warning will display when this is the case.

User input		**Mind the units in which the parameters should be entered:**	
TDI	1,00E-03	[mg.kg$_{bw}^{-1}$.d^{-1}]	
HENRY	1,62E+02	[Pa.m^3.mol^{-1}]	**!Delete cell content if no Henry constant is available.**
K_{oc}	2511,89	[L.kg^{-1}]	
K_{ow}	13803,84	[-]	
SOL	2,72E+01	[mg.L^{-1}]	aqueous solubility
T_{SOL}	2,50E+01	[°C]	temperature at which aqueous solubility is determined

Output			
$MPC_{human\ soil}$	1,363E-02	[mg.kg$_{dwt}^{-1}$]	Expressed in Dutch standard soil

The critical route is: consumption of root crops (MPChuman, soil root)

rivm

chloroethylene

Calculation of MPChuman_comp values based on EUSES 2.0.3 equations for "indirect exposure of humans via the environment".
Four human consumption routes are incorporated: leaf crops, root crops, milk and meat.
Each route contributes to 10% of the TDI (by definition); the lowest of the calculated soil and groundwater concentrations is selected and presented under Output.
Note that pore water concentrations are set equal to the aqueous solubility if the pore water concentration exceeds the aqueous solubility in the model calculations. A warning will display when this is the case.
Note that some bioconcentrations factors are Kow determined. When the Kow is outside of the range of applicability of the respective QSAR (TSCF, BAFmeat and BAFmilk), model calculations are performed with the upper or lower limit of the Kow range for the respective QSAR. A warning will display when this is the case.

User input		**Mind the units in which the parameters should be entered:**	
TDI	6,00E-06	[mg.kg$_{bw}^{-1}$.d^{-1}]	
HENRY	2,56E+03	[Pa.m^3.mol^{-1}]	**!Delete cell content if no Henry constant is available.**
K_{oc}	21,38	[L.kg^{-1}]	
K_{ow}	33,11	[-]	
SOL	2,70E+03	[mg.L^{-1}]	aqueous solubility
T_{SOL}	2,50E+01	[°C]	temperature at which aqueous solubility is determined

Output

$MPC_{human\ soil}$	1,619E-04	[mg.kg$_{dwt}^{-1}$]	Expressed in Dutch standard soil

The critical route is: consumption of root crops (MPChuman, soil root)

Warnings

log Kow is below the range for BAFmilk calculation, log Kow = 3 is used in calculations

1,1-dichloroethylene

Calculation of MPChuman_comp values based on EUSES 2.0.3 equations for "indirect exposure of humans via the environment".
Four human consumption routes are incorporated: leaf crops, root crops, milk and meat.
Each route contributes to 10% of the TDI (by definition); the lowest of the calculated soil and groundwater concentrations is selected and presented under Output.
Note that pore water concentrations are set equal to the aqueous solubility if the pore water concentration exceeds the aqueous solubility in the model calculations. A warning will display when this is the case.
Note that some bioconcentrations factors are Kow determined. When the Kow is outside of the range of applicability of the respective QSAR (TSCF, BAFmeat and BAFmilk), model calculations are performed with the upper or lower limit of the Kow range for the respective QSAR. A warning will display when this is the case.

User input		**Mind the units in which the parameters should be entered:**	
TDI	5,00E-02	[$mg.kg_{bw}^{-1}.d^{-1}$]	
HENRY	3,80E+03	[$Pa.m^3.mol^{-1}$]	**!Delete cell content if no Henry constant is available.**
K_{oc}	66,07	[$L.kg^{-1}$]	
K_{ow}	134,90	[-]	
SOL	2,25E+03	[$mg.L^{-1}$]	aqueous solubility
T_{SOL}	2,50E+01	[°C]	temperature at which aqueous solubility is determined

Output			
$MPC_{human\ soil}$	1,566E+00	[$mg.kg_{dwt}^{-1}$]	Expressed in Dutch standard soil

The critical route is: consumption of root crops (MPChuman, soil root)

Warnings Note: the calculated pore water concentration (leaf) exceeds the aqueous solubility. Aqueous solubility is used in calculations

log Kow is below the range for BAFmilk calculation, log Kow = 3 is used in calculations

rivm

3-chloropropene

Calculation of MPChuman_comp values based on EUSES 2.0.3 equations for "indirect exposure of humans via the environment".
Four human consumption routes are incorporated: leaf crops, root crops, milk and meat.
Each route contributes to 10% of the TDI (by definition); the lowest of the calculated soil and groundwater concentrations is selected and presented under Output.
Note that pore water concentrations are set equal to the aqueous solubility if the pore water concentration exceeds the aqueous solubility in the model calculations. A warning will display when this is the case.
Note that some bioconcentrations factors are Kow determined. When the Kow is outside of the range of applicability of the respective QSAR (TSCF, BAFmeat and BAFmilk), model calculations are performed with the upper or lower limit of the Kow range for the respective QSAR. A warning will display when this is the case.

User input		**Mind the units in which the parameters should be entered:**	
TDI	5,50E-03	[$mg.kg_{bw}^{-1}.d^{-1}$]	
HENRY	1,80E+03	[$Pa.m^3.mol^{-1}$]	**!Delete cell content if no Henry constant is available.**
K_{oc}	20,89	[$L.kg^{-1}$]	
K_{ow}	32,36	[-]	
SOL	2,94E+03	[$mg.L^{-1}$]	aqueous solubility
T_{SOL}	2,50E+01	[°C]	temperature at which aqueous solubility is determined

Output			
$MPC_{human\ soil}$	1,384E-01	[$mg.kg_{dwt}^{-1}$]	Expressed in Dutch standard soil

The critical route is: consumption of root crops (MPChuman, soil root)

Warnings Note: the calculated pore water concentration (leaf) exceeds the aqueous solubility. Aqueous solubility is used in calculations

log Kow is below the range for BAFmilk calculation, log Kow = 3 is used in calculations

2-chlorobutadiene

Calculation of MPChuman_comp values based on EUSES 2.0.3 equations for "indirect exposure of humans via the environment".
Four human consumption routes are incorporated: leaf crops, root crops, milk and meat.
Each route contributes to 10% of the TDI (by definition); the lowest of the calculated soil and groundwater concentrations is selected and presented under Output.
Note that pore water concentrations are set equal to the aqueous solubility if the pore water concentration exceeds the aqueous solubility in the model calculations. A warning will display when this is the case.
Note that some bioconcentrations factors are Kow determined. When the Kow is outside of the range of applicability of the respective QSAR (TSCF, BAFmeat and BAFmilk), model calculations are performed with the upper or lower limit of the Kow range for the respective QSAR. A warning will display when this is the case.

User input		**Mind the units in which the parameters should be entered:**	
TDI	4,10E-05	[$mg.kg_{bw}^{-1}.d^{-1}$]	
HENRY	5,68E+03	[$Pa.m^3.mol^{-1}$]	**!Delete cell content if no Henry constant is available.**
K_{oc}	70,79	[$L.kg^{-1}$]	
K_{ow}	141,25	[-]	
SOL	8,56E+02	[$mg.L^{-1}$]	aqueous solubility
T_{SOL}	2,50E+01	[°C]	temperature at which aqueous solubility is determined

Output

$MPC_{human\ soil}$	1,394E-03	[$mg.kg_{dwt}^{-1}$]	Expressed in Dutch standard soil

The critical route is: consumption of root crops (MPChuman, soil root)

Warnings

log Kow is below the range for BAFmilk calculation, log Kow = 3 is used in calculations

rivm

1,1,1-trichloroethane

Calculation of MPChuman_comp values based on EUSES 2.0.3 equations for "indirect exposure of humans via the environment".
Four human consumption routes are incorporated: leaf crops, root crops, milk and meat.
Each route contributes to 10% of the TDI (by definition); the lowest of the calculated soil and groundwater concentrations is selected and presented under Output.
Note that pore water concentrations are set equal to the aqueous solubility if the pore water concentration exceeds the aqueous solubility in the model calculations. A warning will display when this is the case.
Note that some bioconcentrations factors are Kow determined. When the Kow is outside of the range of applicability of the respective QSAR (TSCF, BAFmeat and BAFmilk), model calculations are performed with the upper or lower limit of the Kow range for the respective QSAR. A warning will display when this is the case.

User input		**Mind the units in which the parameters should be entered:**	
TDI	2,00E+00	[$mg.kg_{bw}^{-1}.d^{-1}$]	
HENRY	1,67E+03	[$Pa.m^3.mol^{-1}$]	**!Delete cell content if no Henry constant is available.**
K_{oc}	104,70	[$L.kg^{-1}$]	
K_{ow}	309,00	[-]	
SOL	1,30E+03	[$mg.L^{-1}$]	aqueous solubility
T_{SOL}	2,50E+01	[°C]	temperature at which aqueous solubility is determined

Output			
$MPC_{human\ soil}$	4,659E+01	[$mg.kg_{dwt}^{-1}$]	Expressed in Dutch standard soil

The critical route is: consumption of root crops (MPChuman, soil root)

Warnings Note: the calculated pore water concentration (leaf) exceeds the aqueous solubility. Aqueous solubility is used in calculations

log Kow is below the range for BAFmilk calculation, log Kow = 3 is used in calculations

1,1,2,2-tetrachloroethane

Calculation of MPChuman_comp values based on EUSES 2.0.3 equations for "indirect exposure of humans via the environment".
Four human consumption routes are incorporated: leaf crops, root crops, milk and meat.
Each route contributes to 10% of the TDI (by definition); the lowest of the calculated soil and groundwater concentrations is selected and presented under Output.
Note that pore water concentrations are set equal to the aqueous solubility if the pore water concentration exceeds the aqueous solubility in the model calculations. A warning will display when this is the case.
Note that some bioconcentrations factors are Kow determined. When the Kow is outside of the range of applicability of the respective QSAR (TSCF, BAFmeat and BAFmilk), model calculations are performed with the upper or lower limit of the Kow range for the respective QSAR. A warning will display when this is the case.

User input		**Mind the units in which the parameters should be entered:**	
TDI	5,00E-02	[$mg.kg_{bw}^{-1}.d^{-1}$]	
HENRY	3,39E+01	[$Pa.m^3.mol^{-1}$]	**!Delete cell content if no Henry constant is available.**
K_{oc}	131,80	[$L.kg^{-1}$]	
K_{ow}	416,90	[-]	
SOL	2,90E+03	[$mg.L^{-1}$]	aqueous solubility
T_{SOL}	2,50E+01	[°C]	temperature at which aqueous solubility is determined

Output			
$MPC_{human\ soil}$	1,079E+00	[$mg.kg_{dwt}^{-1}$]	Expressed in Dutch standard soil

The critical route is: consumption of root crops (MPChuman, soil root)

Warnings

log Kow is below the range for BAFmilk calculation, log Kow = 3 is used in calculations

rivm

1,2-dichloropropane

Calculation of MPChuman_comp values based on EUSES 2.0.3 equations for "indirect exposure of humans via the environment".
Four human consumption routes are incorporated: leaf crops, root crops, milk and meat.
Each route contributes to 10% of the TDI (by definition); the lowest of the calculated soil and groundwater concentrations is selected and presented under Output.
Note that pore water concentrations are set equal to the aqueous solubility if the pore water concentration exceeds the aqueous solubility in the model calculations. A warning will display when this is the case.
Note that some bioconcentrations factors are Kow determined. When the Kow is outside of the range of applicability of the respective QSAR (TSCF, BAFmeat and BAFmilk), model calculations are performed with the upper or lower limit of the Kow range for the respective QSAR. A warning will display when this is the case.

User input		**Mind the units in which the parameters should be entered:**	
TDI	7,00E-02	[$mg.kg_{bw}^{-1}.d^{-1}$]	
HENRY	2,87E+02	[$Pa.m^3.mol^{-1}$]	**!Delete cell content if no Henry constant is available.**
K_{oc}	42,66	[$L.kg^{-1}$]	
K_{ow}	97,72	[-]	
SOL	3,00E+03	[$mg.L^{-1}$]	aqueous solubility
T_{SOL}	2,00E+01	[°C]	temperature at which aqueous solubility is determined

Output			
$MPC_{human\ soil}$	1,619E+00	[$mg.kg_{dwt}^{-1}$]	Expressed in Dutch standard soil

The critical route is: consumption of root crops (MPChuman, soil root)

Warnings Note: the calculated pore water concentration (leaf) exceeds the aqueous solubility. Aqueous solubility is used in calculations

log Kow is below the range for BAFmilk calculation, log Kow = 3 is used in calculations

1,2-dichloroethylene

Calculation of MPChuman_comp values based on EUSES 2.0.3 equations for "indirect exposure of humans via the environment".
Four human consumption routes are incorporated: leaf crops, root crops, milk and meat.
Each route contributes to 10% of the TDI (by definition); the lowest of the calculated soil and groundwater concentrations is selected and presented under Output.
Note that pore water concentrations are set equal to the aqueous solubility if the pore water concentration exceeds the aqueous solubility in the model calculations. A warning will display when this is the case.
Note that some bioconcentrations factors are Kow determined. When the Kow is outside of the range of applicability of the respective QSAR (TSCF, BAFmeat and BAFmilk), model calculations are performed with the upper or lower limit of the Kow range for the respective QSAR. A warning will display when this is the case.

User input		**Mind the units in which the parameters should be entered:**	
TDI	3,00E-02	[$mg.kg_{bw}^{-1}.d^{-1}$]	
HENRY	9,59E+02	[$Pa.m^3.mol^{-1}$]	**!Delete cell content if no Henry constant is available.**
K_{oc}	40,73	[$L.kg^{-1}$]	
K_{ow}	94,40	[-]	
SOL	3,81E+03	[$mg.L^{-1}$]	aqueous solubility
T_{SOL}	2,50E+01	[°C]	temperature at which aqueous solubility is determined

Output			
$MPC_{human\ soil}$	7,077E-01	[$mg.kg_{dwt}^{-1}$]	Expressed in Dutch standard soil

The critical route is: consumption of root crops (MPChuman, soil root)

Warnings Note: the calculated pore water concentration (leaf) exceeds the aqueous solubility. Aqueous solubility is used in calculations

log Kow is below the range for BAFmilk calculation, log Kow = 3 is used in calculations

rivm

1,3-dichloropropene

Calculation of MPChuman_comp values based on EUSES 2.0.3 equations for "indirect exposure of humans via the environment".
Four human consumption routes are incorporated: leaf crops, root crops, milk and meat.
Each route contributes to 10% of the TDI (by definition); the lowest of the calculated soil and groundwater concentrations is selected and presented under Output.
Note that pore water concentrations are set equal to the aqueous solubility if the pore water concentration exceeds the aqueous solubility in the model calculations. A warning will display when this is the case.
Note that some bioconcentrations factors are Kow determined. When the Kow is outside of the range of applicability of the respective QSAR (TSCF, BAFmeat and BAFmilk), model calculations are performed with the upper or lower limit of the Kow range for the respective QSAR. A warning will display when this is the case.

User input		**Mind the units in which the parameters should be entered:**	
TDI	1,00E-05	[$mg.kg_{bw}^{-1}.d^{-1}$]	
HENRY	9,00E+02	[$Pa.m^3.mol^{-1}$]	**!Delete cell content if no Henry constant is available.**
K_{oc}	43,65	[$L.kg^{-1}$]	
K_{ow}	66,10	[-]	
SOL	1,08E+03	[$mg.L^{-1}$]	aqueous solubility
T_{SOL}	2,50E+01	[°C]	temperature at which aqueous solubility is determined

Output			
$MPC_{human\ soil}$	3,026E-04	[$mg.kg_{dwt}^{-1}$]	Expressed in Dutch standard soil

The critical route is: consumption of root crops (MPChuman, soil root)

Warnings

log Kow is below the range for BAFmilk calculation, log Kow = 3 is used in calculations

2,3-dichloropropene

Calculation of MPChuman_comp values based on EUSES 2.0.3 equations for "indirect exposure of humans via the environment".
Four human consumption routes are incorporated: leaf crops, root crops, milk and meat.
Each route contributes to 10% of the TDI (by definition); the lowest of the calculated soil and groundwater concentrations is selected and presented under Output.
Note that pore water concentrations are set equal to the aqueous solubility if the pore water concentration exceeds the aqueous solubility in the model calculations. A warning will display when this is the case.
Note that some bioconcentrations factors are Kow determined. When the Kow is outside of the range of applicability of the respective QSAR (TSCF, BAFmeat and BAFmilk), model calculations are performed with the upper or lower limit of the Kow range for the respective QSAR. A warning will display when this is the case.

User input		**Mind the units in which the parameters should be entered:**	
TDI	1,00E-05	[mg.kg$_{bw}^{-1}$.d^{-1}]	
HENRY	2,48E+03	[Pa.m^3.mol^{-1}]	**!Delete cell content if no Henry constant is available.**
K_{oc}	100,00	[L.kg^{-1}]	
K_{ow}	218,80	[-]	
SOL	1,00E+03	[mg.L^{-1}]	aqueous solubility
T_{SOL}	2,50E+01	[°C]	temperature at which aqueous solubility is determined

Output			
$MPC_{human\ soil}$	3,006E-04	[mg.kg$_{dwt}^{-1}$]	Expressed in Dutch standard soil

The critical route is: consumption of root crops (MPChuman, soil root)

Warnings

log Kow is below the range for BAFmilk calculation, log Kow = 3 is used in calculations

RIVM

National Institute
for Public Health
and the Environment

P.O. Box 1
3720 BA Bilthoven
The Netherlands
www.rivm.com