NATIONAL INSTITUTE OF PUBLIC HEALTH AND ENVIRONMENTAL PROTECTION
BILTHOVEN, THE NETHERLANDS

Report no. 679101 011

TOWARDS INTEGRATED ENVIRONMENTAL QUALITY OBJECTIVES FOR SEVERAL VOLATILE COMPOUNDS

E.J. van de Plassche and G.J.M. Bocktinn

lovember 1993

This research was carried out on behalf of the Directorate for Environmental Protection, Directorate for Chemicals, External Safety, and Radiation Protection, in the frame of the project "Setting integrated environmental quality objectives" (Quality objectives and risks, project no. 679101).

MAILING LIST

1-10	Directoraat Generaal Milieubeheer, Directie Stoffen, Veiligheid en Straling, afdeling Normstelling d.t.v. prof. dr. C.J. v. Leeuwen
11	DG Milieubeheer ir. M.E.E. Enthoven
12	plv. DG Milieubeheer dr. ir. B.C.J. Zoeteman
13	plv. DG Milieubeheer mr. G.J.R. Wolters
14	Directoraat Generaal Milieubeheer, Directie Stoffen, Veiligheid en Straling, afdeling Stoffen t.a.v. ir. M. Bovenkerk
15	Directoraat Generaal Milieubeheer, Directie Bodem t.a.v. plv. directeur drs. A. Deelen
16	Directoraat Generaal Milieubeheer, Directie Drinkwater, Water en Landbouw, afdeling Coördinatie Milieukwaliteit, t.a.v. ir. J. de Rijk
17	Directoraat Generaal Milieubeheer, Directie Lucht en Energie, afdeling Luchtkwaliteit t.a.v. drs. R.J.T. van Lint
18 - 24	Projectgroep IWINS d.t.v. drs. C.A.J. Denneman
25 - 33	Onderzoeksbegeleidingsgroep INS d.t.v. dr. J.H.M. de Bruijn
34 - 40	Projectgroep INS d.t.v. drs. E.J. van de Plassche
41 - 46	Begeleidingsgroep Evenwichtspartitie INS d.t.v. E.J. v.d. Plassche
47 - 61	EEG-OECD-Commissies d.t.v. prof. dr. C.J. v. Leeuwen
62 - 76	OECD SIDS Contact Points d.t.v. drs. E.J. v.d. Plassche
77	Gezondheidsraad
78	Technische Commissie Bodembescherming
79	Coördinatiecommissie Uitvoering Wet Verontreiniging Oppervlaktewateren
80	Raad van de Waterstaat
81	Centrale Raad voor de Milieuhygiëne
82	Stichting Natuur en Milieu
83 - 94	Projectgroep "Effecten van luchtverontreiniging op ecosystemen" d.t.v. dr. M.E.J. van der Weiden,
95	drs. M. v.d. Gaag, Directoraat Generaal Milieubeheer, Directie Drinkwater, Water, Landbouw
96	F.M.W. de Jong, Centrum voor Milieukunde Leiden
97	ir. F. Balk, Adviesbureau BKH
98	drs. A.E.G. Tonneijck, Instituut voor Plantenziektenkundig Onderzoek
99	P. Douben, Department of the Environment, Engeland
100	dr. W.A. Bruggeman, RIZA
101	drs. C. v.d. Guchte, RIZA
102	drs. M.A. Beek, RIZA
103	dr. J.L.M. Hermens, RITOX
104	dr. H.J.M. Verhaar, RITOX
105	ir. P.J. de Bruijn, DHV Raadgevend Ingenieursbureau
106	dr. W. v. Driel, Instituut voor Bodemvruchtbaarheid
107	dr. ir. H. de Heer, ministerie van Landbouw, Natuurbeheer en Visserij, directie Gewasbescherming

108	prof. dr. S.A.L.M. Kooijman, Vrije Universiteit Amsterdam
109	drs. J.J. Middelburg, Rijksuniversiteit Utrecht
110	prof. dr. R.D. Schuiling, Rijksuniversiteit Utrecht
111	dr. ir. C.A.M. van Gestel, Vrije Universiteit Amsterdam
112	prof. dr. N.M. van Straalen, Vrije Universiteit Amsterdam
113	drs. E. Guinée, Haskoning
114	Depot van Nederlandse publikaties en Nederlandse bibliografie
115	Directie RIVM
116	Sectordirecteur Stoffen en Risico's, dr. ir. G. de Mik
117	Sectordirecteur Milieuonderzoek, prof. dr. ir. C. v.d. Akker
118	Sectordirecteur Toekomstverkenningen, ir. F. Langeweg
119	Hoofd Adviescentrum Toxicologie, mw. drs. A.G.A.C. Knaap
120	Hoofd Laboratorium voor Ecotoxicologie, prof. dr. H.A.M. de Kruijf
121	Hoofd Laboratorium voor Water en Drinkwateronderzoek, ir. B.A. Banning
122	Hoofd Laboratorium voor Bodem en Grondwateronderzoek, ir. L.H.M. Kohsiek
123	Hoofd Laboratorium voor Toxicologie, dr. W.H. Könemann
124	Hoofd Laboratorium voor Luchtonderzoek, dr. R.M. v. Aalst
125	dr. W. Slooff
126	ir. W. v. Duijvenbooden
127	dr.ir. D. v.d. Meent
128	ir. C.J. Roghair
129	ir. R. v.d. Berg
130	drs. T. Aldenberg
131	ir. M.A. Vaal
132	dr. P. v. Zoonen
133	dr. W. Slob
134	dr. ir. W.J.G.M. Peijnenburg
135	dr. F.A.A.M. de Leeuw
136	dr. L. v. Bree
137	drs. P.J.T.M. Puijenbroek
138	ing. H.F. Prins
139	drs. H.J.Th. Bloemen
140	M.D. Polder
141	dr. F.X.R. van Leeuwen
142	J.E.M. v. Koten-Vermeulen
143	drs. B.C. Rademaker
144	drs. G.H. Crommentuijn
145	D. Kalf
146 - 147	Auteurs
148	Bureau Projecten- en rapportregistratie
149	Hoofd Bureau Voorlichting en Public Relations, mw. drs. J.A. Lijdsman-Schijvenaars
150	Bibliotheek RIVM
151 - 170	Reserve exemplaren

PREFACE

This report contains results of research carried out in the framework of the project 'Setting integrated environmental quality objectives'. The results have been discussed in the 'Setting integrated environmental quality objectives advisory group'. Members thereof are C.W.M. Bodar (Dutch Health Council) J.H.M. de Bruijn (Ministry of Housing, Physical Planning and Environment), J.H. Canton (National Institute of Public Health and Environmental Protection), C.A.J. Denneman (Ministry of Housing, Physical Planning and Environment), J.W. Everts (Ministry of Transport, Public Works and Water Management, National Institute for Coastal and Marine Management), M.P.M. Janssen (National Institute of Public Health and Environmental Protection), W. Ma (Institute for Forestry and Nature Research), P. Leeuwangh (Winand Staring Centre for Integrated Land, Soil and Water Research), E.J. van de Plassche (National Institute of Public Health and Environmental Protection), P.B.M. Stortelder (National Institute of Inland Water Management), J. Struijs (National Institute of Public Health and Environmental Protection), M. Vossen (National Institute of Inland Water Management), and J. van Wensem (Technical Soil Protection Committee).

CONTENTS

ACKNOWLEDGEMENTS

The following persons are thanked for their contribution to this report:
D. v.d. Meent from the Laboratory of Ecotoxicology of the RIVM: for critically reviewing the report,
W.J.G.M. Peijnenburg from the Laboratory of Ecotoxicology of the RIVM: for his advice on degradation constants in air,
P.J.T.M. van Puijenbroek from the Laboratory of Water and Drinking Water Research of the RIVM: for concentrations in surface water from Cooperating Rhine and Meuse Waterworks,
H.F. Prins from the Laboratory of Soil and Groundwater Research of the RIVM: for concentrations in ground water from the National Groundwater Monitoring Program,
H.J.Th. Bloemen from the Laboratory of Air Research of the RIVM: for concentrations in air,
M. Vossen from the National Institute of Inland Water Management: for concentrations in surface water, suspended solids and sediment measured by the National Institute of Inland Water Management.

SUMMARY

The present report is the final report of the sub-project 'Volatile Compounds' of the project 'Setting Integrated Environmental Quality Objectives for Water, Soil and Air'. Values are derived which can be used to set integrated environmental quality objectives (limit and target values) for 46 volatile compounds. First, Maximum Permissible Concentrations (MPCs) and Negligible Concentrations (Ncs) are derived for air, water, sediment and soil based on (eco)toxicological data. MPCs and NCs in air are derived aiming at the protection of the ecosystem as well as human beings. For some compounds for the compartment air only a preliminary MPC is derived because insufficient (eco)toxicological information is available. For other compounds limit and target values for air have already been set by the Ministry of Housing, Physical Planning and Environment. For sediment no ecotoxicological data are available at all. MPCs and NCs are therefore derived from the ones for water by application of the equilibrium partitioning method.

Thereafter these MPCs, NCs, limit and target values are harmonized. Reason for harmonization is that the concentration at e.g. MPC level in a compartment may not lead to exceeding of the MPC in other compartments. MPCs and NCs for water, sediment and soil are harmonized using the equilibrium partitioning method. For harmonization of the values for water, sediment and soil with the ones for air a procedure had to be developed. Since air may not be at or even near equilibrium with water, sediment and soil due to the rapid refreshment of the atmosphere a procedure is used applying computed steady state concentration ratios instead of equilibrium partitioning. The model SimpleBox is used for these computations. SimpleBox is a multimedia fate model in which the environmental compartments are represented by homogeneous boxes. The model is set to represent the behaviour of chemicals in an environment resembling The Netherlands. By comparing computed steady state concentrations with the derived MPCs and NCs based on (eco)toxicological data it is investigated whether adjustment of the MPCs or NCs is necessary. Based on the calculations using SimpleBox MPCs and NCs for water for 5 compounds had to be adjusted downwards. The harmonization procedure to test the coherence of MPCs and NCs must be considered as a scientifically sound, nevertheless 'non-validated' concept. It is believed that the application of the model SimpleBox and consequently the adjustment of MPC and NC values, is justified by the lack of alternatives.

In Table 1 harmonized MPCs, NC and limit and target values are presented for all compartments. For those compounds for which only a preliminary MPC and NC in air could be derived, harmonization of these values with the ones for water, sediment and soil was not possible. Only MPCs and NCs for water, sediment and soil could be harmonized using the equilibrium partitioning method. MPCs and NCs for water, sediment and soil and preliminary MPCs and NCs in air for these compounds are presented in Table 2.

The derived MPCs, NCs and limit and target values are compared with reported environmental concentrations in The Netherlands in air, surface and ground water, suspended matter, sediment and soil. Based on the data available, MPCs are never exceeded while only for some compounds the NC in one of the compartments is exceeded. For many compounds no measurements have been carried out, however.

Table 1. Overview of harmonized Maximum Permissible (MPC) and Negligible Concentrations (NC) for water ($MPC_{aq.}$ and $NC_{aq.}$), sediment ($MPC_{sed.}$ and $NC_{sed.}$), soil (MPC_{soil} and NC_{soil}), and air (MPC_{air} and NC_{air}) and existing limit and target values for air.

compound	water		sediment		soil		air			
	$MPC_{aq.}$ ($\mu g/l$)	$NC_{aq.}$ ($\mu g/l$)	$MPC_{sed.}$ (mg/kg)	$NC_{sed.}$ (mg/kg)	MPC_{soil} (mg/kg)	NC_{soil} (mg/kg)	MPC_{air} ($\mu g/m^3$)	NC_{air} ($\mu g/m^3$)	limit value ($\mu g/m^3$)	target value ($\mu g/m^3$)
acrylonitrile	7.6	0.076	$6.8*10^{-4}$	$6.8*10^{-6}$	$6.8*10^{-4}$	$6.8*10^{-6}$	10	-	-	0.1
benzene	240	2.4	0.95	0.0095	0.95	0.0095	30	-	-	1
2-chloro-1,3-butadiene	-	-	-	-	-	-	1.0	0.01	-	-
3-chloropropene	3.4	0.034	0.0048	$4.8*10^{-5}$	0.0048	$4.8*10^{-5}$	74	0.74	-	-
1,2-dichloroethane	700	7.0	1.5	0.015	1.5	0.015	100	-	-	1
1,1-dichloroethene	3,400	34	12	0.12	12	0.12	200	2.0	-	-
dichloromethane	20,000	200	36	0.36	36	0.36	1,700	-	-	20
1,2-dichloropropane	76	0.76	0.18	0.0018	4.2	0.042	12	0.12	-	-
1,3-dichloropropene	8.0	0.08	0.023	$2.3*10^{-4}$	0.023	$2.3*10^{-4}$	40	0.40	-	-
ethylene	8,500	85	5.8	0.058	5.8	0.058	-	2	300	-
ethylene oxide	84	0.84	0.0021	$2.1*10^{-5}$	0.0021	$2.1*10^{-5}$	3	-	-	0.03
styrene	570	5.7	25	0.25	25	0.25	800	-	-	8
tetrachloroethene	330	3.3	4.0	0.040	0.16	0.0016	2,500	2,000	-	25
tetrachloromethane	1,100	11	37	0.37	37	0.37	60	-	-	1
toluene	730	7.3	4.2	0.042	1.4	0.014	300	3	-	-
1,1,1-trichloroethane	2,100	21	6.9	0.069	6.9	0.069	4,800	4.8	-	-
trichloroethene	2,400	24	13	0.13	13	0.13	5,000	50	-	50
trichloromethane	590	5.9	1.9	0.019	1.9	0.019	100	-	-	1
vinylchloride	820	8.2	1.4	0.014	1.4	0.014	100	-	-	1

water: $MPC_{aq.}$s and $NC_{aq.}$s for acrylonitrile, 3-chloropropene, 1,3-dichloropropene and ethylene oxide are indicative values.

sediment: all $MPC_{sed.}$ and $NC_{sed.}$ values are based on the equilibrium partitioning method.

soil: MPC_{soil}s and NC_{soil}s for 1,2-dichloropropane, tetrachloroethene and toluene are indicative values based on ecotoxicological data. The MPC_{soil}s and NC_{soil}s for the other compounds are based on the equilibrium partitioning method.

air: NC_{air} for ethylene is an indicative value; MPC_{air} and NC_{air} for 2-chloro-1,3-butadiene are revised preliminary values; MPC_{air}s and NC_{air}s for 3-chloropropene, 1,1-dichloroethene, 1,2-dichloropropane, 1,3-dichloropropene and 1,1,1-trichloroethane are derived in the present report.

Table 2. Overview of (preliminary) Maximum Permissible (MPC) and Negligible Concentrations (NC) for water ($MPC_{aq.}$ and $NC_{aq.}$), sediment ($MPC_{sed.}$ and $NC_{sed.}$), soil (MPC_{soil} and NC_{soil}), and air (preliminary MPC_{air} and NC_{air}).

compound	water		sediment		soil		air	
	$MPC_{aq.}$ ($\mu g/l$)	$NC_{aq.}$ ($\mu g/l$)	$MPC_{sed.}$ (mg/kg)	$NC_{sed.}$ (mg/kg)	MPC_{soil} (mg/kg)	NC_{soil} (mg/kg)	preliminary MPC_{air} ($\mu g/m^3$)	preliminary NC_{air} ($\mu g/m^3$)
1,2-dichlorobenzene	250	2.5	5.5	0.055	0.4	0.004	60	0.60
1,3-dichlorobenzene	250	2.5	5.5	0.055	0.4	0.004	-	-
1,4-dichlorobenzene	250	2.5	5.5	0.055	0.4	0.004	670	6.7
1,1-dichloroethane	700	7.0	1.5	0.015	1.5	0.015	370	3.7
1,2-dichloroethene	6,100	61	22	0.22	22	0.22	36	0.36
1,3-dichloropropane	76	0.76	0.18	0.0018	0.18	0.0018	-	-
2,3-dichloropropene	8.0	0.08	0.044	$4.4*10^{-4}$	0.044	$4.4*10^{-4}$	-	-
ethylbenzene	370	3.7	3.1	0.031	3.1	0.031	39	0.39
hexachlorobenzene	2.4	0.024	1.3	0.013	1.3	0.013	2.3	0.023
hexachloroethane	83	0.83	17	0.17	17	0.17	27	0.27
monochlorobenzene	690	6.9	7.6	0.076	7.6	0.076	42	0.42
2-monochlorotoluene	310	3.1	33	0.33	33	0.33	780	0.78
3-monochlorotoluene	310	3.1	33	0.33	33	0.33	-	-
4-monochlorotoluene	310	3.1	33	0.33	33	0.33	-	-
pentachlorobenzene	7.5	0.075	3.0	0.030	0.3	0.003	8	0.08
pentachloroethane	230	2.3	49	0.49	49	0.49	-	-
1,2,3,4-tetrachlorobenzene	24	0.24	7.2	0.072	0.072	$7.2*10^{-4}$	1.6	0.016
1,2,3,5-tetrachlorobenzene	24	0.24	7.2	0.072	0.072	$7.2*10^{-4}$	1.6	0.016
1,2,4,5-tetrachlorobenzene	24	0.24	7.2	0.072	0.072	$7.2*10^{-4}$	1.6	0.016
1,1,2,2-tetrachloroethane	3,300	33	14	0.14	14	0.14	0.2	0.002
1,2,3-trichlorobenzene	67	0.67	6.7	0.067	0.24	0.0024	4	0.04
1,2,4-trichlorobenzene	67	0.67	6.7	0.067	0.24	0.0024	4	0.04

(continued)

(continuation Table 2)

compound	water		sediment		soil		air	
	$MPC_{aq.}$ ($\mu g/l$)	$NC_{aq.}$ ($\mu g/l$)	$MPC_{sed.}$ (mg/kg)	$NC_{sed.}$ (mg/kg)	MPC_{soil} (mg/kg)	NC_{soil} (mg/kg)	preliminary MPC_{air} ($\mu g/m^3$)	preliminary NC_{air} ($\mu g/m^3$)
1,3,5-trichlorobenzene	67	0.67	6.7	0.067	0.24	0.0024	4	0.04
1,1,2-trichloroethane	7,900	79	39	0.39	39	0.39	18	0.18
2-xylene	380	3.8	14	0.14	14	0.14	340	3.4
3-xylene	380	3.8	14	0.14	14	0.14	1,000	10
4-xylene	380	3.8	14	0.14	14	0.14	1,000	10

MPCs and NCs for water, sediment and soil are harmonized using the equilibrium partitioning method. Preliminary MPCs and NCs in air could not be harmonized with the ones for water, sediment and soil.

MPCs and NCs for 1,1-dichloroethane and 1,3-dichloropropane for water, sediment and soil set equal to the ones for 1,2-dichloroethane and 1,2-dichloropropane, respectively.

sediment: all $MPC_{sed.}$ and $NC_{sed.}$ values are based on the equilibrium partitioning method.

soil: MPC_{soil}s and NC_{soil}s for di-, tri- and tetra- and pentachlorobenzene(s) are indicative values based on ecotoxicological data. The MPC_{soil}s and NC_{soil}s for the other compounds are based on the equilibrium partitioning method.

air: preliminary MPC_{air}s and NC_{air}s are values which should not be used to set limit and target values.

$MPC_{aq.}$, $MPC_{sed.}$ and MPC_{soil} for hexa- and pentachlorobenzene may change because effects due to their accumulation potential will be examined in another project. For the other compounds it is not considered necessary to estimate the risk due to secondary poisoning because they will probably not accumulate in the food-chain due to their physico-chemical properties (low lipophilicity: low log K_{ow}).

SAMENVATTING

Het onderhavige rapport vormt de eindrapportage van het deelproject 'Vluchtige Stoffen' als onderdeel van het project 'Integrale Normstelling Stoffen Water, Bodem en Lucht'. In dit eindrapport zijn voor een aantal vluchtige organische verbindingen waarden afgeleid die gebruikt kunnen worden voor het opstellen van integrale milieukwaliteitsdoelstellingen (grens- of streefwaarden). Allereerst zijn voor water, sediment, bodem en lucht Maximaal Toelaatbare Risiconivo's (MTRs) en Verwaarloosbare Risiconivo's (VRs) afgeleid op basis van (eco)toxicologische gegevens. MTRs en VRs in lucht zijn zowel ter bescherming van het ecosysteem als de mens bepaald. Voor een aantal stoffen kon alleen een voorlopige MTR in lucht worden afgeleid omdat onvoldoende (eco)toxicologische gegevens beschikbaar zijn. Daarnaast zijn voor een aantal stoffen al grens- en streefwaarden in lucht opgesteld door het ministerie van VROM. Voor sediment zijn geen ecotoxicologische gegevens beschikbaar. MTRs en VRs voor sediment zijn daarom afgeleid uit die voor water door toepassing van de evenwichtspartitiemethode.

Vervolgens zijn deze compartimentale MTRs, VRs en grens- en streefwaarden op elkaar afgestemd. De concentratie op bv. MTR-nivo in het ene compartiment mag namelijk niet leiden tot een overschrijding van de MTR in een ander compartiment. Voor het afstemmen van de waarden voor water, sediment en bodem is gebruik gemaakt van de evenwichtspartitiemethode. Deze methode kan voor het afstemmen van de waarden voor water, sediment en bodem met die in lucht niet gebruikt worden aangezien lucht niet in evenwicht is met water, sediment en bodem door de snelle verversing van de lucht. Voor de afstemming met lucht is dan ook een speciale procedure ontwikkeld. Hierbij is gebruik gemaakt van berekende 'steady state' concentratie ratio's door toepassing van het model SimpleBox. SimpleBox is een multimedia model waarmee het gedrag van stoffen in het milieu voorspeld kan worden. De verschillende compartimenten worden hierbij voorgesteld als homogene 'boxen'. Parameters zijn zodanig gekozen dat de schaal van het model representatief is voor Nederland. Door de berekende 'steady state' concentraties te vergelijken met de MTRs en VRs, die gebaseerd zijn op (eco)toxicologische, gegevens is bekeken of bijstelling van deze MTRs en VRs noodzakelijk is. Gebaseerd op berekeningen met dit model zijn voor 5 stoffen de MTRs en VRs voor water naar beneden bijgesteld. Opgemerkt moet worden dat het gebruiken van het model SimpleBox voor afstemming van MTR en VR waarden een wetenschappelijk juist, echter 'niet gevalideerd' concept is. Op dit moment zijn er echter geen alternatieven voor het toepassen van SimpleBox en het vervolgens bijstellen van MTR en VR waarden.

In Tabel 1 zijn afgestemde MTRs, VRs en grens- en streefwaarden voor de verschillende compartimenten weergegeven. Voor die stoffen waarvoor alleen een voorlopige MTR en VR in lucht beschikbaar was, was afstemming met de MTRs en VRs voor water, sediment en bodem niet mogelijk. De MTRs en VRs voor water, sediment en bodem konden alleen onderling afgestemd worden met de evenwichtspartitiemethode. MTRs en VRs voor water, sediment en bodem en voorlopige MTRs en VRs in lucht zijn voor deze stoffen weergeven in Tabel 2.

De al dan niet afgestemde MTRs, VRs en grens- en streefwaarden zijn tevens vergeleken met actuele concentraties in lucht, grond- en oppervlaktewater, gesuspendeerd materiaal, sediment en bodem. Voor geen enkele stof worden de MTRs overschreden terwijl slechts voor enkele stoffen het VR overschreden wordt. Voor veel stoffen zijn echter geen gegevens beschikbaar.

Tabel 1. Overzicht afgestemde Maximaal Toelaatbare Risiconivo's (MTRs) en Verwaarloosbare Risiconivo's (VRs) voor water (MTR_{water} en VR_{water}), sediment ($MTR_{sediment}$ en $VR_{sediment}$), bodem (MTR_{bodem} en VR_{bodem}), en lucht (MTR_{lucht} en VR_{lucht}) en bestaande grens- en streefwaarden in lucht.

stof	water		sediment		bodem		lucht			
	MTR_{water} ($\mu g/l$)	VR_{water} ($\mu g/l$)	$MTR_{sediment}$ (mg/kg)	$VR_{sediment}$ (mg/kg)	MTR_{bodem} (mg/kg)	VR_{bodem} (mg/kg)	MTR_{lucht} ($\mu g/m^3$)	VR_{lucht} ($\mu g/m^3$)	grenswaarde ($\mu g/m^3$)	streefwaarde ($\mu g/m^3$)
acrylonitril	7.6	0.076	$6.8*10^{-4}$	$6.8*10^{-6}$	$6.8*10^{-4}$	$6.8*10^{-6}$	10	-	-	0.1
benzeen	240	2.4	0.95	0.0095	0.95	0.0095	30	-	-	1
2-chloor-1,3-butadieen	-	-	-	-	-	-	1.0	0.01	-	-
3-chloorpropeen	3.4	0.034	0.0048	$4.8*10^{-5}$	0.0048	$4.8*10^{-5}$	74	0.74	-	-
1,2-dichloorethaan	700	7.0	1.5	0.015	1.5	0.015	100	-	-	1
1,1-dichlooretheen	3,400	34	12	0.12	12	0.12	200	2.0	-	-
dichloormethaan	20,000	200	36	0.36	36	0.36	1,700	-	-	20
1,2-dichloorpropaan	76	0.76	0.18	0.0018	4.2	0.042	12	0.12	-	-
1,3-dichloorpropeen	8.0	0.08	0.023	$2.3*10^{-4}$	0.023	$2.3*10^{-4}$	40	0.40	-	-
ethyleen	8,500	85	5.8	0.058	5.8	0.058	-	2	300	-
ethyleen oxide	84	0.84	0.0021	$2.1*10^{-5}$	0.0021	$2.1*10^{-5}$	3	-	-	0.03
styreen	570	5.7	25	0.25	25	0.25	800	-	-	8
tetrachlooretheen	330	3.3	4.0	0.040	0.16	0.0016	2,500	2,000	-	25
tetrachloormethaan	1,100	11	37	0.37	37	0.37	60	-	-	1
tolueen	730	7.3	4.2	0.042	1.4	0.014	300	3	-	-
1,1,1-trichloorethaan	2,100	21	6.9	0.069	6.9	0.069	4,800	4.8	-	-
trichlooretheen	2,400	24	13	0.13	13	0.13	5,000	50	-	50
trichloormethaan	590	5.9	1.9	0.019	1.9	0.019	100	-	-	1
vinylchloride	820	8.2	1.4	0.014	1.4	0.014	100	-	-	1

water: MTR_{water}s en VR_{water}s voor acrylonitril, 3-chloorpropeen, 1,3-dichloorpropeen and ethyleen oxide zijn indicatieve waarden.

sediment: alle $MTR_{sediment}$ en $VR_{sediment}$ waarden afgeleid met de evenwichtspartitiemthode.

bodem: MTR_{bodem}s en VR_{bodem}s voor 1,2-dichloorpropaan, tetrachlooretheen en tolueen zijn indicatieve waarden gebaseerd op ecotoxicologische gegevens. De MTR_{bodem}s en VR_{bodem}s voor de andere stoffen zijn afgeleid met de evenwichtspartitiemethode.

lucht: VR_{lucht} ethyleen: indicatieve waarde; MTR_{lucht} en VR_{lucht} voor 2-chloor-1,3-butadieen zijn bijgestelde voorlopige waardes; MTR_{lucht}s en VR_{lucht}s voor 3-chloorpropeen, 1,1-dichlooretheen, 1,2-dichloorpropaan, 1,3-dichloorpropeen en 1,1,1-trichloorethaan zijn afgeleid in dit rapport.

Tabel 2. Overzicht (voorlopige) Maximaal Toelaatbare Risiconivo's (MTRs) en Verwaarloosbare Risiconivo's (VRs) voor water (MTR_{water} en VR_{water}), sediment ($MTR_{sediment}$ en $VR_{sediment}$), bodem (MTR_{bodem} en VR_{bodem}), en lucht (MTR_{lucht} en VR_{lucht}).

stof	water		sediment		bodem		lucht	
	MTR_{water} ($\mu g/l$)	VR_{water} ($\mu g/l$)	$MTR_{sediment}$ (mg/kg)	$VR_{sediment}$ (mg/kg)	MTR_{bodem} (mg/kg)	VR_{bodem} (mg/kg)	voorlopige MTR_{lucht} ($\mu g/m^3$)	voorlopige VR_{lucht} ($\mu g/m^3$)
1,2-dichloorbenzeen	250	2.5	5.5	0.055	0.4	0.004	60	0.60
1,3-dichloorbenzeen	250	2.5	5.5	0.055	0.4	0.004	-	-
1,4-dichloorbenzeen	250	2.5	5.5	0.055	0.4	0.004	670	6.7
1,1-dichloorethaan	700	7.0 →	1.5	0.015	1.5	0.015	370	3.7
1,2-dichlooretheen	6,100	61 →	22	0.22	22	0.22	36	0.36
1,3-dichloorpropaan	76	0.76 →	0.18	0.0018	0.18	0.0018	-	-
2,3-dichloorpropeen	8.0	0.08 →	0.044	$4.4*10^{-4}$	0.044	$4.4*10^{-4}$	-	-
ethylbenzeen	370	3.7 →	3.1	0.031	3.1	0.031	39	0.39
hexachloorbenzeen	2.4	0.024 →	1.3	0.013	1.3	0.013	2.3	0.023
hexachloorethaan	83	0.83 →	17	0.17	17	0.17	27	0.27
monochloorbenzeen	690	6.9 →	7.6	0.076	7.6	0.076	42	0.42
2-monochloortolueen	310	3.1 →	33	0.33	33	0.33	780	0.78
3-monochloortolueen	310	3.1 →	33	0.33	33	0.33	-	-
4-monochloortolueen	310	3.1 →	33	0.33	33	0.33	-	-
pentachloorbenzeen	7.5	0.075 →	3.0	0.030	0.3	0.003	8	0.08
pentachloorethaan	230	2.3 →	49	0.49	49	0.49	-	-
1,2,3,4-tetrachloorbenzeen	24	0.24 →	7.2	0.072	0.072	$7.2*10^{-4}$	1.6	0.016
1,2,3,5-tetrachloorbenzeen	24	0.24 →	7.2	0.072	0.072	$7.2*10^{-4}$	1.6	0.016
1,2,4,5-tetrachloorbenzeen	24	0.24 →	7.2	0.072	0.072	$7.2*10^{-4}$	1.6	0.016
1,1,2,2-tetrachloorethaan	3,300	33 →	14	0.14	14	0.14	0.2	0.002
1,2,3-trichloorbenzeen	67	0.67 →	6.7	0.067	0.24	0.0024	4	0.04
1,2,4-trichloorbenzeen	67	0.67 →	6.7	0.067	0.24	0.0024	4	0.04

(z.o.z. voor vervolg)

(vervolg Tabel 2)

stof	water		sediment		bodem		lucht	
	MTR_{water} ($\mu g/l$)	VR_{water} ($\mu g/l$)	$MTR_{sediment}$ (mg/kg)	$VR_{sediment}$ (mg/kg)	MTR_{bodem} (mg/kg)	VR_{bodem} (mg/kg)	voorlopige MTR_{lucht} ($\mu g/m^3$)	voorlopige VR_{lucht} ($\mu g/m^3$)
1,3,5-trichloorbenzeen	67	0.67	6.7	0.067	0.24	0.0024	4	0.04
1,1,2-trichloorethaan	7,900	79	39	0.39	39	0.39	18	0.18
2-xyleen	380	3.8	14	0.14	14	0.14	340	3.4
3-xyleen	380	3.8	14	0.14	14	0.14	1,000	10
4-xyleen	380	3.8	14	0.14	14	0.14	1,000	10

MTRs en VRs voor water, sediment en bodem zijn afgestemd door middel van toepassing van de evenwichtspartitiemethode. MTRs en VRs voor water, sediment en bodem zijn echter niet afgestemd met voorlopige MTRs en VRs voor lucht.

MTRs en VRs voor 1,1-dichloorethaan en 1,3-dichloorpropaan voor water, sediment en bodem zijn gelijkgesteld aan die van 1,2-dichloorethaan en 1,2-dichloorpropaan, respectievelijk.

sediment: alle $MTR_{sediment}$ en $VR_{sediment}$ waarden afgeleid met de evenwichtspartitiemthode.

bodem: MTR_{bodem}s en VR_{bodem}s voor di-, tri-, tetra- en pentachloorbenzeen zijn indicatieve waarden gebaseerd op ecotoxicologische gegevens. De MTR_{bodem}s en VR_{bodem}s voor de andere stoffen zijn afgeleid met de evenwichtspartitiemethode.

lucht: voorlopige MTR_{lucht}s en VR_{lucht}s zijn waarden die niet gebruikt kunnen worden voor het afleiden van grens- en streefwaarden.

MTR_{water}, $MTR_{sediment}$ en MTR_{bodem} voor hexa- en pentachloorbenzeen kunnen nog veranderen aangezien nog geen rekening is gehouden met mogelijk nadelige effecten als gevolg van doorvergiftiging. In een afzonderlijk project zal hieraan aandacht besteed worden. Voor de overige stoffen zal geen inschatting gemaakt worden van het risico voor doorvergiftiging aangezien deze stoffen waarschijnlijk niet zullen accumuleren in de voedselketen vanwege hun fysisch-chemische eigenschappen (lage lipofiliteit: lage log K_{ow}).

1 INTRODUCTION

In 1989 the Directorate-General for Environmental Protection started the project "Setting integrated environmental quality objectives". In this project action A-35 of the National Environmental Policy Plan is worked out [1]. Goal is to derive integrated environmental quality objectives for air, ground and surface water, sediment and soil for a great number of compounds, based on the risk philosophy of the Ministry of Housing, Physical Planning and Environment [2]. The project is carried out by the National Institute for Public Health and Environmental Protection. The first project (a) "MILBOWA"[1] resulted in the report "Desire for levels" [3]. In this report a methodology was proposed for deriving Maximum Permissible Concentrations for several compounds like heavy metals, chlorophenols, pesticides and polycyclic aromatic hydrocarbons. Based on this report integrated environmental quality objectives for water, sediment and soil were proposed by the Minister of the Environment from The Netherlands [4].

The second project (b) is divided into three sub-projects: 'Exotic Metals' (b-1), 'Volatile Compounds' (b-2) and 'Secondary Poisoning' (b-3). In project b-1 for nine trace metals, i.e. antimony, barium, beryllium, cobalt, molybdenum, selenium, thallium, tin, and vanadium, values were derived which can be used to set integrated environmental quality objectives for ground and surface water, sediment and soil [5]. For deriving these values almost the same methods were used as described in "Desire for levels" [3]. Hence, Maximum Permissible Concentrations (MPC) and Negligible Concentrations (NC) for water, sediment and soil were determined using extrapolation methods based on ecotoxicological data. Subsequently these MPCs and NCs for the different compartments were harmonized using the equilibrium partitioning method [6, 7, 8]. Reason for harmonization is that the concentration at MPC (or NC) level in one compartment may not lead to exceeding of the MPC (or NC) in other compartments due to transport of the chemical between different compartments. A flow diagram of the different steps leading to integrated environmental quality objectives is given in figure 1.

Criticism of several advisory committees, asked by the Ministry of Housing, Physical Planning and Environment for their opinion on the proposals for integrated environmental quality objectives of the project "MILBOWA", was that no harmonization of the proposed objectives had taken place with the compartment air [9, 10]. No MPCs for the compartment air were derived, however because most of these compounds were not volatile. Next to this, no method was available at that time to harmonize the MPC for air with the ones for water, sediment and soil.

Based on these considerations a project titled "Volatile Compounds" (b-2) was started aiming at the derivation of integrated environmental quality objectives for 46 volatile organic hydrocarbons for water, sediment, soil and air. For the trace elements dealt with in project b-1 no MPCs were derived for the compartment air because it was expected that almost no toxicity data via inhalation will be available for these metals. Besides, the harmonization of MPCs for air with ones for the other compartments is still problematic at the moment for metals.

---

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

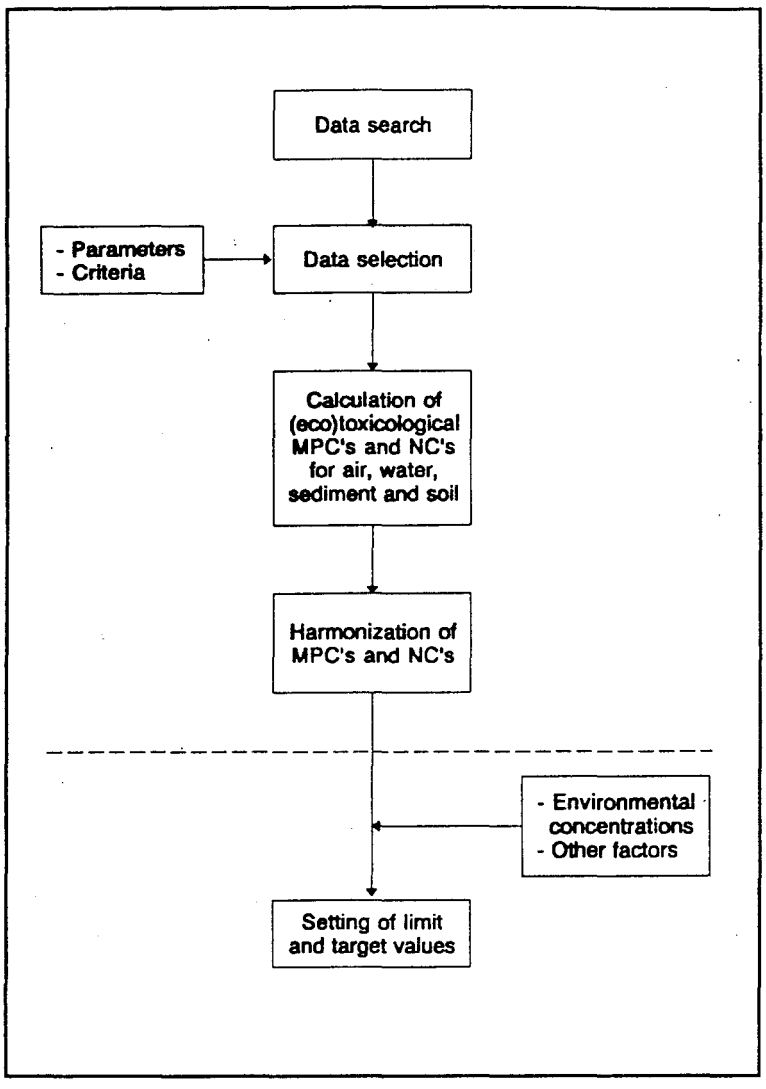

Figure 1. Process of setting integrated environmental quality objectives

The selected volatile compounds of project b-2 are presented in Table 1.

Table 1. Selected substances of the project "Volatile Compounds"

acrylonitrile	3-monochlorotoluene
benzene	4-monochlorotoluene
2-chloro-1,3-butadiene	pentachlorobenzene
3-chloropropene	pentachloroethane
1,2-dichlorobenzene	styrene
1,3-dichlorobenzene	1,2,3,4-tetrachlorobenzene
1,4-dichlorobenzene	1,2,3,5-tetrachlorobenzene

1,1-dichloroethane	1,2,4,5-tetrachlorobenzene
1,2-dichloroethane	1,1,2,2-tetrachloroethane
1,1-dichloroethene	tetrachloroethene
1,2-dichloroethene	tetrachloromethane
dichloromethane	toluene
1,2-dichloropropane	1,2,3-trichlorobenzene
1,3-dichloropropane	1,2,4-trichlorobenzene
1,3-dichloropropene	1,3,5-trichlorobenzene
2,3-dichloropropene	1,1,1-trichloroethane
ethylbenzene	1,1,2-trichloroethane
ethylene	trichloroethene
ethylene oxide	trichloromethane
hexachlorobenzene	vinylchloride
hexachloroethane	2-xylene
monochlorobenzene	3-xylene
2-monochlorotoluene	4-xylene

Within the framework of the project "Volatile compounds" a first starting-point was a workshop organized on October 8, 1991 at the National Institute of Public Health and Environmental Protection titled "Integration of setting quality objectives for air with water and soil" [11]. In this workshop experts from scientific research institutes, governmental institutes and the industry participated. Topics discussed concerned the derivation of MPCs in air for human beings as well as the ecosystem and the harmonization of MPCs derived for water and soil with the ones for air. Approaches presented in this workshop how to deal with these aspects have been worked out in the course of time.

Summarizing, the following activities had to be carried out within the project "Volatile Compounds":

1. deriving MPCs for water, sediment and soil based on ecotoxicological data,
2. deriving MPCs for air based on ecotoxicological and toxicological data aiming at the protection of the ecosystem as well as human beings. Because inhalation via air is such an important exposure route for humans it was decided to derive also a MPC for human beings.
3. harmonization of the MPCs and NCs for the different compartments. For the harmonization of MPCs and NCs for water, soil and sediment the equilibrium partitioning method will be used as already described. In order to harmonize the MPCs and NCs for water, sediment and soil with the ones for air a harmonization procedure was developed. Within this procedure a multimedia box model, called SimpleBox, is used.
4. setting integrated environmental quality objectives (limit and target values).

It was decided by the National Institute of Public Health and Environmental Protection and the Ministry of Housing, Physical Planning and Environment to publish separate reports about these activities. In the present report, which can be regarded as an integration report of the project "Volatile Compounds", harmonized values are derived which can be used to set integrated environmental quality objectives. The last step, setting limit and target values, will be the subject of a separate policy document that will include also integrated environmental quality objectives for

the nine trace metals stated above and a group of pesticides with a potential for secondary poisoning (projects b-1 and b3, respectively).

In Chapter 2 MPC and NC values are derived for water, soil and air based on (eco)toxicological data. In Chapter 3 the procedure used to harmonize the MPC and NC values for the different compartments will be described. In Chapter 4 several physico-chemical properties, needed for the model SimpleBox, for the volatile compounds are discussed. In Chapter 5 MPC and NC values for water, sediment and soil are harmonized using the equilibrium partitioning method. Thereafter the MPC and NC values for air are harmonized with the ones for water and soil in Chapter 6. These harmonized MPC and NC values are compared with actual concentrations in Chapter 7.

2 DERIVING MAXIMUM PERMISSIBLE CONCENTRATIONS AND NEGLIGIBLE CONCENTRATIONS FROM TOXICITY DATA

2.1 Risk limits of substances for human beings and the ecosystem

For deriving environmental quality objectives two risk limits have been defined in The Netherlands in the policy document "Premises for risk management" [2]:

- Maximum Permissible Concentration (MPC),
- Negligible Concentration (NC) defined as 1% of the MPC. The safety factor of 100 is used because of the possibility of combined toxicity due to the presence of other chemicals in the environment.

The aim of quality objectives for ecosystems is that the MPC is set at a level that protects all species in an ecosystem. Using a statistical extrapolation model, a 95% protection level is chosen as a cut-off value. This means theoretically that for 95% of the species the NOEC can be exceeded. An overview of the methods used in The Netherlands is presented by Slooff [7].

In case of human beings a distinction is made between substances without a threshold level, genotoxic carcinogens, and substances with threshold levels. For the former substances the MPC is defined at 10^{-6}/year for mortality to humans. For substances with a threshold level the MPC cannot be defined so strictly because many different effects with various concentration-effect relationships can be experienced. In general the MPC is calculated using results from toxicological studies with mammals or epidemiological studies by application of uncertainty factors to No Observed Adverse Effect Levels (NOAELs) derived from these studies.

In the following paragraphs the derivation of Maximum Permissible Concentrations (MPCs) for water, sediment, soil and air is described, referred to as $MPC_{aq.}$, $MPC_{sed.}$, MPC_{soil}, and MPC_{air}, respectively. In Van de Plassche et al.: "Derivation of Maximum Permissible Concentrations for several volatile compounds for water, sediment and soil" the calculation of the $MPC_{aq.}$, $MPC_{sed.}$ and MPC_{soil} is described in detail [12]. Calculation of the MPC_{air}s is described in Rademaker and Van de Plassche: "The derivation of Maximum Permissible Concentrations for several volatile compounds in air" [13]. A short summary of these reports is given in the following paragraphs.

As already stated in Chapter 1 the MPC_{air}s were derived aiming at the protection of man as well as the ecosystem. The MPCs for water, soil and sediment were derived aiming at the protection of the ecosystem only.

2.2 MPCs and NCs for water

$MPC_{aq.}$s were calculated applying extrapolation methods based on single species toxicity data: if only acute data or less than 4 chronic NOEC values are available the modified EPA method is applied (preliminary effect assessment) [7, 14]. The outcome of this method is called an indicative $MPC_{aq.}$. If 4 or more chronic NOEC values from different taxonomic groups are available the method of Aldenberg & Slob is applied (refined effect assessment) [7, 14, 15]. For chemicals which could be classified as 'inert chemicals' Quantitative Structure-Activity Relationships (QSARs) were used to obtain chronic NOEC values, based on the assumption that

for inert chemicals the expected effect concentration can be calculated on the basis of the octanol/water partition coefficient (K_{ow}) [16]. With QSARs for non-specific toxicity a set of NOEC values for 19 different organisms were obtained. This data set was used to calculate the $MPC_{aq.}$ with the extrapolation method of Aldenberg & Slob. For chemicals which could not be classified as inert ones toxicity data were obtained by literature search.

In order to determine which compounds could be considered as 'inert chemicals' acting by narcosis, a classification scheme presented by Verhaar and Hermens (1991) was used [17]. They defined structural requirements for four classes of compounds: inert, less inert, reactive and specifically acting chemicals. Based on this classification scheme it could be concluded that most of the volatile substances belong to the class of 'inert chemicals'. For these 'inert' compounds NOECs were calculated using QSARs. Additionally, for 27 out of the 46 compounds a comparison was made between the results of the use of QSARs and, what is called the 'traditional approach' by Van de Plassche et al., which uses only toxicity data (L(E)C50 and NOEC values) gathered by literature search [12]. From this comparison it could be concluded that results from both approaches were in good agreement. [12] $MPC_{aq.}$s calculated with the QSAR approach were preferred however, because they are based on toxicity estimations for 19 different organisms.

Only acrylonitrile, 2-chloro-1,3-butadiene, 3-chloropropene, 1,3- and 2,3-dichloropropene and ethylene oxide belong to another class of compounds: they are reactive chemicals. For these compounds toxicity data for freshwater as well as saltwater organisms were gathered by literature search. Data were very scarce for these 6 substances. For 2-chloro-1,3-butadiene and 2,3-dichloropropene no toxicity data were available at all for the aquatic environment. For acrylonitrile, 1,3-dichloropropene and ethylene oxide no chronic data were present so the $MPC_{aq.}$ was calculated using the EPA method based on acute toxicity data. Although 4 chronic NOEC values from different taxonomic groups were present for 3-chloropropene the modified EPA method was applied instead of the method of Aldenberg & Slob because based on acute data it could be concluded that the chronic NOEC values were present for less sensitive taxonomic groups (bacteria, algae and protozoans).

In Table 2.1 $MPC_{aq.}$s and $NC_{aq.}$s for all compounds are presented. Because no toxicity data were available for ground water organisms these $MPC_{aq.}$s and $NC_{aq.}$s are used for surface as well as ground water.

In addition, it has to be stated that secondary poisoning is not taken into account although it is recognized that some of the compounds can bioaccumulate. The risk of adverse effects from bioaccumulating compounds will however be subject of another report in which all compounds, including penta- en hexachlorobenzene, from the project 'Setting environmental quality objectives' that have a potential for secondary poisoning will be dealt with (sub-project b-3; see Chapter 1).

Table 2.1. Maximum Permissible and Negligible Concentrations for water (mg/l)

compound	$MPC_{aq.}$ (μg/l)	$NC_{aq.}$ (μg/l)	lowest NOEC[a] (μg/l)	lowest L(E)C50[a] (μg/l)
acrylonitrile	7.6[b,c]	0.076[b,c]	-	7,600
benzene	2,400	24		
2-chloro-1,3-butadiene	-[d]	-[d]		
3-chloropropene	3.4[b]	0.034	3,200	340
1,2-dichlorobenzene	270[d]	2.7[d]		
1,3-dichlorobenzene	210[d]	2.1[d]		
1,4-dichlorobenzene	260[d]	2.6[d]		
1,1-dichloroethane	7,300	73		
1,2-dichloroethane	14,000	140		
1,1-dichloroethene	3,400	34		
1,2-dichloroethene	6,100	61		
dichloromethane	20,000	200		
1,2-dichloropropane	5,300	53		
1,3-dichloropropane	5,200	52		
1,3-dichloropropene	8.0[b]	0.08[b]	-	800
2,3-dichloropropene	8.0[b,e]	0.08[b,e]		
ethylbenzene	370	3.7		
ethylene	8,500	85		
ethylene oxide	84[b]	0.84[b]	-	84,000
hexachlorobenzene	2.4	0.024		
hexachloroethane	8.3	0.083		
monochlorobenzene	690	6.9		
2-monochlorotoluene	300[f]	3.0[f]		
3-monochlorotoluene	330[f]	3.3[f]		
4-monochlorotoluene	300[f]	3.0[f]		
pentachlorobenzene	7.5	0.075		
pentachloroethane	230	2.3		
styrene	570	5.7		
1,2,3,4-tetrachlorobenzene	23[g]	0.23[g]		
1,2,3,5-tetrachlorobenzene	22[g]	0.22[g]		
1,2,4,5-tetrachlorobenzene	26[g]	0.26[g]		
1,1,2,2-tetrachloroethane	3,300	33		
tetrachloroethene	330	3.3		
tetrachloromethane	1,100	11		
toluene	730	7.3		
1,2,3-trichlorobenzene	64[h]	0.64[h]		
1,2,4-trichlorobenzene	79[h]	0.79[h]		

compound	$MPC_{aq.}$ (μg/l)	$NC_{aq.}$ (μg/l)	lowest NOEC[a] (μg/l)	lowest L(E)C50[a] (μg/l)
1,3,5-trichlorobenzene	57[h]	0.57[h]		
1,1,1-trichloroethane	2,100	21		
1,1,2-trichloroethane	7,900	79		
trichloroethene	2,400	24		
trichloromethane	5,900	59		
vinylchloride	8,200	82		
2-xylene	400[i]	4.0[i]		
3-xylene	330[i]	3.3[i]		
4-xylene	400[i]	4.0[i]		

[a] lowest NOEC and L(E)C50 presented only for those compounds for which the $MPC_{aq.}$ or $NC_{aq.}$ is calculated using the 'traditional approach'.
[b] indicative $MPC_{aq.}$ and $NC_{aq.}$ based on the modified EPA method.
[c] no $MPC_{aq.}$ and $NC_{aq.}$ can be calculated because no toxicity data are available.
[d] overall $MPC_{aq.}$ and $NC_{aq.}$ for dichlorobenzene: 250 and 2.5 μg/l, respectively.
[e] value calculated for 1,3-dichloropropene.
[f] overall $MPC_{aq.}$ and $NC_{aq.}$ for monochlorotoluene: 310 and 3.1 μg/l, respectively.
[g] overall $MPC_{aq.}$ and $NC_{aq.}$ for tetrachlorobenzene: 24 and 0.24 μg/l, respectively.
[h] overall $MPC_{aq.}$ and $NC_{aq.}$ for trichlorobenzene: 67 and 0.67 μg/l, respectively.
[i] overall $MPC_{aq.}$ and $NC_{aq.}$ for xylene: 380 and 3.8 μg/l, respectively.

2.3 MPCs and NCs for soil and sediment

For the derivation of MPC_{soil}s or MPC_{sed}s the QSAR approach cannot be used because almost no QSARs are available for terrestrial organisms. Therefore extrapolation methods based on experimental toxicity data are used (modified EPA and Aldenberg & Slob method). Toxicity data were gathered for all compounds by literature search.

For the compartment soil only for 11 substances toxicity data were present. Next to this, the data for these compounds were available for a limited number of taxonomic groups. Due to this scarcity of data all MPC_{soil}s had to be calculated using the modified EPA method which means that all MPC_{soil}s should be regarded as indicative values [7].

For the chlorobenzenes the toxicity data were inconsistent in a sense that for the tri- and tetrachlorobenzenes the differences within these groups were larger than those between these two groups. This can be explained by a possible specific toxicity of 1,2,3-trichlorobenzene and 1,2,4,5- and 1,2,3,4-tetrachlorobenzenes towards plants [18, 19]. In experiments performed by Hulzebos et al. with *Lactuca sativa* the differences between the isomers were consistent in exposure via soil and nutrient solution. They attributed these differences partly to the number of unsubstituted free vicinal carbon atoms. In Table 2.2 the MPC_{soil}s and NC_{soil}s are presented.

Table 2.2. Maximum Permissible and Negligible Concentrations for soil and the lowest L(E)C50 and NOEC (in mg/kg dry weight). All values have been converted to a standard soil with 10% organic matter.

compound	MPC_{soil}[a] (mg/kg)	NC_{soil}[a] (mg/kg)	lowest NOEC (mg/kg)	lowest L(E)C50 (mg/kg)
1,4-dichlorobenzene	0.4	0.0041	50	390
1,2-dichloropropane	4.2	0.042	-	4,240
pentachlorobenzene	0.3	0.003	50	280
1,2,3,4-tetrachlorobenzene	0.2[b]	0.002[b]	50	160
1,2,3,5-tetrachlorobenzene	0.007[b]	0.00007[b]	-	7
1,2,4,5-tetrachlorobenzene	0.01[b]	0.0001[b]	-	10
tetrachloroethene	0.16	0.0016	-	155
toluene	1.4	0.0014	14	>140
1,2,3-trichlorobenzene	0.005[c]	0.00005[c]	5	5
1,2,4-trichlorobenzene	0.1[c]	0.001[c]	50	127
1,3,5-trichlorobenzene	0.6[c]	0.006[c]	50	615

[a] all MPC_{soil} and NC_{soil}s are indicative ones because the modified EPA method is used.
[b] overall MPC_{soil} and NC_{soil} for tetrachlorobenzenes: 0.072 and 0.00072 mg/kg, respectively.
[c] overall MPC_{soil} and NC_{soil} for trichlorobenzenes: 0.24 and 0.0024 mg/kg, respectively.

As can be seen from this table high assessment factors were applied to toxicity data available: for all compounds, except for toluene for which more toxicity data were available leading to the use of a factor 100, a factor 1,000 was applied to the lowest L(E)C50 due to scarcity of data.

No data were present for sediment dwelling organisms exposed via contaminated sediment. This means that no MPCs for sediment could be derived. MPCs for sediment can be calculated using MPCs for water by application of the equilibrium partitioning method. These calculations will be presented in Chapter 5.

2.4 MPCs and NCs for air

With respect to the derivation of a MPC_{air} the substances of the project "Volatile compounds" were divided into two categories:

Category 1: thirteen compounds for which limit and/or target values for air have already been set by the Ministry of Housing, Physical Planning and the Environment: acrylonitrile, benzene, 1,2-dichloroethane, dichloromethane, ethylene, ethylene oxide, styrene, tetrachloroethene, tetrachloromethane, toluene, trichloroethene, trichloromethane and vinylchloride. The data set for these compounds was updated only, to see if recent studies necessitate a re-evaluation of these values [20]. It was concluded that this re-evaluation was not needed. Limit and/or target values for air

of these compounds and the respective MPCs for water, sediment and soil will be harmonized in the present report in Chapter 6.

For several compounds of this category only a target value exists. Therefore the MPC_{air}, used a.o. as a basis for these target values, is used for harmonization. In Table 2.3 the MPC_{air}s, limit and target values are presented for these compounds. These values have been taken from a working paper from Guinée and Blom, written in the framework of the project 'Volatile Compounds' [21].

Table 2.3. Maximum Permissible Concentrations, limit and target values for air set by the Ministry of Housing, Physical Planning and the Environment

compound	MPC_{air} ($\mu g/m^3$)	limit value ($\mu g/m^3$)	target value ($\mu g/m^3$)
acrylonitrile	10	1	0.1
benzene	30	10	1
1,2-dichloroethane	100	-	1
dichloromethane	1,700	-	20
ethylene	-	300[a]	2[b]
		30[c]	
ethylene oxide	3	-	0.03
styrene	800	-	8
tetrachloroethene	2,500	2,000[d]	25
tetrachloromethane	60	-	1
toluene	300	-	3[e]
trichloroethene	5,000	50[f]	50
trichloromethane	100	-	1
vinylchloride	100	-	1

[a] 1 hour average, 99.99 percentile [22].

[b] 24 hour average determined by Slooff et al. [23]. This value is presented here as an indicative NC_{air}, being more than a factor 100 lower than the target value of 300 $\mu g/m^3$, because according to Slooff this concentration is almost equal to natural background concentrations.

[c] 24 hour average, 99.7 percentile [22].

[d] also a limit value of 8,300 $\mu g/m^3$, 1 hour average, 98 percentile (peak value) has been set.

[e] value presented is not a target value but a NC_{air} derived by Guinée and Blom based on Van Swieten et al. [24].

[f] also a limit value of 300 $\mu g/m^3$, 1 hour average, 98 percentile (peak value) has been set.

Category 2: thirty-four compounds for which no limit and/or target values for air exist in The Netherlands. For these compounds a MPC_{air} was based on ecotoxicological and toxicological data aiming at the protection of the ecosystem as well as human beings, respectively.

Only if the complete toxicological profile of a compound is known a MPC_{air} for human beings can be derived. It was decided that for each compound a minimum toxicological data set must be available containing data on carcinogenicity (inhalation and/or oral), mutagenicity, teratogenicity and reproduction (inhalation and/or oral) and (sub)chronic toxicity data (inhalation). The exposure route of the study on the most critical effect (principal study) had to be inhalatory. Oral studies were used for completing the toxicological profile of a compound. Effect levels were corrected for continuous exposure. Only for 6 compounds the data stated above were available. This means that only for these substances a MPC_{air} could be derived.

Based on the available data 2-chloro-1,3-butadiene was considered to be genotoxic. Carcinogenicity data were inadequate, however. Because a related compound, 1,3-butadiene is mutagenic in vivo and carcinogenic in mice after inhalation, 2-chloro-1,3-butadiene cannot be excluded being a genotoxic carcinogen, which necessitates a non-threshold approach for deriving a MPC_{air}. Adequate carcinogenicity data needed for calculation were not available, however. Based on MPC_{air}s for known genotoxic carcinogenics it was decided to set the MPC_{air} for 2-chloro-1,3-butadiene at 1.0 $\mu g/m^3$.

Based on the available data the other compounds were considered to be not carcinogenic. This justified the use of a threshold approach to derive the MPC_{air} by applying uncertainty factors on the NOAEL or LOAEL from the principal inhalation study. For all compounds an uncertainty factor of 10 * 10 was applied for inter- and intraspecies variation. The magnitude of the other uncertainty factors applied (LOAEL → NOAEL and (sub)chronic → chronic exposure) depended on aspects like the type of effect (nature, severity and biological significance), duration of the study and progression of the effect in time.

For deriving a MPC_{air} for the ecosystem the modified EPA method as proposed by Slooff was used [7]. As in the modified EPA method for the compartments water and soil uncertainty factors are applied on ecotoxicological data (acute L(E)C50 or chronic NOEC values). The magnitude of the uncertainty factor depends on the amount and kind (i.e. acute or chronic) of information available. As for water and soil the MPC_{air}s for the ecosystem calculated with the modified EPA method should be regarded as indicative ones. This accounts especially for air because there is still no accepted method to derive MPC_{air}s and because ecotoxicological data were very scarce: for most compounds only data for mammals were available. It was concluded that the MPC_{air}s for the ecosystem cannot be used as a basis to set environmental quality objectives.

The effect data on mammals were used also for the derivation of the MPC_{air} for human beings. In case of the ecosystem, however only effect parameters considered relevant with respect to the existence of populations are taken into account. In general these are survival, reproduction and growth. In case of human beings also other parameters are used, e.g. histopathological and biochemical changes. In general this leads to lower effect levels. This is the cause for the fact that for all compounds the MPC_{air} for human beings was lower than the one for the ecosystem [20].

If one or more elements of the minimum toxicological data set were missing or if only ecotoxicological data were available only a preliminary MPC_{air} was derived. If no or no reliable inhalation studies were available oral studies were used for deriving a preliminary MPC_{air} aiming at

the protection of human beings. [20] Uncertainty factors were applied rather stringent for deriving a preliminary MPC_{air} for human beings: 10 * 10 for inter- and intraspecies variation, 10 for (sub)chronic → chronic exposure and 10 for LOAEL → NOAEL [20].

For those compounds for which a preliminary MPC_{air} has been derived first more toxicological data must be present before a MPC_{air} can be derived. These values should not be used to derive limit and target values. For 3- and 4-monochlorotoluene and pentachloroethane no toxicity data were available at all, so no preliminary MPC_{air} could be derived. [20]

In Table 2.4 and 2.5 the MPC_{air} and NC_{air} and preliminary MPC_{air} and NC_{air} values are presented, respectively. Also toxicity data on which these values were based are given. LC50 values from Table 2.5 were used for deriving MPC_{air}s aiming at the protection of ecosystems, only.

Table 2.4. Maximum Permissible and Negligible Concentrations for air and the NOAEL or LOAEL on which the MPC_{air} is based (all values are corrected for continuous exposure)

compound	MPC_{air} ($\mu g/m^3$)	NC_{air} ($\mu g/m^3$)	NOAEL (mg/m^3)	LOAEL (mg/m^3)
2-chloro-1,3-butadiene	1.0[a]	0.01[a]		
3-chloropropene	7.4	0.074	7.38	
1,1-dichloroethene	200	2.0	20	
1,2-dichloropropane	12	0.12		12.4
1,3-dichloropropene	40	0.40	4	
1,1,1-trichloroethane	4,800	48	482	

[a] revised preliminary MPC_{air} and NC_{air}

Table 2.5. Preliminary Maximum Permissible (preliminary MPC_{air}) and Negligible Concentrations (preliminary NC_{air}) for air and the NOAEL on which the preliminary MPC_{air} is based (all values are corrected for continuous exposure)

compound	preliminary MPC_{air} ($\mu g/m^3$)	preliminary NC_{air} ($\mu g/m^3$)	NOAEL (mg/m^3)	LC50 (mg/m^3)
1,2-dichlorobenzene	60	0.60	60.4	
1,4-dichlorobenzene	670	6.7	67	
1,1-dichloroethane	370	3.7	366	
hexachloroethane	27	0.27	27	
1,2-dichloroethene	36	0.36	357	

compound	preliminary MPC_{air} ($\mu g/m^3$)	preliminary NC_{air} ($\mu g/m^3$)	NOAEL (mg/m^3)	LC50 (mg/m^3)
hexachlorobenzene	2.3[b,c]	0.023[b,c]	0.23	
1,3-dichloropropane	6,000[a]	60[a]		6,000
2,3-dichloropropene	380[a]	3.8[a]		378
ethylbenzene	39	0.39	39	
monochlorobenzene	42	0.42	42	
2-monochlorotoluene	780	7.8	775	
pentachlorobenzene	8[b,c]	0.08[b,c]	7.9	
tetrachlorobenzene	1.6[b,c]	0.016[b,c]	1.6	
1,1,2,2-tetrachloroethane	0.20	0.0020	0.20	
trichlorobenzene	4	0.040	4.0	
1,1,2-trichloroethane	18[c]	0.18[c]	18.2	
2-xylene	340	3.4	337	
3-xylene	1,000	10	1,000	
4-xylene	1,000	10	1,000	

[a] only effect data available to calculate a preliminary MPC_{air} aiming at the protection of the ecosystem

[b] only effect data available to calculate a preliminary MPC_{air} aiming at the protection of the human beings

[c] based on oral toxicity data

Different values are sometimes present for preliminary MPC_{air}s, MPC_{air}s or target values for different isomers:

- dichlorobenzenes: a preliminary MPC_{air} of 60 $\mu g/m^3$ for 1,2-dichlorobenzene versus a preliminary MPC_{air} of 670 $\mu g/m^3$ for 1,4-dichlorobenzene. Both values are based on inhalation studies. For 1,2-dichlorobenzene an extra uncertainty factor of 10 for (semi)chronic to chronic exposure was applied compared to 1,4-dichlorobenzene. Rademaker et al. concluded that the preliminary MPC_{air} is probably an overestimation because the effects found were almost the same for both isomers and besides these effects did not increase in time in the study with 1,2-dichlorobenzene [20]. Because both values are still preliminary MPC_{air}s it is decided to use both values for harmonization.
- dichloroethane: a preliminary MPC_{air} of 370 $\mu g/m^3$ for 1,1-dichloroethane versus a MPC_{air} of 100 $\mu g/m^3$ for 1,2-dichloroethane. The latter compound is considered a carcinogen while for the derivation of a preliminary MPC_{air} 1,1,-dichloroethane was not considered a carcinogen based on the available data. Both values will therefore be used for harmonization.
- dichloroethene: a MPC_{air} of 200 $\mu g/m^3$ for 1,1-dichloroethene versus a preliminary MPC_{air} of 36 $\mu g/m^3$ for 1,2-dichloroethene. Both values are based on inhalation studies using a threshold approach. In case of 1,2-dichloroethene a higher uncertainty factor was applied, however. Both values will be used for harmonization.
- dichloropropane: a MPC_{air} of 12 $\mu g/m^3$ for 1,2-dichloropropane versus a preliminary MPC_{air} of 6,000 $\mu g/m^3$ for 1,3-dichloropropane. For 1,3-dichloropropane no data were available,

however to derive a MPC_{air} aiming at the protection of human beings. This value is therefore almost certainly too high. Therefore no value for 1,3-dichloropropane will be used for harmonization.

- dichloropropene: a MPC_{air} of 40 $\mu g/m^3$ for 1,3-dichloropropene versus a preliminary MPC_{air} of 380 $\mu g/m^3$ for 2,3-dichloropropene. For 2,3-dichloropropene no data were available, however to derive a MPC_{air} aiming at the protection of human beings. This value is therefore almost certainly too high. Therefore no value for 2,3-dichloropropene will be used for harmonization.
- trichloroethane: a MPC_{air} of 4,800 $\mu g/m^3$ for 1,1,1-trichloroethane versus a preliminary MPC_{air} of 18 $\mu g/m^3$ for 1,1,2-trichloroethane. Both values are based a threshold approach: 1,1,1-trichloroethane on a inhalation study and 1,1,2-trichloroethane on a oral study. In case of 1,1,2-trichloroethane a higher uncertainty factor was applied, however. Both values will be used for harmonization.
- xylenes: preliminary MPC_{air}s of 340, 1,000 and 1,000 were derived for 2-, 3- and 4-xylene, respectively. These differences are considered acceptable. All values will be used for harmonization.

It should be stated that the (preliminary) MPC_{air}s presented in the present paragraph do not account for peak concentrations. In order to do so, the ratio between peak (short term) exposure to high concentrations and chronic exposure to the compound must be known. In order to determine whether peak concentrations actually occur and to calculate this ratio a substantial amount of monitoring data or actual concentrations and data on emission (diffuse or point sources; height of emission; spread of point sources) are needed. These data are not available for the compounds discussed here [20].

3 HARMONIZATION OF ENVIRONMENTAL QUALITY OBJECTIVES

3.1 Introduction

Harmonization of MPCs and NCs for the different compartments is necessary because air is an important transportation medium for many, also relatively non-volatile, chemicals which may affect the quality of water and soil. Also, releases of chemicals to water and soil can, after volatilization, lead to concentrations in air, which may cause adverse effects either to man or to parts of the ecosystem, e.g. plants. Hence, achieving concentrations lower than the MPC[2] for one compartment does not necessarily mean that a "safe" concentration in another compartment can be maintained. This means that the MPCs for air, water, sediment and soil must be set in such a way that they meet a coherence-criterion. This criterion implies that MPCs for one compartment have to be set at a level where full protection to organisms living in other compartments is ensured.

In order to harmonize MPCs for groundwater, surface water, sediment and soil the equilibrium partitioning method is applied like in the other projects of the project "Setting integrated environmental quality objectives" [3, 5]. Rationale behind this method is that in the long term concentrations in water and sediment or in groundwater and soil are expected to approach equilibrium reasonably close. Hence, sediment-water and soil-groundwater partition coefficients are applied to convert MPCs derived for water into objectives for sediment and soil. This procedure is described in Chapter 5.

The equilibrium partitioning method may not be applicable for harmonization of water, sediment and soil MPCs with the ones for air since air may not be at or even near equilibrium with water and soil due to the rapid refreshment of the atmosphere. To overcome this problem, a procedure is used applying computed steady state concentration ratios rather than equilibrium partitioning. The model SimpleBox is used for these computations. Before the harmonization procedure is described a short description of SimpleBox is given in the next paragraph. A detailed description of SimpleBox is given by Van de Meent [25].

3.2 The model SimpleBox

The spreadsheet model SimpleBox is a kind of model that is commonly referred to as the 'Mackay-type': it is a multimedia fate model in which the environmental compartments are represented by homogeneous boxes [26]. The assumption of homogeneity is of course a severe oversimplification of the real environment. Because MPCs are set for the environment in general, rather than for specific situations, this is considered acceptable, however. Within this main assumption of homogeneity the SimpleBox model is generic in a sense that it can be customized to represent specific environmental situations. For the purpose of harmonization of MPCs SimpleBox has been set to represent the behaviour of micropollutants in an open reference

---

[2] For reasons of readability only MPCs is used in this Chapter instead of MPCs and NCs.

environment, resembling The Netherlands. A schematical representation is shown in figure 2.

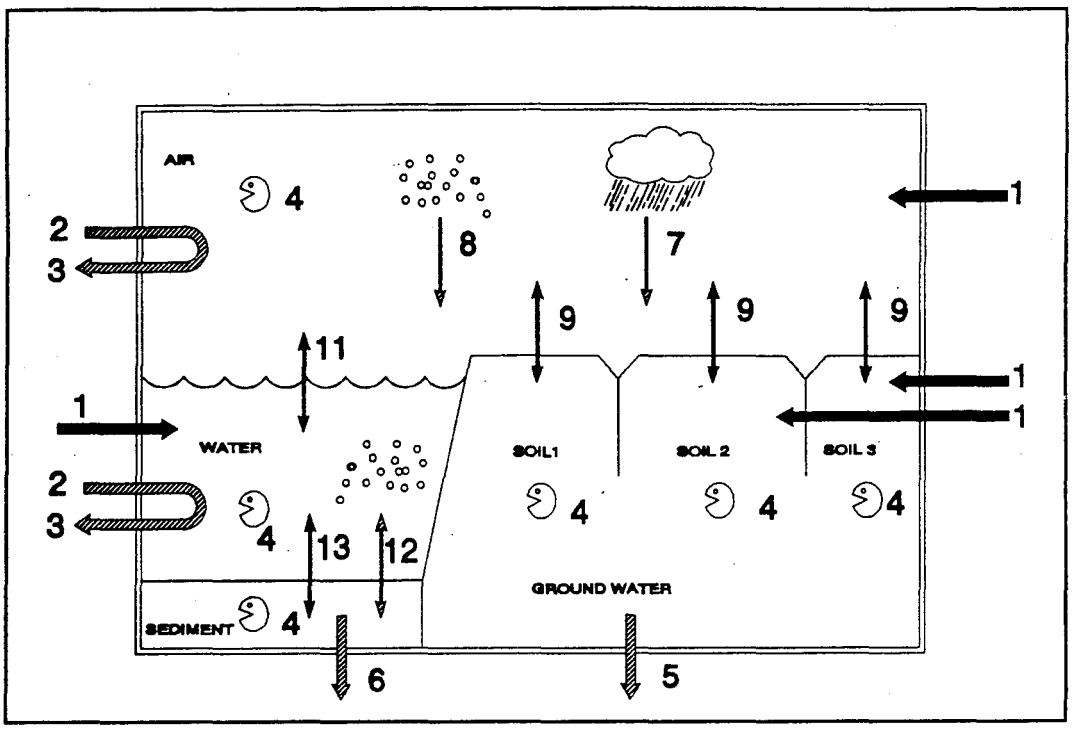

Figure 2. Schematic representation of the SimpleBox model used to compute steady state inter-media concentration ratios. 1=emission, 2=import, 3=export, 4=degradation, 5=leaching, 6=burial, 7=wet deposition with rain, 8=dry deposition with aerosols, 9=air-soil exchange through gas absorption and volatilization, 10=run-off, 11=air-water exchange through gas absorption and volatilization, 12=sedimentation and resuspension, 13=sediment-water exchange through direct sorption and desorption.

The reference environment modelled consists of eight compartments: air, water, suspended particles, sediment, aquatic organisms, and 3 soil compartments (natural, agricultural and industrial soil). Several transport routes of the chemical from one compartment to another are possible. Air and water compartments are continuously being 'renewed' by air and water from 'outside'. Sediment is continuously being 'renewed' as older sediments become buried under fresh deposits by the process of sedimentation. A chemical can enter the system (input) by emission in one of the compartments or by import from 'outside', while losses from the system (output) can occur by degradation, leaching to groundwater or burial in old sediments. Steady state concentrations are calculated, which means that concentrations in all compartments have become constant in time.

3.3 Harmonization procedure

The harmonization procedure used in the present report has been developed by Van de Meent and De Bruijn [27, 28]. In figure 3 the procedure is depicted schematically.

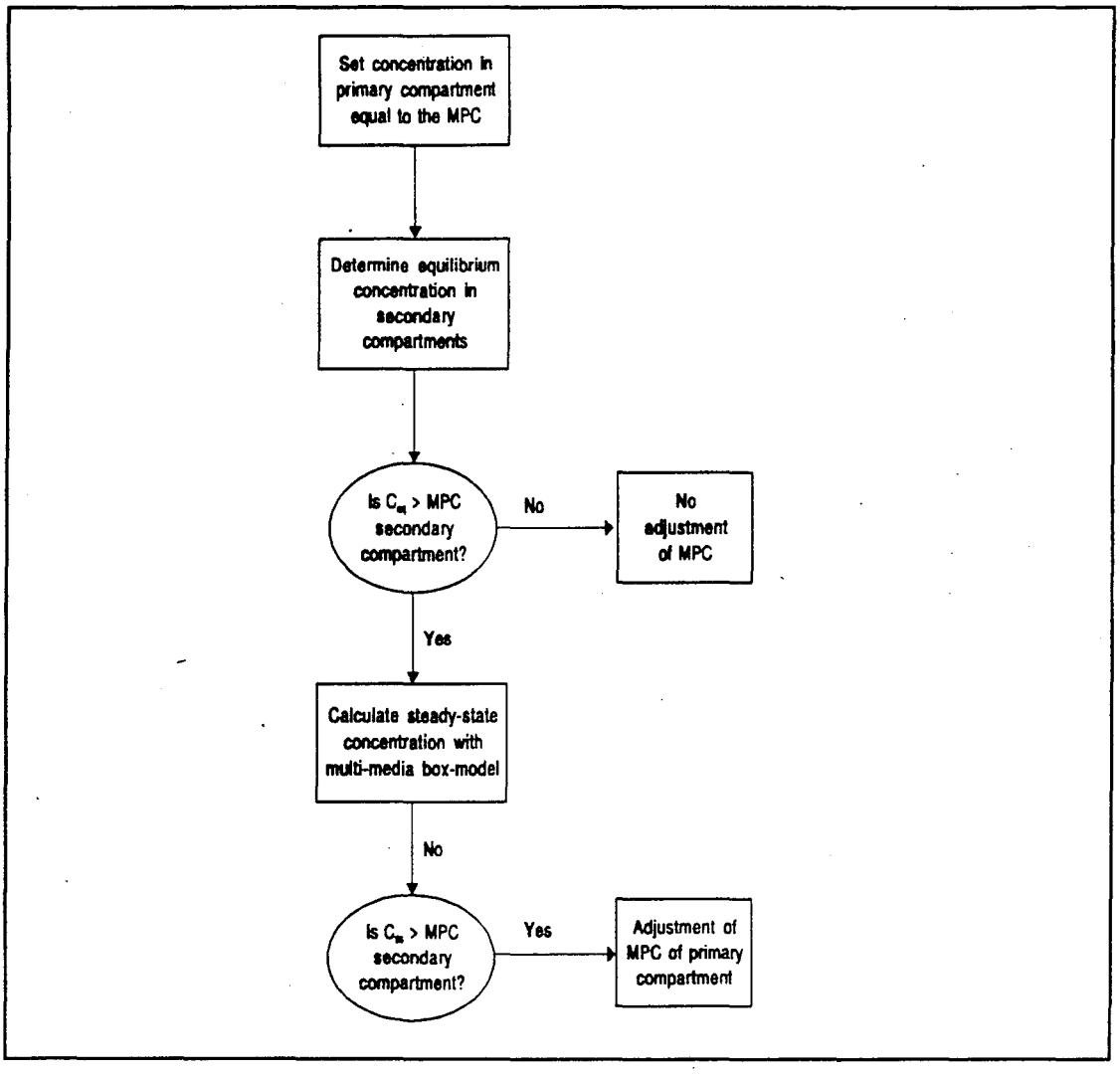

Figure 3. Harmonization procedure for assessing the coherence of MPCs and NCs (in figure only MPC is used instead of MPC or NC; C_{eq}: equilibrium concentration; C_{ss}: steady state concentration)

As can be seen from figure 3 the harmonization procedure is a step-wise approach. The procedure consists of the following steps:

Step 1: Determination of the primary compartment

It is assumed that emissions of the chemical exclusively take place into one of the compartments air, water or soil. Hence, if a chemical may be released into different compartments, several

calculations have to be performed.
One of the essentials of the procedure is that the concentration in the primary compartment is set equal to the MPC in that compartment, so if air is the primary compartment the concentration is set equal to the MPC_{air}.

Step 2: Equilibrium concentrations (C_{eq} in figure 3) in the secondary compartments are calculated

Equilibrium concentrations are considered as maximum achievable concentrations in the secondary compartment. Concentrations higher than the equilibrium concentration are possible if intermedia transport is dominated by mechanisms such as atmospheric deposition or sedimentation. However, this is not expected to be significant for the volatile compounds dealt with in the present report.

The following equilibrium partitioning relationships are used:

$$\frac{C_{air}}{C_{water}} = \frac{H}{R.T}.1000 \qquad (1)$$

$$\frac{C_{soil}}{C_{water}} = Kp_{soil} \qquad (2)$$

$$\frac{C_{air}}{C_{soil}} = \frac{H}{R.T.Kp_{soil}}.1000 \qquad (3)$$

where:

C_{air} :	concentration in air [$mg.m^{-3}$]
C_{water} :	concentration in water [$mg.l^{-1}$]
C_{soil} :	concentration in soil [$mg.kg^{-1}$]
H :	Henry's law constant [$Pa.m^3.mol^{-1}$]
R :	gas constant [8.314 $Pa.m^3.mol^{-1}.K^{-1}$]
T :	temperature [K]
Kp_{soil} :	soil-water partition coefficient [$l.kg^{-1}$]

Calculations are carried out as follows. The concentration in the primary compartment is assumed to be equal to the MPC for that compartment. Using the equations above the equilibrium concentrations in the secondary compartments are calculated.

Step 3: Equilibrium concentrations in the secondary compartments are compared with the MPCs for these compartments

If the equilibrium concentrations are lower than the MPCs, it can be concluded that the MPC for the primary compartment does not lead to exceeding of the MPCs derived for the other compartments. If the equilibrium concentration is higher than the MPC for one or both of the secondary compartments the model SimpleBox is run.

Step 4: Steady state concentrations (C_{ss} in figure 3) in the secondary compartments computed by SimpleBox are compared with MPCs for these compartments

To test if the MPCs for the different compartments are coherent SimpleBox is run as follows. It is assumed that the emissions have been controlled to such a level that the concentration in the

primary compartment has become equal to the MPC. This implies that emissions have remained constant for a sufficiently long period of time that all concentrations in the primary as well as in the secondary compartments have become constant in time. Input by import and emission is treated as follows: concentrations of the chemical in the primary compartment outside the system are assumed to be equal to the MPC in the primary compartment while concentrations in the secondary compartments are set equal to zero. This is only relevant of course if air or water is the primary compartment. This means that if e.g. water is the primary compartment import via water and air is equal to the MPC for water and 0, respectively.

Total emission into the primary compartment then is set by iteration equal to a value, exactly matching the total of all losses from the system minus advective input from the primary compartment outside the system. The result is that the concentration of the chemical in the primary compartment becomes equal to the MPC. Thereafter, the steady state concentrations in the secondary compartments are evaluated. Two different situations are possible:

1. the steady state concentration is lower than the MPC: no adjustment of the MPC of the primary compartment is necessary.
2. the steady state concentration exceeds the MPC: the MPC of the primary compartment should be adjusted to a value that will not lead to problems in the secondary compartments. This will be discussed further in Chapter 6 in which the MPC and NC values for the different compartments are harmonized according to the procedure described in the present paragraph.

4. PHYSICO-CHEMICAL DATA USED

4.1 Introduction

Several physico-chemical properties are needed to run SimpleBox. An overview of these properties for the volatile compounds are presented in Table 4.1. In this chapter the most important ones for the volatile compounds are discussed being the Henry's law constants, degradation in air, soil-water partition coefficients including octanol-water coefficients, degradation in water and soil, vapour pressure and water solubility.

4.2 Henry's law constants

Henry's law constants or Henry coefficients (H_c) and air-water partition coefficients (K_{aw}) describe the equilibrium distribution of a chemical over the gas and water phase:

$$K_{aw} = \frac{H_c}{R*T} = \frac{C_{air}}{C_{water}} \qquad [-] \tag{4}$$

where C_{water} and C_{air} are equilibrium concentrations in water and air (both in $\mu g.m^{-3}$) and R is the gas constant (8.3144 $Pa.m^3.mol^{-1}.K^{-1}$) and T (K) the experimental temperature for which H_c was determined. An overview of the available literature data on H_c values for the volatile compounds is given in Appendix A.

H_cs can be determined experimentally by measuring gas headspace concentration ratios from sets of sealed bottles [29]. An alternative manner is to measure the concentration of the chemical in water as a function of time as it is stripped with a steady stream of gas [30]. This avoids the need for gas phase analysis. If the miscibility of the chemical and water is less than a few mole percent, H_cs can be estimated from experimentally determined water solubilities and vapour pressures [31].

$$H_c = \frac{Vap.Pressure}{Solubility} \qquad [Pa.m^3.mol^{-1}] \tag{5}$$

Ten Hulscher et al. observed a doubling of experimental H_c values (chlorobenzenes, PCBs and PAHs) for every 10 °C temperature increase [32]. Experimental data of Ashworth reveal a similar increase of H_c with temperature for 45 chemicals including most compounds of the project "Volatile Compounds" [33]. In the present report preferably H_c values measured at 10 °C were used. H_cs determined at 20 or 25 °C (or calculated from vapour pressures and water solubility) were lowered with a factor 2 or 3, respectively.
Starting point for collecting H_cs were data presented by Mackay and Shiu [34]. In this extensive review article experimental values published by Ashworth et al. (1988) were not yet included. Ashworth's data were preferred over those of Mackay and Shiu (1981) because the large number of analysis (45 compounds, at 5 temperatures, each determination performed in eight fold) and the fact that both experimental methods described above were employed

Table 4.1 Physico-chemical properties for the volatile compounds

compound	MW (g/mol)	K_{aw} 10 °C	log K_{oc} (l/kg)	log K_{ow}	K_p [a] (l/kg)	k_{deg} (air[b]) (10^{-6}/s)	ready biodeg	VP (kPa)
acrylonitrile	53.06	0.002		0.25	0.089	3.40	y	13.3
benzene	78.11	0.142	1.90	2.19	4.0	1.28	y	12.7
2-chloro-1,3-butadiene	88.50	0.083		2.16[c]	7.2	40.0	n	23.1
3-chloropropene	76.50	0.118		1.45[c]	1.4	10.0	n	38.0
1,2-dichlorobenzene	147.01	0.070	2.64[d]	3.43	22	0.40	n	0.196
1,3-dichlorobenzene	147.01	0.095	2.64[d]	3.53	22	0.72	n	0.307
1,4-dichlorobenzene	147.01	0.091	2.64[d]	3.44	22	0.32	y	0.090
1,1-dichloroethane	98.96	0.158		1.79	3.1	0.10	n	30.2
1,2-dichloroethane	98.96	0.050	1.62	1.48	2.1	0.10[e]	n	8.53
1,1-dichloroethene	96.94	0.663		1.86	3.6	4.0	n	72.4
1,2-dichloroethene	96.94	0.071		1.86	3.6	4.0	n	31.5
dichloromethane	84.93	0.039	1.56	1.25	1.8	0.14	n	46.5
1,2-dichloropropane	112.97	0.053	1.68	1.99	2.4	0.10[e]	n	6.0
1,3-dichloropropane	112.97	0.076		2.00	5.0	0.10[e]	n	6.0
1,3-dichloropropene	110.97	0.029		1.76[c]	2.9	12.6	n	4.5
2,3-dichloropropene	110.97	0.052		2.04[c]	5.5	10[e]	n	7.1
ethylbenzene	106.16	0.140	2.22	3.15	8.3	7.50	n	0.933
ethylene	28.05	3.072		1.13	0.67	8.50	y	4,040
ethylene oxide	44.05	12.66		-0.30	0.025	0.06	n	146
hexachlorobenzene	284.80	0.009	4.04	5.73	550	0.72	n	$1.5*10^{-6}$
hexachloroethane	236.72	0.255	3.61	4.14	200	0.05[f]	n	0.028
monochlorobenzene	112.57	0.105	2.34	2.90	11	0.94	y	1.58
2-monochlorotoluene	126.58	0.206		3.32[c]	105	2.00	n	0.36
3-monochlorotoluene	126.58	0.170		3.28	95	1.17	n	0.36
4-monochlorotoluene	126.58	0.208		3.33	110	2.46	n	0.31
pentachlorobenzene	250.32	0.013		5.18	400[e]	0.72	n	0.0022
pentachloroethane	202.28	0.036		3.63	210	0.05[f]	n	0.453
styrene	104.15	0.177		2.95	45	10[d]	n	0.60
1,2,3,4-tetrachlorobenzene	215.88	0.013	3.78[d]	4.64	300	0.30[e]	n	0.005
1,2,3,5-tetrachlorobenzene	215.88	0.021	3.78[d]	4.66	300	0.30[e]	n	0.010
1,2,4,5-tetrachlorobenzene	215.88	0.017	3.78[d]	4.60	300	0.30[e]	n	0.0007
1,1,2,2-tetrachloroethane	167.85	0.014	1.92	2.39	4.2	0.10	n	0.793
tetrachloroethene	165.82	0.364	2.38	3.40	12	0.17	n	1.87
tetrachloromethane	153.82	0.637		2.83	34	0.05[f]	n	11.9
toluene	92.14	0.164	2.06	2.79	5.7	6.20	y	2.93
1,2,3-trichlorobenzene	181.43	0.056	3.31[d]	4.14	100	0.50[e]	n	0.028
1,2,4-trichlorobenzene	181.43	0.056	3.31[d]	4.05	100	0.50[e]	n	0.061
1,3,5-trichlorobenzene	181.43	0.056	3.31[d]	4.19	100	0.50[e]	n	0.028
1,1,1-trichloroethane	133.41	0.415	1.82	2.49	3.3	0.01	n	13.3
1,1,2-trichloroethane	133.39	0.017	1.99	1.89	4.9	0.33	n	3.0
trichloroethene	131.39	0.149	2.04	2.42	5.5	2.36	n	7.71
trichloromethane	119.38	0.074	1.81	1.97	3.2	0.10	n	21.3
vinylchloride	62.50	0.646		1.52[c]	1.7	6.60	n	33.7
2-xylene	106.16	0.123		3.12	66	14.7	n	0.667
3-xylene	106.16	0.177	2.50	3.20	16	24.5	n	0.80
4-xylene	106.16	0.181	2.72	3.15	26	15.2	n	0.867

[a] calculated from K_{oc} or K_{ow} values assuming an organic carbon content of 5% for soil and sediment. K_p for suspended matter were calculated assuming an organic carbon content of 10%, and are therefore two times higher than the values for soil and sediment.

[b] assuming concentration OH radicals of 10^6 molecules/cm^3

[c] calculated value (C log P)

[d] average value for isomers

[e] estimate

[f] non-degradable; value presented is estimated minimum reactivity [25]

simultaneously as a check. Furthermore, these H_cs were measured for a temperature range (10 °C to 30 °C) whereas Mackay and Shiu's values were usually measured at 25 °C only (the average Dutch water temperature is 12 °C) [35]. In fact Ashworth's data agree well with Mackay and Shiu's data when the temperature correction proposed above is applied, the only exception being values for vinylchloride, 1,1- and 1,2-dichloroethene that are up to 80 times lower than data found by Mackay and Shiu (1981). In view of the considerable discrepancies in the vapour pressures, solubilities and experimental H_cs Mackay and Shiu (1981) did not recommend a value for these compounds. Here the values of Ashworth (1988) are used.

4.3 Degradation in air

Organic compounds can be removed from the troposphere by photolysis and reaction with OH and NO_3 radicals and O_3 (and for certain basic amines and hydrazines and other nitrogen containing heterocycles, by reaction with gas-phase HNO_3) [36]. According to Atkinson (1985) it is widely recognized that the OH radical is the dominant reactive species in the degradation of organic compounds in both the natural and polluted troposphere. The other reactions can dominate over OH radical reaction for certain classes of organics, e.g. photolysis of the alkyl nitrites and nitrosamines, reaction with O_3 for the higher alkenes, reaction with the NO_3 radical for the higher alkenes, dimethyl sulfide and the lower thiols, furan and pyrrole, and the hydroxy-substituted aromatics [36]. Almost none of the compounds considered here fall in one of these classes and therefore degradation reactions other than the reaction with hydroxyl radicals were neglected. The available experimental data concerning kinetics of the reactions of OH radicals with organic compounds under atmospheric conditions have been compiled and evaluated extensively by Atkinson [36]. The loss rates (k_{deg}, fraction of the compound degraded per day) shown in Table 4.1 were calculated from the degradation rate constants recommended by Atkinson (1985) by multiplication with an estimated average OH radical concentration. Because for the propenes degradation through reaction with O_3 and NO_3 radicals might dominate reaction with OH radicals the k_{deg} values for these compounds underestimate actual degradation rates.

In the troposphere, the important direct sources of OH radicals are from the reaction of O atoms formed from the photodissociation of O_3 with water vapour and from the photodissociation of HONO [36]. The other important direct source of OH radicals arises from the reaction of HO_2 radicals with NO yielding a OH radical and a NO_2 molecule. Because OH radicals are formed in the atmosphere under the influence of light, OH radical concentrations exhibit seasonal, alititudinal, diurnal, geographical and altitude variations. Because OH radical half-life is short, high daytime concentrations decrease sharply at night to almost zero. Therefore, degradation reactions with OH radicals are almost completely restricted to the day time. Clearly, average OH radical concentrations are difficult to give; values proposed in the literature vary considerably. Typical annually averaged concentrations during a 24 hour period range from $5x10^5$ to $2x10^6$ molecules/cm^3 for the northern hemisphere [37, 38]. The k_{deg} values shown in Table 1 were calculated assuming an average OH radical concentration of 10^6 molecules/cm^3 recommended by De Leeuw [38].

4.4 Soil-water partitioning

Soil-water partition coefficients (K_ps) describe the equilibrium distribution of a chemical over a solid phase (soil, sediment or suspended matter) and water.

$$K_p = \frac{C_{water}}{C_{soil}} \qquad [l.kg^{-1}] \tag{6}$$

Where C_{water} and C_{soil} are equilibrium concentrations in water and soil (in mg/dm^3 and mg/kg, respectively).
K_p values were preferably based on experimental values. A large number (approximately 5000 values) of experimental organic carbon normalized soil-water partition coefficients (K_{oc} values) were compiled by Gerstl [39]. These data were recently evaluated and complemented by Bockting et al. [40]. The values shown in Table 4.1 are averages of the logarithmic values presented by Bockting et al. Because the variations of K_{oc} (and K_{ow}) values for individual di-, tri- and tetrachlorobenzenes isomers appeared to be insignificant K_{oc} values were averaged. The value for pentachlorobenzene was estimated by interpolation using the values for the other chlorobenzenes.

K_ps were calculated from the K_{oc} according to:

$$K_p = K_{oc} * f_{oc} \qquad [l.kg^{-1}] \tag{7}$$

where f_{oc} is the fraction organic carbon of the soil or sediment. According to Slooff f_{oc} is fixed at 5% [7].

When no experimental K_{oc} values were found K_{oc}s (and K_ps) were derived from K_{ow} values according to an empirical regression equation [7, 8, 41]):

$$K_{oc} = K_{ow} \qquad [l.kg^{-1}] \tag{8}$$

The collection of octanol-water partition coefficients (K_{ow} values) is described in Van de Plassche et al. [12]. Most K_{ow}s were taken from Van Leeuwen et al. [16]. They recommended the use of experimental values obtained by the slow-stirring method. If not available, so called 'star values' selected from the MEDCHEM database were recommended [42]. The MEDCHEM database is considered the most extensive and reliable source for K_{ow}s available. The value that is considered most reliable in the data-base is indicated with a star.
Besides a large number of K_{ow} values from the literature the MEDCHEM database contains a routine for estimation of K_{ow}s based on structural properties of the compound (ClogP method). A description of the database and the ClogP method is given by Leo et al. [43]. K_{ow}s calculated with the ClogP method are less reliable than experimental values, but in an evaluation of the system Verhaar and Hermens concluded that this estimation method normally leads to reasonable values [44].

Acrylonitrile, 2-chloro-1,3-butadiene, dichloroethene, vinylchloride, ethylene, ethylene oxide, ethylbenzene, 3-chloropropene, dichloropropene, 2-monochlorotoluene and styrene were not considered by Van Leeuwen et al. (1992). For these compounds the star values from the MEDCHEM database were selected by Van de Plassche et al. [12].

4.5 Degradation in water and soil

The potential for biodegradation of a compound is often determined in biodegradation tests where the compound is either assigned readily biodegradable or not readily biodegradable [45]. SimpleBox attributes a degradation rate proportional to the concentration of bacteria in water (degradation in soil and sediment is assumed to occur only for the porewater dissolved fraction of the chemical). Pseudo first order rate constants are obtained by extrapolation from the results of standard screening tests for ready biodegradability in water according to a procedure developed by Struijs and Van den Berg [45].

The indicators for biodegradation shown in Table 4.1 were determined using easily obtainable information like reviews etc. If no information on a chemicals degradation potential was available it was assumed that the chemical is not readily biodegradable. It has to be stated that no extensive literature search was carried on this aspect because, as will be shown in Chapter 6, degradation in soil and water is only of secondary importance for the harmonisation of MPCs for these volatile compounds.

4.6 Vapour pressure and water solubility

The vapour pressure of a chemical is used in the model's formulas for estimating the fraction of the chemical that is associated with aerosol particles. Furthermore, when no K_{aw} is available the model estimates a value from the vapour pressure and the solubility (according to equation 5). Because for all chemicals a K_{aw} was entered the vapour pressure was used only for calculating atmospheric deposition. Vapour pressures were selected from various handbooks and review articles on specific compounds.

As stated above the model uses the water solubility of a chemical together with the vapour pressure for estimating K_{aw} values when no value was entered for this parameter. This is the only manner in which the model uses the solubility of a chemical. Because for all chemicals a K_{aw} value was available there was no need to enter solubility data.

5. HARMONIZATION OF MAXIMUM PERMISSIBLE AND NEGLIGIBLE CONCENTRATIONS FOR WATER WITH SEDIMENT AND SOIL

5.1 Procedure

The derivation of MPC and NC values has been described in paragraphs 3.2 and 3.3 for the aquatic and terrestrial compartments, respectively. As was mentioned in paragraph 3.3 only some toxicity data were present for soil organisms while no data at all were available for sediment dwelling organisms. In these cases the calculation of the MPC and NC for soil and sediment is therefore carried out by means of the equilibrium partitioning method using the formula [5]:

$$MPC_{sed./soil} = MPC_{aq.} * K_p$$

where:

K_p = partition coefficient between sediment or soil and water (l/kg)

$MPC_{aq.}$ = maximum permissible concentration derived from toxicity data for aquatic organisms (mg/l)

$MPC_{sed./soil}$ = maximum permissible concentration in soil or sediment (mg/kg dry sediment or soil)

Similar equations can be set up for the NC in sediment and soil. Soil and sediment partition coefficients have been described in Chapter 4. If no toxicity data are available for soil and sediment dwelling organisms and the equilibrium partitioning method is used to calculate MPC and NC values for sediment and soil, harmonization of these values with the values for surface or groundwater is impossible. In this case the equilibrium partitioning method can be used only as an indirect method to derive MPC or NC values based on ecotoxicological data, and not as a method for harmonization. Results of these calculations are presented in paragraph 5.2.

Only for the compounds from Table 3.2, for which MPC_{soil}s and NC_{soil}s have been calculated, harmonized values can be derived. Therefore MPC_{soil}s and NC_{soil}s based on toxicity data and MPC_{soil}s and NC_{soil}s calculated by means of the equilibrium partitioning method are compared. This will be presented in paragraph 5.3.

5.2 Calculation of Maximum Permissible and Negligible Concentrations for sediment and soil using the equilibrium partitioning method

In Table 5.1 MPCs and NCs for soil and sediment are presented using $MPC_{aq.}$s and $NC_{aq.}$s from Table 3.1 and partition coefficients from Table 4.1.

Table 5.1. Maximum Permissible ($MPC_{sed./soil}$) and Negligible Concentrations ($NC_{sed./soil}$) for sediment and soil based on ecotoxicological data for aquatic organisms and equilibrium partitioning (in mg/kg)

compound	$MPC_{aq.}$ (μg/l)	$NC_{aq.}$ (μg/l)	K_p (l/kg)	$MPC_{sed./soil}$ (mg/kg)	$NC_{sed./soil}$ (mg/kg)
acrylonitrile	7.6	0.076	0.089	$6.8*10^{-4}$	$6.8*10^{-6}$
benzene	2,400	24	4.0	9.5	0.095
3-chloropropene	3.4	0.034	1.4	0.0048	$4.8*10^{-5}$
1,2-dichlorobenzene	270	2.7	22	5.9[a]	0.059[a]
1,3-dichlorobenzene	210	2.1	22	4.6[a]	0.046[a]
1,4-dichlorobenzene	260	2.6	22	5.7[a]	0.057[a]
1,1-dichloroethane	7,300	73	3.1	23	0.23
1,2-dichloroethane	14,000	140	2.1	29	0.29
1,1-dichloroethene	3,400	34	3.6	12	0.12
1,2-dichloroethene	6,100	61	3.6	22	0.22
dichloromethane	20,000	200	1.8	36	0.36
1,2-dichloropropane	5,300	53	2.4	13	0.13
1,3-dichloropropane	5,200	52	5.0	26	0.26
1,3-dichloropropene	8.0	0.08	2.9	0.023	$2.3*10^{-4}$
2,3-dichloropropene	8.0	0.08	5.5	0.044	$4.4*10^{-4}$
ethylbenzene	370	3.7	8.3	3.1	0.031
ethylene	8,500	85	0.67	5.8	0.058
ethylene oxide	84	0.84	0.025	0.0021	$2.1*10^{-5}$
hexachlorobenzene	2.4	0.024	550	1.3	0.013
hexachloroethane	83	0.83	200	17	0.17
monochlorobenzene	690	6.9	11	7.6	0.076
2-monochlorotoluene	300	3.0	110	31[b]	0.31[b]
3-monochlorotoluene	330	3.3	95	31[b]	0.31[b]
4-monochlorotoluene	300	3.0	110	32[b]	0.32[b]
pentachlorobenzene	7.5	0.075	400	3.0	0.030
pentachloroethane	230	2.3	210	49	0.49
styrene	570	5.7	45	25	0.25
1,2,3,4-tetrachlorobenzene	23	0.23	300	6.9[c]	0.069[c]
1,2,3,5-tetrachlorobenzene	22	0.22	300	6.6[c]	0.066[c]
1,2,4,5-tetrachlorobenzene	26	0.26	300	7.8[c]	0.078[c]
1,1,2,2-tetrachloroethane	3,300	33	4.2	14	0.14
tetrachloroethene	330	3.3	12	4.0	0.040
tetrachloromethane	1,100	11	34	37	0.37
toluene	730	7.3	5.7	4.2	0.042
1,2,3-trichlorobenzene	64	0.64	100	6.4[d]	0.064[d]

compound	$MPC_{aq.}$ (μg/l)	$NC_{aq.}$ (μg/l)	K_p (l/kg)	$MPC_{sed./soil}$ (mg/kg)	$NC_{sed./soil}$ (mg/kg)
1,2,4-trichlorobenzene	79	0.79	100	7.9[d]	0.079[d]
1,3,5-trichlorobenzene	57	0.57	100	5.7[d]	0.057[d]
1,1,1-trichloroethane	2,100	21	3.3	6.9	0.069
1,1,2-trichloroethane	7,900	79	4.9	39	0.39
trichloroethene	2,400	24	5.5	13	0.13
trichloromethane	5,900	59	3.2	19	0.19
vinylchloride	8,200	82	1.7	14	0.14
2-xylene	400	4.0	66	26[e]	0.26[e]
3-xylene	330	3.3	16	5.2[e]	0.052[e]
4-xylene	400	4.0	26	11[e]	0.11[e]

[a] overall $MPC_{sed./soil}$ and $NC_{sed./soil}$ for dichlorobenzene: 5.5 and 0.055 mg/kg, respectively

[b] overall $MPC_{sed./soil}$ and $NC_{sed./soil}$ for monochlorotoluene: 33 and 0.33 mg/kg, respectively.

[c] overall $MPC_{sed./soil}$ and $NC_{sed./soil}$ for tetrachlorobenzene: 7.2 and 0.072 mg/kg, respectively.

[d] overall $MPC_{sed./soil}$ and $NC_{sed./soil}$ for trichlorobenzene: 6.7 and 0.067 mg/kg, respectively.

[e] overall $MPC_{sed./soil}$ and $NC_{sed./soil}$ for xylene: 14 and 0.14 mg/kg, respectively.

Much research has been carried out on the validity of the assumptions underlying the equilibrium partitioning method for establishing sediment quality criteria. In general it can be concluded that the equilibrium partitioning method works well for nonionic organic chemicals. The assumption that soil and sediment organisms are exposed only via interstitial or pore water is probably not valid for highly hydrophobic chemicals for which uptake by food or sediment cannot be excluded. Therefore the $MPC_{sed./soil}$ and $NC_{sed./soil}$ for e.g. penta- and hexachlorobenzene presented in Table 5.1 may be too high.

5.3 Harmonization of $MPC_{aq.}$ and $NC_{aq.}$ with MPC_{soil} and NC_{soil} for those compounds for which toxicity data for soil organisms were available

In Table 5.2 MPC_{soil} and NC_{soil} based on equilibrium partitioning and toxicity data are presented (based on equilibrium partitioning: from Table 5.1; based on ecotoxicological data: from Table 3.2).

Table 5.2. Maximum Permissible (MPC_{soil}) and Negligible Concentrations (NC_{soil}) based on ecotoxicological data and equilibrium partitioning (in mg/kg).

compound	equilibrium partitioning		ecotoxicological data	
	MPC_{soil} (mg/kg)	NC_{soil} (mg/kg)	MPC_{soil} (mg/kg)	NC_{soil} (mg/kg)
1,4-dichlorobenzene	5.7	0.057	0.4	0.004
1,2-dichloropropane	13	0.13	4.2	0.042
pentachlorobenzene	3.0	0.030	0.3	0.003
1,2,3,4-tetrachlorobenzene	6.9	0.069	0.2	0.002
1,2,3,5-tetrachlorobenzene	6.6	0.066	0.007	0.00007
1,2,4,5-tetrachlorobenzene	7.8	0.078	0.01	0.0001
tetrachlorobenzene[a]	7.1	0.071	0.072	0.00072
tetrachloroethene	4.0	0.040	0.16	0.0016
toluene	4.2	0.042	1.4	0.014
1,2,3-trichlorobenzene	6.4	0.064	0.005	0.00005
1,2,4-trichlorobenzene	7.9	0.079	0.1	0.001
1,3,5-trichlorobenzene	5.7	0.057	0.6	0.006
trichlorobenzene[a]	6.7	0.067	0.24	0.0024

[a] overall MPC_{soil} and NC_{soil}

As can be seen from this Table the values based on ecotoxicological data are always lower than the ones based on the equilibrium partitioning method. Especially for di-, tri- and tetrachlorobenzene the differences are considerable. Differences are a.o. caused by the different methods used for calculation of the $MPC_{aq.}$ and MPC_{soil}. In case of the former value the method of Aldenberg & Slob is used (see paragraph 3.2) leading to $MPC_{aq.}$s being somewhat lower than the lowest calculated NOEC [12]. MPC_{soil} values were calculated using the modified EPA method: for all compounds high assessment factors of 100-1,000 had to be applied to toxicity data (see paragraph 3.3). Despite this, as in the first project "MILBOWA" (see Chapter 1) and according to Slooff, the MPC_{soil} and NC_{soil} based on ecotoxicological data are preferred over the ones based on the equilibrium partitioning method [3, 7].

Comparing the values presented in Tables 5.1 and 5.2 for the individual chlorobenzenes the derivation of the MPC_{soil}s and NC_{soil}s remains problematic for these compounds. First of all, it can be noticed that using the equilibrium partitioning method MPC_{soil}s and NC_{soil}s decrease with increasing degree of chlorination while this is not the case for the values based on toxicity data: a 'turning point' appears after the tetrachlorobenzenes. This can be explained by a reduction in bioavailability in soil tests for the more lipophilic chlorobenzenes. Secondly, there is a considerable variation between the MPC_{soil}s and NC_{soil}s for the three isomers of tri- and tetrachlorobenzene based on ecotoxicological data. As already stated in paragraph 2.3 this is caused by specific toxicity of some isomers towards higher plants. For all isomers an

assessment factor of 1,000 was used to calculate the MPC_{soil} (see Table 2.2). It can be stated that it is unrealistic to use such high assessment factors based on these toxicity data because lower values will not become available due to the above mentioned specific mode of action towards plants. Besides, *L. sativa* was used as test plant. This species is regarded as a sensitive one: in tests with lettuce, tomato and oats with 10 compounds Adema and Henzen found that EC50 values for lettuce and tomato were - on average - 3 times lower than for oats [46]. It is therefore proposed to use the overall MPC_{soil}s and NC_{soil}s, calculated as the geometric mean value of the individual values for the three isomers, for the tri- and tetrachlorobenzenes. Finally it is proposed to use the MPC_{soil} and NC_{soil} based on ecotoxicological data for 1,4-dichlorobenzene also for the other isomers.

Summarizing, the following MPC_{soil}s are proposed: 7.6; 0.4; 0.24; 0.072; 0.3 and 1.3 mg/kg for mono-, di-, tri-, tetra-, penta and hexachlorobenzene, respectively. NC_{soil}s are a factor 100 lower.

6. HARMONIZATION OF MAXIMUM PERMISSIBLE AND NEGLIGIBLE CONCENTRATIONS FOR WATER, SEDIMENT, AND SOIL WITH AIR

6.1 Introduction

In this chapter the MPC and NC values derived for the compartments water, sediment, soil and air are harmonized using the procedure described in paragraph 2.3. Physico-chemical properties used as input parameters for the model SimpleBox have been presented in Chapter 4. In Table 6.1 an overview of the 'not-harmonized' MPC and NC values is presented.

From this Table it can be concluded that harmonization is not possible for many compounds because no MPC and NC have been derived for all compartments. For 2-chloro-1,3-butadiene only MPC and NC values for air are available. For 1,2-dichloroethene, 1,3-dichloropropane, 2,3-dichloropropene, ethylbenzene, hexachloroethane, monochlorotoluene, pentachloroethane, 1,1,2-trichloroethane, 3,- and 4-xylene and all chlorobenzenes no MPC_{air}s and NC_{air}s could be derived. For the other compounds harmonization of all MPCs and NCs is carried out according to the procedure described in Chapter 2.

First step in the harmonization procedure is the determination of the primary compartment. Therefore a broad search was carried out, using Integrated Criteria Documents and data from the Dutch Emission Registration, about emissions of the volatile compounds discussed in the present report. As was expected these compounds are emitted to a large extent to air. Many are also emitted to water, however. Therefore the harmonization procedure was followed for two possible situations, i.e. emission to air and emission to water. It is recognized that the situation emission to water is not a realistic assumption because only a small percentage of the total emissions are to water for most volatile compounds. However, it should be realized that the main issue in this Chapter is whether the MPCs and NCs for the different compartments conflict with each other. So, if the compound is indeed emitted to water the question should be answered that if the concentration in water is equal to the $MPC_{aq.}$ or $NC_{aq.}$, are the MPCs or NCs in the other compartments exceeded?

For the situations emission to air and emission to water first maximum concentrations in the secondary compartments are calculated using equilibrium partitioning. This is presented in the following paragraph.

Table 6.1. Overview of Maximum Permissible (MPC) and Negligible Concentrations (NC) for water ($MPC_{aq.}$ and $NC_{aq.}$), sediment ($MPC_{sed.}$ and $NC_{sed.}$), soil (MPC_{soil} and NC_{soil}), and air (MPC_{air} and NC_{air}) and existing limit and target values for air.

compound	water		sediment		soil		air			
	$MPC_{aq.}$ ($\mu g/l$)	$NC_{aq.}$ ($\mu g/l$)	$MPC_{sed.}$ (mg/kg)	$NC_{sed.}$ (mg/kg)	MPC_{soil} (mg/kg)	NC_{soil} (mg/kg)	MPC_{air} ($\mu g/m^3$)	NC_{air} ($\mu g/m^3$)	limit value ($\mu g/m^3$)	target value ($\mu g/m^3$)
acrylonitrile	7.6	0.076	$6.8*10^{-4}$	$6.8*10^{-6}$	$6.8*10^{-4}$	$6.8*10^{-6}$	10	-	1	0.1
benzene	2,400	24	9.5	0.095	9.5	0.095	30	-	10	1
2-chloro-1,3-butadiene	-	-	-	-	-	-	1.0	0.01	-	-
3-chloropropene	3.4	0.034	0.0048	$4.8*10^{-5}$	0.0048	$4.8*10^{-5}$	7.4	0.074	-	-
1,2-dichlorobenzene	270	2.7	5.9	0.059	0.4	0.004	60	0.60	-	-
1,3-dichlorobenzene	210	2.1	4.6	0.046	0.4	0.004	-	-	-	-
1,4-dichlorobenzene	260	2.6	5.7	0.057	0.4	0.004	670	6.7	-	-
1,1-dichloroethane	7,300	73	23	0.23	23	0.23	370	3.7	-	-
1,2-dichloroethane	14,000	140	29	0.29	29	0.29	100	-	-	1
1,1-dichloroethene	3,400	34	12	0.12	12	0.12	200	2	-	-
1,2-dichloroethene	6,100	61	22	0.22	22	0.22	36	0.36	-	-
dichloromethane	20,000	200	36	0.36	36	0.36	1,700	-	-	20
1,2-dichloropropane	5,300	53	13	0.13	4.2	0.042	12	0.12	-	-
1,3-dichloropropane	5,200	52	26	0.26	26	0.26	6,000	60	-	-
1,3-dichloropropene	8.0	0.08	0.023	$2.3*10^{-4}$	0.023	$2.3*10^{-4}$	40	0.40	-	-
2,3-dichloropropene	8.0	0.08	0.044	$4.4*10^{-4}$	0.044	$4.4*10^{-4}$	380	3.8	-	-
ethylbenzene	370	3.7	3.1	0.031	3.1	0.031	39	0.39	-	-
ethylene	8,500	85	5.8	0.058	5.8	0.058	-	2	300	-
ethylene oxide	84	0.84	0.0021	$2.1*10^{-5}$	0.0021	$2.1*10^{-5}$	3	-	-	0.03
hexachlorobenzene	2.4	0.024	1.3	0.013	1.3	0.013	2.3	0.023	-	-
hexachloroethane	83	0.83	17	0.17	17	0.17	27	0.27	-	-
monochlorobenzene	690	6.9	7.6	0.076	7.6	0.076	42	0.42	-	-
2-monochlorotoluene	300	3.0	31	0.31	31	0.31	780	7.8	-	-
3-monochlorotoluene	330	3.3	31	0.31	31	0.31	-	-	-	-
4-monochlorotoluene	300	3.0	32	0.32	32	0.32	-	-	-	-

compound	water		sediment		soil		air			
	$MPC_{aq.}$ ($\mu g/l$)	$NC_{aq.}$ ($\mu g/l$)	$MPC_{sed.}$ (mg/kg)	$NC_{sed.}$ (mg/kg)	MPC_{soil} (mg/kg)	NC_{soil} (mg/kg)	MPC_{air} ($\mu g/m^3$)	NC_{air} ($\mu g/m^3$)	limit value ($\mu g/m^3$)	target value ($\mu g/m^3$)
pentachlorobenzene	7.5	0.075	3.0	0.030	0.3	0.003	8.0	0.080	-	-
pentachloroethane	230	2.3	49	0.49	49	0.49	-	-	-	-
styrene	570	5.7	25	0.25	25	0.25	800	-	-	8
1,2,3,4-tetrachlorobenzene	23	0.23	6.9	0.069	0.072	$7.2*10^{-4}$	-	-	-	-
1,2,3,5-tetrachlorobenzene	22	0.22	6.6	0.066	0.072	$7.2*10^{-4}$	-	-	-	-
1,2,4,5-tetrachlorobenzene	26	0.26	7.8	0.078	0.072	$7.2*10^{-4}$	1.6	0.016	-	-
1,1,2,2-tetrachloroethane	3,300	33	14	0.14	14	0.14	0.2	0.002	-	-
tetrachloroethene	330	3.3	4.0	0.040	0.16	0.0016	2,500	-	2,000	25
tetrachloromethane	1,100	11	37	0.37	37	0.37	60	-	-	1
toluene	730	7.3	4.2	0.042	1.4	0.014	300	-	-	3
1,2,3-trichlorobenzene	64	0.64	6.4	0.064	0.24	0.0024	4.0	0.040	-	-
1,2,4-trichlorobenzene	79	0.79	7.9	0.079	0.24	0.0024	4.0	0.040	-	-
1,3,5-trichlorobenzene	57	0.57	5.7	0.057	0.24	0.0024	4.0	0.040	-	-
1,1,1-trichloroethane	2,100	21	6.9	0.069	6.9	0.069	4,800	48	-	-
1,1,2-trichloroethane	7,900	79	39	0.39	39	0.39	18	0.18	-	-
trichloroethene	2,400	24	13	0.13	13	0.13	5,000	-	50	50
trichloromethane	5,900	59	19	0.19	19	0.19	100	-	-	1
vinylchloride	8,200	82	14	0.14	14	0.14	100	-	-	1
2-xylene	400	4.0	26	0.26	26	0.26	340	3.4	-	-
3-xylene	330	3.3	5.2	0.052	5.2	0.052	1,000	10	-	-
4-xylene	400	4.0	11	0.11	11	0.11	1,000	10	-	-

water: $MPC_{aq.}$s and $NC_{aq.}$s for acrylonitrile, 3-chloropropene, 1,3- and 2,3-dichloropropene and ethylene oxide are indicative values.

sediment: all $MPC_{sed.}$ and $NC_{sed.}$ values are based on the equilibrium partitioning method.

soil: MPC_{soil}s and NC_{soil}s for 1,2-dichloropropane, tetrachloroethene, toluene, and di-, tri- and tetra- and pentachlorobenzene(s) are indicative values based on ecotoxicological data. The MPC_{soil}s and NC_{soil}s for the other compounds are based on the equilibrium partitioning method.

air: MPC_{air}s and NC_{air}s for all chlorobenzenes, 1,2-dichloroethene, 1,3-dichloropropane, 2,3-dichloropropene, 1,1-dichloroethane, ethylene, ethylbenzene, hexachloroethane, 2-monochlorotoluene, 1,1,2,2-tetrachloroethane, 1,1,2-trichloroethane and xylenes are preliminary values which should not be used to set limit and target values. The MPC_{air} and NC_{air} for 2-chloro-1,3-butadiene are revised preliminary values.

6.2 Harmonization of MPC and NC values: equilibrium concentrations

The following calculations are carried out for the two situations:

- emission to air: it is assumed that the concentration in air is equal to the MPC_{air}. Using equilibrium relationships maximum concentrations (C_{eq}) in soil and water are calculated (for equations see paragraph 3.3). These maximum concentrations in soil and water are compared with the MPC_{soil} and $MPC_{aq.}$.
- emission to water: it is assumed that the concentration in water is equal to the $MPC_{aq.}$. Using equilibrium relationships maximum concentrations (C_{eq}) in soil and air are calculated. These maximum concentrations in soil and air are compared with the MPC_{soil} and MPC_{air}.

Results of the calculations are presented in Table 6.2. Calculations carried out using the NC yield the same results as with the MPC values because the difference between the MPC and NC is for all compartments a factor 100. An exception to this rule are the differences between the MPC_{air}s and the target values for air for benzene, dichloromethane, ethylene, and tetrachloromethane (see Table 6.1). Nevertheless, conclusions based on the NCs for these compounds are the same as for the MPCs. Therefore C_{eq}/NC ratios are not shown here.

The following conclusions can be drawn with respect to the two situations:

- emission to air: as can easily be seen from Table 6.2 maximum concentrations (C_{eq}) in soil and water are always lower than the MPC_{soil} or $MPC_{aq.}$, respectively. This implies that concentrations in air equal to the MPC_{air} or NC_{air} do not lead to problems in other compartments. This accounts also for compounds like acrylonitrile and 1,3-dichloropropene with $C_{eq}/MPC_{aq.}$ or MPC_{soil} ratios of 0.74 and 0.17, respectively, because the equilibrium concentrations are regarded as maximum achievable concentrations.
- emission to water: for this situation the opposite conclusion must be drawn: the maximum concentration (C_{eq}) in air is for all volatile compounds higher than the MPC_{air}. For most compounds the ratio C_{eq}/MPC_{soil} is equal to one.

For those compounds for which no toxicity data were available for soil organisms, emission to soil will lead to the same conclusions as emission to water if equilibrium partitioning is used for harmonization (not if the model SimpleBox is applied). For these compounds the MPC_{soil} and NC_{soil} were derived from the $MPC_{aq.}$ and $NC_{aq.}$ using equilibrium partitioning. The same relationships are used in the harmonization procedure, however (see paragraph 2.3). This is the reason why for these compounds the C_{eq}/MPC_{soil} ratios presented in Table 6.2 are equal to 1.0. For di-, tri-, tetra- and pentachlorobenzene(s), 1,2-dichloropropane, tetrachloroethene and toluene the ratio is higher: these MPC_{soil}s are based on ecotoxicological data.

Hence, following the harmonization procedure steady state concentrations in air were calculated assuming emission to water using the model SimpleBox. Results thereof are described in the following paragraph.

Table 6.2. Harmonization of Maximum Permissible (MPC) ~~and Negligible Concentrations (NC)~~ using equilibrium relationships for two situations: emission to air and emission to water. Ratios between the equilibrium concentration (C_{eq}) and the MPC in the secondary compartment (i.e. water and soil for emission to air and air and soil for emission to water) are presented.

compound	emission to:	C_{eq}/MPC_{air} [a]	$C_{eq}/MPC_{aq.}$	C_{eq}/MPC_{soil}
acrylonitrile	air		0.74	0.74
	water	1.3		1.0
benzene	air		$8.8*10^{-5}$	$8.8*10^{-5}$
	water	$1.1*10^{4}$		1.0
3-chloropropene	air		0.018	0.018
	water	54		1.0
1,2-dichlorobenzene	air		$3.2*10^{-3}$	0.047
	water	320		15
1,4-dichlorobenzene	air		0.028	0.40
	water	35		14
1,1-dichloroethane	air		$3.2*10^{-4}$	$3.2*10^{-4}$
	water	3,100		1.0
1,2-dichloroethane	air		$1.4*10^{-4}$	$1.4*10^{-4}$
	water	7,000		1.0
1,1-dichloroethene	air		$8.9*10^{-5}$	$8.9*10^{-5}$
	water	$1.1*10^{4}$		1.0
1,2-dichloroethene	air		$8.3*10^{-5}$	$8.3*10^{-5}$
	water	$1.2*10^{4}$		1.0
dichloromethane	air		$2.2*10^{-3}$	$2.2*10^{-3}$
	water	450		1.0
1,2-dichloropropane	air		$4.7*10^{-5}$	$1.4*10^{-4}$
	water	$2.1*10^{4}$		3
1,3-dichloropropene	air		0.17	0.17
	water	5.9		1.0
ethylbenzene	air		$7.5*10^{-4}$	$7.5*10^{-4}$
	water	1,300		1.0
ethylene	air		$1.1*10^{-5}$	$1.1*10^{-5}$
	water	$8.7*10^{4}$		1.0
ethylene oxide	air		$2.8*10^{-6}$	$2.8*10^{-6}$
	water	$3.5*10^{5}$		1.0
hexachlorobenzene	air		0.11	0.11
	water	9.1		1.0
hexachloroethane	air		$1.3*10^{-3}$	$1.3*10^{-3}$
	water	780		1.0
monochlorobenzene	air		$5.8*10^{-4}$	$5.8*10^{-4}$
	water	1,700		1.0

compound	emission to:	C_{eq}/MPC_{air}	$C_{eq}/MPC_{aq.}$	C_{eq}/MPC_{soil}
2-monochlorotoluene	air		0.085	0.085
	water	79		1.0
pentachlorobenzene	air		0.085	0.085
	water	12		10
styrene	air		$7.9*10^{-3}$	$7.9*10^{-3}$
	water	130		1.0
tetrachlorobenzene	air		$3.6*10^{-3}$	0.39
	water	280		110
1,1,2,2-tetrachloroethane	air		$4.3*10^{-6}$	$4.3*10^{-6}$
	water	$2.3*10^{5}$		1.0
tetrachloroethene	air		0.021	0.51
	water	48		2.5
tetrachloromethane	air		$8.6*10^{-5}$	$8.6*10^{-5}$
	water	$1.2*10^{4}$		1.0
toluene	air		$2.5*10^{-3}$	$7.5*10^{-3}$
	water	400		3.0
trichlorobenzene	air		$1.3*10^{-3}$	$1.3*10^{-3}$
	water	790		24
1,1,1-trichloroethane	air		$5.5*10^{-3}$	$5.5*10^{-3}$
	water	180		1.0
1,1,2-trichloroethane	air		$1.4*10^{-4}$	$1.4*10^{-4}$
	water	7,400		1.0
trichloroethene	air		0.014	0.014
	water	72		1.0
trichloromethane	air		$2.3*10^{-4}$	$2.3*10^{-4}$
	water	4,400		1.0
vinylchloride	air		$1.9*10^{-5}$	$1.9*10^{-5}$
	water	$5.3*10^{4}$		1.0
2-xylene	air		$6.9*10^{-3}$	$6.9*10^{-3}$
	water	140		1.0
3-xylene	air		0.017	0.017
	water	58		1.0
4-xylene	air		0.014	0.014
	water	72		1.0

[a] preliminary MPC_{air}, MPC_{air} or limit value (see Table 6.1)

6.3 Harmonization of MPC and NC values using SimpleBox

Steady state concentrations in air were computed with SimpleBox[3] assuming emission to water. Model settings applied for the computations are presented in appendix B. As stated in paragraph 3.3 the model is run as follows: it is assumed that emissions have been controlled to such a level that the concentration in water is equal to the $MPC_{aq.}$. Import from outside the system in water is set at $MPC_{aq.}$ level, while import via air is set at zero. Steady state concentrations (C_{ss}) in air and soil are calculated then. Subsequently, these steady state concentrations in air and soil are compared with the (preliminary) MPC_{air} or limit values and MPC_{soil}.

An example of the calculations performed with SimpleBox is given in Table 6.3 which summarizes input and output for toluene. Biota refers to all living organisms in water. The compartment biota is modelled as being in passive, non-equilibrium exchange with water. For the volatile compounds discussed in the present report only a small percentage of the chemical is present in biota.

Table 6.3. Example of the calculations performed with SimpleBox. Input and output are summarized for toluene.

Model version	SimpleBox vs 1.0 (930501), Lotus123 version
Model files	SIMBOX.bat(930501); SIMBOX10.mlt(930501); SIMINT10.exe(930501); SPLITRES.exe(910212)
Date and time of analysis	14/06/93 11:24
Analyst	G.J.M. Beckting
Description of the analysis	

DATA USED

COMPOUND	toluene	SYSTEM	NETH
MOL WEIGHT	92.14181 g.mol-1	SYSTEM AREA	37975 km2
LOG KOW	2.79 -	AREA WATER	4746.875 km2
VAPOR PRESSURE	2.9E+03 Pa	AREA NATURAL SOIL	15760 km2
SOLUBILITY	2.7E-01 g.l-1	AREA AGRICULTURAL SOIL	17069 km2
HENRY'S LAW CONSTANT	3.9E+02 Pa.m3.mol-1	AREA OTHER SOIL	379.75 km2
KP (suspended matter)	11 l.kg-1	RESIDENCE TIME AIR	0.4 d
KP (sediment)	6 l.kg-1	RESIDENCE TIME WATER	63.4 d
KP (natural soil)	6 l.kg-1	EFFLUENT STP	2.8E+06 m3.d-1
KP (agricultural soil)	6 l.kg-1	DILUTION FACTOR	2.59E+28 [-]
KP (other soil)	6 l.kg-1	SLUDGE PRODUCTION STP	0 kg.d-1
DEGRADATION RATE (air)	5.4E-01 d-1	QUALITY STANDARD (water)	7.3E-06 g.l-1
DEGRADATION RATE (water)	1.4E-01 d-1	QUALITY STANDARD (sediment)	4.2E-05 g.kg-1
DEGRADATION RATE (sediment)	1.8E+03 d-1	QUALITY STANDARD (soil)	1.4E-05 g.kg-1
DEGRADATION RATE (soil)	3.2E-01 d-1	QUALITY STANDARD (groundwate	7.3E-06 g.l-1

FATE

* DIRECT EMISSION TO AIR	1.0E-20 t.y-1	* EXPORT WITH AIR	4.3E+04 t.y-1
* DIRECT EMISSION TO WATER	5.8E+04 t.y-1	* EXPORT WITH WATER	6.9E+02 t.y-1
* DIRECT EMISSION TO SOIL	3.0E-20 t.y-1	TOTAL EXPORT	4.38E+04 t.y-1
* EMISSION from STP to AIR	1.0E-20 t.y-1	* BURIAL IN SEDIMENT	-1.4E-07 t.y-1
* EMISSION from STP to WATER	2.0E-20 t.y-1	* LEACHING TO GROUNDWATER	2.1E-02 t.y-1
* EMISSION with WWTP SLUDGE	1.0E-20 t.y-1	TOTAL ACCUMULATION	2.12E-02 t.y-1
TOTAL EMISSIONS	5.83E+04 t.y-1		
		* DEGRADATION in AIR	9.2E+03 t.y-1
* IMPORT with AIR	3.5E-10 t.y-1	* DEGRADATION in WATER	5.3E+03 t.y-1
* IMPORT with WATER	7.9E-06 t.y-1	* DEGRADATION in SEDIMENT	5.1E+00 t.y-1
TOTAL IMPORT	7.88E-06 t.y-1	* DEGRADATION in SOIL	5.4E+00 t.y-1
		TOTAL DEGRADATION	1.45E+04 t.y-1

DISTRIBUTION & RISK

	CONCENTRATION	RISK QUOTIENT	DISTRIBUTION
AIR	1.2E-06 g.m-3	0.41407 -	31.2 %
WATER			
* DISSOLVED	7.3E-06 g.l-1	1.00000 -	68.8 %
* PARTICULATE	8.3E-10 g.l-1		0.0 %
* SEDIMENT	1.2E-10 g.kg-1	0.00000 -	0.0 %
SOIL			
* NATURAL SOIL	1.9E-08 g.kg-1	0.00133 -	0.0 %
* AGRICULTURAL SOIL	6.8E-09 g.kg-1	0.00048 -	0.0 %
* OTHER SOIL	1.9E-08 g.kg-1	0.00133 -	0.0 %
GROUNDWATER			
* NATURAL SOIL	3.3E-09 g.l-1	0.00044 -	0.0 %

[3] SimpleBox version 1.0 is used for the calculations in the present report.

Table 6.4 gives C_{ss}/MPC and C_{ss}/NC ratios calculated using the SimpleBox model assuming emission to water.

Table 6.4. Harmonization of Maximum Permissible (MPC) and Negligible Concentrations (NC) using the model SimpleBox to calculate steady state concentrations assuming emission to water. Ratios between the steady state concentration in air or soil (C_{ss}) and the MPC for air or soil are presented.

compound	C_{ss}/MPC[a] air	C_{ss}/MPC soil
acrylonitrile	0.04	0.003
benzene	16	0.003
3-chloropropene	0.070	0.002
1,2-dichlorobenzene	0.9	0.040
1,4-dichlorobenzene	0.075	0.0087
1,1-dichloroethane	4.1	0.001
1,2-dichloroethane	26	0.004
1,1-dichloroethene	3.2	0.0003
1,2-dichloroethene	29	0.0026
dichloromethane	2.2	0.006
1,2-dichloropropane	76	0.012
1,3-dichloropropene	0.02	0.004
ethylbenzene	1.5	0.0012
ethylene	4.8	0.00005
ethylene oxide	6.0	0.0004
hexachlorobenzene	0.089	0.44
hexachloroethane	0.64	0.0008
monochlorobenzene	3.2	0.0006
2-monochlorotoluene	0.075	0.0009
pentachlorobenzene	0.10	0.089
styrene	0.11	0.001
tetrachlorobenzene	2.1	0.93
1,1,2,2-tetrachloroethane	2.100	0.010
tetrachloroethene	0.03	0.015
tetrachloromethane	3.9	0.0005
toluene	0.41	0.001
trichlorobenzene	2.9	0.089
1,1,1-trichloroethane	0.09	0.001
1,1,2-trichloroethane	61	0.0089

compound	C_{ss}/MPC^a air	soil
trichloroethene	0.09	0.001
trichloromethane	11	0.003
vinylchloride	14	0.0003
2-xylene	0.16	0.001
3-xylene	0.037	0.0006
4-xylene	0.054	0.0008

[a] C_{ss}: steady state concentration in air or soil assuming emission to water.
Calculations using NC or limit values yield the same ratios as shown above because for most compounds the difference between the MPC or limit value and NC or target value is a factor 100. Only for benzene, dichloromethane, ethylene and tetrachloromethane this is not the case (see table 6.1). For these compounds C_{ss}/NC_{air} or limit value ratios are equal to 4.7, 1.8, 7.1 and 2.3.

For both situations all C_{ss}/MPC_{soil} ratios are less than one. This can easily be explained because atmospheric deposition is not an important transport process for the volatile compounds and because the direction of diffusive transfer is towards air.

For 17 out of 35 compounds the steady state concentrations in air are lower than the (preliminary) MPC_{air} or limit values. This means that for these compounds the MPCs for the different compartments can be regarded as a coherent set of values. For the other compounds the C_{ss}/MPC_{air} ratios vary from 0.02 for 1,3-dichloropropene to 2,100 for 1,1,2,2-tetrachloroethane. Based on these calculations it can be concluded that for these compounds the $MPC_{aq.}$ and $NC_{aq.}$ must be adjusted downwards. The problem that arises is how this should be done considering the uncertainties involved in the harmonization procedure and the derivation of the MPCs for the different compartments. Because of these uncertainties a sensitivity analysis was carried out for the model SimpleBox of the calculated ratios between the steady state concentrations in air and the MPC_{air}. This is described in the following paragraph.

6.4 Sensitivity analysis for SimpleBox

When using SimpleBox for harmonization it is important to realize that, whether the MPCs of the different compartments are anticipated to conflict, depends on the model settings used (parameters that characterize the environment and rate constants characterizing intermedia mass transfer and degradation). Hence, it is very important to understand the sensitivity of the model outcome to the choice of these parameters. Goal of the simplified sensitivity analysis presented here was to gain insight into the key parameters that determine the C_{ss}/MPC ratios for air for the volatile compounds. Furthermore, the results can give an idea of the uncertainties in the C_{ss}/MPC ratios for air presented in Table 6.4. The results are only valid for the application of SimpleBox for these volatile compounds where the emission to water is adjusted so that a constant concentration equal to the $MPC_{aq.}$ (or $NC_{aq.}$) is achieved in this compartment (not for predictions

assuming a fixed emission). The sensitivity analysis was carried out by varying physico-chemical properties of the volatile compounds discussed in the present report and by varying system-parameters like the atmospheric mixing height.

The sensitivity analysis was greatly simplified, and its practical value enhanced by starting with calculations for three model-chemicals varying in physico-chemical properties: toluene, 1,1,2,2-tetrachloroethane and benzene. For these chemicals the value of each parameter investigated was varied over one order of magnitude by calculating a low, normal and high value, the normal value being equal to the values presented in Table 4.1. The following physico-chemical parameters were chosen: K_{ow} (soil-water partitioning), H_c (air-water partitioning) and degradation in air (k_{deg}). Next to this, calculations were also carried out under so-called 'worst case' conditions, i.e. a parameter setting that is expected to lead to the highest steady state concentrations in the secondary compartments. A worst-case scenario is chosen with an atmospheric residence time ten times longer (and a ten times lower windspeed) than under normal conditions: 5 instead of 0.5 days, respectively. These parameter settings can be compared with windless weather. This 'worst case' condition is considered a 'realistic worst case'.

For each combination of low, normal and high values the model was run in the same manner as described in Chapter 3 to calculate C_{ss}/MPC_{air} ratios. Combination of the high, low and normal values for the 3 physico-chemical parameters yields 27 (3x3x3) possible C_{ss}/MPC_{air} ratios. In Table 6.5 C_{ss}/MPC_{air} ratios are presented. Calculations not presented here showed that the ratios are not influenced by the degradation constant for soil and water (derived from ready biodegradability tests).

From Table 6.5 it follows that for one magnitude of variation the ratios for toluene, 1,1,2,2-tetrachloroethane and benzene are:

- independent of the K_{ow} value,
- relatively insensitive for H_c
- sensitive for k_{deg} in air, especially for the 'worst case' situation for toluene and benzene (high air residence time).

These observations can be explained easily. The steady state concentration for air related to a given steady state concentration in water is a resultant of the fluxes represented schematically in Figure 4. Here the amount of the chemical leaving The Netherlands (export) depends on the windspeed and the concentrations in air at the Dutch borders (the amount of the chemical entering the Netherlands is equal to zero because concentrations in secondary compartments outside the system were set equal to zero). The flux through volatilization depends on the chemicals vapour pressure, H_c, molecular weight, concentration in water (C_{water}), concentration in air (C_{air}) and parameters defining the physical system (fraction of the system area covered by water and the windspeed). The loss through degradation in the air compartment depends on k_{deg} and C_{air}.

The K_{ow} value (and the degradation in water) do not influence C_{air} because losses through adsorption or degradation in the water compartment are compensated for to achieve that C_{water}

Table 6.5 Sensitivity analysis: schematic representation of the variation of C_{ss}/MPC_{air} ratios for toluene, 1,1,2,2-tetrachloroethane and benzene assuming an uncertainty of one magnitude of variation in 3 physico-chemical parameters.

K_{ow} [a]	H_c (air)	k_{deg}	toluene 'normal'	'worst case'	1,1,2,2-tetrachloroethane 'normal'	'worst case'	benzene 'normal'	'worst case'
		L[b]	0.43	0.37	1,100	1,200	4.4	5.2
	L	N	0.38	0.20	1,100	1,200	4.3	4.2
		H	0.27	0.08	1,100	1,100	3.9	2.5
		L	0.47	0.41	2,100	2,500	4.9	6.0
L	N	N	0.41	0.22	2,100	2,400	4.7	4.7
		H	0.30	0.09	2,100	2,300	4.3	2.8
		L	0.49	0.43	2,900	3,800	5.0	6.2
	H	N	0.43	0.23	2,900	3,700	4.9	4.9
		H	0.31	0.09	2,900	3,400	4.5	3.0
		L	0.43	0.37	1,100	1,200	4.4	5.2
	L	N	0.38	0.20	1,100	1,200	4.3	4.2
		H	0.27	0.08	1,100	1,100	3.9	2.5
		L	0.47	0.41	2,100	2,500	4.9	6.0
N	N	N	0.41	0.22	2,100	2,400	4.7	4.7
		H	0.30	0.09	2,100	2,300	4.3	2.8
		L	0.49	0.43	2,900	3,800	5.0	6.2
	H	N	0.43	0.23	2,900	3,700	4.9	4.9
		H	0.31	0.09	2,900	3,400	4.5	3.0
		L	0.43	0.37	1,100	1,200	4.4	5.2
	L	N	0.38	0.20	1,100	1,200	4.3	4.2
		H	0.27	0.08	1,100	1,100	3.9	2.5
		L	0.47	0.41	2,100	2,500	4.9	6.0
N	N	N	0.41	0.22	2,100	2,400	4.7	4.7
		H	0.30	0.09	2,100	2,300	4.3	2.8
		L	0.49	0.43	2,900	3,800	5.0	6.2
	H	N	0.43	0.23	2,900	3,700	4.9	4.9
		H	0.31	0.09	2,900	3,400	4.5	3.0

[a] and K_p

[b] N (normal) represents the values used for the parameters as shown in Table 4.1; L (low) represents N/V10 and H (high) N*V10

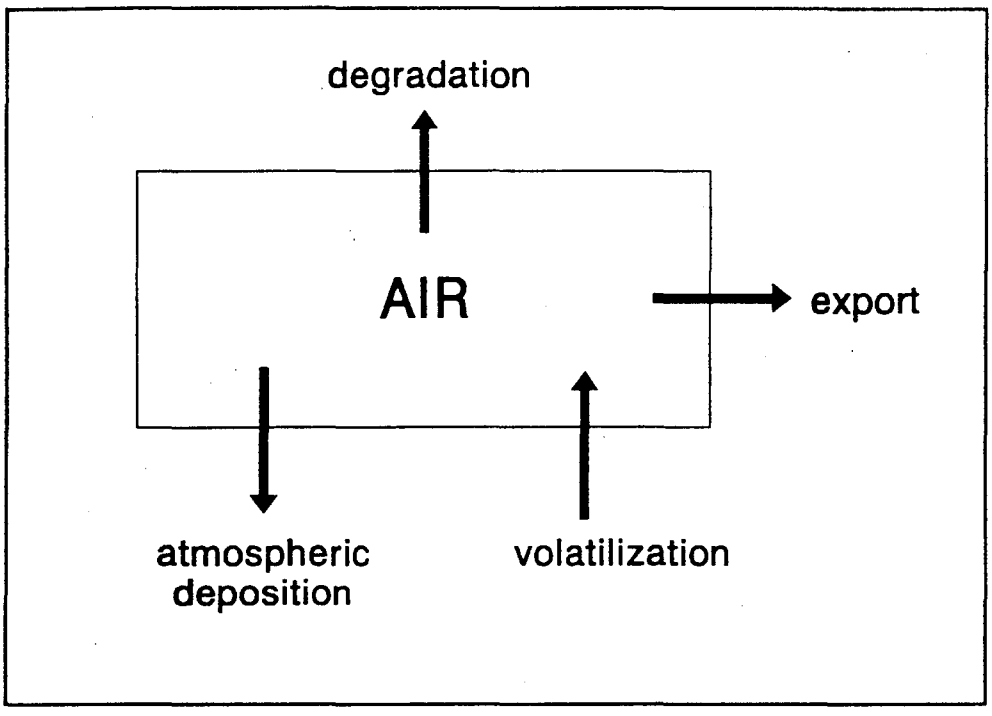

Figure 4. Schematic representation of the fluxes that determine the concentrations in the air compartment (atmospheric deposition is only of minor influence on the air concentrations of the compounds considered in this report).

remains equal to the $MPC_{aq.}$ (or $NC_{aq.}$). The relatively low sensitivity for H_c results from the formulation of the exchange rate water-air in the model. When H_cs increase the exchange rates approach asymptotically a maximum value. This implies that when H_cs are high, which is the case for the compounds considered here, uncertainties of H_c have a relatively small influence on the exchange rate.

It is not surprising that k_{deg} in air is a key parameter for predicting C_{ss}/MPC_{air} or NC_{air} ratios because degradation and export are the main output fluxes for the air compartment. When the windspeed is low, degradation dominates the output and the system is most sensitive for k_{deg} in air.

One might expect that in the 'worst case' situation when the system's residence time for air is high (and the windspeed is low) C_{ss}/MPC or NC_{air} ratios increase dramatically because more time is available for volatilization of the chemical and less clean air enters the system. In the model the overall mass transfer coefficients for gas absorption and volatilization are estimated using the classical two-film resistance model [25]. For calculating the partial mass transfer coefficients at the air- and water-side of the air-water interface either fixed values may be chosen or recipes/equations can be used to calculate these coefficients. Using the latter option the partial mass transfer coefficient at the air-side of the air-water interface depends on the windspeed and the molecular weight, while for the coefficient at the water side a recipe is used in which this coefficient depends on the windspeed [25]. In the present report this option was applied because in this way a lower windspeed ('worst case' situation) leads to a lower volatilization across the air-water interface. This outweighs the effects described above resulting in only small differences in

the C_{ss}/MPC_{air} ratios for the 'normal' and 'worst case' situation.

Further sensitivity analysis showed that C_{ss}/MPC_{air} ratios for air increase linear with the volatilization rate and the fraction of the system area that is water. A linear decrease occurs when the atmospheric mixing height is increased.

Considering the results for the 'worst case' calculations it might be argued that this situation is in fact not a 'worst-case'. However, the outcome of the model calculations for the 'worst case' situation are heavily influenced by the choice of the modelling of the volatilization rate as stated above. Also other 'worst case' situations are imaginable, e.g. meterological conditions characterized by high temperature, high levels of solar radiation (for some compounds this will lead to a higher k_{deg}, however), low windspeeds and higher atmospheric mixing height. With respect to a sensitivity analysis of SimpleBox it may be useful to carry out a Monte Carlo simulation in which parameters like windspeed, air residence time, atmospheric mixing height and physico-chemical properties (k_{deg}) are used. The actual variations occurring for these parameters must then be studied first. This lies outside the scope of the present report, however. Considering the uncertainties calculations with SimpleBox, caused by e.g. the modelling of the volatilization rate, it seems reasonable to assume that there is an uncertainty of a factor 10 in the results presented in Table 6.4.

6.5 Adjustment of MPC and NC values

Another aspect which has to be taken into account when adjusting the $MPC_{aq.}$ and $NC_{aq.}$ values downwards based on the calculations of SimpleBox, are the MPCs themselves. High uncertainty factors were often used to derive MPCs: 100-1,000 for deriving MPC_{air}s and 1,000-10,000 for deriving preliminary MPC_{air}s, both aiming at the protection of human beings (see Tables 2.4 and 2.5) and 10-1,000 in case of the modified EPA method used for calculating, $MPC_{aq.}$s and MPC_{soil}s (see Tables 2.1 and 2.2).

Based on these considerations the $MPC_{aq.}$ and $NC_{aq.}$ were adjusted as follows. If only preliminary MPC_{air} values were available for the compartment air, the $MPC_{aq.}$ and $NC_{aq.}$ were not adjusted because of the uncertainty in the preliminary MPC_{air} values leading to the application of high uncertainty factors. For these compounds first more toxicological information should become available. It is possible that if more information becomes available the applied uncertainty factors can be lowered leading to higher MPC_{air}s and NC_{air}s. Consequently this leads to lower C_{eq} or C_{ss}/MPC_{air} or NC_{air} ratios.

If the MPC_{air} values were not preliminary the $MPC_{aq.}$s and $NC_{aq.}$s were adjusted downwards. Because of the uncertainty of a factor 10 in the calculations presented in Table 6.4 adjustment was only carried out if the steady state concentration in air exceeded the MPC_{air} or NC_{air} with more than a factor 10. Thereafter adjustment was carried out in steps of 10: if the steady state concentration was 10-20 times higher than the MPC_{air} or NC_{air} the $MPC_{aq.}$ and $NC_{aq.}$ are adjusted downwards with a factor 10; if the steady state concentration was 20-30 times higher than the MPC_{air} or NC_{air} the $MPC_{aq.}$ and $NC_{aq.}$ are adjusted downwards with a factor 20 etc.

In Table 6.6 adjusted $MPC_{aq.}$ and $NC_{aq.}$ values are presented. Consequently, if the $MPC_{sed.}$ or $NC_{sed.}$ is based on equilibrium partitioning these values must also be adjusted.

Table 6.6 Harmonized Maximum Permissible and Negligible Concentrations for water together with the 'adjustment factor'

compound	harmonized $MPC_{aq.}$ (μg/l)	adjustment factor	harmonized $NC_{aq.}$ (μg/l)	adjustment factor
acrylonitrile	7.6	1	0.076	1
benzene	240	10	2.4	10
3-chloropropene	3.4	1	0.034	1
1,2-dichlorobenzene	270[a]	1	2.7[a]	1
1,3-dichlorobenzene	210[a]	1	2.1[a]	1
1,4-dichlorobenzene	260[a]	1	2.6[a]	1
1,1-dichloroethane	7,300[a]	1	73[a]	1
1,2-dichloroethane	700	20	7.0	20
1,1-dichloroethene	3,400	1	34	1
1,2-dichloroethene	6,100[a]	1	61[a]	1
dichloromethane	20,000	1	200	1
1,2-dichloropropane	76	70	0.76	70
1,3-dichloropropane	5,200[a]	1	52[a]	1
1,3-dichloropropene	8.0	1	0.08	1
2,3-dichloropropene	8.0[a]	1	0.08[a]	1
ethylbenzene	370[a]	1	3.7[a]	1
ethylene	8,500	1	85	1
ethylene oxide	84	1	0.84	1
hexachlorobenzene	2.4[a]	1	0.024[a]	1
hexachloroethane	83[a]	1	0.83[a]	1
monochlorobenzene	690[a]	1	6.9[a]	1
2-monochlorotoluene	300[a]	1	3.0[a]	1
3-monochlorotoluene	330[a]	1	3.3[a]	1
4-monochlorotoluene	300[a]	1	3.0[a]	1
pentachlorobenzene	7.5[a]	1	0.075[a]	1
pentachloroethane	230[a]	1	2.3[a]	1
styrene	570	1	5.7	1
1,2,3,4-tetrachlorobenzene	23[a]	1	0.23[a]	1
1,2,3,5-tetrachlorobenzene	22[a]	1	0.22[a]	1
1,2,4,5-tetrachlorobenzene	26[a]	1	0.26[a]	1
tetrachloroethene	330	1	3.3	1
tetrachloromethane	1,100	1	11	1
toluene	730	1	0.73	1
1,2,3-trichlorobenzene	64[a]	1	0.64[a]	1
1,2,4-trichlorobenzene	79[a]	1	0.79[a]	1
1,3,5-trichlorobenzene	57[a]	1	0.57[a]	1
1,1,1-trichloroethane	2,100	1	21	1
1,1,2-trichloroethane	7,900[a]	1	79[a]	1
trichloroethene	2,400	1	24	1
trichloromethane	590	10	5.9	10
vinylchloride	820	10	8.2	10
2-xylene	400[a]	1	4.0[a]	1
3-xylene	330[a]	1	3.3[a]	1
4-xylene	400[a]	1	4.0[a]	1

[a] because only a preliminary MPC_{air} or NC_{air} is available no adjustment of the $MPC_{aq.}$ or $NC_{aq.}$ is carried out

As can be seen from Table 6.6 $MPC_{aq.}$s and $NC_{aq.}$s are adjusted for five compounds: benzene, 1,2-dichloroethane, 1,2-dichloropropane, trichloromethane and vinylchloride. Adjusted $MPC_{sed.}$ and $NC_{sed.}$ values are 0.95, 1.5, 0.18, 1.9 1.4 mg/kg and 0.0095, 0.015, 0.0018, 0.019, 0.014 mg/kg, respectively.

It might be remarked that in the 'adjustment procedure' described above preliminary MPC_{air}s and indicative $MPC_{aq.}$s are treated differently. However, if more ecotoxicological information becomes available the $MPC_{aq.}$ will usually increase because lower uncertainty factors will be used in the modified EPA method or because the Aldenberg & Slob method can be used. An increase in the $MPC_{aq.}$ will lead to higher steady state concentrations in air. Therefore the same conclusion must be drawn then as in the present report, i.e. that the $MPC_{aq.}$ must be adjusted downwards leading to the same adjusted $MPC_{aq.}$ as the ones presented in Table 6.6.

In Tables 6.7 and 6.8 values for all compounds are presented. In Table 6.7 for those compounds for which existing limit and target values were available or MPC_{air}s and NC_{air}s were derived in the present report. For these compounds the MPCs for water and soil could be harmonized with the one for air. In Table 6.8 for those compounds for which only preliminary MPC_{air}s and NC_{air}s could be derived or for which even insufficient toxicological information was present to derive a preliminary MPC_{air}. For these compounds harmonization was not possible.

Some of the values in tables 6.7 and 6.8 differ from the ones derived before:

- 1,1-dichloroethane: MPC and NC values for water, sediment and soil were set equal to the ones for 1,2-dichloroethane,
- 1,3-dichloropropane: MPC and NC values for water, sediment and soil were set equal to the ones for 1,2-dichloropropane,
- overall MPC and NC values for water and sediment were calculated for di-, tri- and tetrachlorobenzene, monochlorotoluene and xylene.

Table 6.7. Overview of harmonized Maximum Permissible (MPC) and Negligible Concentrations (NC) for water ($MPC_{aq.}$ and $NC_{aq.}$), sediment ($MPC_{sed.}$ and $NC_{sed.}$), soil (MPC_{soil} and NC_{soil}), and air (MPC_{air} and NC_{air}) and existing limit and target values for air.

compound	water		sediment		soil		air			
	$MPC_{aq.}$ ($\mu g/l$)	$NC_{aq.}$ ($\mu g/l$)	$MPC_{sed.}$ (mg/kg)	$NC_{sed.}$ (mg/kg)	MPC_{soil} (mg/kg)	NC_{soil} (mg/kg)	MPC_{air} ($\mu g/m^3$)	NC_{air} ($\mu g/m^3$)	limit value ($\mu g/m^3$)	target value ($\mu g/m^3$)
acrylonitrile	7.6	0.076	$6.8*10^{-4}$	$6.8*10^{-6}$	$6.8*10^{-4}$	$6.8*10^{-6}$	10	-	-	0.1
benzene	240	2.4	0.95	0.0095	0.95	0.0095	30	-	-	1
2-chloro-1,3-butadiene	-	-	-	-	-	-	1.0	0.01	-	-
3-chloropropene	3.4	0.034	0.0048	$4.8*10^{-5}$	0.0048	$4.8*10^{-5}$	74	0.74	-	-
1,2-dichloroethane	700	7.0	1.5	0.015	1.5	0.015	100	-	-	1
1,1-dichloroethene	3,400	34	12	0.12	12	0.12	200	2.0	-	-
dichloromethane	20,000	200	36	0.36	36	0.36	1,700	-	-	20
1,2-dichloropropane	76	0.76	0.18	0.0018	4.2	0.042	12	0.12	-	-
1,3-dichloropropene	8.0	0.08	0.023	$2.3*10^{-4}$	0.023	$2.3*10^{-4}$	40	0.40	-	-
ethylene	8,500	85	5.8	0.058	5.8	0.058	-	2	300	-
ethylene oxide	84	0.84	0.0021	$2.1*10^{-5}$	0.0021	$2.1*10^{-5}$	3	-	-	0.03
styrene	570	5.7	25	0.25	25	0.25	800	-	-	8
tetrachloroethene	330	3.3	4.0	0.040	0.16	0.0016	2,500	2,000	-	25
tetrachloromethane	1,100	11	37	0.37	37	0.37	60	-	-	1
toluene	730	7.3	4.2	0.042	1.4	0.014	300	3	-	-
1,1,1-trichloroethane	2,100	21	6.9	0.069	6.9	0.069	4,800	4.8	-	-
trichloroethene	2,400	24	13	0.13	13	0.13	5,000	50	-	50
trichloromethane	590	5.9	1.9	0.019	1.9	0.019	100	-	-	1
vinylchloride	820	8.2	1.4	0.014	1.4	0.014	100	-	-	1

water: $MPC_{aq.}$s and $NC_{aq.}$s for acrylonitrile, 3-chloropropene, 1,3-dichloropropene and ethylene oxide are indicative values.
sediment: all $MPC_{sed.}$ and $NC_{sed.}$ values are based on the equilibrium partitioning method.
soil: MPC_{soil}s and NC_{soil}s for 1,2-dichloropropane, tetrachloroethene and toluene are indicative values based on ecotoxicological data. The MPC_{soil}s and NC_{soil}s for the other compounds are based on the equilibrium partitioning method.
air: NC_{air} for ethylene is an indicative value; MPC_{air} and NC_{air} for 2-chloro-1,3-butadiene are revised preliminary values

Table 6.8. Overview of (preliminary) Maximum Permissible (MPC) and Negligible Concentrations (NC) for water ($MPC_{aq.}$ and $NC_{aq.}$), sediment ($MPC_{sed.}$ and $NC_{sed.}$), soil (MPC_{soil} and NC_{soil}), and air (preliminary MPC_{air} and NC_{air}).

compound	water		sediment		soil		air	
	$MPC_{aq.}$ ($\mu g/l$)	$NC_{aq.}$ ($\mu g/l$)	$MPC_{sed.}$ (mg/kg)	$NC_{sed.}$ (mg/kg)	MPC_{soil} (mg/kg)	NC_{soil} (mg/kg)	preliminary MPC_{air} ($\mu g/m^3$)	preliminary NC_{air} ($\mu g/m^3$)
1,2-dichlorobenzene	250	2.5	5.5	0.055	0.4	0.004	60	0.60
1,3-dichlorobenzene	250	2.5	5.5	0.055	0.4	0.004	-	-
1,4-dichlorobenzene	250	2.5	5.5	0.055	0.4	0.004	670	6.7
1,1-dichloroethane	700	7.0	1.5	0.015	1.5	0.015	370	3.7
1,2-dichloroethene	6,100	61	22	0.22	22	0.22	36	0.36
1,3-dichloropropane	76	0.76	0.18	0.0018	0.18	0.0018	-	-
2,3-dichloropropene	8.0	0.08	0.044	$4.4*10^{-4}$	0.044	$4.4*10^{-4}$	-	-
ethylbenzene	370	3.7	3.1	0.031	3.1	0.031	39	0.39
hexachlorobenzene	2.4	0.024	1.3	0.013	1.3	0.013	2.3	0.023
hexachloroethane	83	0.83	17	0.17	17	0.17	27	0.27
monochlorobenzene	690	6.9	7.6	0.076	7.6	0.076	42	0.42
2-monochlorotoluene	310	3.1	33	0.33	33	0.33	780	0.78
3-monochlorotoluene	310	3.1	33	0.33	33	0.33	-	-
4-monochlorotoluene	310	3.1	33	0.33	33	0.33	-	-
pentachlorobenzene	7.5	0.075	3.0	0.030	0.3	0.003	8	0.08
pentachloroethane	230	2.3	49	0.49	49	0.49	-	-
1,2,3,4-tetrachlorobenzene	24	0.24	7.2	0.072	0.072	$7.2*10^{-4}$	1.6	0.016
1,2,3,5-tetrachlorobenzene	24	0.24	7.2	0.072	0.072	$7.2*10^{-4}$	1.6	0.016
1,2,4,5-tetrachlorobenzene	24	0.24	7.2	0.072	0.072	$7.2*10^{-4}$	1.6	0.016
1,1,2,2-tetrachloroethane	3,300	33	14	0.14	14	0.14	0.2	0.002
1,2,3-trichlorobenzene	67	0.67	6.7	0.067	0.24	0.0024	4	0.04
1,2,4-trichlorobenzene	67	0.67	6.7	0.067	0.24	0.0024	4	0.04
1,3,5-trichlorobenzene	67	0.67	6.7	0.067	0.24	0.0024	4	0.04

compound	water		sediment		soil		air	
	$MPC_{aq.}$ ($\mu g/l$)	$NC_{aq.}$ ($\mu g/l$)	$MPC_{sed.}$ (mg/kg)	$NC_{sed.}$ (mg/kg)	MPC_{soil} (mg/kg)	NC_{soil} (mg/kg)	preliminary MPC_{air} ($\mu g/m^3$)	preliminary NC_{air} ($\mu g/m^3$)
1,1,2-trichloroethane	7,900	79	39	0.39	39	0.39	18	0.18
2-xylene	380	3.8	14	0.14	14	0.14	340	3.4
3-xylene	380	3.8	14	0.14	14	0.14	1,000	10
4-xylene	380	3.8	14	0.14	14	0.14	1,000	10

MPCs and NCs for 1,1-dichloroethane and 1,3-dichloropropane for water, sediment and soil set equal to the ones for 1,2-dichloroethane and 1,2-dichloropropane, respectively.

sediment: all $MPC_{sed.}$ and $NC_{sed.}$ values are based on the equilibrium partitioning method.

soil: MPC_{soil}s and NC_{soil}s for di-, tri- and tetrachlorobenzenes are indicative values based on ecotoxicological data. The MPC_{soil}s and NC_{soil}s for the other compounds are based on the equilibrium partitioning method.

air: preliminary MPC_{air}s and NC_{air}s are values which should not be used to set limit and target values.

$MPC_{aq.}$, $MPC_{sed.}$ and MPC_{soil} for hexa- and pentachlorobenzene may change because effects due to their accumulation potential will be examined in another project.

7. ENVIRONMENTAL CONCENTRATIONS MEASURED IN THE NETHERLANDS

Data on environmental concentrations in the Netherlands were collected for all compartments. A summary of reported concentrations is presented in Table 7.1. In the following paragraphs the data are discussed and compared with the values presented in Tables 6.7 and 6.8.

7.1 Environmental concentrations in air

The underlying data for air are presented in Appendix C. For each location year averages are calculated from 12-16 weekly samples taken in the period 1991 to 1992 by the RIVM [47]. Clearly, for almost all compounds concentrations at urban and street locations (neglected for the calculation of the rural averages shown in Table 7.1) are higher than in rural areas. The spatial distribution of the concentrations in the rural areas agrees with the pattern of a large number of airborne pollutants: an increase of the average concentration going from the north to the south of The Netherlands [47].

Unfortunately, approximately half of the compounds considered in this report were not included in the monitoring programme of the RIVM. The value for ethylene shown in Table 7.1 is based on data supplied by Bloemen [48]. The value for 1,1,2,2-tetrachloroethane might not be representative for actual rural levels because only measurements performed in the period of 1982-1983 at an urban location were available.

Comparing the actual concentrations presented in Table 7.1 with the values derived in Chapter 6 the following can be concluded. Actual concentrations are lower than the $MPC_{a,r}$s or limit values for all compounds. With respect to the $NC_{a,r}$ and target values it can be concluded that these values are exceeded for benzene (factor 1.6), 1,2-dichloropropane (factor 4.3), ethylene (factor 1.8) and toluene (factor 1.2). For acrylonitrile, 2-chloro-1,3-butadiene, 3-chloropropene, 1,1-dichloroethane, 1,1-dichloroethene, dichloromethane, 1,3-dichloropropene, ethylene oxide and vinylchloride no concentrations in air were available, however.

Comparing the actual concentrations with the preliminary $MPC_{a,r}$s and $NC_{a,r}$s it can be concluded that the preliminary $MPC_{a,r}$s are always much higher than the actual concentrations. With respect to the preliminary $NC_{a,r}$s only the one for ethylbenzene is somewhat exceeded: a factor 1.6. For 1,1-dichloroethane, 1,2-dichloroethene, hexachlorobenzene, hexachloroethane, monochlorotoluene, pentachlorobenzene and tetrachlorobenzene no data were available, however.

7.2 Environmental concentrations in surface water

The underlying data for surface water collected by the Cooperating Rhine and Meuse Waterworks in 1990 and 1991 are presented in Appendix D. Concentrations were measured at several locations, a.o. Rhine River (Lobith), Meuse River (Eysden and Keizersveer), Lek River (Hagestein) and Lake IJssel (Andijk). For 24 compounds data were available. In all cases the median as well as the 90 percentile are lower than the NC_{aq} derived in Chapter 6, usually more than a factor 10.

Concentrations in surface water in The Netherlands are also measured by the National Institute of Inland Water Management. Because of the structure of their data base concentrations are not presented in this report but the $MPC_{aq.}$ and $NC_{aq.}$ values as derived in Chapter 6 have been compared by the National Institute of Inland Water Management with the 90 percentile and the maximum concentrations for state and non-state water bodies, respectively [49].

For state water bodies measurements from 1988-1992 were used. 21 Of the volatile compounds have been measured regularly at the 7 main locations: benzene, 1,2-, 1,3, and 1,4-dichlorobenzene, 1,2,4,5-tetrachlorobenzene, toluene, ethylbenzene, trichlorobenzenes (total), hexachlorobenzene, 1,2-dichloroethane, 1,1,1-trichloroethane, trichloromethane, tetrachloromethane, trichloroethene, tetrachloroethene, xylene (total of 2- and 3-xylene) and styrene. For the di-, tri- and tetrachlorobenzenes only data for 1988 were available. After 1988 these compounds have been measured in particulate matter, only. All 90 percentile concentrations are far below the $NC_{aq.}$, at least more than a factor 4. Only for some individual measurements the $NC_{aq.}$ was exceeded, i.e. for 1,2-dichloroethane (2 measurements), tetrachloroethene (1 measurement), toluene (1 measurement) and xylene (1 measurement).

For non-state water bodies measurements from 1990 were used. Only for 5 compounds data were available: benzene, toluene, xylene, ethylbenzene and hexachlorobenzene for 16, 16, 14, 14 and 89 locations, respectively. Only hexachlorobenzene has been measured at a sufficient number of locations. All maximum concentrations are below the $NC_{aq.}$: for hexachlorobenzene more than a factor 4 and for the other compounds more than a factor 10.

7.3 Environmental concentrations in particulate matter

Concentrations in particulate matter are also measured by the National Institute of Inland Water Management [49]. Only data for state water bodies are available. 10 Compounds were measured from 1988 until 1991 at 16 locations: di-, tri-, tetra- and hexachlorobenzene(s). All 90 percentile concentrations are lower than the $MPC_{sed.}$. The $NC_{sed.}$ is only exceeded for hexachlorobenzene at three locations (factor 1-2). For the other compounds the $NC_{sed.}$ is always at least a factor 3 lower.

7.4 Environmental concentrations in sediment

Concentrations in sediment have been measured by the National Institute of Inland Water Management [49]. For state water bodies only data for hexachlorobenzene were available measured until 1991 (total of 2801 measurements). The $MPC_{sed.}$ was never exceeded while the $NC_{sed.}$ was exceeded for 13% of the measurements. Also for non-state water bodies only data for hexachlorobenzene were available (total of 2428 measurements). The $MPC_{sed.}$ was never exceeded while the $NC_{sed.}$ was exceeded for 2% of the measurements, only.

7.5 Environmental concentrations in soil

For soil only for hexachlorobenzene data were available [18]. In the framework of the Dutch Soil Quality Monitoring Programma soil samples were taken at 40 locations in The Netherlands at 0-10 and 10-30 cm, representing 10 different combinations of land use/soil type. Concentrations in grassland, farmland and orchard were <0.5-34 μg/kg and <0.5-17 μg/kg for 0-10 and 10-30 cm, respectively. Concentrations in forests were all below the detection limit of 0.5 μg/kg. Concentrations in soil are far below the MPC_{soil} for hexachlorobenzene. However, the NC_{soil} is sometimes exceeded in grassland, farmland and orchard (maximum factor 2.6) but not in forests.

7.6 Environmental concentrations in groundwater

The underlying data for groundwater are presented in Appendix E. Data were collected from a data-base present at the National Institute of Public Health and Environmental Protection containing data from the National Groundwater Quality Monitoring Network and the Provincial Groundwater Quality Monitoring Network. From three periods data were available: 1979/1984, 1987/1988 and 1990/1991. In appendix E data are presented for three soil types: sand, clay and peat for two different depths: 5-15 and 15-30 meter. Measurements lower than the detection limit were included in the calculations of the mean, maximum and 90 percentile.

For all compounds except 2-chloro-1,3-butadiene; 3-chloropropene; 1,1-dichloroethene; 2,3-dichloropropene; ethylene; ethylene oxide; hexachlorobenzene; hexachloroethane; monochlorotoluene; pentachlorobenzene; pentachloroethane; tetrachlorobenzene; 1,1,2,2-tetrachloroethane and vinylchloride data were available. For all compounds 90 percentile concentrations were much lower than the $MPC_{aq.}$. For tetrachloroethene the maxium concentration in sand at 5-15 m was higher than the $MPC_{aq.}$ in 1987/1988. Compared to the other data for this compound this value must be considered as an outlier. For 1,2-dichloropropane high concentrations have been measured in the periods 1979/1984 and 1987/1988. Formulations of the soil desinfectant 1,3-dichloropropene contained until 35% of this persistent compound. At the moment this percentage has been reduced to less than 0.5% [50]. For most compounds concentrations were also lower than the $NC_{aq.}$. For the following compounds the $NC_{aq.}$ was exceeded:

- benzene: maximum concentration for sand at 5-15 m; however only by a factor 1.2 (from 1987/1988),
- 1,2-dichloroethane: maximum concentration for sand at 5-15 m by a factor 2.7 (from 1987/1988),
- 1,2-dichloropropane: using the most recent data from 1990/1991 in clay and sand 90 percentiles at both depths are slightly higher than the $NC_{aq.}$,
- toluene: maximum concentration for clay at 15-30 m; however only by a factor 1.7 (from 1987/1988),
- trichloromethane: maximum concentration in sand and peat at 5-15 m by a factor 1.2 and 14, respectively.

Table 7.1. Summary of reported concentrations in groundwater, surface water, and air measured in The Netherlands.

compound	surface water[a] median (μg/l)	90 percentile (μg/l)	air average ($\mu g/m^3$)
benzene	<0.10	<0.10-0.10	1.60
1,2-dichlorobenzene	<0.10		0.018
1,3-dichlorobenzene	<0.10	<0.10	0.003
1,4-dichlorobenzene	0.10[b]		<0.00005
1,2-dichloroethane	<0.10-<2.0	0.10-<2.0	0.10
1,1-dichloroethene	<0.10		
1,2-dichloroethene	<0.10-0.20[c]		
dichloromethane	<0.50-<2.0	<0.50-<2.0	
1,2-dichloropropane	<0.10-<0.40	<0.40-<0.50	0.52
ethylbenzene	<0.10-<0.20	<0.10-<0.20	0.63
ethylene			3.57
hexachlorobenzene	<0.010	<0.010-<0.020	
monochlorobenzene	<0.10	<0.10	0.0023
styrene			0.16
1,1,2,2-tetrachloroethane	<0.10-0.20	<0.10	0.0007[d]
tetrachloroethene	0.060-0.22	<0.010-0.59	0.29
tetrachloromethane	<0.010-0.20	0.060-0.91	0.64
toluene	<0.10	0.16	3.58
1,2,3-trichlorobenzene			0.0037
1,2,4-trichlorobenzene			0.0007
1,3,5-trichlorobenzene			0.0003
trichlorobenzene	<0.10[e]		
1,1,1-trichloroethane	0.040-0.20	<0.10-0.64	1.02
1,1,2-trichloroethane	<0.10	<0.10	<0.5
trichloroethene	<0.020-0.23	<0.10-0.83	0.43
trichloromethane	<0.050-0.10	<0.10-0.70	0.10
2-xylene	<0.20	<0.20	0.74
3-xylene	<0.20	<0.20	1.35
4-xylene	<0.20	<0.20	0.42

[a] data from Cooperating Rhine and Meuse Waterworks
[c] two results from one measurement
[b] result from one measurement
[d] data from urban area; not recent
[e] results from two measurements (both values <0.10 μg/l)

8. DISCUSSION AND CONCLUSIONS

8.1 Derivation of Maximum Permissible Concentrations

In the present report MPCs have been derived for water, soil and air based on (eco)toxicological information (see Chapter 3). With respect to availability of ecotoxicological data it can be stated that data for organisms exposed via sediment, soil and air were lacking. For the volatile compounds dealt with in the present report particularly data on plants and organisms like insects and maybe birds exposed via air are important to obtain, because these are organisms at risk regarding exposure to air. This field of ecotoxicology is at the moment in 'status nascendi'. Only for plants test methods are available at the moment. In the near future projects will start within the National Institute of Public Health and Environmental Protection and the Research Institute for Plant Protection to develop ecotoxicological test methods and to test several of the compounds dealt with here.

For deriving a MPC_{air} aiming at the protection of human beings a minimum toxicological data set was formulated (see paragraph 2.3). Only for 6 compounds all elements of this data set were present. From their literature search Rademaker et al. concluded that in most cases chronic inhalation and reproduction tests are lacking [13].

For air MPCs were derived aiming at the protection of man as well as the environment, although it is recognized that at the moment there is no accepted method for deriving MPC_{air}s for the ecosystem. As stated in Chapter 1 MPC_{air}s were also derived for human beings because exposure via air is such an important route. It is recognized of course that human beings can also be exposed via water and soil. However, because for volatile compounds exposure via these routes is of minor importance it is considered acceptable to derive no MPCs for soil and water for human beings.

It should be reminded that these MPCs do not take into account adverse effects due to secondary poisoning. In another project this will be dealt with for penta- and hexachlorobenzene because of their high lipophilicity. An aquatic and a terrestrial food chain will be examined: water → fish or mussel → fish- or mussel-eating birds and mammals and soil → earthworms → worm-eating birds and mammals.

8.2 Harmonization procedure

The procedure used for harmonization of MPC and NC values for the different compartments has been presented in Chapter 2. Crucial in this procedure is the use of the model SimpleBox. As stated before in Chapter 6 such 'Mackay-type' models are applied for specific purposes. As Mackay states himself "They are useful for predicting the likely behaviour of chemicals which may be newly introduced into commerce, or which may be subject to production increases, or introduction into new environments" [26]. Or as Van de Meent states: "Models like SimpleBox are meant to be used in a generic way. To explain why, in what way and to what extent the fate of different chemicals in a multimedia environment may be different. Or to explain why, in what way and to what extent the fate of one chemical may be different in different environmental situations" [25]. In environmental science they are applied to gain insight into the effects of processes like transportation and transformation between air, water and soil. This means that the outcome of

such model calculations are used as a resource and not as absolute results. In the present report SimpleBox is used for a completely different goal, however, i.e. to test whether independently derived MPCs and NCs for air, water and soil are coherent. In this case the outcome of the model computations, i.e. steady state concentrations in soil and air, resulted in an adjustment of the MPC and NC values for water for several compounds (see Table 6.6). With respect to the use of SimpleBox several items need to be discussed.

First of all the model itself. It has been argued sufficiently in paragraph 2.1 that steady state computations rather than the equilibrium calculations are needed for harmonization of the MPC and NC values for water and soil with the ones for air. The SimpleBox model applied then, consists of parameters that characterize the environment and parameters that describe intermedia partitioning of the chemical. The first parameters were set in such a way that the environment modelled resembled The Netherlands. Of course, many of these parameters are a severe generalization of reality, e.g. the atmospheric mixing height which is set at 1,000 m or a single hydraulic retention time of c. 63 days. It should be realized, however that SimpleBox is used here for harmonization purposes and not to calculate actually occurring concentrations. Important is the scale at which the calculations are carried out: in the present report The Netherlands. The outcome might be different if other scales are used, e.g. Rhine River basin or Europe. It would be interesting to carry out such calculations because it might well be that harmonized values derived here conflict with each other on the scales stated above.

Secondly, several processes are modelled in SimpleBox using the second set of parameters. As stated in paragraph 6.4 a model-setting was chosen in which at low windspeed the volatilization rate from the water phase decreases. This decrease depended also on the molecular weight of the compound. Calculations, which are not shown here, indicated that this choice influenced the C_{ss}/MPC_{air} or NC_{air} ratios considerably.

At the moment the modelling of volatilization from the water phase is a subject of scientific debate. Some authors prefer a fixed value for the partial mass transfer coefficients at the water-side and air-side of the air-water interface, which means that the volatilization rate is independent from the windspeed [25]. The volatilization rate remains an uncertain factor in the calculations. It is logical that if the residence time of air in the system decreases, the windspeed also decreases. In SimpleBox this is the average windspeed at 10 m above the surface [25]. However, the exact consequences for transport processes at the air-water interphase, where different micrometerological conditions occur, are unclear.

Thirdly, parameters that describe the properties of the chemical are used as input in SimpleBox. As stated in Chapter 6 for the volatile compounds the volatilization rate from the water phase and the degradation rate in air can be regarded as the key parameters. Few data were available on degradation in air. Only degradation by OH radicals is taken into account because it is widely recognized that this degradation route is the most important one. This can be seen, however, as a 'worst case' approach because for some chemicals other mechanisms might contribute to degradation. Next to this the k_{deg} had to be estimated for several compounds. More research into this aspect is needed.

Next to this the way in which SimpleBox is applied here should be discussed. Import of the chemical from outside the system was assumed to occur via the primary compartment, only. For the situation emission to water, the concentration in water from outside was set equal to the $MPC_{aq.}$, while the concentration in air from outside was set equal to zero. It can be remarked that this is not a realistic assumption. However, from calculations not shown here it could be concluded that setting the concentration in air from outside equal to the MPC_{air} didn't influence the C_{ss}/MPC_{air} ratios, as presented in Table 6.4, especially for compounds with already high

ratios.

One of the underlying assumptions of the harmonization procedure is that emissions have remained constant for a sufficiently long period of time that the concentrations in all compartments have become constant in time, i.e. a steady state situation has arisen. In the present report calculations with SimpleBox were carried out at MPC and NC level (see Table 6.4). With respect to calculations at NC level it can be argued that NCs or target values derived from them may be compared with the steady state concentrations calculated by the model because of the fact that these NCs or target values are meant to reflect what is in policy terms called the long term objective for the environment. In the long term concentrations in the environment should be reached at which risks for man and the ecosystem are negligible [1]. It seems reasonable to assume that when the environmental policy is successful with respect to maintaining concentrations at NC level, a steady state situation may have been reached.

With respect to calculations at MPC level the situation may be different. MPCs or limit values derived thereof, must be reached within a specific timescale (years). According to the environmental policy in The Netherlands these limit values should not be exceeded. Therefore, the principle of setting a time limit for reaching concentrations lower than the limit value is in conflict with the procedure for harmonization of quality objectives on the basis of longer term environmental policy that leads to steady state concentrations. However, since for the volatile compounds discussed here dynamic model calculations show that this steady state situation is reached fairly quick (days), it is allowed to use these steady state concentrations also for harmonization at MPC level. For future applications of the model with other types of compounds, e.g. metals, this may be different.

Summarizing, it is recognized that many uncertainties are still present in the harmonization procedure applied in the present report for these volatile compounds. Much work remains to be done with respect to the further development and improvement of the model SimpleBox as well as to further testing of the procedure itself, e.g. testing other type of compounds than the volatile ones dealt with here. It should be emphasized that, until now, models like SimpleBox have been applied mainly for scientific purposes. The concept has proved to be useful as a tool to gain insight into the environmental fate of chemicals due to intermedia transport- and transformation processes. Although the environmental science on which the model is built is well established, the validity of the multimedia box modelling concept to serve specific purposes, as the present one, has never been tested adequately. The harmonization procedure described in paragraph 3.3 to test the coherence of MPCs and NCs must therefore be considered as a scientifically sound, nevertheless 'non-validated' concept. It is believed that the application of the model SimpleBox and consequently the adjustment of MPC and NC values, is justified by the lack of alternatives.

8.3 Use of preliminary $MPC_{a,t,r}$s

For several compounds only preliminary $MPC_{a,t,r}$s could be derived due to a lack of toxicological information (see Table 2.5). As stated already these values should not be used to set limit and target values for air. However, they can still be used for other purposes with the restriction that they are based on toxicological as well as ecotoxicological data. This means that the preliminary $MPC_{a,t,r}$s for 1,3-dichloropropane and 2,3-dichloropropene should be excluded (see Table 2.5).

First of all they could be used as a means to assess the air quality by comparing them with actual concentrations as has been done in paragraph 7.1. Secondly, they can be used for an

initial harmonization: outcome of the model calculations with SimpleBox can be used as an indication about the coherence of the MPC values. In Table 6.4 C_{ss}/MPC_{air} ratios have been presented for the compounds for which preliminary MPC_{air}s have been derived. Based on the adjustment procedure described in paragraph 6.5 the $MPC_{aq.}$s for 1,2-dichloroethene, 1,1,2,2-tetrachloroethane and 1,1,2-trichloroethane must be adjusted with a factor 20, 2100 and 60, respectively. For the other compounds ratios are less than one which means that the MPCs and NCs can be regarded as a coherent set of values. This can be underpinned further, because if more toxicological information becomes available probably a higher MPC_{air} will be derived compared to the preliminary MPC_{air}, caused by the use of lower uncertainty factors. With respect to the 3 compounds for which steady state concentrations in air are higher than the preliminary MPC_{air} the following can be remarked:

- 1,2-dichloroethene and 1,1,2-trichloroethane: preliminary MPC_{air}s are lower than the isomers: 0.18 times lower than the MPC_{air} for 1,1-dichloroethene and 0.004 times lower than the one for 1,1,1-trichloroethane, respectively. The preliminary MPC_{air} for 1,1,2-trichloroethane is based on oral toxicity data using an uncertainty factor of 1,000, while the MPC_{air} for 1,1,1-trichloroethane is based on inhalation toxicity data using an uncertainty factor of 100 [20]. The preliminary MPC_{air} for 1,2-dichloroethene is based on inhalation toxicity data using an uncertainty factor of 10,000, while the MPC_{air} for 1,1-dichloroethene is based on inhalation toxicity data using an uncertainty factor of 100 [20]. It is possible that if more toxicological data become available for 1,2-dichloroethene and 1,1,2-trichloroethane derived MPC_{air}s will be higher than the preliminary MPC_{air}s and steady state concentrations in air will be lower than these MPC_{air}s.
- 1,1,2,2-tetrachloroethane: the preliminary MPC_{air} for this compound is lower than all the other ones including the MPC_{air}s and limit values presented in Table 2.4, even lower than compounds which are considered as genotoxic carcinogens. The preliminary MPC_{air} may be an overestimation, but it cannot be excluded that the MPCs for the different compartments are not coherent.

8.4 Environmental concentrations

Conclusion from the comparison of the available actual concentrations with MPCs, NC, limit or target values is that for most compounds these levels are not exceeded. Often data were not available, however. For soil, sediment and surface water this is not regarded as a problem because these compartments are not the ones considered 'at risk', due to the volatile properties of the compounds discussed in the present report. Exceptions are penta- and hexachlorobenzene: due to their low water solubility these compounds have a potential to accumulate in sediments or soil.

Air and maybe also groundwater can be considered as compartments at risk for the volatile compounds dealt with in the present report. Because several compounds do not degrade, or degrade at a very low rate, in the environment and have a low adsorbing capacity they may end up in groundwater as a result of spills or amospheric depostion. Before measurements are carried out for these compartments, of course aspects like toxicity (level of the MPC or NC of the compound considered compared to MPC or NC levels of other compounds) production volume and use in The Netherlands should be taken into account.

9. REFERENCES

1. National Environmental Policy Plan (1989). To choose or to lose. Second Chamber, session 1988-1989, 21137, no. 1-2.

2. Premises for risk management (1989). Risk limits in the context of environmental policy. Second Chamber, session 1988-1989, 21137, no. 5.

3. Van de Meent, D., Aldenberg, T., Canton, J.H., Van Gestel, C.A.M., and Slooff, W. (1990). Desire for levels. Background study for the policy document "Setting environmental quality standards for water and soil". RIVM report No. 670101 002.

4. Notitie milieukwaliteitsdoelstellingen bodem en water (1991). Tweede Kamer, vergaderjaar 1990-1991, 21990, no 1 (in Dutch).

5. Van de Plassche, E.J., and De Bruijn, J.H.M. (1992). Towards integrated environmental quality objectives for surface water, ground water, sediment and soil for nine trace metals. RIVM report No. 679101 005.

6. Van der Kooij, L.A., Van de Meent, D., Van Leeuwen, C.J., and Bruggeman, W.A. (1991). Deriving quality criteria for water and sediment from the results of aquatic toxicity tests and production standards: application of the equilibrium partitioning method. Wat. Res. **25**, 679-705.

7. Slooff, W., et al. (1992). RIVM guidance document. Ecotoxicological effect assessment: deriving Maximum Tolerable Concentrations (MTC) from single-species toxicity data. RIVM report No. 719102 018.

8. Di Toro, D.M., Zarba, C.S., Hansen, D.J., Berry, W.J., Schwartz, R.C., Cowan, C.E., Pavlou, S.P., Allen, H.E., Thomas, N.A., and Paquin, P.R. (1991). Technical basis for establishing sediment quality criteria for nonionic organic chemicals using equilibrium partitioning. Environ. Toxicol. Chem. **10**, 1541-1583.

9. Advies Commissie voor de Waterverontreiniging inzake de Nota Milieukwaliteits-doelstellingen Bodem en Water. Raad van de Waterstaat, 23-05-1991, Den Haag (in Dutch).

10. Advies notitie Milieukwaliteitsdoelstellingen bodem en water. Coördinatiecommissie Uitvoering Wet Verontreiniging Oppervlaktewateren, 22-04-1991, Den Haag (in Dutch).

11. Directoraat-Generaal Milieubeheer, Directie Stoffen en Risicobeheersing (1991). Integratie normstelling voor lucht met bodem en water. Verslag van de Workshop van 8 oktober 1991 gehouden in het kader van het Project Integrale Normstelling Stoffen (in Dutch).

12. Van de Plassche, E.J., Polder, M.D., and Canton, J.H. (1993). Derivation of Maximum Permissible Concentrations for several volatile compounds for water, sediment and soil. RIVM report No. 679101 008.

13. Rademaker, B.C. and Van de Plassche, E.J. (1993). The derivation of Maximum Permissible Concentrations of several volatile compounds in air. RIVM report No. 679101 010.

14. OECD (1992). Report of the OECD workshop on the extrapolation of laboratory aquatic toxicity data to the real environment. OECD Environment Monographs No. 59, Paris.

15. Aldenberg, T., and Slob, W. (1993). Confidence limits for hazardous concentrations based on logistically distributed NOEC toxicity data. Eotox. Environ. Saf. **25**, 48-63.

16. Van Leeuwen, C.J., Van der Zandt, P.T.J., Aldenberg, T., Verhaar, H.J.M., and Hermens, J.L.M. (1992). Application of QSARs, extrapolation and equilibrium partitioning in aquatic effects assessment. I. Narcotic industrial pollutants. Environ. Toxicol. Chem. **11**, 267-282.

17. Verhaar, H.J.M., and Hermens, J.L.M. (1991). Quantitative structure-activity relationships of environmental pollutants: an outline for application within hazard assessment of new and existing chemicals. RITOX, Utrecht.

18. Slooff, W., Bremmer, H.J., Hesse, J.M., and Matthijsen, A.J.C.M. (eds.) (1991). Integrated Criteria Document Chlorobenzenes. RIVM report No. 710401 015.

19. Hulzebos, E.M., Adema, D.M.M., Dirven-van Breemen, E.M., Henzen, L., Van Dis, W.A., Herbold, H.A., Hoekstra, J.A., Baerselman, R., and Van Gestel, C.A.M. (1993). Phytotoxicity studies with *Lactuca sativa* in soil and nutrient solution. Environ. Toxicol. Chem. **12**, 1079-1094.

20. Rademaker, B.C., Guineé, E.P., and Van de Plassche, E.J. (1993). The derivation of preliminary Maximum Permissible Concentrations of volatile compounds in air. RIVM report No. 679101 009.

21. Maximum Permissible Concentrations, Negligible Concentrations, limit and target values for several volatile compounds. Notation for project "Setting integrated environmental quality objectives" by E. Guinée and T. Blom (ministry of Housing, Physical Planning and the Environment), 23-03-1993 (in Dutch).

22. Indicatief Meerjarenprogramma Lucht 1985-1989. Tweede Kamer, sessie 18605, no. 1-2 (in Dutch).

23. Slooff, W. (1991). Exploratory report ethylene. RIVM report No. 710410 010.

24. Van Swieten, C.W.M., Hauwert, P.C.M., and Keulen, R.W. (1992). Evaluatie en berekening luchtkwaliteit trends van 8 prioritaire stoffen. TNO-report no. R92/118 (in Dutch).

25. Van de Meent, D. (1993). SIMPLEBOX: a generic multimedia fate evaluation model. RIVM report No. 672720 001.

26. Mackay, D. (1991). Multimedia environmental models: the fugacity approach. Lewis Publishers, Inc., Chelsea, Michigan.

27. Van de Meent, D., and De Bruijn, J.H.M. (submitted). A modelling procedure to evaluate the coherence of independently derived environmental quality objectives for air, water and soil. Environ. Toxicol. Chem.

28. De Bruijn, J., Guinée, E., and Van de Meent, D. (1993). Rekening houden met atmosferische depositie in normstelling en bodembeleid. In: Proceedings symposium "Atmosferische depositie en bodemkwaliteit". VVM, Vereniging Lucht en TCB, Den Haag, pp 55-67 (in Dutch).

29. Lincoff, A.H., and Gossett, J.M. (1984). The determination of Henry's law constant for volatile organics by equilibrium partitioning in closed systems. In: Gas transfer at water surfaces. Brusasert, W. and Girka, G.H. (eds.) Reidel, Dordrecht.

30. Mackay, D., Shiu, W.Y., and Sutherland, R.P. (1979). Determination of Henry's law constants for hydrophobic pollutants. Environ. Sci. Technol. **13**, 333-337.

31. Suntio, L.R., Shiu, W.Y., Mackay, D., Seber, J.N., and Glotteity, D. (1988). Critical review of Henry's law constants for pesticides. Rev. Environ. Contam. Toxicol. **103** ,1-59.

32. Ten Hulscher, Th.E.M., Van der Velde, L.E., and Bruggeman, W.A. (1992). Temperature dependence of Henry's law constants for selected chlorobenzenes, polychlorinated biphenyls and polycyclic aromatic hydrocarbons. Environ. Toxicol. Chem. **11**, 1595-1603.

33. Ashworth, R.A. (1988). Air-water partitioning coefficients of organics in dilute aqueous solutions. J. Hazardous Materials **18**, 25-36.

34. MacKay, D., and Shiu, W.Y. (1981). A critical review of Henry's law constants for chemicals of environmental interest. J. Phys. Chem. Ref. Data. **10**, (4), 1175-1199.

35. DGW/RIZA (1990) Jaarboek van afvoeren, waterstanden, golven en waterkwaliteit. 1990. Dienst Getijdewateren en RIZA, Rijkswaterstaat, Den Haag/Lelystad (in Dutch).

36. Atkinson, R. (1985). Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds under atmospheric conditions. Chem. Rev. **85**, 69-201.

37. Crutzen, P.J. (1982). In: Atmospheric chemistry. Goldberg, D.G. (eds.) Ann Arbor Press, MI, pp. 318-328.

38. De Leeuw, F. (1993). Assessment of the atmospheric hazards and risks of new chemicals. RIVM report No. 679102 017.

39. Gerstl, Z. (1990). Estimation of organic chemical sorption by soils. J. Contaminant Hydrology **6**, 357-375.

40. Bockting, G.J.M., Van de Plassche, E.J., Struijs, J., and Canton, J.H. (1993). Soil-water partition coefficients for organic compounds. RIVM report. 679101 013.

41. OECD (1992). Report of the OECD workshop on effects assessment of chemicals in sediment. OECD Environment Monograph No. 60. Paris.

42. MEDCHEM database (1992) Database and calculation method for K_{ow} values. Developed at Pomona College, Claremont, California.

43. Leo, A., Hansch, C., and Elkins, D. (1971). Partition coefficients and their uses. Chemical Rev. **71**, (6), 525-616.

44. Verhaar, H.J.M., en Hermens, J.L.M. (1990). QSAR System. Een evaluatie. Deel 2: Beschrijving van de afzonderlijke modulen van het QSAR Systeem, inklusief validering aan de hand van een toetsingsset. RITOX rapport, Rijks Universiteit Utrecht (in Dutch).

45. Struijs, J., and Van den Berg, R. (submitted). Standardized biodegradability tests: extrapolation to aerobic environments. Wat. Res.

46. Adema, D.M.M. and L. Henzen (1989). A comparison of plant toxicities of some industrial chemicals in soil culture and soilless culture. Ecotox. Environ. Saf. **18**, 219-229.

47. RIVM (1991). Milieudiagnose 1991, II Luchtkwaliteit. RIVM report No. 222101 022 (in Dutch).

48. Bloemen, H. (1993). Personal communication, RIVM, Bilthoven.

49. Vossen, M. and A. Wilting (1993). Toetsing van actuele concentraties vluchtige verbindingen aan in INS-kader afgeleide MTR- en VR-waarden. RIZA, Werkdocument 93.108X (in Dutch).

50. Lagas, P., Van Maaren, H.L.J., Van Zoonen, P., Baumann, R.A., and Heusinkveld, H.A.G. (1991). Onderzoek naar het vóórkomen van bestrijdingsmiddelen in het grondwater van Nederland. RIVM report No. 725803 003 (in Dutch).

APPENDIX A. HENRY's LAW CONSTANTS (kPa.m^3/mol)

Compound	Experimental				Calculated from Vap. Pressure and Solubility							Recommeded	Remark
	[1]	[2]	[3]	[9]	[4]	[4]	[5]	[6]	[7]	[8]	[10]		
	10 °C	10 °C	10 °C	10 °C	25 °C	25 °C		20 °C	20 °C	25 °C	20 °C	10 °C	
toluene		0.386			0.673	0.654						0.39 [2]	
2-chlorotoluene (o)								0.970				0.49 [6]	calc., temp. corrected*
3-chlorotoluene (m)								0.800				0.40 [6]	calc., temp. corrected
4-chlorotoluene (p)								0.980				0.49 [6]	calc., temp. corrected
benzene		0.334			0.562	0.557						0.33 [2]	
ethylbenzene		0.330			0.854	0.829						0.33 [2]	
monochlorobenzene		0.247			0.348	0.363						0.25 [2]	
1,2-dichlorobenzene		0.165			0.193	0.195						0.17 [2]	
1,3-dichlorobenzene		0.224			0.193	0.366						0.22 [2]	
1,4-dichlorobenzene		0.215			0.240	0.160						0.21 [2]	
1,2,3-trichlorobenzene					0.127	0.234						0.13 [2,4]	assumed equal to 1,2,4-CB
1,2,4-trichlorobenzene		0.131				0.379						0.13 [2,4]	
1,3,5-trichlorobenzene						0.161						0.13 [2,4]	assumed equal to 1,2,4-CB
1,2,3,4-tetrachlorobenzene			0.031			0.261						0.03 [3]	
1,2,3,5-tetrachlorobenzene			0.050		0.159	0.593						0.05 [3]	
1,2,4,5-tetrachlorobenzene						0.261						0.04 [3]	average of tetra-CB
pentachlorobenzene			0.030			0.977	−0.49					0.03 [3]	
hexachlorobenzene			0.021			0.005 (20 °C)						0.02 [3]	
1,1-dichloroethane		0.373				0.585						0.37 [2]	
1,2-dichloroethane		0.119			0.099	0.108						0.12 [2]	
1,1,1-trichloroethane		0.978			3.470 (20 °C)	3.060						0.98 [2]	
1,1,2-trichloroethane		0.040				0.122						0.04 [2]	
1,1,2,2-tetrachloroethane		0.033				0.047						0.03 [2]	
pentachloroethane						0.253						0.08 [4]	calc., temp. corrected
hexachloroethane		0.601			1.302							0.60 [2]	
dichloromethane					0.272	0.256						0.09 [4]	temp. corr.
trichloromethane (chloroform)		0.174			0.322	0.385						0.17 [2]	
tetrachloromethane		1.500			2.160	2.271						1.50 [2]	
ethene						21.700						7.23 [4]	calc., temp. corrected
chloroethene (vinylchloride)		1.520			117.600 (10 °C)	105.600 (10 °C)						1.52 [2]	
1,1-dichloroethene		1.560			15.610 (20 °C)	13.320						1.56 [2]	
1,2-dichloroethene		0.167				0.715						0.17 [2]	average of cis and trans
trichloroethene	0.158	0.545			0.904	1.240						0.35 [1,2]	
tetrachloroethene		0.857			1.239	1.985						0.86 [2]	
1,2-dichloropropane		0.124				0.365						0.12 [2]	
1,3-dichloropropane						0.180 (10 °C)						0.18 [4]	calc.
3-chloropropene										0.833		0.28 [8]	calc., temp. corrected
1,3-dichloropropene										0.208		0.07 [8]	calc., average cis and trans
2,3-dichloropropene										0.365		0.12 [8]	calc., temp. corrected

HENRY's LAW CONSTANTS (kPa.m^3/mol)

Compound	Experimental					Calculated from Vap. Pressure and Solubility						Recommeded	Remark
	[1]	[2]	[3]	[9]	[4]	[4]	[5]	[6]	[7]	[8]	[10]		
	10 °C	10 °C	10 °C	10 °C	25 °C	25 °C		20 °C	20 °C	25 °C	20 °C	10 °C	
1,2–xylene (o)		0.289				0.511						0.29 [2]	
1,3–xylene (m)		0.416				0.733						0.42 [2]	
1,4–xylene (p)		0.426				0.702						0.43 [2]	
acrylonitril									0.008			0.004 [7]	calc., temp. corrected
ethyleneoxyde				29.80 **								29.80 [9]	
styrene							1.249					0.42 [5]	calc., temp. corrected
2–chloro–1,3–butadiene											0.392	0.20 [4]	calc., temp. corrected

* Lowered by factor 2 (20 °C) or 3 (25 °C).
** Derived from experimentally measured volatilization rates.

[1] Nicholson, B.C., Maguire, B.P., Bursill, D.B. (1984) Henry's law constants for the trihalomethanes: Effects of water composition and temperature. Environ. Sci. Technol. 18:518-521.
[2] Ashworth, R.A. (1988) Air-water partitioning coefficients of organics in dilute aqueous solutions. J. Hazardous Materials 18:25-36.
[3] Ten Hulscher, Th.E.M., Van der Velde, L.E. and Bruggeman, W.A. (1992) Temperature dependence of Henry's law constants for selected chlorobenzenes, polychlorinated biphenyls and polycyclic aromatic hydrocarbons. Environ. Toxicol. Chem. 11:1595-1603.
[4] MacKay, D. and Shiu, W.Y. (1981) A critical review of Henry's law constants for chemicals of environmental interest. J. Phys. Chem. Ref. Data. 10(4):1175-1199.
[5] Thomas, R.G. (1990) Chapter 15 in: Lyman, W.J. et al. Handbook of physical chemical property estimation methods. American Chemical Society, Washington, DC.
[6] BUA (1989) Bundes Umwelt Ambt. Gesellschaft Deutscher Chemiker-Advisory Committee on Existing Chemicals of Environmental Relevance. Chlorotoluenes, BUA report.
[7] Ministerie van VROM (1984) Criteriadocument over acrylonitril. Publikatiereeks lucht 29. Staatsdrukkerij, Den Haag.
[8] Krijgsheld, K.R. and Van der Gen, A. (1986) Assessment of the impact of the emission of certain organochlorine compounds on the aquatic environment. Part II Allylchloride, 1,3- and 2,3-dichloropropene. Chemosphere 15:861-880.
[9] Conway, R.A., Waggy, G.T., Spiegel, M.H., Berglund, R.L. (1983) Environmental fate and effects of ethylene oxide. Environ. Sci. Technol. 17: 102-112.
[10] ASTER (1993) Assessment Tools for Evaluation of Risk. Environmental Research Laboratories, US Environmental Protection Agency, Duluth.

APPENDIX B. MODEL SETTINGS AND INPUT PARAMETERS FOR SIMPLEBOX

In this appendix model settings and input parameters for SimpleBox, used for the calculations as presented in paragraph 6.3 are given.

Environment characteristics	
volume: air	$3.80 * 10^{13}$ m^3
volume: water	$1.42 * 10^{10}$ m^3
volume: suspended matter	$8.90 * 10^{5}$ m^3
volume: biota	$5.93 * 10^{5}$ m^3
volume: sediment	$1.42 * 10^{8}$ m^3
volume: soil 1	$7.88 * 10^{8}$ m^3
volume: soil 2	$3.42 * 10^{9}$ m^3
volume: soil 3	$1.90 * 10^{7}$ m^3
system area	$3.80 * 10^{10}$ m^2
fraction area water	12.5 %
fraction area soil 1	41.5 %
fraction area soil 2	45.0 %
fraction area soil 3	1.0 %
atmospheric mixing height (air)	1000 m
depth (water)	3 m
depth (sediment)	0.03 m
depth soil 1 and 3	0.05 m
depth soil 2	0.20 m
concentration suspended matter	$1.5 * 10^{-2}$ kg/m^3
concentration biota	$1.0 * 10^{-3}$ kg/m^3
RHO (suspended matter)	$1.14 * 10^{3}$ kg/m^3
RHO (biota)	$1.01 * 10^{3}$ kg/m^3
RHO (sediment)	$1.28 * 10^{3}$ kg/m^3
RHO (soil 1, 2, 3)	$1.50 * 10^{3}$ kg/m^3
fraction water (suspended matter)	90 %
fraction water (biota)	99 %
fraction water (sediment)	80 %
fraction air (soil)	20 %
fraction water (soil)	30 %
fraction solid (soil)	50 %
RHO (solid phase)	$2.40 * 10^{3}$ kg/m^3
residence time (air)	0.50 d[a]
windspeed	5.0 m/s[b]
hydraulic residence time (water)	63.4 d
sum of discharges streams crossing system boundaries	$2.6 * 10^{3}$ m^3/s
sum runoff from soils into water compartment	$4.0 * 10^{2}$ m^3/s

Compound properties	
compound name	
formula	
molecular weight	(g/mol)
K_{ow}	
vapour pressure	(Pa)
water solubility	(mg/l)
result test ready biodegradability	yes/no
K_{aw} (air-water)	
air-water interface temperature	12 °C
K_p (suspended matter-water)	l/kg
C_{org} (suspended matter)	10 %
K_p (sediment-water)	l/kg
C_{org} (sediment)	5 %
K_p (soil-water)	l/kg
C_{org} (soil 1, 2, 3)	5 %
BCF (fish)	l/kg
percentage fat (fish)	5 %

C_{org}	organic carbon content
soil 1	natural soil
soil 2	agricultural soil
soil 3	industrially used soil

APPENDIX C. CONCENTRATIONS IN AIR MEASURED IN THE NETHERLANDS ($\mu g/m^3$)

Compound	1991 street Apeldoorn [1]	1991 urban Dordrecht [1]	1991 urban Rotterdam [1]	1991 rural Wijnandsrade [1]	1991 rural Zegveld [1]	1991 rural Witteveen [1]	1992 rural Houtakker [2]	1986 suburban Bilthoven [2]	1991/1991 rural Moerdijk [3]	1982/1983 urban Vlaardingen [4]	average rural
toluene	21.40	8.51	9.37	7.03	3.00	1.47	2.8	5.5			3.58
2-chlorotoluene (o)											
3-chlorotoluene (m)											
4-chlorotoluene (p)											
benzene	5.94	3.14	3.73	2.83	1.28	0.87	1.4	2.8			1.60
ethylbenzene	3.65	1.73	2.07	1.17	0.52	0.24	0.6	1.0			0.63
monochlorobenzene	0.012	0.001	0.022	0.000	0.000	0.007		<0.5			0.0023
1,2-dichlorobenzene	0.138	0.024	0.064	0.029	0.022	0.003		<0.5			0.0180
1,3-dichlorobenzene	0.013	0.003	0.000	0.000	0.009	0.000		<0.5			0.0030
1,4-dichlorobenzene	0.198	0.099	0.170	0.000	0.000	0.000		<0.5			0.0000
1,2,3-trichlorobenzene	0.130	0.010	0.000	0.010	0.001	0.000		<0.5			0.0037
1,2,4-trichlorobenzene	0.023	0.006	0.002	0.001	0.001	0.000		<0.5			0.0007
1,3,5-trichlorobenzene	0.015	0.003	0.049	0.000	0.001	0.000		<0.5			0.0003
1,2,3,4-tetrachlorobenzene											
1,2,3,5-tetrachlorobenzene											
1,2,4,5-tetrachlorobenzene											
pentachlorobenzene											
hexachlorobenzene											
1,1-dichloroethane											
1,2-dichloroethane	1.13	0.33	0.85	0.29	0.00	0.00		2.0			0.10
1,1,1-trichloroethane	2.17	1.38	1.53	1.25	0.97	0.85		1.6			1.02
1,1,2-trichloroethane								<0.5			<0.5
1,1,2,2-tetrachloroethane										0.0007	0.0007
pentachloroethane											
hexachloroethane											
dichloromethane											
trichloromethane (chloroform)	0.13	0.14	0.16	0.11	0.08	0.12		0.3			0.10
tetrachloromethane	1.62	0.95	0.90	0.91	0.50	0.52		0.7			0.64
ethene							1.6		5.53		3.57
chloroethene (vinylchloride)											
1,1-dichloroethene											
1,2-dichloroethene											
trichloroethene	0.95	0.61	0.71	0.72	0.40	0.18		0.6			0.43
tetrachloroethene	0.78	0.45	0.53	0.42	0.26	0.18		0.8			0.29
1,2-dichloropropane	2.66	1.66	1.20	1.08	0.31	0.17		0.3			0.52
1,3-dichloropropane											
3-chloropropene											

CONCENTRATIONS IN AIR MEASURED IN THE NETHERLANDS ($\mu g/m^3$)

Compound	1991 street Apeldoorn [1]	1991 urban Dordrecht [1]	1991 urban Rotterdam [1]	1991 rural Wijnandsrade [1]	1991 rural Zegveld [1]	1991 rural Witteveen [1]	1992 rural Houtakker [2]	1986 suburban Bilthoven [2]	1991/1991 rural Moerdijk [3]	1982/1983 urban Vlaardingen [4]	average rural
1,3-dichloropropene											
2,3-dichloropropene											
1,2-xylene (o)	4.24	1.88	2.21	1.21	0.52	0.24	1.0	0.9			0.74
1,3-xylene (m)	7.88	4.02	4.72	2.43	1.07	0.54	1.1 *	2.2 *			1.35
1,4-xylene (p)	2.65	1.04	1.22	0.81	0.33	0.11	1.1 *	2.2 *			0.42
acrylonitril											
ethyleneoxyde											
styrene	0.62	0.30	0.45	0.27	0.10	0.12					0.16
2-chloro-1,3-butadiene											

* sum of 1.3- and 1.4-xylene
** urban, no rural value available

[1] RIVM (1991) Milieudiagnose 1991, II Luchtkwaliteit, Rapportnummer 222101022, Bilthoven.
[2] Bloemen, H. (1993) personal communication, RIVM, Bilthoven.
[3] Thijsse, Th.R. (1993) Koolwaterstoffen in Noord-Brabant. Bepaling van de grootschalige koolwaterstofniveaus over de provincie in de periode maart 1991 tot en met februari 1992. IMW-TNO-rapport (in preparation), Delft.
[4] Thijsse, Th.R. en Huygen, C.(1985) Grootschalige achtergrondconcentraties van spoorelementen en verbindingen in Nederlandse buitenlucht. TNO-rapport R 85/272, Delft.

APPENDIX D. CONCENTRATIONS IN SURFACE WATER MEASURED IN THE NETHERLANDS

Monitoring data from the Cooperating Rhine and Meuse Waterworks (in Dutch: RIWA) for 1990 and 1991. Data are presented per compound and per location. The following data selection was carried out:

- only one analysis result present for a location:this result is given,
- 2 analysis results present for a location: minimum and maximum is given,
- more than 2 and less than 10 analysis results present for a location: median is given,
- 10 or more analysis results present for a location: median, 10 and 90 percentile is given.

compound	location	concentration (µg/l)					
		one result	minimum	maximum	median	10 percentile	90 percentile
benzene	IJsselmeer (Andijk)				<0.10		
	Maas (Eysden)	0.10					
	Lek (Hagestein)				<0.10	<0.10	<0.10
	Lek (Hagestein)				<0.10	<0.10	0.10
	Maas (Keizersveer)				<0.10	<0.10	<0.10
1,2-dichlorobenzene	Maas (Eysden)				<0.10		
	Lek (Hagestein)				<0.10		
	Lek (Hagestein)				<0.10		
1,3-dichlorobenzene	Maas (Eysden)	<0.10					
	Lek (Hagestein)		<0.10	<0.10			
	Lek (Hagestein)				<0.10	<0.10	<0.10
1,4-dichlorobenzene	Maas (Eysden)	0.10					
dichlorobenzene	Maas (Eysden)	<0.10					

compound	location	concentration (µg/l) one result	minimum	maximum	median	10 percentile	90 percentile
1,2-dichloroethane	Maas (Eysden)				0.10	<0.10	0.10
	Lek (Hagestein)	<0.10					
	Maas (Keizersveer)	<0.10					
	IJsselmeer (Andijk)				<2.0	<2.0	<2.0
	afgedamde Maas (Brakel)				<2.0	<2.0	<2.0
	Maas (Eysden)				<2.0	<2.0	<2.0
	Lek (Hagestein)				<0.10	<0.10	0.10
	Maas (Keizersveer)				<2.0	<2.0	<2.0
1,1-dichloroethene	Maas (Eysden)				<0.10		
1,2-dichloroethene	Maas (Eysden)	0.20					
	Maas (Keizersveer)	<0.10					
dichloromethane	IJsselmeer (Andijk)				<2.0	<2.0	<2.0
	afgedamde Maas (Brakel)				<0.50	<0.50	<0.50
	Maas (Eysden)				<0.50	<0.50	1.3
	Maas (Keizersveer)				<0.50	<0.50	<0.50
1,2-dichloropropane	afgedamde Maas (Brakel)				<0.40	<0.40	<0.40
	Maas (Eysden)				<0.40	<0.40	<0.40
	Haringvliet (Stellendam)				<0.10	<0.10	<0.50
	Maas (Keizersveer)				<0.40	<0.40	<0.40
ethylbenzene	IJsselmeer (Andijk)				<0.10		
	Lek (Hagestein)				<0.10	<0.10	<0.10
	Maas (Keizersveer)	0.10					
	Lek (Hagestein)				<0.10		

compound	location	concentration (µg/l) one result	minimum	maximum	median	10 percentile	90 percentile
ethylbenzene	Maas (Keizersveer)				<0.20	<0.20	<0.20
hexachlorobenzene	IJsselmeer (Andijk)				<0.010	<0.010	<0.020
	Maas (Belfeld)				<0.010	<0.010	<0.010
	afgedamde Maas (Brakel)				<0.010	<0.010	<0.010
	Maas (Eysden)				<0.010	<0.005	<0.010
	Gat v/d Kerksloot (Inlaat de Gijster)				<0.010		
	Lek (Hagestein)				<0.010		
	Haringvliet (Stellendam)				<0.010	<0.005	<0.010
	Maas (Keizersveer)				<0.010	<0.005	<0.010
	Rijn (Lobith)				<0.010	<0.010	<0.010
	Lekkanaal (Nieuwegein)				<0.010	<0.010	<0.010
monochlorobenzene	IJsselmeer (Andijk)				<0.10		
	Lek (Hagestein)				<0.10		
	Maas (Keizersveer)				<0.10	<0.10	<0.10
1,1,2,2-tetrachloroethane	IJsselmeer (Andijk)				0.20		
	Maas (Keizersveer)		<0.10	0.10			
	IJsselmeer (Andijk)				<0.10	<0.10	<0.10
	Maas (Eysden)	<0.10					
	Lek (Hagestein)		0.10	0.10			
	Haringvliet (Stellendam)	<0.10					
tetrachloroethene	Maas (Eysden)				0.20	<0.10	0.30
	Lek (Hagestein)				<0.10	<0.10	<0.10
	Maas (Keizersveer)				0.10	<0.10	0.10
	Rijn (Lobith)	<0.10					

compound	location	concentration (µg/l) one result	minimum	maximum	median	10 percentile	90 percentile
tetrachloroethene	IJsselmeer (Andijk)				<0.10	<0.10	<0.10
	afgedamde Maas (Brakel)				<0.010	<0.010	<0.010
	Maas (Eysden)				0.22	0.030	0.59
	Lek (Hagestein)				<0.10	<0.10	0.10
	Haringvliet (Stellendam)				<0.10	<0.10	<0.50
	Maas (Keizersveer)				0.060	<0.010	0.18
	Rijn (Lobith)				<0.10	<0.10	0.10
trichlorobenzene	Maas (Eysden)		<0.10	<0.10			
1,1,1-trichloroethane	Maas (Eysden)				0.10		
	Lek (Hagestein)	<0.10					
	IJsselmeer (Andijk)				<0.10	<0.10	<0.10
	afgedamde Maas (Brakel)				<0.10		
	Maas (Eysden)				0.20	<0.010	0.64
	Lek (Hagestein)				<0.10	<0.10	0.10
	Haringvliet (Stellendam)	<0.10					
	Maas (Keizersveer)				0.040	<0.10	0.16
	Rijn (Lobith)				<0.10	<0.10	<0.10
1,1,2-trichloroethane	Maas (Eysden)				<0.10		
	Lek (Hagestein)	<0.10					
	IJsselmeer (Andijk)				<0.10	<0.10	<0.10
	Maas (Eysden)	<0.10					
	Lek (Hagestein)				<0.10		
	Haringvliet (Stellendam)	<0.10					
trichloroethene	Maas (Eysden)				0.10	<0.10	0.20

compound	location	concentration (µg/l) one result	minimum	maximum	median	10 percentile	90 percentile
trichloroethene	Lek (Hagestein)				<0.10		
	Maas (Keizersveer)				0.10		
	IJsselmeer (Andijk)				<0.10	<0.10	<0.10
	afgedamde Maas (Brakel)				<0.020	<0.020	0.50
	Maas (Eysden)				0.23	<0.020	0.83
	Lek (Hagestein)				<0.10	<0.10	0.10
	Haringvliet (Stellendam)				<0.10	<0.10	<0.50
	Maas (Keizersveer)				<0.020	<0.020	0.24
	Rijn (Lobith)				<0.10	<0.10	<0.10
trichloromethane	IJsselmeer (Andijk)				0.10		
	Maas (Eysden)				<0.10		
	Lek (Hagestein)		<0.10	0.40			
	Maas (Keizersveer)		0.10	0.30			
	IJsselmeer (Andijk)				<0.10	<0.10	<0.10
	afgedamde Maas (Brakel)				<0.050	<0.050	0.22
	Maas (Eysden)				0.10	<0.050	0.28
	Lek (Hagestein)				0.10	<0.10	0.70
	Haringvliet (Stellendam)	<0.10					
	Maas (Keizersveer)				<0.050	<0.050	0.10
	Rijn (Lobith)				0.20	0.10	0.30
tetrachloromethane	IJsselmeer (Andijk)				<0.10	<0.10	<0.10
	afgedamde Maas (Brakel)				<0.10	<0.010	0.91
	Maas (Eysden)				0.020	<0.010	0.32
	Lek (Hagestein)				0.20		
	Haringvliet (Stellendam)	<0.10					
	Maas (Keizersveer)				<0.010	<0.010	0.060

compound	location	concentration (µg/l) one result	minimum	maximum	median	10 percentile	90 percentile
tetrachloromethane	Rijn (Lobith)				<0.10	<0.10	<0.10
toluene	Maas (Keizersveer)				<0.10	<0.10	0.16
2-xylene	Maas (Keizersveer)				<0.20	<0.20	<0.20
3- and 4-xylene	Maas (Keizersveer)				<0.20	<0.20	<0.20

APPENDIX E. CONCENTRATIONS IN GROUNDWATER MEASURED IN THE NETHERLANDS

Only when data were present from the Provincial Grounwater Quality Monitoring Network this is indicated, i.e. for 1,2-dichloropropane and 1,3-dichloropropene. Otherwise data are from the National Groundwater Monitoring Network. Measurements have been carried out in several periods: data are presented for each period separately. The mean, maximum and 90 percentile is presented for sand, clay and peat for two levels: 5-15 and 15-30 meter. Measurements lower than the detection limit were included for calculation of the mean, maximum and 90 percentile. It should be stated that detection limits have changed in time for several compounds.

compound	soil type	depth (m)	concentration (μg/l) mean	maximum	90 percentile
acrylonitrile[a]	sand	5-15	1,000	1,000	1,000
	clay	5-15	1,000	1,000	1,000 (50 percentile)
benzene[a]	sand	5-15	0.33	2.90	0.50
		15-30	0.22	0.50	0.20
	clay	5-15	0.29	0.80	0.50
		15-30	0.24	1.10	0.20
	peat	5-15	0.31	1.20	0.30
		15-30	0.21	0.30	0.20
1,2-dichlorobenzene[a]	sand	5-15	0.39	0.50	0.50
		15-30	0.50	0.50	0.50
	clay	5-15	0.44	0.50	0.50
		15-30	0.50	0.50	0.50
	peat	5-15	0.48	0.50	0.50
		15-30	0.50	0.50	0.50
1,3-dichlorobenzene[a]	sand	5-15	0.39	0.50	0.50
		15-30	0.50	0.50	0.50
	clay	5-15	0.44	0.50	0.50
		15-30	0.50	0.50	0.50
	peat	5-15	0.48	0.50	0.50
		15-30	0.50	0.50	0.50

compound	soil type	depth (m)	concentration (µg/l) mean	maximum	90 percentile
1,4-dichlorobenzene[a]	sand	5-15	0.39	0.50	0.50
		15-30	0.50	0.50	0.50
	clay	5-15	0.44	0.50	0.50
		15-30	0.50	0.50	0.50
	peat	5-15	0.48	0.50	0.50
		15-30	0.50	0.50	0.50
1,1-dichloroethane[a]	sand	5-15	1.01	1.40	1.00
		15-30	1.00	1.20	1.00
	clay	5-15	1.00	1.00	1.00
		15-30	1.00	1.00	1.00
	peat	5-15	1.00	1.00	1.00
		15-30	1.00	1.00	1.00
1,2-dichloroethane[a]	sand	5-15	1.00	19.00	1.00
		15-30	1.00	1.20	1.00
	clay	5-15	1.30	6.00	1.00
		15-30	1.06	2.40	1.00
	peat	5-15	0.98	1.00	1.00
		15-30	1.00	1.00	1.00
1,2-dichloroethane[b]	sand	5-15	10.00	10.00	10.00
		15-30	10.00	10.00	10.00
	clay	5-15	10.00	10.00	10.00
		15-30	10.38	17.50	10.00
	peat	5-15	10.00	10.00	10.00 (80 percentile)
		15-30	10.00	10.00	10.00 (80 percentile)
1,2-dichloroethene[b]	sand	5-15	10.00	10.00	10.00
		15-30	10.00	10.00	10.00
	clay	5-15	10.00	10.00	10.00
		15-30	10.00	10.00	10.00
	peat	5-15	8.04	10.00	10.00 (80 percentile)
		15-30	10.00	10.00	10.00 (80 percentile)

compound	soil type	depth (m)	concentration (μg/l) mean	maximum	90 percentile
dichloromethane[a]	sand	5-15	1.00	1.00	1.00
		15-30	1.00	1.00	1.00
	clay	5-15	1.00	1.00	1.00
		15-30	1.00	1.00	1.00
	peat	5-15	1.00	1.00	1.00
		15-30	1.00	1.00	1.00
dichloromethane[b]	sand	5-15	9.19	10.00	10.00
		15-30	10.00	10.00	10.00
	clay	5-15	9.15	10.00	10.00
		15-30	10.00	10.00	10.00
	peat	5-15	10.00	10.00	10.00 (80 percentile)
		15-30	10.00	10.00	10.00 (80 percentile)
1,2-dichloropropane[c]	sand	5-15	4.92	165	1.90
		5-15	1.00	1.00	1.00
		15-30	0.80	1.54	0.86 (80 percentile)
	clay	5-15	0.58	1.87	0.87
		5-15	1.00	1.00	1.00 (70 percentile)
		15-30	0.42	0.55	0.40
	peat	5-15	0.40	0.40	0.40
1,2-dichloropropane[b]	sand	5-15	13.55	69.20	10.00
		15-30	10.00	10.00	10.00
	clay	5-15	10.00	10.00	10.00
		15-30	10.23	13.00	10.00
	peat	5-15	52.93	224.64	10.00 (80 percentile)
		15-30	10.00	10.00	10.00 (80 percentile)
1,2-dichloropropane[a]	sand	5-15	1.02	2.10	1.00
		15-30	1.00	1.00	1.00
	clay	5-15	1.00	1.00	1.00
		15-30	1.00	1.00	1.00
	peat	5-15	3.83	35.00	1.00
		15-30	1.00	1.00	1.00

compound	soil type	depth (m)	concentration (μg/l) mean	maximum	90 percentile
1,3-dichloropropane[a]	sand	5-15	0.76	1.00	1.00
		15-30	1.00	1.00	1.00
	clay	5-15	0.84	1.00	1.00
		15-30	1.00	1.00	1.00
	peat	5-15	0.96	1.00	1.00
		15-30	1.00	1.00	1.00
1,3-dichloropropene[d]	sand	5-15	0.05	0.05	0.05
(cis and trans)	clay	5-15	0.05	0.05	0.05
ethylbenzene[a]	sand	5-15	0.51	1.00	0.50
		15-30	0.50	0.50	0.50
	clay	5-15	0.50	0.50	0.50
		15-30	0.51	0.70	0.50
	peat	5-15	0.63	2.10	0.50
		15-30	0.50	0.50	0.50
monochlorobenzene[a]	sand	5-15	0.50	0.50	0.50
		15-30	0.50	0.50	0.50
	clay	5-15	0.50	0.50	0.50
		15-30	0.50	0.50	0.50
	peat	5-15	0.50	0.50	0.50
		15-30	0.50	0.50	0.50
styrene[a]	sand	5-15	0.50	0.50	0.50
		15-30	0.50	0.50	0.50
	clay	5-15	0.50	0.50	0.50
		15-30	0.50	0.50	0.50
	peat	5-15	0.54	1.00	0.50
		15-30	0.50	0.50	0.50
tetrachloroethene[a]	sand	5-15	67.19	5,500.00	1.00
		15-30	1.31	19.00	1.00
	clay	5-15	0.84	1.00	1.00
		15-30	1.00	1.00	1.00
	peat	5-15	0.96	1.00	1.00
		15-30	1.00	1.00	1.00

compound	soil type	depth (m)	concentration (μg/l) mean	maximum	90 percentile
tetrachloroethene[b]	sand	5-15	8.05	191.75	0.03
		15-30	0.46	6.00	0.15
	clay	5-15	0.02	0.05	0.03
		15-30	0.06	0.40	0.07
	peat	5-15	0.01	0.02	0.02 (80 percentile)
		15-30	0.42	2.00	0.07 (80 percentile)
tetrachloromethane[b]	sand	5-15	0.02	0.20	0.01
		15-30	0.03	0.15	0.05
	clay	5-15	0.01	0.01	0.01
		15-30	0.01	0.01	0.01
	peat	5-15	0.01	0.01	0.01 (80 percentile)
		15-30	0.01	0.01	0.01 (80 percentile)
toluene[a]	sand	5-15	0.68	6.00	0.95
		15-30	0.54	1.40	0.60
	clay	5-15	0.70	1.80	1.00
		15-30	1.03	12.00	0.60
	peat	5-15	1.19	6.80	1.10
		15-30	0.54	0.80	0.50
1,2,3-trichlorobenzene[a]	sand	5-15	0.06	0.10	0.10
		15-30	0.05	0.05	0.05
	clay	5-15	0.06	0.10	0.10
		15-30	0.05	0.05	0.05
	peat	5-15	0.05	0.07	0.05
		15-30	0.05	0.05	0.05
1,2,4-trichlorobenzene[a]	sand	5-15	0.06	0.10	0.10
		15-30	0.05	0.05	0.05
	clay	5-15	0.06	0.10	0.05
		15-30	0.05	0.05	0.05
	peat	5-15	0.05	0.07	0.05
		15-30	0.05	0.05	0.05

compound	soil type	depth (m)	concentration (µg/l) mean	maximum	90 percentile
1,2,5-trichlorobenzene[a]	sand	5-15	0.06	0.10	0.10
		15-30	0.05	0.05	0.05
	clay	5-15	0.06	0.10	0.10
		15-30	0.05	0.05	0.05
	peat	5-15	0.05	0.07	0.05
		15-30	0.05	0.05	0.05
1,1,1-trichloroethane[a]	sand	5-15	0.75	1.00	1.00
		15-30	1.00	1.00	1.00
	clay	5-15	0.84	1.00	1.00
		15-30	1.00	1.00	1.00
	peat	5-15	0.96	1.00	1.00
		15-30	1.00	1.00	1.00
1,1,1-trichloroethane[b]	sand	5-15	0.10	0.27	0.10
		5-15	1.00	1.00	
		15-30	0.40	2.50	0.21
		15-30	1.00	1.00	1.00
	clay	5-15	3.94	30.2	0.80
		5-15	1.00	1.00	
		15-30	1.74	15	0.85
		15-30	1.00	1.00	1.00
	peat	5-15	0.07	0.10	0.10 (80 percentile)
		5-15	1.00	1.00	1.00 (80 percentile)
		15-30	0.09	0.10	0.10 (80 percentile)
		15-30	1.00	1.00	1.00 (80 percentile)
1,1,2-trichloroethane[a]	sand	5-15	0.75	1.00	1.00
		15-30	1.00	1.00	1.00
	clay	5-15	0.84	1.00	1.00
		15-30	1.00	1.00	1.00
	peat	5-15	0.96	1.00	1.00
		15-30	1.00	1.00	1.00

compound	soil type	depth (m)	concentration (μg/l) mean	maximum	90 percentile
trichloroethene[a]	sand	5-15	1.04	20.00	1.00
		15-30	1.06	4.70	1.00
	clay	5-15	0.84	1.00	1.00
		15-30	1.00	1.00	1.00
	peat	5-15	0.96	1.00	1.00
		15-30	1.00	1.00	1.00
trichloroethene[b]	sand	5-15	0.14	0.95	0.10
		15-30	0.77	9.30	0.10
	clay	5-15	0.15	0.50	0.17
		15-30	0.19	0.55	0.37
	peat	5-15	0.08	0.11	0.10 (80 percentile)
		15-30	0.44	1.50	0.50 (80 percentile)
trichloromethane[b]	sand	5-15	0.86	6.83	2.00
		15-30	0.46	5.20	0.10
	clay	5-15	0.13	0.31	0.10
		15-30	0.11	0.18	0.10
	peat	5-15	16.05	79.45	0.51 (80 percentile)
		15-30	0.10	0.10	0.10 (80 percentile)
1,2-xylene[b]	sand	5-15	0.61	9.00	0.50
		15-30	0.50	0.50	0.50
	clay	5-15	0.51	0.80	0.50
		15-30	0.50	0.50	0.50
	peat	5-15	0.68	2.70	0.50
		15-30	0.50	0.50	0.50
1,3- and 1,4-xylene[b]	sand	5-15	0.58	1.90	0.55
		15-30	0.51	0.90	0.50
	clay	5-15	0.58	1.70	0.50
		15-30	0.53	1.00	0.50
	peat	5-15	1.06	6.60	0.70
		15-30	0.51	0.60	0.50

a measurements from 1987/1988
b measurements from 1979/1984
c measurements from 1990/1991: national and provincial network
d measurements from 1990: national and provincial network