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**Calculation of human-toxicological serious soil
contamination concentrations and proposals for
intervention values for clean-up of soil and groundwater:
Third series of compounds**

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PREFACE

The Directorate General of Environment has commissioned the National Institute of Public Health and Environmental Protection (RIVM) to provide a scientific basis for parts of the Soil Protection Act. An important aspect is the updating of the intervention values for soil clean-up (the former C values).

After a thorough review of 80 chemicals, proposals and procedures for determination were accepted and implemented by the Dutch Parliament (Second Chamber 1993/94, 22727, no.'s 5 and 7). May 1994, intervention values for these 80 substances came into force ('Circular on intervention values for contaminated land', Staatscourant 1994, no.95). Following the first series of 80 chemicals, intervention values were then proposed for the second series of compounds (Van den Berg, 1995). This report represents values proposed for the third series of compounds.

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SUMMARY

Recently implemented have been the thoroughly revised intervention values for soil clean-up. In this report, proposals will be presented for intervention values for 15 additional compounds on the basis of an ecotoxicological and a human-toxicological evaluation. For all compounds the human-toxicological serious soil contamination concentration was calculated using the CSOIL model and the human-toxicological maximum permissible risk levels. The ecotoxicological serious soil contamination concentration was determined by the methodology of Denneman and Van Gestel (1990, 1991), updated by Crommentuijn *et al.* (1994). Proposals for intervention values are determined by means of integrating the ecotoxicological and the human-toxicological serious soil contamination concentrations.

The ecotoxicological serious soil contamination concentrations and the Maximum Permissible Risk levels in this report have been described in detail in report nos. 715810008 and 715810009, respectively.

The proposals for the intervention values are derived according to the procedures described for the first and second series of compounds in a number of previous reports.

Depending on sensitivity and reliability of the input parameters, various efforts have been made to obtain reliable input parameter values. In this report, intervention values for soil and groundwater are proposed for silver, ethylene glycol, diethylene glycol, acrylonitrile, formaldehyde, methanol, 1-butanol, butylacetate, methyl *tert*-butyl ether, 1,1-dichloroethane, 1,1,1-trichloroethane, *cis*-& *trans*-1,2-dichloroethene and a mixture of aromatic solvents (containing high concentrations of C₃ en C₄ alkyl benzenes). For dodecylbenzene a risk evaluation is executed but no intervention value is proposed because of lack of an ecotoxicological serious soil contamination concentration and reliable physicochemical data.

SAMENVATTING

Onlangs zijn voor een groot aantal stoffen de nieuwe interventiewaarden bodemsanering van kracht geworden. In dit rapport worden voorstellen gedaan voor humaan-toxicologisch en ecotoxicologisch onderbouwde interventiewaarden voor een 15-tal nog niet eerder in dit kader beoordeelde stoffen. Voor al deze stoffen is een humaantoxicologische ernstige bodemverontreinigingsconcentratie berekend met behulp van het computermodel CSOIL en het humaan-toxicologisch maximaal toelaatbaar risico. De ecotoxicologische ernstige bodemverontreinigingsconcentratie is bepaald met behulp van de methode van Denneman en Van Gestel (1990, 1991), welke herzien is door Crommentuijn *et al.* (1994). De voorgestelde interventiewaarden komen tot stand door integratie van de ecotoxicologische en de humaan-toxicologische ernstige bodemverontreinigingsconcentratie.

De ecotoxicologische ernstige bodemverontreinigingsconcentraties and humaan-toxicologische maximaal toelaatbare risico's in dit rapport zijn in detail beschreven in respectievelijk rapport 715810008 en 715810009.

De voorstellen zijn tot stand gekomen volgens de methoden die bij de eerste set van stoffen zijn gebruikt en in een aantal rapporten zijn vastgelegd. Afhankelijk van de gevoeligheid en betrouwbaarheid van de inputparameters is meer of minder inspanning geleverd om betrouwbare inputparameterwaarden te verkrijgen. Er worden voorstellen gedaan voor interventiewaarden bodem- en grondwatersanering voor zilver, ethyleenglycol, diethyleenglycol, acrylonitril, formaldehyde, methanol, 1-butanol, butylacetaat, methyl *tert*-butyl ether, 1,1-dichlooroethaan, 1,1,1-trichloorethaan, *cis*- & *trans*-1,2-dichloretheen en een mengsel van aromatische oplosmiddelen dat hoge concentraties aan C₃ en C₄ alkylbenzenen bevat. Voor dodecylbenzeen is een risicoevaluatie uitgevoerd maar er is geen voorstel voor een interventiewaarde gedaan, bij gebrek aan een ecotoxicologische ernstige bodem verontreinigingsconcentratie en aan betrouwbare fysisch-chemische gegevens.

1 INTRODUCTION

This report describes the derivation of human-toxicological serious soil contamination concentrations (HUM-TOX SCCs) for 15 additional compounds and the integration of these concentrations with the ecotoxicological serious soil contamination concentrations (ECOTOX SCCs). The HUM-TOX SCC is derived by using physicochemical data and human-toxicological maximum permissible risk values (MPRs) for calculations with the CSOIL-model. Figure 1 shows the relation between the different steps, resulting in proposals for intervention values. These different steps are described in separate reports. The shaded box (Figure 1) is described in the present report. The derivation of the HC50 and the ECOTOX SCC for the compounds discussed has been described in the report of Crommentuijn *et al.* (1995). The derivation of the MPRs is given in the report of Janssen *et al.* (1995). All relevant information for the derivation of the HUM-TOX SCC and the integration of the ECOTOX SCC and HUM-TOX SCC has been included in the present report.

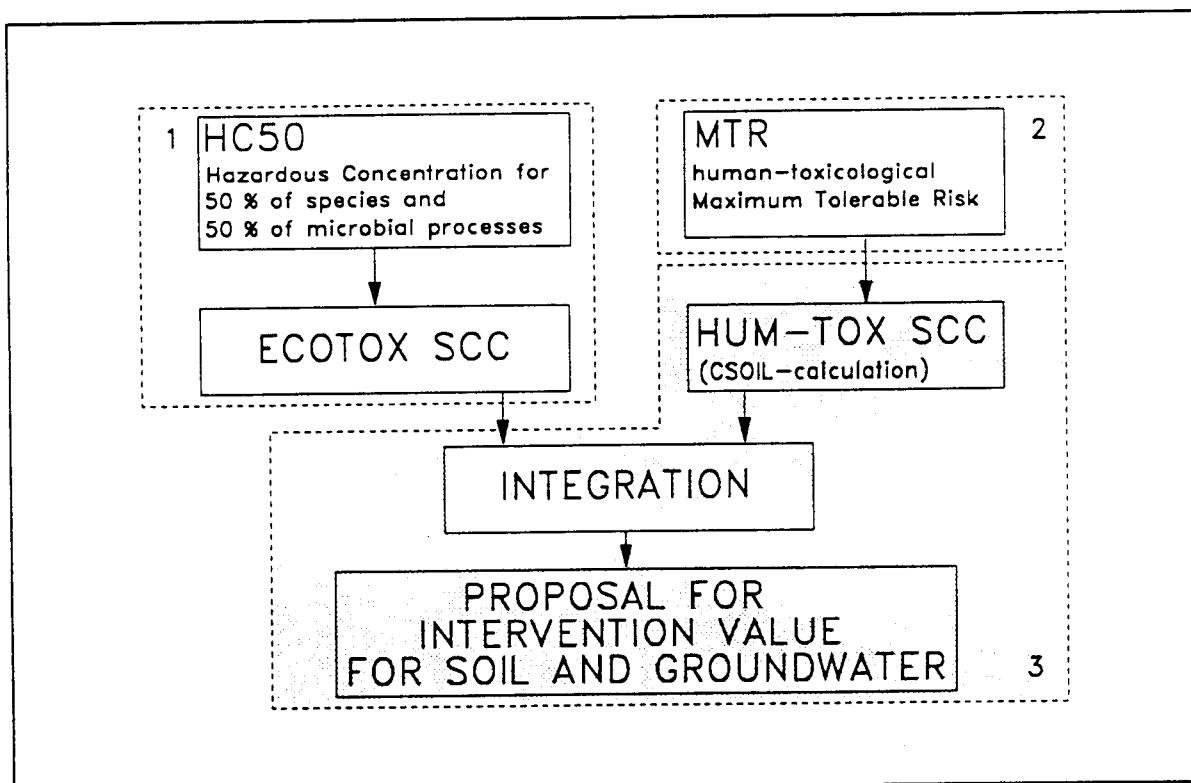


Figure 1. Diagram of pathways leading to proposals for intervention values of soil and groundwater.

1. Report of Crommentuijn *et al.* (1995) no.715810008
2. Report of Janssen *et al.* (1995) no.715810009
3. This report no.715810010

The compounds discussed in this report are: silver as 'metal'; ethylene glycol, diethylene glycol, acrylonitrile, formaldehyde, methanol, 1-butanol, 1-butylacetate, methyl *tert*-butyl ether as organic solvents; dodecylbenzene and aromatic solvents containing C₃ & C₄ alkyl benzenes as aromatic compounds and 1,1,1-trichloroethane, 1,1-dichloroethane and *cis*-and *trans*-1,2-dichloroethene as chlorinated hydrocarbons. These compounds are used for several industrial activities and frequently found on contaminated sites.

Chapter 2 describes the physicochemical properties used for the calculation of the HUM-TOX SCC. In Chapter 3 the ECOTOX SCCs of the compounds, derived by Crommentuijn *et al.* (1995), are given. In Chapter 4 the human-toxicological maximum permissible risk levels derived by Janssen *et al.* (1995) are shown and Chapter 5 describes the human exposure and determination of the HUM-TOX SCCs. Finally, in Chapter 6 the integration of the values results in proposals for intervention values for soil and groundwater.

The proposals for the intervention values will be reviewed by the Technical Soil Protection Committee (TCB) and will be subject to a political discussion before they are implemented as intervention values.

2 PHYSICOCHEMICAL PROPERTIES

2.1 Description of the physicochemical properties

This section describes all physicochemical properties used for the calculation of the HUM-TOX SCC.

2.1.1 Soil-water partition coefficient

The soil-water partition coefficient (K_d) is the ratio between the concentration of a compound in the solid phase of the soil and its equilibrium concentration in the porewater, assuming linearity. The K_d for metals is empirically determined. For organic compounds the K_d is derived from the K_{oc} (the organic carbon normalized soil-water partition coefficient, described in 2.1.7) according to the CSOIL formulas in Appendix IX.

2.1.2 Bioconcentration factor

If vegetables grow on contaminated land, accumulation of compounds (metals) in the plant may occur due to root uptake and dry deposition on the plant. The affinity for accumulation due to root uptake is expressed by the bioconcentration factor (BCF), defined as the ratio of the mass fraction of a compound per kg plant dry weight and per kg soil dry weight (Bockting & Van den Berg, 1992). The BCFs in this report are derived from Baes *et al.* (1984). Accumulation of organic compounds may occur as well, but the root uptake is calculated according to the equations in Appendix IX.

2.1.3 Vapour pressure

The vapour pressure is a measure of the tendency of a substance to pass from a solid or a liquid to a vapour state. It is the pressure of the gas in equilibrium with the liquid or the solid at a given temperature.

Vapour pressures are found in handbooks like Verschueren (1983) and MacKay *et al.* (1992) and review articles like MacKay and Shiu (1981). All vapour pressures were corrected for soil temperature (10°C) according to Lide *et al.* (1993); Chang (1990) and Sawyer & McCarty (1989). In comparison with the first 92 compounds considered, for which vapour pressures of 20 or 25°C were used as input parameters, this temperature correction, results in more reliable output values. The temperature correction will be implemented in the procedure for the derivation of the HUM-TOX SCCs.

2.1.4 Solubility

Solubility data have been collected from review articles (Mackay and Shiu, 1981), handbooks (Verschueren, 1983; Chemiekaarten, 1991; MacKay *et al.* 1992) and databases (MEDCHEM, 1992; Cesars, 1989). Water solubility is a function of the temperature of the water and compound specific. For all compounds, a temperature correction was applied when necessary to obtain the solubility at soil temperature (10°C). For the application of this correction the vapour pressure

at 10°C and the Henry's law constant at 10°C were used. H_c 's at 10°C were obtained by using the temperature correction from Wolff & Van der Heide (1982).

2.1.5 Henry's law constant

The proportionality constant between the vapour pressure of a solute above an aqueous solution and the concentration in solution is called the Henry's law constant (H_c) (Fetter, 1993). The dimensionless H_c (at 20°C) is used in the CSOIL model to calculate the exposure to contaminants during showering (Van den Berg, 1995). The H_c was calculated as the ratio between the vapour pressure and the solubility. Calculated H_c 's have been compared to empirical H_c 's collected from extensive review articles by MacKay and Shiu (1981) and Gosset (1987). Like the temperature correction for vapour pressure, the correction for solubility has not been applied to the first series of compounds considered.

2.1.6 Octanol-water partition coefficient (K_{ow})

The octanol-water partition coefficient is a measure of the hydrophobicity of a compound. The organic compound is shaken with a mixture of n-octanol and water, and the proportion dissolving into each phase is measured. The octanol-water partition coefficient is the ratio of the concentration in the octanol to the concentration in water (Fetter, 1992).

K_{ow} 's were selected from Verschueren (1983), Chemiekaarten (1991), the MEDCHEM database (1992) and some review articles. The K_{ow} 's mentioned have been calculated by Leo *et al.* (1971) using several equations. In addition, the MEDCHEM database and review articles contain a large number of empirical K_{ow} values.

2.1.7 Organic carbon normalized soil-water partition coefficient (K_{oc})

The sorption of organic compounds onto a mineral surface or to the organic carbon of the soil is almost exclusively onto the organic carbon fraction (foc) if it constitutes at least 1% of the soil on a weight basis (Karickhoff *et al.*, 1979). Under these circumstances a partition coefficient with respect to the organic fraction (K_{oc}), can be defined as the K_d divided by foc (fraction organic carbon) (Fetter, 1993).

For the compounds in these series K_{oc} values were mainly obtained from MacKay and Shiu (1981). K_{oc} 's were also obtained from the report of Bockting *et al.* (1993) and other reviews. For most of these compounds it is extremely difficult to find a reliable K_{oc} . Therefore, additional K_{oc} 's were derived from the K_{ow} and/or solubility (S) according to Karickhoff (1981), using equations 1 and 2:

$$K_{oc} = 0.411 * K_{ow} \quad (1)$$

where K_{oc} = organic carbon normalized soil-water partition coefficient ($\text{L}\cdot\text{kg}^{-1}$)
 K_{ow} = octanol-water partition coefficient

$$\log K_{oc} = -0.921 \log S - 0.00953 (\text{MP-25}) - 1.405 \quad (2)$$

where S = molefraction of compound in water (-)
 MP= melting point compound ($^{\circ}\text{C}$)

In equation 2 the term 0.00953 (MP-25) is a correction for crystal energy for organic compounds (Karickhoff, 1981). This correction, a function of the melting point of a compound, is needed for polar functional groups and very high melting points (Karickhoff, 1981).

When the properties of a compound did not restrict the use of Karickhoff's equations, equations 1 and 2 were used for insufficient datasets. The sensitivity of the K_{oc} was considered for each compound. When the K_{oc} appeared to be very sensitive to the model output, more effort was made to find a reliable parameter value.

2.1.8 Permeation coefficient

The permeation coefficient is a measure of the transport of a compound through a membrane, here specified as a polyvinylethylene tube (expressed in square meters per day).

For the calculation of organic compound permeation from water or air into pipelines, compound-specific permeation coefficients are needed. No database exists in which the relevant data are given. Only the reports of Vonk (1985) and Van der Heijden and Hofman (1986) provide information on a limited number of compounds. Based on comparable compounds, with consideration of structure and size, values for these coefficients were estimated. It should be mentioned that the exposure pathways through drinking-water uptake are of minor importance, so that improvement of the estimation method of permeation coefficients is not found necessary. A permeation coefficient of $1 * 10^{-7} \text{ m}^2 \cdot \text{d}^{-1}$ has been used for all industrial solvents and aromatic compounds (Veenendaal *et al.*, 1985). For dodecylbenzene, a permeation coefficient of $0.5 * 10^{-7}$ was used. For a few chlorinated hydrocarbons (1,1,1-trichloroethane and 1,2-dichloroethene) other permeation coefficients were used. These coefficients were calculated using the diffusion coefficient ($D_w = 4.9 * 10^{-8} [\text{m}^2 \cdot \text{day}^{-1}]$) of 1,2-dichloroethane. The permeation coefficients are shown in Table 1.

Table 1 Permeation coefficients for 1,1,1-trichloroethane and *cis*- & *trans*-1,2-dichloroethene

Compound	Permeation coefficient (in $\text{m}^2 \cdot \text{day}^{-1}$)
1,1,1 trichloroethane	$2 * 10^{-6}$
1,1-dichloroethane	$3 * 10^{-7}$
<i>cis</i> - and <i>trans</i> -1,2-dichloroethene	$4 * 10^{-8}$

2.1.9 Acid dissociation

Dissociation of organic acid will result in negatively charged species. These species are more mobile in soils than their parent compounds. At a pH of 6 (for a standard soil), acid-dissociation is not relevant for any of the compounds mentioned here, so no negatively charged species will be present.

2.2 Collection of the physicochemical properties

Calculations of the HUM-TOX SCC have uncertainties, due to sensitivity to the physicochemical input parameters. In this respect, sensitivity of the parameter values is considered for all compounds together with reliability of the parameter values. When an input value appears to be very sensitive and is not well founded, more effort has been made to find a reliable parameter value. The K_{oc} , vapour pressure and solubility have a more-or-less large impact on the calculated HUM-TOX SCC, depending on the characteristics of the compound. For most compounds in this study, parameter values obtained are very reliable; in these cases no further investigation of sensitivity of the HUM-TOX SCC is needed. However, for several compounds, like ethylene glycol and methanol, empirical K_{oc} 's were not very well founded.

2.2.1 Silver

In spite of several mobile complexes, silver apparently is immobile in soils if the pH is higher than 4 due to sorption onto soil complexes (Kabata-Pendias, 1992). Therefore, high porewater concentrations of silver are unlikely to occur. Baes *et al.* (1984) determined a K_d for silver, based on a review in the literature. Unfortunately, little information is available on the partitioning behaviour of silver in soils. A partition coefficient (K_d) for silver has been adopted from Jones *et al.* (1986) and Baes *et al.* (1984).

Trace element contents of plants grown on contaminated soil show a large variation depending on plant and soil specific factors. A review of the available literature on this subject and a summary of the most important factors was presented by Bockting & Van den Berg (1992). It is likely that the very low solubility of silver reduces uptake by plants considerably. Klein (1978) concluded that silver tends to accumulate mainly in the roots and that the element is excluded from the plant foliage even when present in soils at high concentrations. It was found that as much as 90% of the silver added to a nutrient solution can be immobilized in the roots of *Lolium perenne* and *Trifolium repens* (Adriano, 1986). Unfortunately, no concentrations in the soil are given, which makes it impossible to calculate bioconcentration factors (BCFs) from these studies.

No data were found on vegetables from silver-contaminated soils. Due to lack of information the BCF factors were derived from Baes *et al.* (1984). In this study, the BCF_{root} (the ratio of the mass fraction of a compound per kg root and per kg soil) and BCF_{shoot} (the ratio of the mass fraction of a compound per kg shoot and per kg soil) for silver were separately derived, primarily by considering the elemental structure, because few references on direct determination for this element were available. The assumption was made that the variation in BCF from silver and the element directly above silver in the periodic system, which is copper, is similar identical. Because the BCF_{shoot} is an uncertain value it does not seem meaningful to derive a BCF for

potatoes analogous to Bockting and Van den Berg (1992), where the BCF for potatoes was chosen as a factor two below the BCF_{shoot}, which is the BCF for other vegetables.

The selected physicochemical properties of silver are summarized in Table 2. The underlying data are shown in Appendix I.

Table 2 Physicochemical data for silver

silver		
CAS reg.number	7440-22-4	
molecular weight	107.9	g.mol ⁻¹
K _d	128	l.kg ⁻¹
BCF _{root}	0.1	mg.kg ⁻¹ c _{root} /c _{soil} (dry weight)
BCF _{shoot}	0.4	mg.kg ⁻¹ c _{shoot} /c _{soil} (dry weight)

2.2.2 Organic solvents

The selected physicochemical properties for a number of industrial organic solvents are summarized in Table 3. The underlying data can be found in Appendix II.

Table 3 Selected physicochemical data for industrial solvents

ethylene glycol		
CAS registration number	107-21-1	
molecular weight	62.1	(g.mol ⁻¹)
water solubility	1.6*10 ⁴	(mol.m ⁻³)
log K _{ow}	-1.6	
K _o	0 ¹¹	(l.kg ⁻¹)
vapour pressure (10°C)	6	(Pa)
Henry's law constant (10°C)	1.59*10 ⁻⁷	(-)
diethylene glycol		
CAS registration number	111-46-6	
molecular weight	106.1	(g.mol ⁻¹)
water solubility	4.8*10 ⁴	(mol.m ⁻³)
log K _{ow}	-1.8	
K _o	2149 ¹¹	(l.kg ⁻¹)
vapour pressure	1.33	(Pa)
Henry's law constant (10°C)	1.18*10 ⁻⁸	(-)

acrylonitrile

CAS registration number	107-13-1	
molecular weight	53.1	(g.mol ⁻¹)
water solubility (10°C)	981	(mol.m ⁻³)
log K _{ow}	-0.3	
K _{oc}	8.76	(l.kg ⁻¹)
vapour pressure (10°C)	7890	(Pa)
Henry's law constant (10°C)	3.42*10 ⁻³	(-)

formaldehyde

CAS registration number	50-00-0	
molecular weight	30	(g.mol ⁻¹)
water solubility	2.4*10 ⁴	(mol.m ⁻³)
log K _{ow}	0.12	
K _{oc}	0 ¹²¹	(l.kg ⁻¹)
vapour pressure (10°C)	288072	(Pa)
Henry's law constant (10°C)	5.1*10 ⁻³	(-)

methanol

CAS registration number	67-56-1	
molecular weight	32	(g.mol ⁻¹)
water solubility	3.3*10 ⁴	(mol.m ⁻³)
log K _{ow}	-0.7	
K _{oc}	0 ¹²¹	(l.kg ⁻¹)
vapour pressure (10°C)	7180	(Pa)
Henry's law constant (10°C)	9.13*10 ⁻⁵	(-)

1-butanol

CAS registration number	71-36-3	
molecular weight	74.1	(g.mol ⁻¹)
water solubility (10°C)	612	(mol.m ⁻³)
log K _{ow}	0.9	
K _{oc}	5.8	(l.kg ⁻¹)
vapour pressure (10°C)	300	(Pa)
Henry's law constant (10°C)	2.08*10 ⁻⁴	(-)

1-butylacetate

CAS registration number	123-86-4	
molecular weight	116.2	(g.mol ⁻¹)
water solubility (10°C)	91	(mol.m ⁻³)
K _{ow}	1.78	
K _{oc}	38 ²¹	(l.kg ⁻¹)
vapour pressure (10°C)	796	(Pa)
Henry's law constant (10°C)	3.72*10 ⁻³	(-)

methyl *tert*-butyl ether

CAS registration number	1634-04-4	
molecular weight	88.2	(g.mol ⁻¹)
water solubility (10°C)	328	(mol.m ⁻³)
log K _{ow}	0.94	
K _{oc}	13.4 ²¹	(l.kg ⁻¹)
vapour pressure (10°C)	17618	(Pa)
Henry's law constant (10°C)	2.28*10 ⁻²	(-)

¹⁾ sensitive parameter for calculation of the HUM-TOX SCC²⁾ unreliable parameter

2.2.3 Aromatic compounds

Table 4 summaries the selected physicochemical properties of dodecylbenzene and of a mixture of alkylbenzenes originating from petrol (gasoline) or from other petroleum products. The mixture contains high concentrations of C₃ and C₄ alkyl benzenes. For the determination of the parameters for the alkyl benzenes the average composition of the mixture is considered. This composition was derived from 'C-9 aromatic naphtha' as given by the International Research and Development Corporation (1988). The physicochemical properties were determined for the most frequently found individual compounds. Considering the fraction of the individual compounds in the mixture, the weight geometrical mean of the physicochemical characteristics of the individual compounds was then calculated. The underlying data and calculations are shown in Appendices III and IV. As well for dodecylbenzene as for the mixture of aromatic solvents no sufficient K_{oc}'s were available.

Table 4 *The selected physicochemical properties for dodecylbenzene and a mixture of aromatic solvents (containing high concentrations of C₃ en C₄ alkyl benzenes)*

dodecylbenzene

CAS registration number	123-01-3	
molecular weight	246.4	(g.mol ⁻¹)
water solubility	7.7*10 ⁻⁷	(mol.m ⁻³)
log K _{ow}	>8.46	
K _{oc}	not available	(l.kg ⁻¹)
vapour pressure	0.032	(Pa)
Henry's law constant	not available	

aromatic solvents¹⁾

molecular weight	120.9	(g.mol ⁻¹)
water solubility (10°C)	0.39	(mol.m ⁻³)
log K _{ow}	3.80	
K _{oc}	not available	(l.kg ⁻¹)
vapour pressure (10°C)	182	(Pa)
Henry's law constant (10°C)	1.98*10 ⁻¹	(-)

¹⁾ Composition 'C9 aromatic naphtha' as given by IRDC (1988): *o*-xylene 3.2%, *i*-propylbenzene 2.74%, *n*-propylbenzene 3.97%, 1-methyl-4-ethylbenzene 7.05%, 1-methyl-3-ethylbenzene 15.1%, 1-methyl-2-ethylbenzene 5.44%, 1,3,5-trimethylbenzene 8.37%, 1,2,4-trimethylbenzene 40.5%, 1,2,4-trimethylbenzene 40.5%, 1,2,3-trimethylbenzene 6.18%, >=C10s 6.19%. Note that the C₅&C₁₀ alkyl benzenes as given by IRDC are C₃ and C₄ alkyl benzenes in the notation used in the report.

2.2.4 Chlorinated hydrocarbons

In Table 5 the selected physicochemical properties are given for some chlorinated hydrocarbons. The underlying data are shown in Appendix V.

Table 5 *The selected physicochemical properties for 1,1-dichloroethane, 1,1,1-trichloroethane, cis-1,2-dichloroethene and trans-1,2-dichloroethene*

1,1-dichloroethane

CAS registration number	75-34-3	
molecular weight	99	(g.mol ⁻¹)
water solubility (10°C)	43.5	(mol.m ⁻³)
log K _{ow}	1.79	
K _{oc}	27.5	(l.kg ⁻¹)
vapour pressure (10°C)	15217	(Pa)
Henry's law constant (10°C)	1.49*10 ⁻¹	(-)

1,1,1-trichloroethane

CAS registration number	71-55-6	
molecular weight	133.4	(g.mol ⁻¹)
water solubility (10°C)	6	(mol.m ⁻³)
log K _{ow}	2.8	
K _{oc}	93	(l.kg ⁻¹)
vapour pressure (10°C)	8215	(Pa)
Henry's law constant (10°C)	5.82*10 ⁻¹	(-)

1,2-dichloroethene (cis)

CAS registration number	540-59-0	
molecular weight	96.95	(g.mol ⁻¹)
water solubility (10°C)	8	(mol.m ⁻³)
log K _{ow}	1.27	
K _{oc}	65.6	(l.kg ⁻¹)
vapour pressure (10°C)	15461	(Pa)
Henry's law constant (10°C)	8.21*10 ⁻¹	(-)

1,2-dichloroethene (trans)

CAS registration number	540-59-0	
molecular weight	96.95	(g.mol ⁻¹)
water solubility (10°C)	6	(mol.m ⁻³)
log K _{ow}	1.09	
K _{oc}	64.6	(l.kg ⁻¹)
vapour pressure (10°C)	20973	(Pa)
Henry's law constant (10°C)	1.49	(-)

3 ECOTOXICOLOGICAL SERIOUS SOIL CONTAMINATION CONCENTRATION

The methodology to derive the ECOTOX SCC, as described by Denneman and Van Gestel (1990, 1991) and Denneman (1993), has been updated by Crommentuijn *et al.* (1994). The recommendations given by the Technical Soil Protection Committee (TCB, 1992) and the scientific information and methods which have become available in recent years were taken into account. Crommentuijn *et al.* (1994) describe the methodology for derivation of ecotoxicological criteria for the serious soil contamination concentration. The ecotoxicological criterium for serious soil contamination is that there is a serious danger for a soil ecosystem when 50% of the species and 50% of the microbial processes are threatened. This will be the case when the NOEC (No-Observed-Effect-Concentration) for effects on vital life-functions of species (like survival, growth and reproduction) and microbial- and enzymatic processes are exceeded. If a substance has a potential for secondary poisoning, the possible adverse effects due to secondary poisoning are incorporated in the criterion.

The methodology used to derive the ecotoxicological criterion for serious soil contamination is described in a stepwise protocol. The first step of the protocol describes which data are needed. The second step gives the formulas for normalisation and standardisation of the data on terrestrial species and microbial processes. After normalisation and standardisation of these data in step 3 a selection of the data is made. Step 4 describes the method used to calculate an HC50(terrestrial species) and HC50(microbial processes). The method used to derive the HC50(birds) and HC50(mammals) to check if there is a risk for secondary poisoning is described in step 5.

If not enough data on terrestrial species and microbial processes are available to derive a reliable criterium for serious soil contamination, the HC50(terrestrial species) and HC50(microbial processes) are compared with a partition-HC50 using data on the toxicity of aquatic species. If no data on terrestrial species and microbial processes are available only a partition-HC50 can be derived. The methods used to derive partition-HC50s are described in steps 6, 7, 8 and 9 of the protocol. In step 10 the derivation of the ecotoxicological criterium for serious soil contamination from the HC50-values is described. The stepwise approach makes it possible to identify the methods used and the uncertainties introduced. The advantage is that new knowledge, available in the future, can be incorporated. Crommentuijn *et al.* (1994) outlines the extensive description.

The proposals for the ECOTOX SCC for the third series of compounds (Crommentuijn *et al.*, 1995) are summarized in Table 6. In general, the HC50 values are based on terrestrial toxicity, microbial toxicity and aquatic toxicity data, with the terrestrial toxicity data yielding the most reliable ECOTOX SCC (reliability qualified as 'high'). In most cases no terrestrial or microbial data were available for the compounds described here, except for silver (microbial data available, reliability qualified as 'moderate'). Through recalculation by means of an equilibrium partitioning coefficient (using the partition coefficients K_d , K_{ow} or K_{oc} from Tables 2 to 5) the aquatic toxicity data are used for the determination of the ECOTOX SCC. However, because of differences in bioavailability and composition of the species in surface water and porewater this results in an ECOTOX SCC of low reliability.

Table 6 Proposals for the ecotoxicological serious soil contamination concentration (ECOTOX SCC) for a standard soil (10% organic matter, 25% lutum), with reliability indicated, based on terrestrial, microbial and aquatic (recalculated for partitioning) ecotoxicological data (Crommentuijn et al., 1995)

Compound	Aquatic-Eq.part. HC50 value [mg.kg ⁻¹]	Recommended ECOTOX SCC [mg.kg ⁻¹]	Reliability ^{a)} ECOTOX SCC
silver	15 ^{c)}	15	moderate
1,1 dichloroethane	42	42	low
1,1,1 trichloroethane	88	88	low
<i>cis</i> -1,2 dichloroethene	238	238	low
<i>trans</i> -1,2-dichloroethene	238	238	low
ethylene glycol	90	90	low
diethylene glycol	450000	450000	low
acrylonitrile	1.3	1.3	low
formaldehyde	0.30	0.30	low
methanol	33	33	low
1-butanol	26	26	low
1-butyacetate	95	95	low
methyl <i>tert</i> -butyl ether	125	125	low
dodecylbenzene	n.a.	n.a.	n.a.
aromatic solvents	211 ^{b)}	211	low

^{a)} reliability (range: low-moderate-high)

^{b)} weighted mean of ECOTOX SCC of trimethylbenzenes (HC50=199, 92%) and tetramethylbenzenes (HC50 =346, 8%), considering the composition of C₉ aromatic naphtha (see 2.2.3).

^{c)} For all compounds terrestrial and microbial ecotoxicological HC50 are lacking, except for silver, for which a microbial ecotoxicological value is available.

n.a. = not available

4 HUMAN-TOXICOLOGICAL MAXIMUM PERMISSIBLE RISK LEVELS

In agreement with 'Premises for risk management' (VROM, 1988), soil quality leading to exposures exceeding the 'Maximum Permissible Risk' (MPR) is chosen as the human-toxicological basis for the derivation of the HUM-TOX SCC. For non-genotoxic carcinogens and non-carcinogenic compounds the maximum permissible risk is defined as the toxicologically tolerable daily intake (TDI). This is the quantity of a compound to which humans can be orally exposed daily without experiencing adverse effects on health. For genotoxic carcinogens the 'maximum permissible risk' is defined as the quantity of a compound with a risk of one additional case of a lethal tumour in 10,000 lifelong-exposed individuals (VROM, 1988).

For each of the compounds in this study a *toxicity profile* for human health evaluation was prepared. The profiles are presented in Janssen *et al.* (1995). The profiles give a summary of the available toxicity data; the data presented have been limited to that directly relevant for derivation of the TDI or cancer risks. In the profiles additional information was added about absorption factors (dermal, inhalation and, for volatile compounds, oral) and about existing guideline values in the Netherlands.

As explained in the report of Janssen *et al.* (1995), finalized and officially published review documents are used in the toxicological evaluation of the individual compounds wherever this is possible. Intensive literature researches for original publications were performed for 1-butylacetate, methyl *tert*-butyl ether, dodecylbenzene and aromatic solvents, no adequate review documents being available for these compounds. The results of these searches were used selectively: only the key publications were selected for inclusion in the profile. For 1,1-dichloroethane, 1,2-dichloroethene (*cis/trans*) and 1,1,1-trichloroethane limited searches were done for original publications supplementary to the data in the review documents available for these 3 compounds. For the remaining compounds adequate review documents (RIVM basis records, evaluations by IPCS, WHO or US-EPA) were available to serve as a basis for the profile. Wherever necessary, the original publications of studies given in these reviews were consulted and reevaluated.

The method used to prepare the toxicity profiles agrees with the approach described earlier by Vermeire *et al.* (1991). The description of the concepts and procedures used for the toxicological evaluation of compounds will be updated in a separate guidance document (Janssen, 1995), in which a detailed discussion of concepts and procedures is presented. Table 7 gives the human-toxicological MPRs of the 15 compounds described in this report (Janssen *et al.*, 1995).

Table 7 Human-toxicological maximum permissible risk levels (MPRs) for 15 compounds for deriving serious soil contamination concentration from human-toxicological data

Compound	TDI/ADI ^a ($\mu\text{g} \cdot \text{kg}_{\text{bw}}^{-1} \cdot \text{d}^{-1}$)	Safety factor	TCA ^b ($\mu\text{g} \cdot \text{m}^{-3}$)	Safety factor	Background exposure ^c ($\mu\text{g} \cdot \text{kg}_{\text{bw}}^{-1} \cdot \text{d}^{-1}$)
I. Metals					
silver	5	3	- ^e		0.06-1.3
III. Aromatic compounds					
dodecylbenzene	5	1000	- ^e		0
aromatic solvents	170(PTDI) ^g	- ^h	800	100	0
V. Chlorinated hydrocarbons					
1,1-dichloroethane	80(PTDI) ^g	- ^h	370(PTCA) ^g	1000	0.05
1,1,1-trichloroethane	80(PTDI) ^g	- ^h	380	1000	0.7
cis-1,2-dichloroethene	6	5000	30(PTCA) ^g	- ^h	0.15
trans-1,2-dichloroethene	17	1000	80(PTCA) ^g	- ^h	0.15
VII. Miscellaneous compounds					
(Organic solvents)					
ethylene glycol	400 ^d	100	- ^e		0
diethylene glycol	400 ^d	100	- ^e		0
acrylonitrile	0.1 ^f	- ^h	10 ^f		0.028
formaldehyde	150	100	1.2	100	unknown
methanol	500	1000	1100	100	500
1-butanol	125	1000	550(PTCA) ^g	- ^h	unknown
1-butyacetate	200(PTDI) ^g	- ^h	1000	100	1
methyl-t-butyl ether	900	1000	500	1000	unknown

source: (Janssen *et al.*, 1995)

^a Tolerable Daily Intake or Acceptable Daily Intake: in the present context denoted as MPR value. Where only provisional data are available this is explicitly stated in the table (abbreviation PTDI added)

^b Tolerable Concentration in Air (long-term exposure). Where only provisional data are available this is explicitly stated in the table (abbreviation PTCA added)

^c Values given should be considered as rough estimates of prevalent exposures

^d Combined value for mono- and diethylene glycol (applies to sum of concentrations when both compounds are present).

^e Inhalatory uptake not considered relevant in present context.

^f Based on carcinogenicity as endpoint; excess lifetime risk per 10,000 persons 1

^g Tentative value, derived via route-to-route calculation.

^h Route-to-route calculation used; safety factor as given for the other route.

5 EXPOSURE ASSESSMENT - HUMAN-TOXICOLOGICAL SERIOUS SOIL CONTAMINATION CONCENTRATION

A human exposure model (CSOIL) based on literature and reviews of other models (Van den Berg, 1995) has been described. In this model, exposure via all relevant exposure pathways, including the description of the relevant transfer processes, has been quantified. For the calculation of the HUM-TOX SCC, a standard exposure data set has been defined, in which all exposure pathways are considered. The original CSOIL model (Van den Berg & Roels, 1991) has been adjusted for a number of aspects which have been discussed with the TCB and other experts. The full adjusted set of CSOIL equations is given in Appendix IX. Figure 2 shows the direct and indirect exposure routes used in the CSOIL model, through which humans may be exposed to soil contamination. The exposure through fish, meat and milk was not considered.

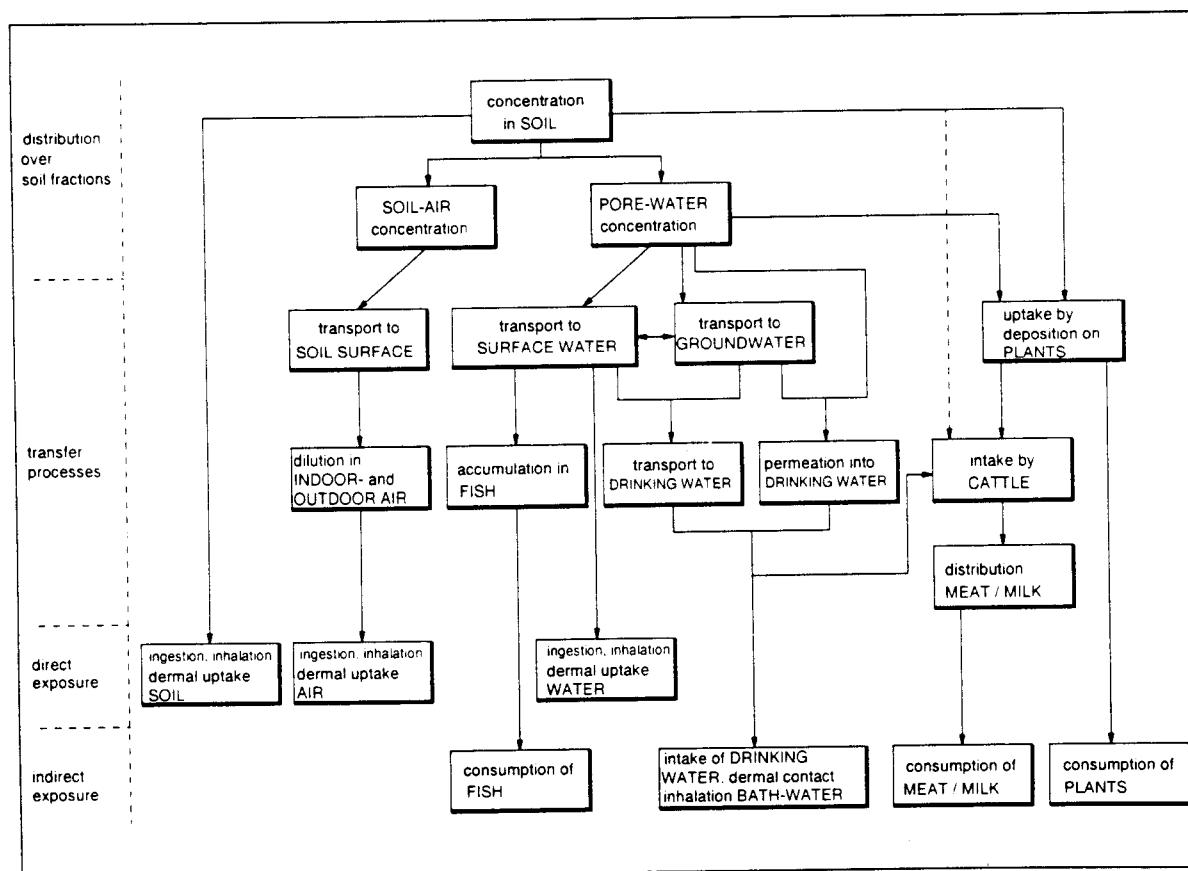


Figure 2. Schematic view of exposure routes in the case of soil pollution (Van den Berg, 1995).

On the basis of the selected physicochemical data, discussed in Chapter 2, and the human-toxicological MPR values given in Chapter 4, the CSOIL model has been used to calculate the HUM-TOX SCC. The proposed HUM-TOX SCC is the concentration of a contaminant in the soil which gives an exposure dose equal to the human-toxicological MPR value for the standard scenario. The standard scenario is defined as the lifetime exposure for humans in a residential area (house with garden). In Figure 3 the relationship is shown between the concentration in the soil and the total dose of a compound (here cadmium). The doses for a child and an adult are used to calculate the mean dose per human during a lifetime. The MPR value is also shown. Background exposure is not taken into account.

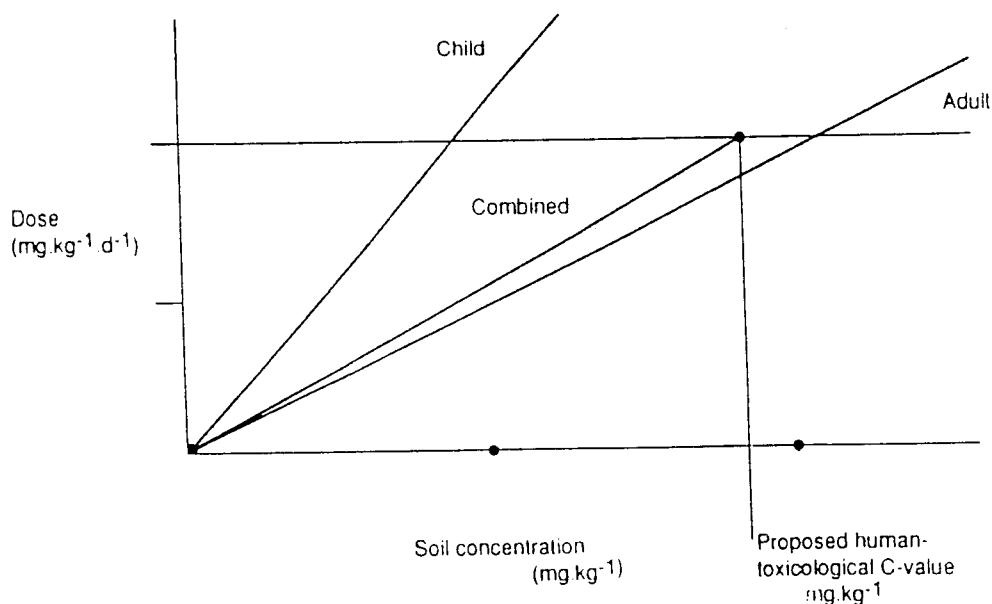


Figure 3. Relationship between concentration of cadmium in soil and the doses. Where the curve that presents the mean dose exceeds the MTR (here $0.001 \text{ mg} \cdot \text{kg}^{-1} \cdot \text{d}^{-1}$) the HUM-TOX SCC is exceeded.

In Table 8 the results of the calculations (HUM-TOX SCCs) for the compounds considered in this report are listed. Tables 2 to 5 and Table 7 present the input data of the model calculations per compound. The CSOIL calculations for all compounds mentioned are shown in Appendix VII. For the calculations of the distribution of a compound over the different soil phases (solid phase, porewater and soil air) the selected vapour pressures, solubilities and $\log K_{oc}$'s, given in Tables 2 to 5 have been used. For the calculation of the exposure of organic compounds through vegetables the $\log K_{ow}$ has been used (Appendix IX). The major exposure routes are discussed below.

Looking at the relative contribution of the exposure routes for a lifetime it can be seen that for silver, the major exposure route is ingestion via vegetables (this route accounts for more than 90 % of the total exposure). Ingestion of soil is also relevant, but is of minor importance (8%). For acrylonitrile, formaldehyde, methanol and methyl *tert*-butyl ether the percentage exposure via inhalation of indoor air contributes more than the percentage exposure via ingestion of vegetables. The ingestion via vegetables is of major importance when considering ethylene glycol and butanol. For diethylene glycol both routes account for about 50 % of the total exposure.

Permeation through a polyvinylethylene tube is not important for any of the compounds, except for ethylene glycol for which there is 6% contribution to exposure due to permeation into drinking water. The aromatic compounds are a group for which exposure via inhalation of indoor air is most important (58%), together with ingestion via vegetables (40%). The halogenated hydrocarbons are characterized by large exposure through indoor air, which accounts for more than 90 % of the total exposure for 1,1-dichloroethane, 1,1,1-trichloroethane and *cis*- and *trans*-1,2-dichloroethene.

Table 8

Proposals for the human-toxicological serious soil contamination concentration (HUM-TOX SCC) with uncertainty scores for a standard soil (10% organic matter, 25% lutum) based on the human MPR values (Table 7) and human exposure calculations with CSOIL (Appendix VII)

Compound	Toxicological MPR value [$\mu\text{g} \cdot \text{kg}_{\text{bw}}^{-1} \cdot \text{d}^{-1}$]	HUM- TOX.SCC [$\text{mg} \cdot \text{kg}_{\text{dw}}^{-1}$]	US ¹
silver	5	282	3
1,1-dichloroethane	80	15.1	2
1,1,1-trichloroethane	80	14.6	2
<i>cis</i> -1,2-dichloroethene	6	0.51	4
<i>trans</i> -1,2-dichloroethene	17	0.81	4
ethylene glycol	400	209	6
diethylene glycol	400	$122 \cdot 10^3$	6
acrylonitrile	0.1	0.093	4
formaldehyde	150	25.2	6
methanol	500	164	4
1-butanol	125	103	4
1-butyacetate	200	469	2
methyl <i>t</i> -butyl ether	900	423	4
dodecylbenzene	5	1010	4
aromatic solvents	170	1450	2

¹ Uncertainty scores have also been determined for the HUM-TOX SCC values in accordance with the ECOTOX SCCs. These scores have been determined as the product of separate scores for the human reference dose and the exposure assessment (Van den Berg and Roels, 1991). The higher the score, the less the uncertainty.

For a number of compounds Tolerable Concentrations in Air (TCAs) have been determined. If the calculated indoor air concentration exceeds the TCA, the HUM-TOX SCC value has to be adjusted, in this case for methyl *tert*-butyl ether and formaldehyde (Table 9)

Table 9 *TCA (Tolerable Toxic Concentration in Air) compared with indoor air concentration (Cia), calculated with CSOIL (Appendix VII) and the resulting corrected human-toxicological serious soil contamination concentration (HUM-TOX SCC) for methyl *tert*-butyl ether and formaldehyde.*

Compound	TCA [$\mu\text{g.m}^{-3}$]	CSOIL calculated HUM-TOX SCC [mg.kg_{dw}^{-1}]	Cia [$\mu\text{g.m}^{-3}$]	Corrected HUM-TOX SCC [mg.kg_{dw}^{-1}]
methyl <i>tert</i> -butyl ether	500	423	2540	83
formaldehyde	1.2	25.2	385.4	0.079

6 THE INTEGRATION OF INTERVENTION VALUES IN PROPOSALS

6.1 Intervention value for soil

Both the ECOTOX and the HUM-TOX SCC values, as well as the uncertainties in their derivation, are integrated into the intervention value. For all compounds described in this report, the most stringent of the two SCC values is chosen. In principle, for cases in which the most stringent value has a much lower uncertainty score, the less stringent value is chosen. This could be the case when an uncertainty score is low in contrast with high. The same weight is given to the HUM-TOX as to the ECOTOX SCC. For comparison of the ECOTOX SCC and the HUM-TOX SCC it is necessary to give a qualification to the quantitative values of the HUM-TOX uncertainty scores. Uncertainty scores (as in Table 8) of 1 to 3 are qualified as 'low', 4-6 are considered as 'moderate' and 7-9 as 'high'. Table 10 presents all relevant information about HUM-TOX and ECOTOX SCC values, uncertainty scores and proposed intervention values.

It should be noted that the physicochemical behaviour of dodecylbenzene cannot be compared with any of the other compounds described here. The compound is extremely insoluble in water, and from the available data (see Appendix III) no reliable vapour pressure can be chosen. Also, no ECOTOX SCC is available. Because of the very high K_{ow} value, the calculation of exposure through plant-uptake (Appendix IX, formulas for calculation of plant content) is probably overestimated (65 % of the total exposure) and thus unreliable. It is assumed that, on basis of the physicochemical properties of dodecylbenzene, the most important exposure route for this compound is ingestion of soil. By using the CSOIL formulas for quantification of exposure (Appendix IX), a concentration in the soil, considering ingestion of soil as the main exposure route, can be calculated. The calculated value (3300 mg.kg^{-1} dry weight) can be considered as the value that in no case should be exceeded. However, this value should not be referred to as intervention value.

6.2 Intervention value for groundwater

The proposed intervention values for groundwater have been derived from the proposed intervention values for soil, using the equilibrium theory for soil-water partitioning. Because of problems encountered in determining soil-water partition coefficients (for which wide varieties in values are possible), dilution of groundwater, soil heterogeneity and the lack of equilibrium, intervention values for groundwater are set at a lower level than calculated using the equilibrium theory. Intervention values for groundwater (in accordance with the procedure of Van den Berg & Roels (1991) were derived by decreasing the calculated equilibrium concentration (Table 8) by a factor of 10.

Exposure through direct use of groundwater was excluded in the model. For this reason, it was investigated if direct consumption of polluted drinking water up to the intervention value results in exceedance of the MPR value, in case this would be the only exposure route. In the case of acrylonitrile, formaldehyde, methanol, butanol and butylacetate this could occur. As a consequence, the intervention values for groundwater were lowered to the human MPR value for drinking water. However, because of the uncertainties in soil-water partition coefficients and the approach used for determination of intervention values for groundwater (division by a factor of 10), the intervention values for soil have not been adjusted.

The proposed intervention values for groundwater are shown in Table 10.

Table 10

Proposals for the intervention values for a standard soil (10% organic matter, 25% lutum) and groundwater, with uncertainty scores, based on ECOTOX SCCs (Table 6) and HUM-TOX SCCs (Table 7)

Compound	ECOTOX SCC	US ^a [mg.kg ⁻¹ dry weight]	HUM- TOX SCC.	US ^a [mg.kg ⁻¹ dry weight]	Proposed int.value soil [mg.kg ⁻¹ dry weight]	Proposed int.value groundwater [µg.l ⁻¹]
I Metals and trace elements						
silver	15	mod	282	low	15	12
V Chlorinated hydrocarbons						
1,1-dichloroethane	42	low	15	low	15	870
1,1,1-trichloroethane	88	low	15	low	15	260
cis-1,2-dichloroethene	238	low	0.51	mod	0.5	13
trans-1,2-dichloroethene	238	low	0.81	mod	1	20
VII Other pollutants						
ethylene glycol	90	low	209	mod	100	5*10 ³
diethylene glycol	450*10 ³	low	122*10 ³	mod	120*10 ³	13*10 ³ c
acrylonitrile	1.3	low	0.093	mod	0.1	3c
formaldehyde	0.30	low	0.079 ^d	mod	0.1	48c
methanol	33	low	164	mod	33	24*10 ³
butanol	26	low	103	mod	26	5600
butylacetate	95	low	469	low	95	4100
methyl <i>tert</i> -butyl ether	125	low	83 ^e	mod	83	9200
III Aromatic compounds						
dodecylbenzene	n.a.	n.a.	1010	mod	1000 ^e	0.02 ^e
aromatic solvents	211	low	1450	low	200 ^b	150 ^b

n.a = not available

^a uncertainty score (higher score, less uncertainty)

^b chosen as value for the total group of aromatic solvents

^c corrected for direct uptake as drinking water

^d corrected for concentration in indoor air

^e based only on HUM-TOX SCC

6.3 Comparison to quality objectives

Existing quality objectives for soil and groundwater (VROM, 1991) are taken into consideration in relation to the proposed intervention values.

The intervention value should not be lower than the target value or limit value (for newly formed sediment). For as far as target and limit values exist for the compounds considered, the proposed intervention values are not below the target values for soil or the limit values for newly formed sediments (Beleidsstandpunt MILBOWA) for any of the compounds.

A pre-requisite for use of the values is that they can be determined in chemical analysis at the required levels. Therefore, the proposed values have been compared with detection limits (Appendix X). Except for acrylonitrile and formaldehyde, all proposed values are above these detection levels. For acrylonitrile, the detection limit is about 0.1 mg.kg^{-1} for soil dry matter and about 0.1 mg.l^{-1} for groundwater. For formaldehyde only the detection limit for groundwater is determined (0.1 mg.l^{-1}). An additional problem is that not all laboratories have standard analytical procedures for these two compounds. Another important consideration is that for formaldehyde the background exposure in air ranges from 7 to $12 \mu\text{g.m}^{-3}$ (WHO, 1989). This concentration appears to be higher than the Tolerable Concentration in Air ($1.2 \mu\text{g.m}^{-3}$) (Table 9).

6.4 Discussion

6.4.1 Application and occurrence of compounds

The compounds considered are used in various industries (Nieuwkoop, 1993; Chemiekaarten, 1991). Chlorinated hydrocarbons have a very broad field of application, for example, as solvents in the paint and lacquer industry, in chemical laundry-works and in the graphical industry. They are also applied in the metal industry for cleaning of surfaces. The alcohols methanol and butanol are, along with applications, used in the paint and lacquer industry as well. Glycols are used as softeners in the metal industry and as anti-freeze. Formaldehyde is used as a disinfectant and for artificial resins. Butylacetate is also used in the synthetics industry. Acrylonitrile is used as a fumigant and methyl *tert*-butyl ether as a petrol octane improver. Dodecylbenzene is used as an insulation fluid in cable manufacturing.

The occurrence of the compounds in soils is mainly caused by leaking during storage and usage, and by drainage of waste water. A lot of these contaminations took place in the early twentieth century.

Silver is used in the photochemical industry as silver chloride or silver bromide in an emulsion, which is used for film material. In the present industrial process, the silver is recovered from the used liquid, while several decades ago the silver was drained via waste water.

6.4.2 Reliability of proposed values

Considering the uncertainty in the proposed intervention values, several aspects should be taken into account. Uncertainties may be caused by an uncertain MPR value, unreliable physicochemical input data and physicochemical input data that are sensitive to the output of the CSOIL model. Also the increasing influence of environmental behaviour dependent on the nature of a compound contributes to the uncertainty in the CSOIL model and thus to the uncertainty in the output.

For several compounds the intervention value is derived from the ECOTOX SCC with low reliability (Table 10). This is the case for butylacetate, methanol and butanol. The low reliability of the intervention values for the glycols and for methyl *tert*-butyl ether are caused by the sensitivity and uncertainty in physicochemical input parameters (Table 3). Because of the great uncertainty in MPRs for 1,1-dichloroethane and 1,1,1-trichloroethane (Table 7) the intervention values for these compounds have a low reliability. The proposals for the other compounds can be considered as moderately reliable as a result of the availability of reliable data.

The intervention value for silver is derived from the ECOTOX SCC, with moderate reliability. The reliability of HUM-TOX SCC is much lower because the BCFs are not reliable.

The intervention value of the aromatic solvents, containing a mixture of C₃ and C₄ alkyl benzenes, has a low reliability, mainly due to the uncertainty in the composition of the mixture, which can differ from place to place.

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Appendix I: Physicochemical data for silver

Element	K _d l.kg ⁻¹	Accumulation in plants contents (mg.kg ⁻¹) dry weight	BCF
silver	45 364 128	Baes <i>et al.</i> (1984) Jones <i>et al.</i> (1986) (geometric mean)	0.1 0.4
			roots of vegetables (Baes <i>et al.</i>, 1984) shoots of vegetables (Baes <i>et al.</i>, 1984)

Values used for further calculations are printed in bold.

Appendix II: Physicochemical data for organic solvents

Compound	Solubility mol.m ⁻³		$\log K_{ow}$	K_{ow} 1.kg ⁻¹
ethylene glycol	1.6*10⁴	(Verschueren, 1983)	-1.9 (Verschueren, 1983) -1.9 (Chemiekaarten, 1991) -1.36(MEDCHEM, 1992)	0 (Lokke, 1984)
			-1.6 arithmetical mean	
diethylene glycol	9.4*10 ³ 2.47*10⁴	(Verschueren, 1983) (MEDCHEM, 1992)	-2.0 (Verschueren, 1983) -2.0 (Chemiekaarten, 1991) -1.3 (MEDCHEM, 1992)	2149 (Podoll, 1087)
			-1.8 arithmetical mean	
	4.8*10⁴	geometric mean		
acrylonitrile	73 g.l ⁻¹ (20°C) (Chemiekaarten, 1991) 75 g.l ⁻¹ (25°C) (Howard, 1991) 79 g.l ⁻¹ (20°C) (EPA, 1986) 138g.l ⁻¹ (25°C) (MEDCHEM, 1992) 73.5g.l ⁻¹ (20°C) (Cesars, 1985)		-0.9 (Verschueren, 1983) 0.25 (MEDCHEM)	12.6 (Walton <i>et al.</i> , 1992) 10.2 (Walton <i>et al.</i> , 1992) 8.9 (Kenega, 1980) 5 (AERIS database) 7.1 (EPA, 1986)
			-0.3 arithmetical mean	
	1597 geometric mean (mol.m ⁻³) of values at 20°C			8.76 geometric mean
	981 geometric mean (mol.m ⁻³) at 10°C			
formaldehyde	3.3*10 ⁴ 1.8*10 ⁴ (20°C) (Cesars, 1985)	(Verschueren, 1983)	0 (Chemiekaarten, 1991) 0 (Verschueren, 1983) 0.35 (MEDCHEM, 1992)	0
		2.4*10⁴ geometric mean		0.12 arithmetical mean
methanol	3.1*10 ⁴	(Verschueren, 1983)	-0.82 -0.66 (Verschueren, 1983)	0 (Lokke, 1984)
	3.6*10 ⁴	(MEDCHEM, 1992)	-0.77 (MEDCHEM, 1992) (Chemiekaarten, 1991)	
	3.3*10⁴ geometric mean		-0.7 arithmetical mean	
1-butanol	1080 (20°C) (Chemiekaarten, 1991) 1039 (20°C) (Verschueren, 1983) 977 (25°C) (MEDCHEM, 1992)		0.9 (Chemiekaarten, 1991) 0.9 (Verschueren, 1983)	3.2 (Gerstl & Helling, 1987) 3.3 (from K_{ow}) 18.3 (from S)
			0.9 arithmetical mean	
	1031 geometric mean			5.8 geometric mean
	612 geometric mean at 10°C			
1-butylacetate	60.2 (20°C) (Chemiekaarten, 1991) 120.4 (20°C) (Verschueren, 1983) 463 (Windholz, 1989) 42.9 (25°C) (MEDCHEM, 1992)		1.78 (MEDCHEM, 1992)	24.8 (from kow) 58.8 (from S)
				38 geometric mean
	109.5 geometric mean			
	91 geometric mean at 10°C			

Values used for further calculations are printed in bold.

Appendix II continued: Physicochemical data for organic solvents

Compound	Solubility mol.m ⁻³	log K _{ow}	K _{in} l.kg ⁻¹
methyl <i>t</i> -butyl ether	578 (20°C) (Chemiekaarten, 1991) 412 (25°C) (MEDCHEM, 1992)	0.94 (MEDCHEM, 1992)	11.5 (Hansch <i>et al.</i> , 1968)
	488 geometric mean		3.6 (from kow)
	328 geometric mean at 10°C		57.5(from S)
			13.4 geometric mean

Values used for further calculations are printed in bold.

Appendix II continued: Vapour pressures and Henry's law constants for organic solvents

Compound	Vapour pressure [Pa]		Henry's law constant [-]
ethylene glycol	6.7 (20°C) 12 (20°C)	(Verschueren, 1983) (Chemiekaarten, 1991)	1.59*10⁻⁷ at 10°C
	9 geometric mean (20°C) 6 (10°C)		
diethylene glycol	1 (30°C) < 1.33 (20°C)	(Chemiekaarten, 1991) (Verschueren, 1983)	1.18*10⁻⁸ at 10°C
	1.33		
acrylonitrile	11330.5 (20°C) 11000 (20°C) 13300 (20°C)	(Verschueren, 1983) (Chemiekaarten, 1991) (Cesars, 1985)	3.42*10⁻³ at 10°C
	11835 geometric mean at 20°C 7890 geometric mean at 10°C		
formaldehyde	437000 (20°C) 427272 (20°C)	(Cesars, 1985) (Lide <i>et al.</i> , 1993)	5.1*10⁻³ at 10°C
	432108 geometric mean at 20°C 288072 geometric mean at 10°C		
methanol	12700 (20°C) 12263 (20°C)	(Chemiekaarten, 1991) (Verschueren, 1983)	9.13*10⁻⁵ at 10°C
	12480 geometric mean at 20°C 7180 geometric mean at 10°C		
1-butanol	587 (20°C) 700 (20°C)	(Verschueren, 1983) (Chemiekaarten, 1991)	2.08*10⁻⁴ at 10°C
	641 geometric mean at 20°C 300 geometric mean at 10°C		
1-butylacetate	1333 (20°C) 1070 (20°C)	(Verschueren, 1983) (Chemiekaarten, 1991)	3.72*10⁻³ at 10°C
	1194 geometric mean at 20°C 796 geometric mean at 10°C		
methyl <i>tert</i> -butyl ether	32700 (25°C) 34000 (25°C)	(Chemiekaarten, 1991) (MEDCHEM, 1992)	2.28*10⁻² at 10°C
	33344 geometric mean at 25°C 17618 geometric mean at 10°C		

Values used for further calculations are printed in bold.

Appendix III: Physicochemical data for dodecylbenzene and aromatic compounds

Compound	Solubility mol.m ⁻³		log K _{ow}
dodecylbenzene	Insoluble	(Chemiekaarten, 1991)	
7.7*10⁻⁷ (MEDCHEM, 1992) 8.46 (QSAR calculation)			
aromatic solvents (containing C ₆ C ₆ alkylbenzenes)			
1,2,3-trimethylbenzene	0.63	(Mackay <i>et al.</i> , 1992)	3.82
1,2,4-trimethylbenzene	0.45 0.47	(Mackay and Shiu, 1981) (Verschueren, 1983)	
	0.46 geometric mean		3.85
1,3,5-trimethylbenzene	0.57 0.81 (25°C) 0.40 (25°C) 0.17	(Mackay <i>et al.</i> , 1992) (Mackay and Shiu, 1981) (Mackay and Shiu, 1981) (KIWA, 1985)	
	0.42 geometric mean		3.84
1-ethyl-2-methylbenzene	0.77 (25°C) 0.62	(Mackay and Shiu, 1981) (Howard, 1991)	
	0.69 geometric mean		3.63
1-ethyl-4-methylbenzene	0.79	(Mackay and Shiu, 1981) (Howard, 1991)	3.63
1-ethyl-3-methylbenzene	0.28	(Howard, 1991)	3.67
1,2,3,4-tetramethyl benzene	0.12	(Howard, 1991)	4.32
1,2,3,5-tetramethyl benzene	0.10	(Howard, 1991)	4.39
1,2,4,5-tetramethyl benzene	0.026 0.026 0.026	(Mackay <i>et al.</i> , 1992) (Mackay and Shiu, 1981) (Howard, 1991)	4.42
	0.03 geometric mean		4.42
1-iso-propylbenzene	0.42 (20°C) (Verschueren, 1983)		3.66
n-propylbenzene	0.50 (15°C) (Verschueren, 1983)		3.63

Values used for further calculations are printed in bold.

Appendix III continued:
Vapour pressures and Henry's law constants for dodecylbenzene and aromatic compounds

Compound	Vapour pressure [Pa]	Henry's law constant
dodecylbenzene	<10 (20°C) 0.032	(Chemiekaarten, 1991) MEDCHEM (estimated from log K _{ow}) 0.032
aromatic solvents containing C ₆ &C ₇ alkyl-benzenes		
1,2,3-trimethylbenzene	206 202 170	(Mackay <i>et al.</i> , 1992) (Mackay and Shiu, 1981) (KIWA, 1985)
	191 geometric mean	
1,2,4-trimethylbenzene	279 271 220	(Mackay <i>et al.</i> , 1992) (Mackay and Shiu, 1981) (KIWA, 1985)
	255 geometric mean	
1,3,5-trimethylbenzene	331 328 (25°C)	(Mackay <i>et al.</i> , 1992) (Mackay and Shiu, 1981)
	329 geometric mean	
1-ethyl-2-methylbenzene	330	(Mackay and Shiu, 1981)
1-ethyl-4-methylbenzene	393	(Mackay and Shiu, 1981)
1-ethyl-3-methylbenzene	391	(Mackay and Shiu, 1981)
1,2,3,4-tetramethyl benzene	49	(Mackay <i>et al.</i> , 1992)
1,2,3,5-tetramethyl benzene	67	(Mackay <i>et al.</i> , 1992)
1,2,4,5-tetramethyl benzene	71 66 (25°C)	(Mackay <i>et al.</i> , 1992) (Mackay and Shiu, 1981)
	68 geometric mean	
iso-propylbenzene	426	(Verschueren, 1983)
n-propylbenzene	333	(Verschueren, 1983)

Values used for further calculations are printed bold.

Appendix IV: Calculation of parameter values for mixture of aromatic compounds containing high concentrations of C₃ & C₄ alkyl benzenes

steps:

- 1.classification of parameters in groups
- 2.determination of one parameter value per group (geometric mean)
- 3.weight geometric mean of compounds in mixture, according to composition C, naphtha (IRDC, 1988)
- 4.correction for soil temperature (10°C)

step 1 + 2:

compound	$\Sigma \%$	M in g.mol ⁻¹	S in mol.m ⁻³	V _p in Pa	log K _{ow}
1,2,3 trimethylbenzene		120.2	0.63	191	3.82
1,2,4 trimethylbenzene		"	0.46	255	3.85
1,3,5 trimethylbenzene		"	0.42	329	3.84
trimethylbenzenes	60	120.2	0.50	252	3.84

compound	$\Sigma \%$	M in g.mol ⁻¹	S in mol.m ⁻³	V _p in Pa	log K _{ow}
1-ethyl-2-methylbenzene		120.2	0.69	330	3.63
1-ethyl-4-methylbenzene		"	0.79	393	3.63
1-ethyl-3-methylbenzene		"	0.28	391	3.67
ethyl-methylbenzenes	30	120.2	0.53	370	3.64

compound	$\Sigma \%$	M in g.mol ⁻¹	S in mol.m ⁻³	V _p in Pa	log K _{ow}
1,2,3,4-tetramethylbenzene		134.2	0.12	49	4.32
1,2,3,5-tetramethylbenzene		"	0.10	67	4.39
1,2,4,5-tetramethylbenzene		"	0.03	68	4.42
tetramethylbenzenes	5	134.2	0.07	61	4.38

compound	$\Sigma \%$	M in g.mol ⁻¹	S in mol.m ⁻³	V _p in Pa	log K _{ow}
1-isopropylbenzene		120.2	0.42	426	3.66
n-propylbenzene	"	0.50	333	3.63	
propylbenzenes	5	120.2	0.46	377	3.65

step 3+4:

geometric mean M= $10^{[(60*\log 120.2)+(30*\log 120.2)+(5*\log 134.2)+(5*\log 120.2)/100]} = 120.9 \text{ g.mol}^{-1}$

geometric mean S_{20°C}= $10^{[(60*\log 0.50)+(30*\log 0.53)+(5*\log 0.07)+(5*\log 0.46)/100]} = 0.46 \text{ mol.m}^{-3}$; S_{10°C}= 0.39 mol.m⁻³

geometric mean V_{p20°C}= $10^{[(60*\log 252)+(30*\log 370)+(5*\log 61)+(5*\log 377)/100]} = 269 \text{ Pa}$; V_{p10°C}= 179 Pa

arithmetical mean log K_{ow}= $10^{[(60* 3.84)+(30* 3.64)+(5* 4.38)+(5* 3.65)/100]} = 3.80$

Henry's law constant at 20°C (calculated from V_p, S, T and R)= 250*10⁻³

Appendix V Physicochemical data for chlorinated hydrocarbons.

Compound	Solubility mol.m ⁻³		log K _{ow}	K _a l.kg ⁻¹
1,1-dichloroethane	55.6 (20°C) 51.5 (25°C) 55.5 (20°C)	(Verschueren, 1983) (Mackay and Shiu, 1981) (Mackay and Shiu, 1981)	1.79 (EPA, 1986; MEDCHEM, 1992) 30 (EPA, 1986) 25.3 (from K _{ow}) (592 from S)	
		54.2 geometric mean 43.5 geometric mean at 10°C		27.5 geometric mean (without cal. from S)
1,1,1-trichloroethane	33.0 (20°C) 5.5 (25°C) 7.1 (25°C) 3.6 (25°C) 5.0 (25°C)	(Verschueren, 1983) (Mackay and Shiu, 1981) (Mackay and Shiu, 1981) (Mackay and Shiu, 1981) (Mackay and Shiu, 1981)	2.47 (Karickhoff, 1981) 2.17 (Keuning and Janssen, 1987) 2.50 (EPA, 1986) 4.50 (Derde Nota Waterhuish.) 2.49 (Van de Plassche & Bockting, 1993)	93 (n=15) Ollingher & Ahlert, 1988 Huang <i>et al.</i> , 1987 Grathwohl, 1990 Huang & Ganjidoost, 1990 Chiou <i>et al.</i> , 1979 Bockting <i>et al.</i> , 1993
		7.5 geometric mean 6.0 geometric mean at 10°C	2.8 arithmetical mean	
cis-1,2-dichloroethene	8.3 (20°C) 36.1 (25°C)	(Verschueren, 1983) (Mackay and Shiu, 1981)	0.48 (EPA, 1986) 1.48 (Keuning & Janssen, 1987) 1.86 (Van de Plassche & Bockting, 1993)	58.9 (EPA, 1986) 7.6 (from K _{ow}) 632 (from S)
		17.3 geometric mean 8.0 geometric mean at 10°C	1.27 arithmetical mean	65.6 geometric mean
trans-1,2-dichloroethene	6.2 (20°C) 65.0 (25°C)	(Verschueren, 1983) (Mackay and Shiu, 1981)	0.70 (EPA, 1986) 1.48 (Keuning & Janssen, 1987)	49.0 (EPA, 1986) 20 (from K _{ow}) 276 (from S)
		20.1 geometric mean 6 geometric mean at 10°C	1.09 arithmetical mean	64.6 geometric mean

Values used for further calculations are printed in bold.

Appendix V continued: Vapour pressures and Henry's law constants for chlorinated hydrocarbons

Compound	Vapour pressure [Pa]	Henry's law constant [-]
1,1-dichloroethane	23994 (20°C) (Verschueren, 1983) 30100 (25°C) (Mackay and Shiu, 1981) 24420 (20°C) (Mackay and Shiu, 1981) 24000 (20°C) (Chemiekaarten, 1991)	1.49*10⁻¹ (10°C)
	24137 geometric mean values at 20°C 15217 geometric mean at 10°C	
1,1,1-trichloroethane	13330 (20°C) (Verschueren, 1983) 16530 (25°C) (Mackay and Shiu, 1981) 13200 (20°C) (Mackay and Shiu, 1981) 13330 (20°C) (Mackay and Shiu, 1981) 12800 (20°C) (Mackay and Shiu, 1981)	5.82*10⁻¹ (10°C)
	13163 geometric mean values at 20°C 8215 geometric mean at 10°C	
<i>cis</i> -1,2-dichloroethene	26660 (25°C) (Verschueren, 1983) 27460 (25°C) (Mackay and Shiu, 1981)	8.21*10⁻¹ (10°C)
	27057 geometric mean at 25°C 15461 geometric mean at 10°C	
<i>trans</i> -1,2-dichloroethene	26660 (14°C) (Verschueren, 1983) 34650 (25°C) (Mackay and Shiu, 1981)	1.49 (10°C)
	20973 geometric mean of values at 10°C	

Values used for further calculations are printed in bold.

Appendix VI: References for Appendices I to V

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**Appendix VII:
CSOIL calculations of the human-toxicological serious soil contamination concentration**

TUSSENBEREKENINGEN C-USERTERTRAN23C-SOILCSOIL68 WK1

03-Apr-95
UITVOERER: zilver
SCNr.: 2
UITVOERTABEL 1 BIOTESTELLING KIND [mg/kg 1 g/d]

symbool	waarde eenheid	beschrijving	verdeelcoëff grondwater benetende lucht water verdeelcoëff invoere lucht water verdeelcoëff. gehalte in bodem water CpW => S
Za	-	fugaciteitscap. cst. a. fugaciteitscap. cst. w. fugaciteitscap. cst. s.	
Zw	-	[m0/m3 Pa]	
Zs	-	[m0/m3 Pa]	
Kd	1.28E+02 [kg/dm3]		
Klw	0.00E+00 [-]		
Cop	-	[mg/g]	
Pa	0.00E+00 [-]		
Pw	1.04E-03 [-]		
Ps	9.89E-01 [-]		
Dsa	-	[m2/n]	
Dsw	-	[m2/n]	
Du	-	[m2/n]	
Mt	-	[m/s]	
KG	-	[-]	
Klw_sh	-	[-]	
Kwa	-	[-]	

CONCENTRATIES IN BODEMFASEN

grondw.	bodemvo. [g/m3]	bodemvo. [g/m3]
Cow	0.00E+00	2.20E+00

LUCHTFLUXEN [g/m2/h]

grenslag	vapo.	diffusie buiten	diffusie binnen	total binnen
J2'	J3'	J4'	J5'	J6'

LUCHTCONCENTRATIES [mg/m3]	buten	kruijt	kruijt vloer.
Cova	0.00E+00	0.00E+00	0.00E+00

UITVOERTABEL 2 BIOTESTELLING VOLWASSENE [mg/kg 1 g/d]	ING GROND	DERM GROND BINNEN BUITEN	PERM GEWAS BINNENL. BUITENL.	INH GROND BINNENL. BUITENL.	ING GEWAS BINNENL. BUITENL.	INH VLEES	DERM DOUCHEN	PERM DOUCHEN	INH VLEES	ING MELK	ING EIERN	ING MELK	ING EIERN	TOTAL (excl. diel. producten)
	dic 2.82E-03	deo 0.00E+00	deo 0.00E+00	ipc 4.42E-06	ivco 0.00E+00	wc 0.57E-03	dwc 0.00E+00	iwmc 0.00E+00	dawc 0.00E+00	isawc 0.00E+00	isawc 0.00E+00	isawc 0.00E+00	isawc 0.00E+00	1.24E-02

UITVOERTABEL 3 BIOTESTELLING LEVENSLANG-GEMIDDELD [mg/kg 1 g/d]	ING GROND	DERM GROND BINNEN BUITEN	PERM GEWAS BINNENL. BUITENL.	INH GROND BINNENL. BUITENL.	ING GEWAS BINNENL. BUITENL.	INH VLEES	DERM DOUCHEN	PERM DOUCHEN	INH VLEES	ING MELK	ING EIERN	ING MELK	ING EIERN	TOTAL (excl. diel. producten)
	dia 2.02E-04	daa 0.00E+00	daa 0.00E+00	ivb 2.32E-06	ivb 0.00E+00	wl 4.10E-03	dwi 0.00E+00	iwvb 0.00E+00	dawb 0.00E+00	isawb 0.00E+00	isawb 0.00E+00	isawb 0.00E+00	isawb 0.00E+00	4.31E-03

UITVOERTABEL 4 BIOTESTELLINGSCOEFFICIENTEN LEVENSLANG-GEMIDDELD [1000/d]	ING GROND	DERM GROND BINNEN BUITEN	PERM GEWAS BINNENL. BUITENL.	INH GROND BINNENL. BUITENL.	ING GEWAS BINNENL. BUITENL.	INH VLEES	DERM DOUCHEN	PERM DOUCHEN	INH VLEES	ING MELK	ING EIERN	ING MELK	ING EIERN	TOTAL (excl. diel. producten)
	di 4.27E-04	deb 0.00E+00	deb 0.00E+00	ipb 2.68E-06	ipb 0.00E+00	wl 4.57E-03	dwi 0.00E+00	iwlb 0.00E+00	dawb 0.00E+00	isawb 0.00E+00	isawb 0.00E+00	isawb 0.00E+00	isawb 0.00E+00	5.00E-03

UITVOERTABEL 5 PROCENTUELE BIJDRAGE ROUTES KIND, VOLW., LEVENSLANG-GEMIDDELD	ING GROND	DERM GROND BINNEN BUITEN	PERM GEWAS BINNENL. BUITENL.	INH GROND BINNENL. BUITENL.	ING GEWAS BINNENL. BUITENL.	INH VLEES	DERM DOUCHEN	PERM DOUCHEN	INH VLEES	ING MELK	ING EIERN	ING MELK	ING EIERN	TOTAL (excl. diel. producten)
	1.51E-03	0.00E+00	0.00E+00	9.51E-06	0.00E+00	0.00E+00	1.62E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.77E-02

UITVOERTABEL 6 INTERVENTIEWAARDE GRONDGRONDWATER EN HUMAAN-TOX MAXIMUM CONCENTRATIE GRONDWATER	CS	IW	Cmax	Cgw	GRONDWATER	Brinbekthconc	TCL	Toelaatbare Conc. Lucht	GRONDWATER	Conc. Lucht	ingec	ingec	ingec	TOTAL
			[mg/kg]	[mg/kg]	[ug/dm3]	[mg/m3]		[mg/m3]			n.v.t.	n.v.t.	n.v.t.	

UITVOERTABEL 6	CS	IW	Cmax	Cgw	GRONDWATER	Brinbekthconc	TCL	Toelaatbare Conc. Lucht	GRONDWATER	Conc. Lucht	ingec	ingec	ingec	TOTAL
	282.447	282.447	157.051	220.432	157.051	0.0000					n.v.t.	n.v.t.	n.v.t.	

PERMEATE DRINKWATER(EIDING)

concentratie drinkwater backamertucht [mg/dm3]	concentratie drankwater [mg/kg dw]	Cpd0	Cps0	Cpd0p	3.60E-02
CdW	2.82E+01	1.13E+02			

TUSSENBEREKENINGEN CUSERPETRA123CSoilCSoil68 WK1
03-Apr-95

VERDELING OVER DE BODEMFASSEN diethyleen glycol SCNr. 2

beschrijving waarde eenheid

Z _a	4.25E-04 [mol/m ³ Pa]	fugaciteitscap cat a.
Z _w	3.61E-04 [mol/m ³ Pa]	fugaciteitscap cat w
Z _s	1.12E-07 [mol/m ³ Pa]	fugaciteitscap cat s
Kd	1.25E-02 [kg/dm ³]	verdelingscoff grond/water bekende lucht/water verdeelingscoff. invoer lucht/water verdeelingscoff gehele in bodem waarder CpW > S
Kw_BEREKE	1.18E-08 [-]	
Kw	1.18E-08 [-]	
Cp1	6.35E-08 [mg/kg]	
P _a	1.26E-11 [-]	massafractie a. (bodemlucht)
P _w	1.07E-03 [-]	massafractie w. (bodemwater)
P _s	9.98E-01 [-]	massafractie s. (vaste fase vd bodem)
Dsa	8.91E-04 [m ² /h]	diff coeff bodemlucht
Dew	8.91E-08 [m ² /h]	diff coeff bodemrocht
Du	4.76E-10 [m ² /h]	diff coeff bodem
KL	3.58E-05 [m/s]	water massa transport coeff
KG	3.42E-03 [m/s]	kicht/water verdeelingscoeff
Kw_sh	2.19E-08 [-]	bij badwater temperatuur
Kw _a	4.50E-07 [-]	mate van verdamping v d stof

CONCENTRATIES IN BODEMFASSEN

grondw.	bodeml. bodemvo.
[g/dm ³]	[g/m ³]
C _{gw}	C _{pW}

C_{gw} 8.80E-04 1.15E-05 9.80E-02C_{pW} 7.62E-06

1.51E-03 1.06E-04 9.51E-06

2.64E-05 4.04E-06 1.50E-03

1.16E-04 1.83E-01 1.16E-04

3.25E-03 4.84E-06 6.38E-04

1.30E-02 1.16E-03 1.42E-02

1.85E-01 9.32E-04 3.06E-05

UITVOER diethyleen glycol SCNr. 2

UITVOERTABEL 1

BLUITSTELLING KIND [mg/kg | g/d]

ING DERM GROND BINNEN

dhc 1.22E+00 2.50E-03 4.99E-02

ingr 1.92E-03 5.02E-03 2.63E-05

ingc 4.11E-01 2.98E-02 1.06E-06

ingv 1.40E-05 4.94E-05 7.81E-05

ingb 3.50E-06 3.50E-06 3.50E-06

TCH 1.72E+00

ING EIEREN (excl diel producten)

ING MELK

ING VLEES

ING GEWAS

ING BUITENL.

ING INH.

ING GROND

ING BINNEN

ING DERM

ING GROND

ING BINNEN

ING BUITENL.

ING INH.

ING GROND

UITSENBEREKENINGEN:USERPETRA123CSOLICSON68 WK1												RIVM report no. 715810010			
04-Apr-95												C:\USER\PTERA123\CSOLICSON68 WK1			
04-Apr-95												UITVOER acrylnitril			
04-Apr-95												SCNr- 2			
ERTDELING OVER DE BODEMFASSEN												UITVOERTABEL 1			
SCNr-		beschrijving		waarde		eenheid		ING GROND		DERM GROND BINNEN		INH GROND		BLOOTSTELLING KIND [mg/kg 19/d]	
acrylnitril		verdeling over de bodemfasen		0.6		4.25E-04 [mol/m³ Pa]		Ihgcietscap crd. a		ING GEWAS		PERM DRINKW.		ING VLEES	
		verdeling over de bodemfasen		0.6		1.24E-01 [mol/m³ Pa]		Ihgcietscap crd. a		ING GEWAS		DAMPEN DOUCHEN		ING MELK	
		verdeling over de bodemfasen		0.6		1.58E-01 [mol/m³ Pa]		Ihgcietscap crd. a		ING GEWAS		DERM DOUCHEN		ING EIERN	
		verdeling over de bodemfasen		0.6		5.08E-01 [kg/dm³]		verdelingsoef. grond-water		ING GEWAS		DAMPEN DOUCHEN		ING EIERN (end dieel producten)	
		verdelingsoef. grond-water		0.6		3.42E-03 [kg]		verdelingsoef. grond-water		ING GEWAS		DAMPEN DOUCHEN		TCH 1.78E-04	
		verdelingsoef. grond-water		0.6		3.35E-03 [kg]		verdelingsoef. grond-water		ING GEWAS		DAMPEN DOUCHEN		TCH 1.78E-04	
UITVOERTABEL 2												UITVOERTABEL 2			
SCNr-		beschrijving		waarde		ING GROND		DERM GROND		INH GROND		BLOOTSTELLING VOLWASSENEN [mg/kg 19/d]		UITVOERTABEL 2	
acrylnitril		verdelingsoef. grond-water		0.6		9.26E-07		Ihgcietscap crd. a		ING GROND		BLOOTSTELLING VOLWASSENEN [mg/kg 19/d]		UITVOERTABEL 2	
		verdelingsoef. grond-water		0.6		1.90E-09		Ihgcietscap crd. a		ING GROND		BLOOTSTELLING VOLWASSENEN [mg/kg 19/d]		UITVOERTABEL 2	
		verdelingsoef. grond-water		0.6		3.76E-08		Ihgcietscap crd. a		ING GROND		BLOOTSTELLING VOLWASSENEN [mg/kg 19/d]		UITVOERTABEL 2	
UITVOERTABEL 3												UITVOERTABEL 3			
SCNr-		beschrijving		waarde		ING GROND		DERM GROND		INH GROND		BLOOTSTELLING LEVENSLANG-GEMIDDELD [mg/kg 19/d]		UITVOERTABEL 3	
acrylnitril		verdelingsoef. grond-water		0.6		6.61E-08		Ihgcietscap crd. a		ING GROND		BLOOTSTELLING LEVENSLANG-GEMIDDELD [mg/kg 19/d]		UITVOERTABEL 3	
		verdelingsoef. grond-water		0.6		5.94E-10		Ihgcietscap crd. a		ING GROND		BLOOTSTELLING LEVENSLANG-GEMIDDELD [mg/kg 19/d]		UITVOERTABEL 3	
UITVOERTABEL 4												UITVOERTABEL 4			
SCNr-		beschrijving		waarde		ING GROND		DERM GROND		INH GROND		BLOOTSTELLINGSCOEFFICIENTEN LEVENSLANG-GEMIDDELD [1000/d]		UITVOERTABEL 4	
acrylnitril		verdelingsoef. grond-water		0.6		1.51E-03		Ihgcietscap crd. a		ING GROND		BLOOTSTELLINGSCOEFFICIENTEN LEVENSLANG-GEMIDDELD [1000/d]		UITVOERTABEL 4	
		verdelingsoef. grond-water		0.6		9.85E-09		Ihgcietscap crd. a		ING GROND		BLOOTSTELLINGSCOEFFICIENTEN LEVENSLANG-GEMIDDELD [1000/d]		UITVOERTABEL 4	
UITVOERTABEL 5												UITVOERTABEL 5			
SCNr-		beschrijving		waarde		ING GROND		DERM GROND		INH GROND		PROCENTUELE BLUDRAGE ROUTES KIND, VOLW., LEVENSlang-GEMIDDELD		UITVOERTABEL 5	
acrylnitril		verdelingsoef. grond-water		0.6		1.40E-07		Ihgcietscap crd. a		ING GROND		PROCENTUELE BLUDRAGE ROUTES KIND, VOLW., LEVENSlang-GEMIDDELD		UITVOERTABEL 5	
		verdelingsoef. grond-water		0.6		7.06E-10		Ihgcietscap crd. a		ING GROND		PROCENTUELE BLUDRAGE ROUTES KIND, VOLW., LEVENSlang-GEMIDDELD		UITVOERTABEL 5	
UITVOERTABEL 6												UITVOERTABEL 6			
SCNr-		beschrijving		waarde		ING GROND		DERM GROND		INH GROND		INTERVENTIEWAARDE GRONDGRONDWATER EN HUMAAN-TOX MAXIMUM CONCENTRATIE GRONDWATER		UITVOERTABEL 6	
acrylnitril		verdelingsoef. grond-water		0.6		1.44E+01		Ihgcietscap crd. a		ING GROND		INTERVENTIEWAARDE GRONDGRONDWATER EN HUMAAN-TOX MAXIMUM CONCENTRATIE GRONDWATER		UITVOERTABEL 6	
		verdelingsoef. grond-water		0.6		4.93E-04		Ihgcietscap crd. a		ING GROND		INTERVENTIEWAARDE GRONDGRONDWATER EN HUMAAN-TOX MAXIMUM CONCENTRATIE GRONDWATER		UITVOERTABEL 6	
GEHALTEN IN PLANTEN												GEHALTEN IN PLANTEN			
SCNr-		beschrijving		waarde		ING GROND		DERM GROND		INH GROND		GEHALTEN IN PLANTEN		GEHALTEN IN PLANTEN	
acrylnitril		verdelingsoef. grond-water		0.6		4.25E-03		Ihgcietscap crd. a		ING GROND		GEHALTEN IN PLANTEN		GEHALTEN IN PLANTEN	
		verdelingsoef. grond-water		0.6		6.01E-07		Ihgcietscap crd. a		ING GROND		GEHALTEN IN PLANTEN		GEHALTEN IN PLANTEN	
PERMEATIE DRINKWATERLEIDING												PERMEATIE DRINKWATERLEIDING			
SCNr-		beschrijving		waarde		ING GROND		DERM GROND		INH GROND		PERMEATIE DRINKWATERLEIDING		PERMEATIE DRINKWATERLEIDING	
acrylnitril		verdelingsoef. grond-water		0.6		3.43E-09		Ihgcietscap crd. a		ING GROND		PERMEATIE DRINKWATERLEIDING		PERMEATIE DRINKWATERLEIDING	
concentratie drinkwater backermaat												concentratie drinkwater backermaat			
SCNr-		beschrijving		waarde		ING GROND		DERM GROND		INH GROND		concentratie drinkwater backermaat		concentratie drinkwater backermaat	
acrylnitril		verdelingsoef. grond-water		0.6		1.21E-01		Ihgcietscap crd. a		ING GROND		concentratie drinkwater backermaat		concentratie drinkwater backermaat	
04-Apr-95												04-Apr-95			

TUSSENBEREKENINGEN-CUSERPETRA1230SOILCSOIL 68 WK1		04-Apr-95	UITVOER	buitend	SCAFN.	2
VF RIFELING OVER DE BODEMASEN						
symbool	waarde eenheid	beschrijving				
Za	4 25E-04 [mol/m ³ Pa]	fugacieftscap. cat. a				
Zw	2 04E+00 [mol/m ³ Pa]	fugacieftscap. cat. w				
Zs	1 72E+00 [mol/m ³ Pa]	fugacieftscap. cat. s				
Kd	3 36E-01 [kg/dm ³]	verdelingscoëff grond-water				
Klw	2 08E-04 [-]	beleidende lucht-water verdelingscoëff.				
Cop.	2 64E-04 [-]	invoer lucht-water verdelingscoëff				
Pw	5 91E-05 [-]	gehalte in bodem waarbij Cpw >= S				
Pw	2 84E-01 [-]	massafactie a (bodemlucht)				
Pw	7 16E-01 [-]	massafactie w (bodemvocht)				
Dsa	1 07E-03 [m ² /h]	diff. coeff. bodemlucht				
Dsw	1 07E-07 [m ² /h]	diff. coeff. bodemvocht				
Du	4 66E-07 [m ² /h]	diff. coeff. bodem				
kl	4 28E-05 [m ² /s]	water massa transport coëff				
kG	4 09E-03 [m ² /s]	damp massa transport coëff				
Khw_sh	4 90E-04 [-]	lucht-water verdelingscoëff				
Kws	1 15E-02 [-]	bij bodemwater temperatuur				
		mate van verdamping v.d. stof				

CONCENTRATIES IN BODEMASEN

grondw	bodemlvo	bodemvo	total	total	total	
[kg/dm ³]	[g/m ³]	[g/m ³]	binnen	buiten	binnen	
C _{gw}	C _{pw}	C _{pw}				
2 20E+04	4 58E-02	2 20E+02				

LUCHTFLUXEN [g/m²/h]

grenslag	evapo.	diffusie	total	total	total	
	buitend	binnen	buiten	binnen	buiten	
J2	J3	J4	J5	Jo	Ji	
3 34E-01	9 17E-04	5 79E-05	9 85E-05	9 75E-04	1 01E-03	

LUCHTCONCENTRATIES [g/m³]

buitend	knipr.	binnend	

C_{ba} Co_c C_{ba} C_{ba}C_{ba} C_{ba} C_{ba} C_{ba}

spore-makien	bladgew	org. stoffen/nog. vaste	bloed
[mg/kg dw]	[mg/kg dw]	[mg/kg vg]	[mg/kg vg]
Cpr1	Cpr1	Cp0	Cpdep
		2 13E+02	1 11E+02

PERMEATE DRINKWATERLEIDING

concentratie	concentratie	concentratie	concentratie
[mg/dm ³]	[mg/dm ³]	[mg/dm ³]	[mg/dm ³]
Cdw	Cdw	Cdw	Cdw
1 00E-01	5 77E-06		

PERMEATE DRINKWATERLEIDING	concentratie drinkwater backmerkruft [mg/dm ³]	concentratie backmerkruft [g/m ³]	CBK Cdw Cdw Cdw Cdw Cdw
—	—	—	—

VERDELING OVER DE BODEMFASEN

SCNr.: 2

03-Apr-95

03-Apr-95

methylbenzyllether

SCNr.: 2

03-Apr-95

beschrijving

beschrijving

beschrijving

waarde enheid

waarde enheid

waarde enheid

symbol

symbol

symbol

fugaciteitscap. cst. *

fugaciteitscap. cst. *

fugaciteitscap. cst. *

Za 4.25E+04 [mol/m³ Pa]

Za 1.86E-02 [mol/m³ Pa]

Za 3.59E-02 [mol/m³ Pa]

Kw BERKE

2.28E+02 [-]

Kw 2.90E-02 [-]

Cap1 2.63E-04 [mg/kg]

verdelingscoeff. grond-water

bekende lucht-water verdelingscoeff.

inover lucht-water verdelingscoeff.

gehalte in bodem wasrh (pw >= 5

massafract. s. (bodemlucht)

massafract. w. (bodemvocht)

massafract. s. (vaste less vd bodem)

diff coeff bodemlucht

diff coeff bodemvocht

diff coeff bodem

diff coeff bodem

water massa transport coeff

damp massa transport coeff

lucht-water verdelingscoeff

bij beweert temperatuur

mate van verdamping vd stof

Kw_a 7.71E+01 [kg/dm³]

Das 9.77E-04 [m²/h]

Daw 9.77E-08 [m²/h]

Du 1.65E-05 [m²/h]

Kw_l 3.02E-05 [m²/a]

KG 3.75E-03 [m²/a]

Kw_sh 5.39E-02 [-]

Kw_w 1.97E-01 [-]

CONCENTRATES IN BODEMFASEN

grondw. bodeml. bodemvo.

[ug/dm³] [g/m³]

Cgw Csa 4.66E+04 1.06E+01

Cpw 4.66E+02

LUCHTFLUXEN [g/m²/h]

grondvlag evapo.

diffusie buiten

totaal buiten

binnen

totaal binnen

buiten

binnen

buiten

volw. kind

J2' 1.94E+01 8.35E-03 1.39E-02 J6 1.50E-02 Jj

7.11E-05 6.38E-05

Coa CoBc Cba 2.54E-02 2.54E-03

LUCHTCONCENTRATIES [g/m³]

buitenl. kruipr. binnenv. volw.

spore-melkblaad gew. bladgew. [mg/kg dw]

[mg/kg vg]

GEHALDEN IN PLANTEN

Cps1 Cps0 Cpd0

4.57E+02 2.44E+02 5.39E+02

PERMEATIE DRINKWATERLEIDING

concentratie drinkwater backenmeelvocht [mg/dm³]

Cdw Cbk 2.12E-01 2.09E-04

UITVOERTABEL 1

UITVOER

methylethylketon

SCNr.: 2

BLOOTSTELLING KIND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

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BLOOTSTELLING GROND [mg/kg g/d]

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BLOOTSTELLING BINNEN [mg/kg g/d]

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BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

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BLOOTSTELLING GROND [mg/kg g/d]

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BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

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BLOOTSTELLING GROND [mg/kg g/d]

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BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

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BLOOTSTELLING INH [mg/kg g/d]

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BLOOTSTELLING GROND [mg/kg g/d]

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BLOOTSTELLING BINNEN [mg/kg g/d]

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BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

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BLOOTSTELLING BINNEN [mg/kg g/d]

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BLOOTSTELLING BUITEN [mg/kg g/d]

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BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

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BLOOTSTELLING BINNEN [mg/kg g/d]

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BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BINNEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING BUITEN [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING INH [mg/kg g/d]

SCNr.: 2

BLOOTSTELLING GROND [mg/kg g/d]

INSENBERKENINGEN C:USERIPETRAN2/3CSOILCSOIL60 WK1

VERDIENING OVER DE BODEMFASEN

doorkruisen

SCNR-

synthool

2

warde enheid

beschrijving

08-Jun-95

UNTOER

dodehydrazine

SCNR-

2

BLOOTSTELLING KIND [mg/kg (1/d)]

UITVOERTABEL 1

ING.

GROND

DERM.

GROND

INH.

BINNENL.

BUITENL.

PERM.

DRINKW.

DAMPEN

DERM.

DOUCHEN

VLEES

ING.

MELK

EIEREN

ING.

TOTAL

(excl. dierl.

productien)

Za

4.25E-04

[mol/m³ Pa]

1.7E+01

[1]

Zw

2.1E-05

[mol/m³ Pa]

4.1E-02

[mol/m³ Pa]

Zs

4.1E-02

[mol/m³ Pa]

Kd

6.0E-08

[kg/dm³]

Kiw BERKE

1.7E+01

[1]

Cop

1.30E+03

[mg/kg]

Pa

3.43E-07

[1]

Pw

1.94E-08

[1]

Ps

1.00E+00

[1]

Dsa

5.85E-04

[m²/h]

Dsw

5.85E-08

[m²/h]

Dtr

1.00E-09

[m²/h]

KL

2.35E-05

[m/s]

KG

2.24E-03

[m/s]

Kiw

3.20E-01

[1]

Kwa

1.4E-01

[1]

verdelingscoef. grond/water

borekende lucht/water verdelingscoef.

invloer lucht/water verdelingscoef.

gehalte in bodem waarbij Cpw >> S

massificatie a. (bodemlucht)

massificatie w. (bodemvocht)

massificatie s. (vaste fasen vd bodem)

diff. coef. bodemlucht

diff. coef. bodenvocht

diff. coef. bodem

water massa transport coef.

damp massa transport coef.

lucht/water verdelingscoef.

bij hardwater temperatuur

mate van verdampering v.d. slot

CONCENTRATIES IN BODEMFASEN

grondw.

bodemvo-

[kg/dm³]

[g/m³]

Cdw

Csa

2.60E-03

1.47E-02

1.4E-04

0.00

0.00

0.00

0.00

0.00

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08-Jun-95

UNTOER

dodehydrazine

SCNR-

2

BLOOTSTELLING VOLWASSENEN [mg/kg (1/d)]

UITVOERTABEL 2

ING.

GROND

DERM.

GROND

INH.

BINNENL.

BUITENL.

PERM.

GEWAS

DRINKW.

DAMPEN

DERM.

DOUCHEN

VLEES

ING.

MELK

EIEREN

ING.

GROND

DERM.

GROND

INH.

BINNENL.

BUITENL.

PERM.

GEWAS

DRINKW.

DAMPEN

DERM.

DOUCHEN

VLEES

ING.

MELK

EIEREN

ING.

TOTAL

(excl. dierl.

productien)

Za

4.25E-04

[mol/m³ Pa]

1.7E+01

[1]

Zw

2.1E-05

[mol/m³ Pa]

4.1E-02

[mol/m³ Pa]

Zs

4.1E-02

[mol/m³ Pa]

Kd

6.0E-08

[kg/dm³]

Kiw BERKE

1.7E+01

[1]

Cop

1.30E+03

[mg/kg]

Pa

3.43E-07

[1]

Pw

1.94E-08

[1]

Ps

1.00E+00

[1]

Dsa

5.85E-04

[m²/h]

Dsw

5.85E-08

[m²/h]

Dtr

1.00E-09

[m²/h]

KL

2.35E-05

[m/s]

KG

2.24E-03

[m/s]

Kiw

3.20E-01

[1]

Kwa

1.4E-01

[1]

verdelingscoef. grond/water

invoer lucht/water verdelingscoef.

gehalte in bodem waarbij Cpw >> S

massificatie a. (bodemlucht)

massificatie w. (bodemvocht)

massificatie s. (vaste fasen vd bodem)

diff. coef. bodemlucht

diff. coef. bodenvucht

diff. coef. bodem

water massa transport coef.

damp massa transport coef.

lucht/water verdelingscoef.

bij hardwater temperatuur

mate van verdampering v.d. slot

verdekkende lucht/water verdelingscoef.

gehalte in bodem waarbij Cpw >> S

massificatie a. (bodemlucht)

massificatie w. (bodemvocht)

massificatie s. (vaste fasen vd bodem)

diff. coef. bodemlucht

diff. coef. bodenvucht

diff. coef. bodem

water massa transport coef.

damp massa transport coef.

lucht/water verdelingscoef.

bij hardwater temperatuur

mate van verdampering v.d. slot

verdekkende lucht/water verdelingscoef.

gehalte in bodem waarbij Cpw >> S

massificatie a. (bodemlucht)

massificatie w. (bodemvocht)

massificatie s. (vaste fasen vd bodem)

diff. coef. bodemlucht

diff. coef. bodenvucht

diff. coef. bodem

water massa transport coef.

damp massa transport coef.

lucht/water verdelingscoef.

bij hardwater temperatuur

mate van verdampering v.d. slot

C:\USER\PEI\HAI\23CSSU1\CSU1L88.WK1

T1 ISSENBERGER NINGEN C VSEFANETBAV123CCSOH VCSOH 08 WK1

THE JOURNAL OF CLIMATE

RIVM report no. 715810010											
VERDELING OVER DE BODENFASEN		atomaarische oplosmiddelen		SCNR=		UITVOERTABEL 1		UITVOERTABEL 2		UITVOERTABEL 3	
symbol	waarde enheid	beschrijving				BLOOTSTELLING KIND [mg/kg g d]	BLOOTSTELLING VOLWASSENE [mg/kg g d]	BLOOTSTELLING LEVENSLANG GEMIDDELD [mg/kg g d]	BLOOTSTELLING LEVENSLANG GEMIDDELD [mg/kg g d]		
Za	4.25E-04 [mol/m ³ Pa]	fugaciteitscap. cst. a.				ING. GROND	DERM. GROND BINNENL. BUITENL.	ING. GEWAS	PERM. DRINKW.	DAMPEN DOUCHEN	ING. VLEES
Zw	2.18E-03 [mol/m ³ Pa]	fugaciteitscap. cst. w.				1.45E-02	1.0C	1.92E-01	4.83E-04	1.74E-03	4.85E-03
Zs	8.19E-01 [mol/m ³ Pa]	fugaciteitscap. cst. s.				2.96E-05	5.89E-04	2.20E-05	1.52E-01	2.92E-04	2.18E-04
Kd	1.50E-02 [kg/dm ³]	verdelingscoeff. grond-water				dac1	daao	1.94E-01	4.83E-04	1.53E-01	4.86E-03
Kw BEREKE	1.95E-01 [-]	bekende lucht-water verdelingscoeff.				1.95E-01	1.95E-01	1.94E-01	1.94E-01	1.94E-01	1.94E-01
Kw	1.95E-01 [-]	inwend. lucht-water verdelingscoeff.				1.95E-01	1.95E-01	1.94E-01	1.94E-01	1.94E-01	1.94E-01
Cop	7.10E-03 [mg/kg]	inhoud in bodem water Cpw >= S				1.03E-03	1.13E-04	1.29E-05	9.25E-02	5.40E-05	6.12E-02
Pa	1.72E-04 [-]	massatractie a. (bodemlucht)				daaa	1.92E-06	1.13E-04	1.29E-05	9.25E-02	5.40E-05
Pw	8.86E-04 [-]	massatractie w. (bodemvocht)				1.03E-03	1.13E-04	1.29E-05	9.25E-02	5.40E-05	6.12E-02
Ps	9.99E-01 [-]	massatractie s. (vastolase vd bodem)				daao	1.92E-06	1.13E-04	1.29E-05	9.25E-02	5.40E-05
Dsa	8.36E-04 [m ² /h]	diff. coeff. bodemlucht				1.95E-01	1.95E-01	1.94E-01	1.94E-01	1.94E-01	1.94E-01
Dsw	8.35E-08 [m ² /h]	diff. coeff. bodenvocht				1.95E-01	1.95E-01	1.94E-01	1.94E-01	1.94E-01	1.94E-01
Du	7.21E-07 [m ² /h]	diff. coeff. bodem				1.95E-01	1.95E-01	1.94E-01	1.94E-01	1.94E-01	1.94E-01
KL	3.36E-05 [m/s]	water massa transport coeff.				1.95E-01	1.95E-01	1.94E-01	1.94E-01	1.94E-01	1.94E-01
KG	3.20E-03 [m/s]	damp massa transport coeff.				1.95E-01	1.95E-01	1.94E-01	1.94E-01	1.94E-01	1.94E-01
Kw sh	3.62E-01 [-]	lucht-water verdelingscoeff.				1.95E-01	1.95E-01	1.94E-01	1.94E-01	1.94E-01	1.94E-01
Kwa	1.95E-01 [-]	bij bodemwater temperatuur mate van verdamping v.d. stol				1.95E-01	1.95E-01	1.94E-01	1.94E-01	1.94E-01	1.94E-01

CONCENTRATIONS IN BODMEASIN

UITVOERTABEL 4 BLOOTSTELLINGSCOEFFICIENTEN LEVENSlang GEMIDDELD (100kg)						
	ING. GROND BINNEN	DERM. GROND BINNEN	ING. GROND BUITEN	PERM. GEWAS	DAMPEN DOUCHEN	ING. MELK VLEES
grondw. [$\mu\text{g}/\text{dm}^3$]	1.5E-03	7.62E-06	1.06E-04	9.51E-06	6.75E-02	6.28E-05
bodemw. [g/m^3]	9.60E+02	1.8E+00	9.60E+00	1.77E-02	9.64E-05	1.86E-05

LICHTENBERG

卷之三

As Ca->Cl dan georganisirde interventiowarden.									
	TCL	TCL	TCL	TCL	TCL	TCL	TCL	TCL	TCL
	Torkathare Conc. Lucht [mg/m ³]	W GROND [mg/m ³]	W GROND [mg/m ³]	W GROND [mg/m ³]	W GROND [mg/m ³]	W GROND [mg/m ³]	W GROND [mg/m ³]	W GROND [mg/m ³]	W GROND [mg/m ³]
Craa	Coac	Cha	Cia						
3.90E-06	8.00E-06	3.40E-03	3.40E-04						
1445.292	1445.292	5.359.744	989.900	949.900					
sporen metalen	knobgew.	0.09	stofvervuiling, verh. wortel bladgew.						
[mg/kg dw]	[mg/kg dw]	[mg/kg vgi]	[mg/kg vgi]						

卷之三

卷之三

concentratie drinkwater badkamerlucht

[mg/dm³] [g/m³]

Cdw Cbk
4.38E-03 4.28E-06

symbool	warde eenheid	beschrijving	2	ING.	DERM.	PERM.	DAMPEN.	ING.	ING.	TOTAAL
				GROND	GROND	DRINKW.	DOUCHEN	VLEES	MELK	(excl. dien. producten)
Za	4.25E-04 [mol/m ³ Pa]	fugaciteitscap. cst. a.			INH.	INH.				
Zw	7.30E-04 [mol/m ³ Pa]	fugaciteitscap. cst. w.			BINNENL.	BUITENL.				
Zs	9.86E-03 [mol/m ³ Pa]	fugaciteitscap. cst. s.			GROND	GROND				
Kd	5.39E-00 [kg/dm ³]	verdelingscoef. grond-water			BUITEN	BUITEN				
Kw BERKEK	5.02E-01 [-]	verdeelende lucht-water verdelingscoef. in over lucht/water voordeelingscoef. gehaakt in bodem waarbij C _{lw} >= S								
Kw	5.82E-01 [-]									
C _{d1}	4.99E-03 [mg/kg]									
Pa	1.38E-02 [-]	massafractie a. (bodemlucht)								
Pw	2.38E-02 [-]	massafractie w. (bodemlucht)								
Ps	9.62E-01 [-]	massafractie s. (vaste fase vd bodem)								
Dsa	7.95E-04 [m ² /h]	diff. coef. bodemlucht								
Dsw	7.95E-08 [m ² /h]	diff. coef. bodemvocht								
Du	5.61E-05 [m ² /h]	diff. coef. bodem								
KL	3.19E-05 [m/s]	water massa transport coef.								
KG	3.05E-03 [m/s]	damp massa transport coef.								
KW sh	1.98E-00 [-]	lucht/water verdelingscoef. bij badwater temperatuur								
Kwa	1.90E-01 [-]	mate van verdamping v d slof								

CONCENTRATIES IN BODEMFASEN

grondw.	bodemvo.	diffusie	totaal	ING.	DERM.	PERM.	DAMPEN.	ING.	ING.	TOTAAL
[kg/m ³]	[g/m ³]	buiten	buiten	GROND	GROND	DRINKW.	DOUCHEN	VLEES	MELK	(excl. dien. producten)
C _{gw}	C _{sa}	C _{pw}								
2.60E+02	1.51E+00	2.60E+00								

LUCHTFLUXEN [g/m ² /h]	grenslaag	evapo.	diffusie	totaal	ING.	DERM.	PERM.	DAMPEN.	ING.	TOTAAL
				buiten	GROND	GROND	DRINKW.	DOUCHEN	VLEES	(excl. dien. producten)
J ²	J ³	J ⁴	J ⁵	J ₆	ING.	DERM.	PERM.	DAMPEN.	ING.	TOTAAL
8.21E+00	1.08E-05	9.60E-04	1.60E-03	9.71E-04	1.61E-03					

LUCHTCONCENTRATIES [g/m ³]	buitenl.	kind	ING.	DERM.	PERM.	DAMPEN.	ING.	ING.	TOTAAL	
			GROND	GROND	GROND	GROND	GROND	GROND	(excl. dien. producten)	
J ₂	J ³	J ⁴	J ⁵	J ₆	ING.	DERM.	PERM.	DAMPEN.	ING.	TOTAAL
0.21E+00	1.08E-05	9.60E-04	1.60E-03	9.71E-04	1.61E-03					

GEHALTEN IN PLANTEN	org stoffen/and org verb.	ING.	DERM.	PERM.	DAMPEN.	ING.	ING.	TOTAAL
	wortel	blad	vrucht	vrucht	vrucht	vrucht	vrucht	(excl. dien. producten)
C _{pa1}	C _{ps1}	C _{pw1}	C _{pw0}					
Co _a	Co _{ac}	C _{ha}	2.58E-04					
2.90E-06	6.02E-06	2.58E-03						

PERMEATIE DRINKWATERLEIDING

concentratie concentratie drinkwater badkamerlucht [mg/m³] [mg/m³]C_{dw}

2.37E-02 2.24E-05

0.3800 0.25/A

n.v.t. n.v.t. n.v.t.

Als C_{dw}>C_{lw} dan geconcentreerde drinkwaterleiding:Totaaltoelate Conc Lucht W GROUNDWATER [mg/m³] [kg/dm³]C_{lw}

0.3800 0.25/A

n.v.t. n.v.t. n.v.t.

TUSSENBEREKENINGEN C: USERPETRA1123(CSOILCSOIL68 WK1
VERDELING OVER DE BODEMFASEN 12-dochtoorethen (cis) SCNr.: 2

symbol	warde eenheid	beschrijving	UITVOER	12-dochtoorethen (cis)	SCNr.: 2
Za	4.25E-04 [mol/m3 Pa]	hogactitescap. cst. a.			
Zw	5.17E-04 [mol/m3 Pa]	hogactitescap. cst. w.			
Zs	4.92E-03 [mol/m3 Pa]	hogactitescap. cst. s.			
Kd	3.80E-00 [kg/dm3]	verdelingscoeff. grondwater			
Klw	8.21E-01 [-]	berekende lucht-water verdelingscoeff.			
Copl	3.14E+03 [mg/kg]	invoer lucht-water verdelingscoeff.			
Pa	2.71E-02 [-]	gehalte in bodem waterl. Cpw >= S			
Pw	3.20E-02 [-]	massalucht a. (bodemvocht)			
Ps	9.40E-01 [-]	massalucht a. w. (bodemvocht)			
Dsa	9.32E-04 [m2/h]	massalucht s. (vaste lasse vd bodem)			
Dsw	9.32E-08 [m2/h]	difl. coeff. bodemvocht			
Du	1.26E-04 [m2/h]	difl. coeff. bodemvocht			
KL	3.48E-05 [m/s]	water massa transport coeff.			
KG	3.58E-03 [m/s]	damp massa transport coeff.			
KW sh	1.53E+00 [-]	lucht water verdelingscoeff.			
Kwa	2.23E-01 [-]	bij bodwater temperatuur			
		mate van verdamping v.d. slot			

CONCENTRATIES IN BODEMFASEN

grenslag,	bodeml.	bodenvo.	
[kg/dm3]	[g/m3]	[g/m3]	
Cgw	Csa	Cow	
1.26E-01	1.04E-01	1.26E-01	

LUCHTFLUXEN [@/m2/h]

grenslag	evapo.	diffusie	totaal	totaal	
		buiten	binnen	buiten	
J2*	J3*	J4*	J5*	J6*	J7*
6.61E-01	5.26E-07	7.73E-05	1.28E-04	7.78E-06	1.29E-04

LUCHTCONCENTRATIES [@/m3]	buitenv.	kruipt.	kind	vlow
Coaa	Coac	Cba	Cia	
2.40E-07	4.82E-07	2.07E-04	2.07E-05	

GEHALDEN IN PLANTEN

Spore-maleien	bladgew.	org stofen/anorg verb.	
[mg/kg dw]	[mg/kg dw]	[mg/kg vgl]	
Cpr1	Cps1	Cpr0	Cpdop
		1.40E-01	8.50E-02

BLOOTSTELLING KIND [mg/kg (g/d)]					
ING.	DERM.	GROND.	GROND.	BINNENL.	ING.
5.11E-06	1.05E-08	2.04E-07	8.00E-09	9.24E-03	2.91E-05

UITVOERTABEL 2

BLOOTSTELLING VOLWASSENE [mg/kg (g/d)]					
ING.	DERM.	GROND.	GROND.	BINNENL.	ING.

UITVOERTABEL 3

BLOOTSTELLING LEVENSLANG-GEMIDDELD [1000gd]					
ING.	DERM.	GROND.	GROND.	BINNENL.	ING.

UITVOERTABEL 4

BLOOTSTELLINGSCOEFFICIENTEN LEVENSLANG-GEMIDDELD [1000gd]					
ING.	DERM.	GROND.	GROND.	BINNENL.	ING.

UITVOERTABEL 5

PROCENTUELE BIJDRAGE ROUTES KIND, VOLW., LEVENSLANG-GEMIDDELD					
ING.	DERM.	GROND.	GROND.	BINNENL.	ING.

UITVOERTABEL 6

INTERVENTIEWAARDEN GROND/GROENWATER EN HUMAAN-TOX. MAXIMUM CONCENTRATIE GRONDWATER					
CS	IW	Cmax	Cgw	IW	Cia

UITVOERTABEL 7

As Cia>TCL dan geconcentreerde intervreten:					
TCL	IW GROENWATER	Cia	Benachrichtigc.	IW GROENWATER	[mg/dm3]

PERMEATE DRINKWATERLEIDING

concentratie concentratie drinkwater badkamerlucht [mg/dm3] [g/m3]					
Cow	Cbk	Cps1	Cpd0	Cpd1	Cpd2

Appendix VIII:

RIVM reports related to potential (intervention values) and actual risks due to soil contamination

Berg, R. van den & Roels, J.M. (1991) Beoordeling van risico's voor mens en milieu bij blootstelling aan bodemverontreiniging. Integratie van deelaspecten. RIVM-report no. 725201007, dated February 1991.

Contains: for the 1st series of compounds: integration of ecotoxicological criteria with the results of CSOIL calculations based on the human-toxicological criteria, yielding proposal for soil intervention values; note that several of the then proposed values have been modified at a later stage.

Berg, R. van den (1995) Blootstelling van de mens aan bodemverontreiniging. Een kwalitatieve en kwantitatieve analyse leidend tot voorstellen voor humaan-toxicologische C-toetsingswaarden (beperkt herziene versie). RIVM-report no. 725201006, dated March 1995. **Modified version of the original report from 1991.**

Contains: description of the formulas that constitutes the CSOIL model, the model used to estimate human exposure in case of soil contamination; based on the human-toxicological criteria (MPR-values) for the 1st series of compounds. CSOIL is used to derive human-toxicological intervention values; table 2 to this report gives 'new' modified human-toxicological intervention values.

Berg, R. van den, Bockting, G.J.M., Crommentuyn, G.H. & Janssen, P.J.C.M. (1994) Proposals for intervention values for soil clean-up: Second series of compounds. RIVM-report no. 715810004, dated December 1994.

Contains: physicochemical properties, results of CSOIL calculations, derivation of the serious-soil-contamination-concentrations (SCC) using the ecotoxicological and human-toxicological criteria; integration of values yielding proposal for intervention values; this 2nd series consists of 12 compounds.

Bockting, G.J.M., Swartjes, F.A., Koolenbrander, L.G.M. & Berg, R. van den (1994) Beoordelingsmethodiek bodemkwaliteit ten behoeve van bouwvergunningaanvragen. Deel I. Bodemgebruiksspecifieke beoordelingsmethodiek voor de humane blootstelling. RIVM-report no. 715810001, dated June 1994.

Contains: methodology for estimating actual human exposure using formulas from the CSOIL model and measurements in contact media; several standard soil use categories are defined using standard assumptions as to human exposure; this method is part of a system for the evaluation of soil quality in dealing with requests for official building permits to be granted by local authorities.

Crommentuyn, G.H., Plassche, E.J. van de & Canton, J.H. (1994) Guidance document on the derivation of ecotoxicological criteria for serious soil contamination in view of the intervention value for soil clean-up. RIVM-report no. 950011003, dated November 1994.

Contains: description of the methodology used to derive ecotoxicological criteria in a stepwise protocol: data needs, formulas for normalisation & standardisation, data selection & method for calculation of the several HC50-values.

Denneman, C.A.J. & Gestel, C.A.M. van (1990) Bodemverontreiniging en bodemecosystemen: voorstel voor C-(toetsings)waarden op basis van ecotoxicologische risico's. RIVM-report no. 725201001, dated April 1990.

Contains: ecotoxicological criteria for 1st series of compounds; only data for soil organisms taken into consideration; the separate data for the individual compounds are presented in the appendix to this report

Denneman, C.A.J. & Gestel, C.A.M. van (1991) Afleiding van C-waarden voor bodemecosystemen op basis van aquatisch ecotoxicologische gegevens. RIVM-report no. 725201008, dated September 1991.

Contains: for the 1st series of compounds aquatic ecotoxicological data and QSARs were now also taken into consideration for derivation of C-values for water; from the latter values soil C-values were calculated and compared to the soil C-values previously derived leading to changes for several compounds.

Kreule, P., Berg, R. van den, Waitz, M.F.W. & Swartjes, F.A. (1995) Calculation of human-toxicological serious soil contamination concentrations and proposals for intervention values for clean-up of soil and groundwater: Third series of compounds. RIVM-report no. 715810010

Contains: physicochemical properties, results of CSOIL calculations, derivation of the serious-soil-contamination-concentrations (SCC) using the ecotoxicological and human-toxicological criteria; integration of values yielding proposal for intervention values; this 3rd series consists of 15 compounds.

Linders, J.B.H.J. (1990) Risicobeoordeling bij de mens bij blootstelling aan stoffen. Uitgangspunten en veronderstellingen. RIVM-report no. 725201003, dated August 1990.

Contains: description of calculation formulas to be used for estimation of human exposure via several routes in case of soil contamination; the formulas in this report were used in the compilation of the CSOIL-model as reported in the RIVM-report by van den Berg (1995).

Notenboom, J., Eijsackers, H.J.P. & Swartjes, F.A. (1995) Beoordelingssystematiek ten behoeve van bouwvergunningaanvragen. Deel III. Methodiek ter bepaling van het actuele risico voor het ecosysteem. RIVM-report no. 715810003, dated januari 1995.

Contains: method for determination of risks for ecosystems used during the evaluation of soil quality in dealing with requests for official building permits to be granted by local authorities.

Swartjes, F.A., Koolenbrander, L.G.M. & Bockting, G.J.M. (1994) Beoordelingssystematiek bodemkwaliteit ten behoeve van bouwvergunningaanvragen. Deel II. Methodiek ter bepaling van het verspreidingsrisico. RIVM-report no. 715810002, dated June 1994.

Contains: method for classification of calculated fluxes into 3 classes of increasing risk of contaminant dispersal; this classification provides a pragmatic assessment of the risk of dispersal; this method is part of a system for the evaluation of soil quality in dealing with requests for official building permits to be granted by local authorities.

Vermeire, T.G., Apeldoorn, M.E. van, Fouw, J.C. de & Janssen, P.J.C.M. (1991) Voorstel voor de humaantoxicologische onderbouwing van C-(toetsings)waarden. RIVM-report no. 725201005, dated February 1991.

Contains: human-toxicological criteria (MPR-values) for 1st series of compounds. this 1st series consists of 55 compounds or groups of compounds; includes description of the method used to derive the MPR-values.

Vermeire, T.G. (1993) Voorstel voor de humaantoxicologische onderbouwing van C-(toetsings)waarden. Betreft addendum op rapport 725201005. RIVM-report no. 715801001, dated May 1993.

Contains: reevaluation of the Maximum Permissible Intake values for 9 (groups of) compounds from the set dealt with in the Vermeire et al.-report from 1991.

Appendix IX.

Formulas for the calculation of proposals for human-toxicological serious soil contamination concentrations and actual risks.

Attention! These formulas have been adjusted on the basis of the 1992 TCB recommendations; the information on the uptake of heavy metals by plants has been adjusted to Bockting and Van den Berg, 1992 as well as other information. Mistakes have been corrected.

The consequences in the shape of the proposals for the human toxicological intervention values formulated on this basis are shown in annex 1.11. The proposals for the final intervention values as presented in the Memorandum Intervention Values Soil Clean Up (VROM, 1993) to Parliament, are also given here.

- Appendix 1 Formulas fugacity calculations.
- Appendix 2 Formulas air flux calculations.
- Appendix 3 Formulas dilution air flux outdoor
- Appendix 4 Formulas air concentration calculation .
- Appendix 5 Formulas crop content.
- Appendix 6 Formulas calculation concentration in drinking water after permeation.
- Appendix 7 Formulas for the calculation of the air concentration in the bathroom during showering.
- Appendix 8 Formulas for the quantification of the exposure.
- Appendix 9 Primary set of data.
- Appendix 10 Conversion formulas.

EXTRA REFERENCES

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De accumulatie van sporemetalen in groenten geteeld op verontreinigde bodems. Een literatuurstudie.
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- Fast, T.J., Kliest, J. en Wiel H. van de, 1987
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Voorstel voor de humaan-toxicologische onderbouwing van C-toetsingswaarden. Addendum op rapport 725201005. RIVM-rapportnr. 715801001. RIVM, Bilthoven.

Appendix 1. Formulas fugacity calculations.

organic substances

$$Z_a = 1 / (R * T)$$

Z_a : fugacity capacity constant air [mol.m⁻³.Pa⁻¹]
 R : gas constant [8.3144 Pa.m³.mol⁻¹.K⁻¹]
 T : temperature [K]

$$Z_w = S/V_p$$

Z_w : fugacity constant water mol.m⁻³.Pa⁻¹
 S : water-solubility [mol.m⁻³]
 V_p : vapour pressure pure substance [Pa]

$$Z_s = K_d * S_D * Z_w/V_s$$

Z_s : fugacity capacity constant soil [mol.m⁻³.Pa⁻¹]
 K_d : distribution coefficient soil-water [(mol.kg⁻¹ dry soil)/(mol.dm⁻³)]
 S_D : mass volume of the dry soil [kg dry soil.dm⁻³ humid soil]
 V_s : volume fraction solid phase [-]

$$V_s = 1 - \text{porosity}$$

$$= 1 - V_a - V_w$$

V_a : volume fraction air [-]
 V_w : volume fraction water [-]

$$K_d = K_{oc} * f_{oc}$$

K_{oc} : distribution coefficient soil-water corrected for organic carbon [(mol.kg⁻¹ org. C)/(mol.dm⁻³)]
 f_{oc} : fraction organic carbon [kg org.C.kg⁻¹ dry soil]

$$K_{oc} = 0.411 * K_{ow} \text{ or: } \log K_{oc} = 0.989 * \log K_{ow} - 0.346$$

K_{ow} : octanol-water distribution coefficient [(mol.dm⁻³)/(mol.dm⁻³)]

$$K_{lw} = Z_a / Z_w$$

$$= V_p / (S * R * T)$$

K_{lw} : air-water distribution coefficient [(mol.m⁻³ air)/(mol.m⁻³ water)] [-]

for dissociating substances

$$K_d = K_d * f_{nd}$$

fnD : fraction non-dissociated substance

$$\text{fnD} = 1 / (1 + 10^{[\text{pH} - \text{pKa}]})$$

pH : acid content of the soil (4-8, as default: 6)
 pKa : acid dissociation constant of the substance

Calculation mass fractions

$$\begin{aligned}\text{Pa} &= (\text{Za} * \text{Va}) / (\text{Za} * \text{Va} + \text{Zw} * \text{Vw} + \text{Zs} * \text{Vs}) \\ \text{Pw} &= (\text{Zw} * \text{Vw}) / (\text{Za} * \text{Va} + \text{Zw} * \text{Vw} + \text{Zs} * \text{Vs}) \\ \text{Ps} &= (\text{Zs} * \text{Vs}) / (\text{Za} * \text{Va} + \text{Zw} * \text{Vw} + \text{Zs} * \text{Vs})\end{aligned}$$

Pa : mass fraction in soil air	[-]
Pw : mass fraction in soil moisture	[-]
Ps : mass fraction in solid phase soil	[-]

inorganic substances

Za = 0; Csa = 0; Pa = 0

Pw = 1; Ps = 0

metals and arsenic

Za = 0; Csa = 0; Pa = 0

Pw = Vw / (Vw + Kd * SD)

Ps = 1 - Pw

calculation concentrations

$$\text{Csa} = \text{Cs} * \text{SD} * \text{Pa} / \text{Va}$$

Csa : soil air concentration	[mol.dm ⁻³ or g.m ⁻³]
Cs : initial soil content (total content in gas, water and solid phase) dry soil or mg.kg ⁻¹	[mg.kg ⁻¹]
Cpw = Cs * SD * Pw / Vw	

if : Cpw > S then: Cpw = S
 $\text{Csa} = \text{S} * \text{Vw} * \text{Pa} / (\text{Pw} * \text{Va})$

Cpw : soil moisture concentration [mol.dm⁻³ or g.m⁻³]

Appendix 2. Formulas air flux calculations.

$D_{sa} = V_a^{10/3} * Da / (l-V_s)^2$ with $Da = .036 * (76/M)^{1/2}$	
D_{sa} : diffusion coefficient in the soil-gas phase	[m ² .h ⁻¹]
Da : diffusion coefficient in free air	[m ² .h ⁻¹]
M : molecular mass	[g.mol ⁻¹]
$D_{sw} = V_w^{10/3} * Dw / (l-V_s)^2$ with $Dw = 3.6 * 10^{-6} * (76/M)^{1/2}$	
D_{sw} : diffusion coefficient in the soil-water phase	[m ² .h ⁻¹]
Dw : diffusion coefficient in free water	[m ² .h ⁻¹]
$D_u = (P_a * D_{sa} / V_a) + (P_w * D_{sw} / V_w)$	
D_u : diffusion coefficient in the soil	[m ² .h ⁻¹]
$J_2 = Da * C_{sa}/d$	
$J_3 = C_{pw} * E_v / 24$	
$J_4 = D_u * C_s * SD / dp$	
$J_5 = D_u * C_s * SD / (dp - Bh)$	
if : $C_{pw} > S$ then : $J_4 = D_u * S * V_w / (dp * P_w)$	
if : $C_{pw} > S$ then : $J_5 = D_u * S * V_w / [(dp - Bh) * P_w]$	
J_2 : boundary layer flux	[g.m ⁻² .h ⁻¹]
J_3 : water-evaporation flux	[g.m ⁻¹ .h ⁻¹]
J_4 : diffusion flux water-soil to surface level	[g.m ⁻² h ⁻¹]
J_5 : diffusion flux water-soil to crawl space	[g.m ⁻² h ⁻¹]
E_v : flux of evaporating water	[Fast et al., 1987: 0.0001 m ³ .m ⁻² .d ⁻¹]
d : thickness boundary layer	[Jury et al., 1985: 0.005 m]
dp : mean depth of the contamination	[1.25 m]
Bh : height of the crawl space	[0.5 m]
if : $J_3+J_4 < J_2$ then: $J_o = J_4 + J_3$	
if : $J_3+J_4 \geq J_2$ then: $J_o = J_2$	
if : $J_3+J_5 < J_2$ then: $J_i = J_5 + J_3$	
if : $J_3+J_5 \geq J_2$ then: $J_i = J_2$	
J_o : total soil flux to outdoor air	[g.m ⁻² .h ⁻¹]
J_i : total soil flux to crawl space	[g.m ⁻² .h ⁻¹]

Appendix 3. Formulas dilution air flux outdoor.

SOILRISK (applied in CSOIL)

$$V_f = V_g * S_z / L_p$$

Vf	: dilution velocity	[m.h ⁻¹]
Vfa	: dilution velocity adult	[m.h ⁻¹]
Vfc	: dilution velocity child	[m.h ⁻¹]
Vg	: mean wind velocity	[m.h ⁻¹]
Sz	: vertical Pasquill dispersion coefficient, related to Pasquill weather stability class D	[m]
Lp	: diameter contaminated soil	[100 m]

$$V_g = (V_x + V')/2$$

Vx	: wind velocity at x m altitude	[m.h ⁻¹]
V'	: friction velocity	[m.h ⁻¹]

$$V_x = \ln [Z/Z_o] * V' / k$$

Z	: breathing altitude	[x m]
Zo	: roughness of the surface area (residential area)	[1.0 -]
k	: Karman constant	[0.4 -]

$$V' = k * V_{10} / \ln (Z_{10}/Z_o)$$

Z10	: altitude	[10 m]
V10	: wind velocity at 10 m altitude	[18000 m.h ⁻¹]

$$S_z = C_o * 0.20 * L_p^{0.76}$$

$$C_o = (10 * Z_o)^{0.53} * L_p^{-0.22}$$

C_o : correction factor for the roughness length [-]

model calculation for L_p = 100 m:

	children	adults
Z	= 1.0	1.5 [m]
V'	= 3127	3127 [m.h ⁻¹]
V1	= 0	3170 [m.h ⁻¹]
Vg	= 1563	3148 [m.h ⁻¹]
Co	= 1.56	1.56 [-]
Sz	= 10.31	10.31 [m]
Vfc	= 161.3	[m.h ⁻¹]

$$V_{fa} = 324.6 \text{ [m.h}^{-1}\text{]}$$

HESP

$$V_f = 1 / [1/Kg - l/Kgs - \ln(Y/Xa) / (Prc * V')]$$

Vf	: dilution velocity	[m.h ⁻¹]
J	: flux from the soil	[g.m ⁻² .h ⁻¹]
Kg	: gas phase mass transport coefficient	[m.h ⁻¹]
Kgs	: mass transport coefficient for diffuse sublayer	[m.h ⁻¹]
Y	: breathing zone altitude above soil surface	[1.5 m]
Xa	: thickness of the air boundary layer	[m]
Prc	: Prandtl constant	[0.4 -]
V'	: friction velocity air	[m.h ⁻¹]

$$Kg = 0.029 * V10^{0.78} * L^{-0.11} * Sc^{-0.67}$$

V10	: wind velocity at 10 m altitude	[27000 m.h ⁻¹]
L	: length of the intestinal surface	[300 m]
Sc	: Schmidt-figure for the gas phase	[-]

$$Sc = u / (P * Da)$$

u	: air viscosity	[65.8 g.m ⁻¹ .h ⁻¹]
P	: air density	[1280 g.m ⁻³]
Da	: air density coefficient	[m ² .h ⁻¹]

$$Kgs = Da / Xa$$

$$Xa = 26 * Sc^{1/3} * V_k / V'$$

V _k	: kinetic viscosity of air	[0.05137 m ² .h ⁻¹]
----------------	----------------------------	--

$$V' = (V10 * k) / \ln [(h+sr)/sr]$$

k	: Karman constant	[0.4 -]
h	: altitude	[10 m]
sr	: surface roughness	[0.28 -]

calculation for Da: 0.0295 m².h⁻¹:

Sc	= 1.74 [-]
Kg	= 30.53 [m.h ⁻¹]
Xa	= 0.00037 [m]
Kgs	= 79.67 [m.h ⁻¹]
V'	= 2997 [m.h ⁻¹]
Vf	= 75.4 [m.h ⁻¹]

Appendix 4. Formulas air concentration calculation.

$$Coaa = Jo / Vfa$$

Coaa : concentration in the outdoor air for an adult at 1.5 m altitude

[g.m⁻³]
[m.h⁻¹]

$$Coac = Jo / Vfc$$

Coac : concentration in the outdoor air for a child at 1 m altitude

[g.m⁻³]
[m.h⁻¹]

$$Cba = Ji * Bo / (Bv * Vv)$$

Cba : concentration in the crawl space air

[g.m⁻³]
[50 m²]

Bo : surface area of the crawl space

[25 m³]
[1.25 h⁻¹]

Bv : volume of the crawl space

Vv : ventilation multiplication
(experimental data (Fast et al., 1987): min. 0.03 - max. 7.4 - av. 1.25)

$$Cia = fbi * Cba$$

Cia : concentration in the indoor air

[g.m⁻³]
[0.1 -]

fbi : contribution on the crawl space to the indoor air as fraction

(experimental data (Fast et al., 1987): min. 0 - max. 0.68 - av. 0.11 - 95
perc. 0.39)

if : Cia < Coac then: Cia = Coac

Appendix 5. Formulas crop content.

Deposition

$$Cdp = TSPo * DRo * frs * Cs * [fin / (Yv * fEi)] * \{ 1 - (1 - \exp [- fEi * te]) / (fEi * te) \}$$

Cdp	: crop content caused by deposition	[mg subst.kg ⁻¹ dw crop]
fin	: fraction interception by crop	[0.4 -]
Yv	: crop yield	[0.28 kg dw.m ⁻²]
fEi	: efflorescence constant	[0.033 d ⁻¹]
TSPo	: concentration particles in outdoor air	[0.07 mg.m ⁻³]
frs	: fraction particles in soil	[0.5 -]
DRo	: deposition velocity	[1 cm.s ⁻¹ = 864 m.d ⁻¹]
te	: growing period crop	[180 d]

$$Cdp = 1.089 * 10^{-3} * Cs \quad [\text{mg.kg}^{-1} \text{ dw crop}]$$

Crop content

Metals

root crops:

$$Cpr = BCFr * Cs$$

Cpr	: content of the root crop	[mg subst.kg ⁻¹ dw crop]
BCFr	: bioconcentration factor root	[(mg subst.kg ⁻¹ dw crop)/(mg subst.kg ⁻¹ dry soil)]

leafy crops:

$$Cps = BCFs * Cs + Cdp$$

Cps	: content of the leafy crop	[mg subst.kg ⁻¹ dw crop]
BCFs	: bioconcentration factor crop	[(mg subst.kg ⁻¹ dw crop)/(mg subst.kg ⁻¹ dry soil)]

if no BCFr or BCFs are given:

$$\ln BCFr/s = 2.67 - 1.12 * \ln Kd$$

Other inorganic substances

based on high water-solubility: concentration in pore water = concentration in plant moisture

root crops:

$$Cpr' = Cpw * (l-fdwr)$$

Cpr' : content of the root crop

fdwr = ratio dry weight-fresh weight root crops

[mg subst.kg⁻¹ fresh weight crop]

[0.202 kg dw.kg⁻¹ fresh]

$$BCFr' = (1 - fdwr)$$

BCFr' : bioconcentration factor root

[(mg subst.kg⁻¹ fresh crop)/(mg subst.dm⁻³ soil moisture)]

leafy crops:

$$Cps' = Cpw * (l-fdws) + Cdp * fdws$$

Cps' : content of the leafy crop

fdws = ratio dry weight -fresh weight leafy crops

[mg subst.kg⁻¹ fresh weight crop]

[0.117 kg dw.kg⁻¹ fresh]

$$BCFs' = (l-fdws)$$

BCFs' : bioconcentration factor stem

[(mg subst.kg⁻¹ fresh crop)/(mg subst.dm⁻³ soil moisture)]

Organic substances

roots:

$$BCFr = 10^{(0.77 * \log Kow - 1.52)} + 0.82$$

BCFr' : bioconcentration factor root

[(mg subst.kg⁻¹ fresh crop)/(mg subst.dm⁻³ soil moisture)]

$$Cpr' = BCFr' * Cpw$$

Cpr' : content of the root crop

[mg subst.kg⁻¹ fresh weight crop]

stems:

$$BCFs' : [10^{(0.95 * \log Kow - 2.05)} + 0.82] * [0.784 * 10^{(-0.434 * (\log Kow - 1.78)^2 / 2.44)}]$$

BCFs' : bioconcentration factor stem

[(mg subst.kg⁻¹ fresh crop)/(mg subst.dm⁻³ soil moisture)]

$$Cps' = BCFs' * Cpw + Cdp * fdws$$

Cps' : content of the leafy crop

[mg subst.kg⁻¹ fresh weight crop]

Appendix 6. Formulas calculation concentration in drinking water after permeation.

$$C_{max} = C_{pw} * 2 * D_{pe} * t / (r * d)$$

C _{max}	: maximum concentration in the drinking water after t days stagnation	[mg.dm ⁻³]
D _{pe}	: permeation coefficient	[m ² .d ⁻¹]
t	: time period of water stagnation	[Vonk, 1985: 8 h = 1/3 d]
r	: radius of the pipe	[0.0098 m]
d	: thickness of pipe wall	[0.0027 m]

24 hrs permeation:

$$C_{dw} = C_{max} * 3 * \pi * r^2 * L / Q_{wd}$$

C _{dw}	: 24-hrs mean drinking water concentration	[mg.dm ⁻³]
t	: in this case 24 h = 1 d, hence correction factor 3	
L	: length of the pipe along which permeation can occur = size location	[100 m]
Q _{wd}	: mean daily water consumption	[500 dm ³]

$$C_{dw} = 4.56 * 10^3 * D_{pe} * C_{pw}$$

Appendix 7. Formulas for the calculation of air concentration in the bathroom during showering.

$$k_{wa} = [(H_{sh}/RT_{sh}) * kL * kG]/[(H_{sh}/RT_{sh}) * kG + kL] * [Ad/Vd] * tf$$

k_{wa}	: degree of evaporation of the contaminant	[-]
(H_{sh}/RT_{sh})	: air-water distribution coefficient at a temperature of 313 K (T_{sh})	[-]
T_{sh}	: water temperature shower water	[313 K]
kL	: water mass transport coefficient	[m.s ⁻¹]
kG	: vapour mass transport coefficient	[m.s ⁻¹]
Ad	: surface area water drop	[m ²]
Vd	: volume water drop	[m ³]
tf	: dropping time drop	[l s]

temperature correction for the Henry-constant:

$$\ln H_{sh} = \ln (K_{lw} * R * T_0) + 0.024 * (T_{sh} - T_0)$$

H_{sh}	: Henry-constant at a temperature of 313 K (T_{sh})	[Pa.m ³ .mol ⁻¹]
H_0	: Henry-constant for the reference situation ($T_0 = 283-293$ K)	[Pa.m ³ .mol ⁻¹]

$$Ad = 4 * \pi * r^2$$

$$Vd = 4/3 * \pi * r^3$$

$$Ad/Vd = 3 / r$$

r : radius of the drop [0.5 mm = 0.0005 m]

kL	= $K_l * (44/M)^{1/2} / 3600$	[m.s ⁻¹]
kG	= $K_g * (18/M)^{1/2} / 3600$	[m.s ⁻¹]

K_l	: liquid phase exchange velocity	[0.2 m.h ⁻¹]
K_g	: gas phase mass transport coefficient	[29.88 m.h ⁻¹]

$$C_{bk} = k_{wa} * V_{wb} * C_{dw} / (2 * V_{bk})$$

C_{bk}	: concentration in the bathroom air	[g subst.m ⁻³]
V_{wb}	: volume water consumption	[0.15 m ³]
V_{bk}	: volume bathroom	[l*b*h = 3*2*2.5 = 15 m ³]

$$C_{bk} = k_{wa} * C_{dw} * 5 * 10^{-3}$$

Appendix 8. Formulas quantification exposure.

Soil ingestion

$$DI = AID * Cs * fa/W$$

DI	: uptake via soil-ingestion	[mg subst.kg ⁻¹ .d ⁻¹]
AID	: daily intake amount soil	[kg dry subst.d ⁻¹]
	adults : $50 * 10^{-6}$	
	children : $150 * 10^{-6}$	
W	: body weight	[-]
fa	: relative absorption factor, set at 1	[mg.kg ⁻¹]
Cs	: content in the soil	

$$DIA = 50 * 10^{-6} * Cs/Wa$$

$$DIC = 150 * 10^{-6} * Cs / Wc$$

Dermal contact soil

Outdoor exposure via soil, indoor via soil in dust; during sleep no exposure.

$$DA = A exp * fm * DAE * DAR * Cs * t * tf * frs / W$$

DA	: uptake via dermal contact with soil	[mg.kg ⁻¹ .d ⁻¹]
A exp	: exposed surface area	[m ²]

	indoor	outdoor
adult	0.09	0.17
children	0.05	0.28

fm : matrix factor

DAE : degree of coverage

	indoor	outdoor
adults	0.056	3.75
children	0.056	0.51

DAR : absorption velocity

adults	0.005
children	0.01

t : duration of exposure

	indoor	outdoor
adults	8	8
children	8	8

tf : time fraction exposure

correction of daily to annual average exposure

	indoor	outdoor
adults	1.857	0.143
children	1.143	0.357

frs : fraction soil in dust

frsi: indoor: 0.8

$$\begin{aligned} DAa &= 5.92 * 10^{-6} * Cs / Wa \\ DAC &= 6.43 * 10^{-6} * Cs / Wc \end{aligned}$$

Inhalation of soil (particles)

$$IP = ITSP * Cs * fr * fa/W$$

IP	: uptake of inhaled soil particles	[mg.kg ⁻¹ .d ⁻¹]
ITSP	: amount of inhaled soil particles	[kg.d ⁻¹]
fr	: retention factor particles in lung	[0.75 -]

$$ITSP = TSP * frs * AV * t * ft$$

TSP	: amount of air-suspended particles	[mg.m ⁻³]
	TSPo: outdoor: 70 ug.m ⁻³	
	TSPi: indoor: 0.75 * 70 = 52,5 ug.m ⁻³	

frs	: soil-fraction in particles in the air	[-]
	frso: outdoor: 0.5	
	frsi: indoor: 0.8	

AV	: breathing volume	[m ³ d ⁻¹]
	AVa: adults : 20 = 0.83 m ³ .h ⁻¹	
	AVc: children : 7.6 = 0.32 m ³ .h ⁻¹	

t	: duration of exposure	[h]
	indoor outdoor	

adults	8	8
--------	---	---

children	16	8
----------	----	---

tf	: time fraction exposure	[-]
	correction from daily to annual average exposure	

	indoor outdoor	
--	-------------------	--

adults	2.856	0.143
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children	1.322	0.357
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$$IPa = 0.625 * 10^{-6} * Cs / Wa$$

$$IPc = 0.235 * 10^{-6} * Cs / Wc$$

Inhalation of air

$$IV = [AV * Cia * tfi * ti + AV * Coa * tfo * to] * fa * 10^3 / W$$

IV	: uptake of contamination via vapours	mg.kg ⁻¹ .d ⁻¹]
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Cia	: concentration in the indoor air	[g.m ⁻³]
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Coa	: concentration in the outdoor air	[g.m ⁻³]
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Coaa	: concentration in the outdoor air for an adult	[g.m ⁻³]
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Coac	: concentration in the outdoor air for a child	[g.m ⁻³]
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ti/to : daily duration of exposure indoor resp. outdoor [h]
 tfi/tfo : annual average time fractions for stay indoor resp. outdoor [-]

$$\text{IVa} = (22.86 * \text{Cia} + 1.14 * \text{Coaa}) * 0.83 * 1000 / \text{Wa}$$

$$\text{IVc} = (21.14 * \text{Cia} + 2.86 * \text{Coac}) * 0.32 * 1000 / \text{Wc}$$

Ingestion of crops: leafy and root crops

metals

$$\text{VI} = (\text{Qfvk} * \text{Cpr} + \text{Qfvb} * \text{Cps}) * \text{fv} * \text{fa} / \text{W}$$

VI : uptake of contaminant via crop [mg.kg⁻¹.d⁻¹]
 Qfvk : daily consumption of root crops [kg dry weight.d⁻¹]
 adults : 0.02761
 children : 0.01511
 Qfvb : daily consumption of leafy crops [kg dry weight.d⁻¹]
 adults : 0.01843
 children : 0.00890
 fv : fraction contaminated food [0.1 -]
 Cpr : content of the root crop [mg subst.kg⁻¹ dw crop]
 Cps : content of the leafy crop [mg subst.kg⁻¹ dw crop]

$$\text{VIa} = (0.002761 * \text{Cpr} + 0.001843 * \text{Cps}) / \text{Wa}$$

$$\text{VIc} = (0.001511 * \text{Cpr} + 0.000890 * \text{Cps}) / \text{Wc}$$

other (in)organic substances

$$\text{VI} = (\text{Qfvk}' * \text{Cpr}' + \text{Qfvb}' * \text{Cps}') * \text{fv} * \text{fa} / \text{W}$$

Qfvk' : daily consumption of root crops [kg fresh weight.d⁻¹]
 adults : 0.1367
 children : 0.0748
 Qfvb' : daily consumption of leafy crops [kg fresh weight.d⁻¹]
 adults : 0.1578
 children : 0.0761
 Cpr' : content of the root crop [mg subst.kg⁻¹ fresh weight crop]
 Cps' : content of the leafy crop [mg subst.kg⁻¹ fresh weight crop]

$$\text{VIa} = (0.01367 * \text{Cpr}' + 0.01578 * \text{Cps}') / \text{Wa}$$

$$\text{VIc} = (0.00748 * \text{Cpr}' + 0.00761 * \text{Cps}') / \text{Wc}$$

Ingestion of drinking water

$$DIw = Qdw * Cdw * fa / W$$

DIw : intake of contaminated drinking water by drinking [mg.kg⁻¹.d⁻¹]

Qdw : daily drinking water intake [m³.d⁻¹]

adults : 0.002 = 2 dm³.d⁻¹

children : 0.001 = 1 dm³.d⁻¹

Cdw : drinking water concentration [mg dm⁻³ = g.m⁻³]

$$DIwa = 2 * Cdw / Wa$$

$$DIwc = 1 * Cdw / Wc$$

Inhalation of vapours during showering

$$IVw = Cbk * AV * td * fa * 1000 / W$$

IVw : intake contamination by inhaling vapour during showering [mg.kg⁻¹.d⁻¹]

Cbk : concentration in the bathroom air [g.m⁻³]

td : duration of stay in the bathroom [h]

15 min. showering + 15 min. drying/dressing = [0.5 h]

$$IVwa = 2.08 * Cdw * kwa / Wa$$

$$IVwc = 0.792 * Cdw * kwa / Wc$$

Dermal contact during showering

$$DAw = A_{to} * f_{exp} * DAR * tdc * (1-kwa) * Cdw * fa / W$$

DAw : uptake as a result of dermal contact during showering [mg.kg⁻¹.d⁻¹]

A_{to} : exposure surface area = entire body [m²]

adults : 1.8

children : 0.95

f_{exp} : fraction exposed skin [0.4 -]

DAR : dermal absorption velocity [(mg.m⁻²)/(mg.dm⁻³).h⁻¹]

tdc : contact time = showering time [0.25 h.d⁻¹]

(1-kwa) : substance remaining in water after evaporation [-]

DAR = P1 * P2 according to Fiserova-Bergerova and Pierce (1989), with:

$$P1 = (0.038 + 0.153 * Kow)$$

P1 = 5000 * P1 / (5000 + P1), maximization according to Braun

$$P2 = \exp(-0.016 * M) / 1.5$$

$$DAwa = 0.18 * DAR * (1-kwa) * Cdw / Wa$$

$$DAwc = 0.095 * DAR * (1-kwa) * Cdw / Wc$$

(Dermal contact during bathing)

$$DA_w = A_{to} * DAR * tb * Cd_w * fa / W$$

DAR : dermal absorption velocity [10 (mg.m⁻²)/(mg.dm⁻³.h⁻¹)]

or the DAR indicated earlier

tb : contact time = duration of bathing [0.5 h.d⁻¹]

Total exposure

$$TAD = DIA + DAA + IPA + IVa + VIa + DIWa + IVwa + DAwa$$

$$TCH = DIC + DAC + IPC + IVc + VIc + DIWc + IVwc + DAwc$$

TAD : daily exposure adult [mg.kg⁻¹.d⁻¹]

TCH : daily exposure child [mg.kg⁻¹.d⁻¹]

$$DOSIS = (6 * TCH + 64 * TAD) / 70$$

DOSIS : life-time mean daily exposure [mg.kg⁻¹.d⁻¹]

Appendix 9. Primary set of data.

Necessary set of data in order to be able to calculate potential exposure.

S	: water-solubility	[mol.m ⁻³] or [mg.l ⁻¹]
Vp	: vapour pressure pure substance or	[Pa] or [atm] or [mm Hg]
Klw	: air-water distribution coefficient (this may also be calculated from the other data, see annex 1.10)	[-]
M	: molecular mass	[g.mol ⁻¹]
Kow	: octanol-water distribution coefficient (for organic substances) or	
Kd	: soil-water distribution coefficient (for metals)	[dm ³ .kg ⁻¹]
Dpe	: permeation coefficient	[m ² .d ⁻¹]

Appendix 1.10 Conversion formulas

$$K_{lw} = V_p / (S * R * T)$$

$$V_p = K_{lw} * S * R * T$$

$$R_1 = 8.3144 \text{ Pa.m}^3.\text{mol}^{-1}.\text{K}^{-1}$$

$$R_2 = 8.206 * 10^5 \text{ m}^3.\text{atm}.\text{mol}^{-1}.\text{K}^{-1}$$

if H is given as [Pa.m³.mol⁻¹] then: $K_{lw} = H / (R_1 * T)$

if H is given as [atm.m³.mol⁻¹] then: $K_{lw} = H / (R_2 * T)$ or:
 $K_{lw} = H * 1.013 * 10^5 / (R_1 * T)$

1 mm Hg-pressure = 133.33 Pa = $1.316 * 10^{-3}$ atm

if S is given in [mg.l⁻¹] then: $S = S / M \text{ [mol.m}^{-3}\text{]}$

M : molecular mass [g.mol⁻¹]

foc = 0.58 * fom or fom = 1.724 * foc or OS = 172.4 * foc

fom : fraction organic substance mass

OS : percentage organic substance

source: (Van den Berg, 1995)

Appendix X Detection limits for third series compounds.

The height of detection limits for compounds depends on the analytical methods used, the matrix (e.g soil, water) and on the sample volume. Therefore detection limits are chosen which are general for the environmental laboratories in the Netherlands. A selection was made and can be seen in the following tables:

Detection limits soil

compound	detection limit soil mg.kg ⁻¹ ds + analytical method ¹⁾	detection limit soil mg.kg ⁻¹ ds + analytical method ²⁾
silver	1 (ICP) 0.1 (GC/ECD)	5 (AAS) 0.05 (GC/ECD)
1,1-dichloroethane		
1,1,1-trichloro- ethene	0.1 (GC/ECD)	0.05 (GC/ECD)
<i>cis/trans</i>		
1,2-dichloroethene	0.1 (GC/ECD)	0.05 (GC/ECD)
ethyleneglycol	5 (GC)	0.1 (GC/FID)
diethyleneglycol	5 (GC)	0.1 (GC/FID)
acrylonitrile	0.1 (GC)	-
formaldehyde	-	-
methanol	5 (GC/FID)	1 (GC/FID)
butanol	0.5 (GC)	1 (GC/FID)
butylacetate	0.5 (GC)	1 (GC)
methyl <i>tert</i> -butyl ether	0.5 (GC)	1 (GC)
dodecylbenzene	-	-
aromatic solvents	0.05 (GC)	

¹⁾Tauw Environmental Laboratory, 1994 (8th edition, draft)

²⁾IWACO Prijslijst, februari 1995

-- no standard method for determination of the compound

Note:

- AAS =Atomic Absorption Spectrometer
- GC =Gas Chromatography
- ECD =Electron Capture Detection
- FID =Flame Ionisation Detection

GC (Gas Chromatography) analysis can be amplified with MS (Mass Spectrometry)

Detection limits groundwater

compound	detection limit gr.water [*] µg.l ⁻¹ + analytical method ¹⁾	detection limit gr.water µg.l ⁻¹ + analytical method ²⁾
silver	2/4 (ICP) 5 (GC/ECD)	2 (AAS) 0.5 (GC/ECD)
1,1-dichloroethane		
1,1,1-trichloro- ethene	1 (GC/ECD)	0.5 (GC/ECD)
<i>cis/trans</i> 1,2-dichloroethene	1 (GC/ECD) 5000 (GC/FID)	0.5 (GC/ECD) 1000 (GC/FID)
ethyleneglycol	5000 (GC)	1000 (GC/FID)
diethyleneglycol	100 (GC)	-
acrylonitrile	100 (GC)	-
formaldehyde	5000 (GC/FID)	1000 (GC/FID)
methanol	500 (GC)	1000 (GC/FID)
butanol	500 (GC)	1000 (GC)
butylacetate		
methyl <i>tert</i> -butyl ether	500 (GC)	1000 (GC)
dodecylbenzene	-	-
aromatic solvents	0.2 (GC)	

^{*}=groundwater¹⁾Tauw Environmental Laboratory, 1994 (8th edition, concept)²⁾IWACO Prijslijst, febr 1995

Most laboratoria do not have a standard analytical method for the determination of acrylonitrile and formaldehyde. The Laboratory for Organic Analytical Chemistry (RIVM) have developed methods for the determination of these compounds, but the required amount of sample may be different than the standard sample volume as proposed in NVN 5740*) and NEN (Dutch Final Norms).

*) NVN 5740= Dutch Prenorm: Soil, Investigation strategy for exploratory survey