research for
man and environment

RIJKSINSTITUUT VOOR VOLKSGEZONDHEID EN MILIEU
NATIONAL INSTITUTE OF PUBLIC HEALTH AND THE ENVIRONMENT

RIVM report 711701021

Evaluation and revision of the CSOIL parameter set

Proposed parameter set for human exposure modelling and deriving Intervention Values for the first series of compounds

P.F. Otte, J.P.A. Lijzen, J.G. Otte, F.A. Swartjes
and C.W. Versluijs.

March 2001

This investigation has been performed by account of The Ministry of Housing Spatial Planning and the Environment, Directorate General for the Environment (DGM), Directorate of Soil, Water and Rural Areas, within the framework of RIVM project 711701, Risks in relation to Soil Quality.

RIVM, P.O. Box 1, 3720 BA Bilthoven, telephone: 31 - 30 - 274 91 11; fax: 31 - 30 - 274 29 71

Abstract

Intervention Values are generic soil quality standards used to classify historically contaminated soils, sediments and groundwater (i.e. before 1987) as seriously contaminated in the framework of the Dutch Soil Protection Act. In 1994 Intervention Values were published for 70 (groups of) compounds. Intervention values are based on potential risks for both human health and ecosystems. Human toxicological Serious Risk Concentrations for soil, sediment and groundwater (SRC_{human}) are determined using the human exposure model CSOIL.

This report presents an evaluation and revision of the CSOIL parameter set as part of the technical evaluation of the Intervention Values. The evaluation of the CSOIL parameter set comprises the physicochemical data of all compounds for the first series, as well as the soil, site and exposure parameters. The evaluation results in a revised CSOIL data set with an improved underpinning and traceability of the data set. Another improvement concerns the revision of the soil-water partition coefficients. The report also provides insight into the impact of the revised data set on the SRC_{human} and resulted in a better insight into the uncertainties and variation of the model input parameters.

Preface

The Intervention Values for Soil/Sediment and Groundwater contamination were published in 1994 as part of the Dutch Soil Protection Act (VROM, 1994). To provide an up-to-date scientific basis for these values, the Directorate General of Environment commissioned the project ‘Technical Evaluation of Intervention Values for soil contamination’ to the National Institute of Public Health and the Environment (RIVM).

All the elements of this project are contained in several subprojects for revising human-toxicological and ecotoxicological risk limits for soil, sediment and groundwater. Human-toxicological risk limits for soil are derived with the human exposure model CSOIL, the parameter set of which has been evaluated and revised here. Other reports on the technical evaluation of Intervention Values are:

- Ecotoxicological Serious Risk Concentrations for soil, sediment and (ground)water: updated proposals for first series of compounds (RIVM report 711701020; Verbruggen et al., 2001).
- Evaluation of the most relevant model concepts for human exposure; proposals for updating the most relevant exposure routes of CSOIL (RIVM report 711701022; Rikken et al., 2001).
- Risk assessment of historical soil contamination with cyanides, origin, potential human exposure and evaluation of Intervention Values (RIVM report 711701019; Köster, 2001);
- Proposal for revised Intervention Values for petroleum hydrocarbons on base of fractions of petroleum hydrocarbons (RIVM report 711701015; Franken et al., 1999).
- Re-evaluation of human-toxicological Maximum Permissible Risk levels (RIVM report 711701025; Baars et al., 2001).
- Accumulation of metal in plants as a function of soil type (RIVM report 711701024; Versluijs and Otte, in prep.).
- Revision of the Intervention Value for lead; evaluation of the Intervention Values derived for Soil/Sediment and Groundwater (RIVM report 711701013; Lijzen et al., 1999).

The integration of the results obtained in the subprojects mentioned and the derivation of the proposed risk levels are reported in:

- Technical evaluation of the Intervention Values for Soil/Sediment and Groundwater. Human and ecotoxicological risk assessment and derivation of risk limits for soil, aquatic sediment and groundwater (RIVM report 711701023; Lijzen et al., 2001).

We owe gratitude to the ‘Expert group on human-toxicological risk assessment’ for the information, advice and remarks on this report. Experts include J. Vegter, TCB; T. Crommentuijn, DGM-BWL; J.A. van Zorge, DGM-SAS; C.J.M. van de Bogaard, DGM-IMH; T. Fast; D.H.J. van de Weerdt, GGD Regio IJssel-Vecht; R. van Doorn, GGD Rotterdam; J. Dolfing, Alterra; P.W. van Vliet, Gezondheidsraad; C. van de Guchte, RIZA; J. Wezenbeek, Grontmij; A. Boshoven, IWACO b.v.; W. Veerkamp, VNO/NCW-BMRO; Th. Vermeire, RIVM-CSR; and J. Lijzen, RIVM-LBG. We are also grateful to the ‘Expert group on ecotoxicological risk assessment’: J. Van Wensem, TCB; D. Sijm and T. Traas, RIVM-CSR; J. Appelman, CTB; T. Brock, Alterra; S. Dogger, Gezondheidsraad; J.H. Faber, Alterra; K.H. den Haan, VNO/NCW-BMRO; M. Koene, Stichting Natuur en Milieu; A. Peijnenburg, RIKZ; E. Sneller, RIZA; W.J.M. van Tilborg, VNO/NCW-BMRO.

Contents

Samenvatting

In het kader van de Wet Bodembescherming zijn in 1994 de Interventiewaarden bodemsanering voor de eerste tranche van circa 70 stoffen en stofgroepen vastgesteld. Interventiewaarden zijn generieke risicogrenzen voor de bodem/sediment- en grondwaterkwaliteit, en zijn gebaseerd op het potentiële risico voor de mens en voor ecosystemen. Ze worden gebruikt om bodem-, sediment- of grondwaterverontreiniging te classificeren als ‘ernstig verontreinigd’.
Het Directoraat-Generaal Milieubeheer heeft het RIVM opdracht gegeven voor een technisch-wetenschappelijke evaluatie van deze Interventiewaarden op basis van recente (toxiciteit)data en nieuwe inzichten in risicobeoordeling. De uiteindelijke doelstelling is het doen van voorstellen voor nieuwe risicogrenswaarden.
Het project ‘Technische Evaluatie Interventiewaarden bodemsanering’ bestaat uit verschillende deelstudies die elk een aspect van de evaluatie en herziening omvatten. Eén van de deelaspecten is de afleiding van potentiële humaan-toxicologische risicogrenzen voor bodem en grondwater (SRC_{humaan}). De afleiding gebeurt met het blootstellingsmodel CSOIL, dat uitgaat van het blootstellingscenario ‘*wonen met tuin*’. Dit rapport beschrijft de evaluatie en herziening van zowel de bodem-, lokatie- en blootstellingsparameters van dit blootstellingsmodel als de parameters die de stofeigenschappen beschrijven. De evaluatie van het humaan-toxicologisch Maximum Toelaatbaar Risico (MPR_{humaan}) is gerapporteerd door Baars et al. (2001). De CSOIL parameterset wordt ten dele gebruikt voor de afleiding van potentiële humaan-toxicologische risicogrenzen voor sediment met het model SEDISOIL en voor de afleiding van eco-toxicologische risicogrenzen(SRC_{eco}).

De berekening van de humane blootstelling aan verontreinigde bodem gebeurt op basis van een vastgelegd modelconcept en blootstellingscenario. Het gedrag van verontreinigingen, de blootgestelde mens en het scenario worden beschreven met behulp van een groot aantal parameters. Op basis van verschillende analyses en berekeningen zijn de meest relevante modelparameters geïdentificeerd.
Met betrekking tot de fysisch-chemische parameters zijn dit voor metalen de bodem-plant bioconcentratie factor (BCF) en de partitiecoeffcient bodem-water (Kp). Met betrekking tot organische contaminanten zijn belangrijke fysisch-chemische parameters de partitiecoëfficiënt voor octanol-water (Kow) en de partitiecoefficient organisch koolstof-water (Koc). Voor een aantal stoffen kunnen tevens de wateroplosbaarheid (S) en de dampdruk (Vp) van belang zijn. Daarnaast zijn op basis van een onzekerheids- en gevoeligheidsanalyse een aantal bodem-, locatie- en blootstellingparameters als belangrijk voor de evaluatie aangemerkt.

Voor alle relevante fysisch-chemische parameters zijn nieuwe aanvullende data gezocht. De data betreffende oplosbaarheid en dampdruk zijn voor de als standaard gedefinieerde bodemtemperatuur (283 K) gecorrigeerd. Voor de octanol-water partitiecoëfficiënt (Kow) zijn, na een beoordeling van de data, de LOGPSTAR waarden uit de Medchem (1996) database geselecteerd. In tegenstelling tot de huidige Koc data van 1995, zijn de herziene Koc waarden gebaseerd op experimentele waarden. De vaststelling van generieke bioconcentratiefactoren (BCF) voor metaalopname door moestuingewassen is voor een belangrijk deel gebaseerd op de resultaten van het project ‘Accumulatie van metalen in groentegewassen’ (Versluijs en Otte, in voorbereiding). De Kp waarden voor de verschillende metalen zijn geselecteerd na de evaluatie van enkele veel gebruikte datasets. Zowel voor de BCF als de Kp voor metalen is nagegaan in hoeverre bodemeigenschappen

zoals het percentage lutum en organisch koolstof en de pH de waarden beïnvloeden. Om de onderbouwing voor de afleiding van zogenaamde somwaarden te verbeteren is de CSOIL stoffenset uitgebreid met meer PAK's, PCB's, chloorbenzenen, chloorfenolen, ftalaten en oliefracties (Total Petroleum Hydrocarbons).
Voor de bodemparameters zijn nieuwe waarden vastgesteld voor de fractie porielucht en de bulkdichtheid en andere waarden voor het organisch stof gehalte, lutum en pH ter overweging gegeven. Met betrekking tot de route inhalatie van binnenlucht zijn enkele locatieparameters gewijzigd en enkele toegevoegd ten gevolge van conceptuele aanpassingen. Verder is een aantal parameters gewijzigd met betrekking tot de blootstelling via de consumptie van groentegewassen uit eigen tuin (consumptiehoeveelheid) en met betrekking tot de route ingestie van grond (inname hoeveelheid).

De verschillen tussen de huidige fysisch-chemische dataset uit 1995 en de herziene dataset zijn geanalyseerd, waarbij bovendien het effect van de herziening op de afleiding van de humane risicogrenzen in beeld is gebracht. Hieruit blijkt dat met name de herziening van de partitiecoëfficiënt voor organisch koolstof-water (Koc) bijdraagt tot een veranderde blootstelling en daarmee tot een andere SRC_{humaan} voor bodem.
Met de herziening van de locatie- en blootstellingparameters, zoals opgenomen in CSOIL voor het standaard scenario *'wonen met tuin'* is de CSOIL dataset geactualiseerd en beter onderbouwd. Het effect van de herziening van deze groep parameters is voor de meeste stoffen minder groot dan het effect van de herziening van de fysisch-chemische data.
Het gezamenlijk effect van de herziening van de verschillende aspecten betreffende de afleiding van het humaan risico (humaan-toxicologische risicogrenswaarden, modelconcept en modelparameters) wordt beschouwd in de rapportage van Lijzen et al. (2001).

De evaluatie en herziening van de CSOIL parameterset hebben geleid tot een beter onderbouwde, beter herleidbare en geactualiseerde dataset. Voor enkele stoffen bestaat nog substantiële onzekerheid betreffende de fysisch-chemische data ten behoeve van de potentiële risicobeoordeling. Het betreft hier met name vinylchloride (Vp en H), aldrin en dieldrin (beide Koc). Overwogen moet worden om aanvullend onderzoek of metingen te verrichten.
Het onderzoek heeft geleid tot een beter inzicht in de spreiding en onzekerheden van de verschillende parameters. Deze spreiding is vaak inherent aan het karakter van de parameter (de 'natuurlijke' en 'ruimtelijke' spreiding).
Op basis van de herziene dataset dient te worden overwogen om in de toekomst de blootstelling van de mens uit te drukken in een kansverdeling. Hiermee kan het effect van de onzekerheid van verschillende fysisch-chemische-, locatie- en blootstellingsparameters op de blootstelling op een goede manier in beeld worden gebracht. Bovendien kan een indruk worden verkregen over het risico dat wordt gelopen wanneer de humaan toxicologische toelaatbare blootstelling wordt over- of onderschreden.
De herziene dataset wordt ten dele ook gebruikt voor de afleiding van ecotoxicologische risicogrenzen voor de afleiding van humaan-toxicologische risicogrenzen voor sediment met het model SEDISOIL. Een verdere harmonisatie met gerelateerde activiteiten is wenselijk hoewel verschillen in doelstellingen, vertrekpunten en selectiecriteria een mogelijk obstakel kunnen zijn.

Summary

In 1994 the Intervention Values for soil contamination were published for the first series of about 70 (groups of) compounds in the framework of the Dutch Soil Protection Act. Intervention Values, based on the potential risk for both human and ecotoxicological risk, are generic soil quality standards used to classify historical soil contamination as ‘seriously contaminated’. The Intervention Values for all compounds of the first series were evaluated in line with the most recent views on risk assessment and (toxicological) data to yield proposals for new risk limit values.
The project on ‘Technical Evaluation of Intervention Values’ consists of separate studies, each dealing with one aspect of evaluation and revision of Intervention Values.
One of these is the derivation of human-toxicological serious risk concentrations (SRC_{human}) for soil, sediment and groundwater. For the derivation of SRC_{human} this means the calculation of the *‘lifetime average exposure’* of the *‘average individual’* in a *‘standard situation’*. To derive the SRC_{human}, the CSOIL exposure model is used with a defined exposure scenario called *‘residential with garden’*.

This study was set up to evaluate and revise the model parameter set of the exposure model, CSOIL, while the evaluation and revision of the human-toxicological Maximum Permissible Risk levels (MPR) is described in Baars et al. (2001). The CSOIL parameter set is in part also used for the derivation of SRC_{human} for sediments with the exposure model SEDISOIL and for the derivation of ecotoxicological risk limits (SRC_{eco}).

The calculation of human toxicological potential exposure to contaminated soil is based on several starting points like *realistic case* risk level and the standard exposure scenario, *residential with garden*. The behaviour and characteristics of humans, the scenario used and the contaminants are described with a set of parameters. The most relevant parameters for the calculation of human exposure to contaminated soil and groundwater are identified on the basis of model analysis. For organic contaminants important physicochemical parameters are the partition coefficient octanol-water (Kow) and the partition coefficient organic carbon-water (Koc). For volatile contaminants, the water solubility (S) and vapour pressure (Vp) may also be of importance. For metals, the soil-to-plant bioconcentration factor (BCF) and the partition coefficients, soil/sediment-water (Kp), are critical. For soil, site and exposure parameters, all the parameters describing the exposure routes, ‘ingestion of soil’, ‘inhalation of indoor air’ and ‘consumption of home-grown crops’ were evaluated.

New data are selected for all physicochemical parameters. Solubility (S) and vapour pressure (Vp) data are corrected for default soil temperature (283 K). After assessment of the retrieved data for partition coefficients octanol-water (Kow), it was agreed to use the LOGPSTAR data selected from the Medchem database (1996). The selected Koc data is based mainly on experimental data, in contrast with the current Koc data set. The selection of generic soil to plant bioconcentration factors (BCF) is based on the results of a RIVM study on ‘Accumulation of metals by vegetables and potatoes’ (Versluijs and Otte, in prep.). The revised Kp values for metals are selected after an evaluation of some frequently used sets. The relationship with standard soil characteristics (pH, clay and organic carbon) is considered for both BCF and Kp metals. To strenghten the basis for the derivation of so-called sum values, the physicochemical data set is extended with data for more PAH and PCB congeners,

phthalates, chlorobenzenes, chlorophenols and Total Petroleum Hydrocarbon (TPH) fractions.
Revised values are determined for pore air and dry bulk density. Other values for organic carbon and lutum content and pH are selected for consideration.
New parameters for the exposure routes 'inhalation of indoor air', 'consumption of home-grown crops' (consumption amounts) and 'ingestion of soil' (ingestion amounts) are introduced and revised.

The differences between current and revised data sets are analysed and a picture is given about the impact of the revised data set on the SRC_{human}. Here especially the revision of the Koc contributes to changes of SRC_{human} levels. With the evaluation and revision of the soil, site and exposure parameters the CSOIL data set is actualised, transparent and well founded. The effects of the revised soil, site and exposure parameters on the derived SRC_{human} levels are less important compared with the effects caused by the revised physicochemical data. The combined effects of all revisions (CSOIL input parameter set, model concepts and MPRs) on the derived SRC_{human} levels are considered in the report of Lijzen et al. (2001).

The evaluation and revision of the CSOIL parameter set resulted in a well-founded, state-of-the-art data set.
For vinylchloride uncertainty still remained about the selected values for vapour pressure and Henry's law constant. Because both parameters are critical for the derived SRC_{human}, an additional study was recommended. This also applies to the Kow and Koc values selected for aldrin and dieldrin.
The study has resulted in better insight into the uncertainties and variation of the model input parameters. The variation is often inherent to the character of the parameter (the 'nature' and spatial variation).

On the basis of this information it is recommended in the future to deal quantitatively with uncertainties and to express the human exposure in a distribution of probability.
This allows the demonstration of the combined effects of all the uncertainties of the different parameters on the calculated exposure. Moreover it is possible to get an impression about the risk at exposure levels above or below the maximum permissible intake.
The revised data is also used (in part) for the derivation of ecotoxicological risk levels (SRC_{eco}). A further harmonisation with other related activities is desirable although it is realised that differences in objectives, starting points and selection criteria constitute a possible obstacle.

1 Introduction

1.1. Scope and objectives

The project ‘Technical Evaluation of Intervention Values’ targeted the overall evaluation of the Intervention Values for soil contamination belonging to the first series of compounds. The first series of Intervention Values for contaminated soil, sediment and groundwater was established in 1994 (VROM, 1994). For an overview of the methods used see Swartjes (1999). Since the publication of the Intervention Values, the policy towards contaminated soil, groundwater and sediments has been changed (BEVER, 1999; VROM, 1999). Useful responses on specific (groups of) compounds came from the group of users of the Intervention Values, e.g. the competent authorities (municipalities of large cities, provinces, the district Water Boards and Department of Public Works) and consultancy firms. In addition, new scientific views, more data, exposure models or calculation methods could have become available in this time period. To integrate this new information in the Intervention Value, a technical evaluation of the Intervention Values was considered necessary. Besides, the wish of the Dutch Lower House is to evaluate these risk-based standards about once every five years. The main purpose of the technical evaluation is to derive risk limits (as a basis for Intervention Values) according to the most recent views on the exposure assessment to soil contaminants, by means of evaluating the exposure models, underlying input data, and human-toxicological and ecotoxicological data.

The other activities within the project ‘Technical Evaluation of Intervention Values for soil contamination’ are mentioned in the preface of this report. The integration of the results and the derivation of the proposed risk levels are reported in Lijzen et al. (2001).

Figure 1.1 shows the derivation of human-toxicological serious risk concentrations (SRC_{human}) for soils and groundwater, as carried out by the CSOIL human exposure model. The model calculates the human exposure to contaminated soil via various routes according a defined concept and with the use of approximately 100 input parameters. The concept (Figure 1.3) of the CSOIL model has been assessed and evaluated in the report ‘Evaluation of the most relevant model concepts for human exposure’ (Rikken et al., 2001).
The exposure of humans to contaminated sediments and the derivation of SRC_{human} for sediments were carried out with the SEDISOIL exposure model (Figure 1.2). This model uses a part of the CSOIL input data set, which accounts for a limited number of physicochemical data used for the derivation of ecotoxicological serious risk concentrations (SRC_{eco}, Table 2.1). The SEDISOIL model, developed in 1996, (Bockting et al.) was recently evaluated by RIVM and RIZA (Otte et al., 2000). Where appropriate, attention will be given in the report before you to points of similarity and noteworthy differences between both models will be indicated.

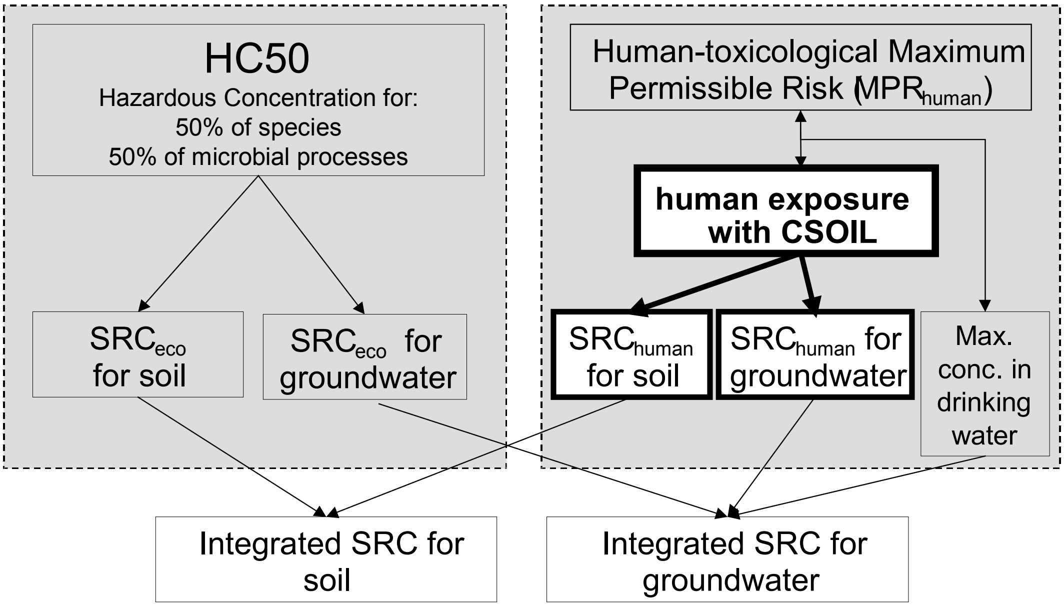


Figure 1.1: General diagram showing the derivation of the integrated risk limits (Integrated Serious Risk Concentrations)

The aim of this study is to evaluate the most relevant CSOIL input parameters so as to improve:

- The quality of input data;
- The consistency and traceability of the process used for CSOIL input parameter selection;
- Insight on the uncertainty.

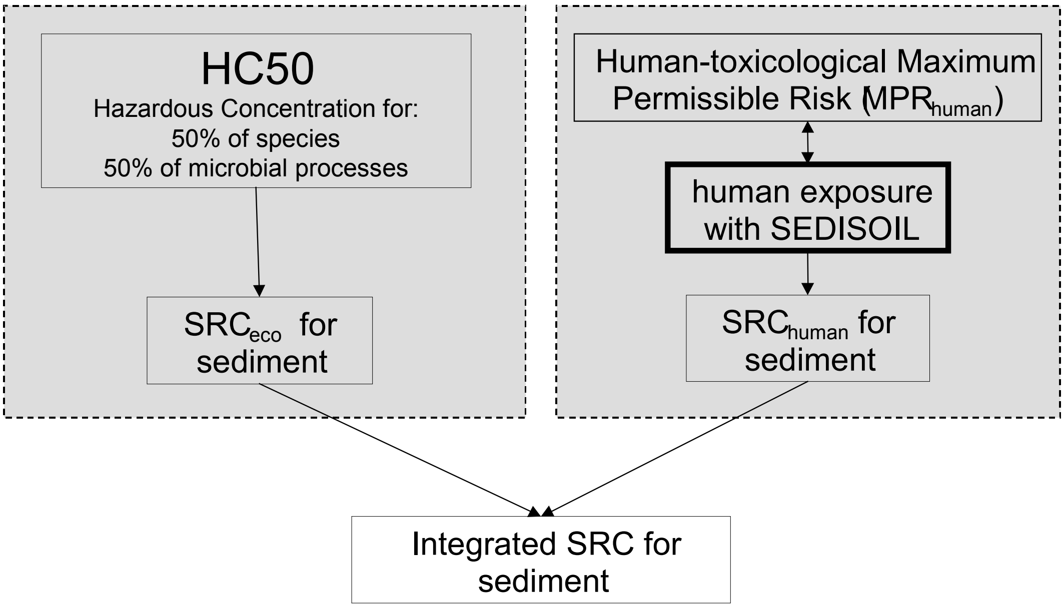


Figure 1.2: Diagram showing the derivation of risk limits (integrated values) for aquatic sediment (SRC= Serious Risk Concentration).

This report provides the background information for the evaluation of all relevant input parameters used to calculate human exposure to contaminated soil with the CSOIL exposure model. This evaluation has resulted in a revised parameter set for all compounds of the first series of Intervention Values.

1.2. CSOIL human exposure model

The CSOIL model concept (Figure 1.3) consists roughly of three parts: first, the description of the behaviour of the compound in the soil and the partitioning over the soil phases; second, the description and parameterisation of the different exposure routes, and finally, the quantification of the lifetime average exposure. On the basis of this concept the input parameters can be roughly divided into:

- compound-specific input parameters; mainly physicochemical properties;
- site and soil properties related to potential exposure and
- exposure parameters which describe the receptor characteristics and behaviour.

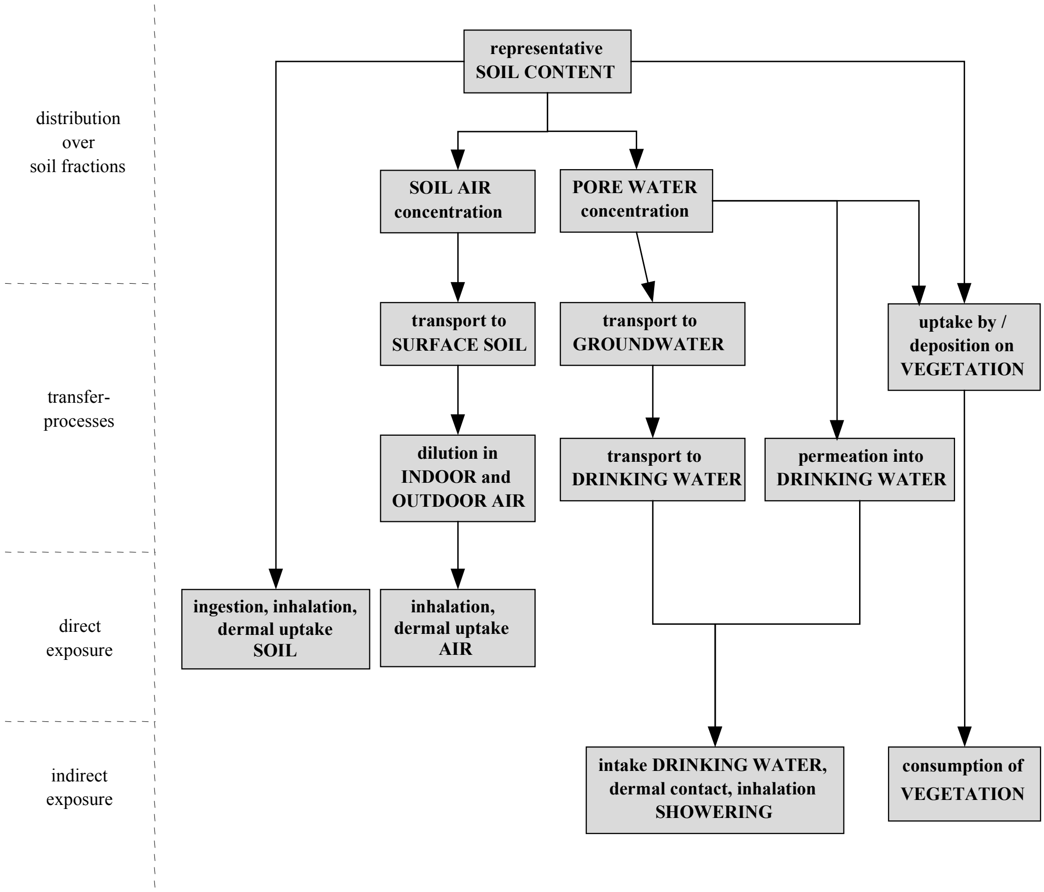


Figure 1.3: Diagram showing the exposure routes of CSOIL.

1.3. Starting points for the evaluation and selection of input parameter values

The uncertainty of the derived risk limits and the underlying political decisions or assumptions are discussed in the integration report (Lijzen et al., 2001). The potential risk is directional for the derivation of Intervention Values. Referring to the derivation of SRC_{human} levels, this will mean calculating the *'lifetime average exposure'* of the *'average individual'* in a *'standard situation'* and determine, among other factors, the proposals for adjusting the current CSOIL data set.

The standard exposure scenario called ‘residential with garden’ describes the ‘standard situation’. The scenario is the starting point for the risk assessment and is not discussed. A consequence of the formulated starting points will be the selection of average parameter values. This prevents the accumulation of conservative values, which can lead to an overestimation of the human exposure. However, for the selection of certain parameter values other criteria or considerations may also be valuable. The discrimination between the uncertainty of a parameter caused by measurement errors and its intrinsic variability might be important. In other cases, selecting a conservative value in favour of the average value might be preferable. These and similar considerations will be discussed in this report.

The most important sources of uncertainty on the compound-specific input parameters are tabulated in Table 1.1. Vissenberg and Swartjes (1996) investigated the uncertainty of soil, site and exposure parameters.

Table 1.1 Most important sources of uncertainty for different parameters

Input parameter	**Uncertainty source**	**Approach**
M S Vp Kow H	Measurement error	Consensus on the method used for data selection. In principle, the geometric mean is selected as input parameter value
Koc	Measurement error Site-specific nature Concentration effects	Consensus on the method used for selection and preconditions
Kp metals	Measurement error Site-specific nature Concentration effects	Average values obtained by Multiple Linear Regression of field data or the geometric mean of selected field data Consensus on preconditions
BCF metal accumulation for plants	Measurement errors Soil type Crop-specific Climate Matrix effects Concentration effects	Average values obtained by Multiple Linear Regression of field data or the geometric mean of selected field data Consensus on preconditions

1.4. Reading guide

Chapter 2 discusses the CSOIL model performance and the determination of the most relevant input parameters, with Chapter 3 describing the selection of compound-specific input parameter values, method used and the revised parameter set. The evaluation and revision of non-compound-specific parameter values (e.g. exposure parameters, and site and soil properties) are described in Chapter 4. Chapter 5 recapitulates the revised data set, which here is also compared with the present CSOIL input parameter set. Significant differences are explained.

2 Selection of parameters to be evaluated

The input parameter set comprises approximately a hundred parameters, partially compound-specific. Hence, in evaluating the input parameter set it is necessary to put emphasis on the parameter(s) having an important effect on the resulting SRC_{human}. Van den Berg (1995) reported the existing CSOIL input parameter set. This chapter overviews the current input parameter values and gives a broad outline of how the input parameters influence the calculation of human exposure. Based on these findings the most relevant parameters are selected for evaluation.

The criterion used to identify the most relevant parameters is the effect of the input parameter value on the calculated human exposure (model sensitivity). In addition the parameters relevant for the determination of the Intervention Values for groundwater will be evaluated.

The results and conclusions from the sensitivity and uncertainty analysis by Vissenberg and Swartjes (1996) and two reports of Van den Berg (1995; 1997) are used to evaluate the present CSOIL data set. The sensitivity and uncertainty analysis of Vissenberg and Swartjes (1996) considers the most relevant exposure, site and soil parameters. Compound-specific parameters were left out of the analysis. For the priority assessment of the compound-specific parameters, carrying out a sensitivity and uncertainty analysis prior to the evaluation was considered. However, due to the following this analysis was considered impracticable.

1. Parallel with the evaluation of the CSOIL input parameter set, the evaluation of the CSOIL concepts was started. The findings from the sensitivity and uncertainty analysis with the current CSOIL model concept will be of limited value for the improved CSOIL model concept.
2. The program language of the current CSOIL model hampers the execution of uncertainty and sensitivity analysis with the available Monte-Carlo computer programs.
3. Information about the uncertainty of the current 1995 CSOIL parameter values was poor.

Section 2.1 focuses on the compound-specific parameters and section 2.2 on the exposure, site and soil parameters.

2.1. Physicochemical parameters – compound-specific

The current physicochemical- and compound-specific properties used for the determination of SRC_{human} levels for soil are given in Table 2.1. The physicochemical properties, which are also used for the determination of SRChuman levels for sediments and groundwater and for SRCeco risk levels, are indicated.

Table 2.1: Physicochemical- and compound-specific input parameters

Physicochemical properties	**SRC$_{eco, soil}$**	**SRC$_{eco, sediment}$**	**SRC$_{human, soil}$**	**SRC$_{human, groundwater}$**	**SRC$_{human, sediment}$ 1)**
Molecular weight (M)			used		used
Solubility (S)			used		used
Vapour pressure (Vp)			used		
Henry's law constant (H)			used		
Acid dissociation constant (pKa)			used		used
Octanol-water coefficient (Kow)			used		used
Organic carbon normalised soil-water partition coefficient (Koc)	used	used	used	used	used
Bio Concentration Factor vegetables for metals (BCF)			used		
Bio Concentration Factor fish for metals (BCF) 2)					used
Soil-water partition coefficient (Kp metals) 2)	used	used	used	used	used
Permeation coefficient (Pe)			used		
Relative oral absorption factor for soil (Fag)			used		used

1) For a description of the derivation of human risk limits for sediments and the used exposure model SEDISOIL see the report of Otte et al. (2000a).

2) The selection of the BCF fish for metals and the Kp metals for sediments are described in the report of Otte et al. (2000a)

The relative absorption factor (fa) will be discussed in general, as this parameter is not subject of this study.

2.1.1. Molecular weight (M)

The calculated human exposure is influenced by the molecular weight of the compound. For seven compounds Van den Berg (1997) reported input errors.

2.1.2. Solubility (S)

Solubility was evaluated for organic compounds, not for inorganic chemicals
The calculation of the exposure to metals from contaminated soils is based on the total soil concentration of the element. The chemical form in which the metal is present and consequently the solubility is not considered.
For those compounds that belong to the group inorganic compounds (cyanides, thiocyanates, bromide, chloride and fluoride) it is considered that the total compound is present in the water phase of the soil. For cyanides a specific evaluation was executed and reported by Köster (2001).

Regarding organic compounds, the CSOIL model concept uses solubility for the calculation of the Henry's law constant (H). In particular the exposure via inhalation of air is directly influenced by the solubility.
The current solubility values, as selected by Van den Berg (1995), are mainly based on Verschueren and Kolkhuis Tanke (1989) and on values extracted from the ASTER database. Moreover solubility values were taken from RIVM Integrated Criteria Documents for hexaclorocyclohexanes, chlorobenzenes, polycyclic aromatic hydrocarbons, chlorophenoles and phthalates (Van den Berg, 1997).

Solubility has significant effect on the exposure to contaminated soil via inhalation. There is no direct effect on the exposure via crop consumption as the concentration in the pore water

is determined by the partition coefficient. Only in case of pore water concentrations exceeding the solubility an effect may be found.
It is concluded that the value of the solubility is significant for the exposure via inhalation of air and, for compounds with low solubility, the exposure via crop consumption.

2.1.3. Vapour pressure (Vp)

The vapour pressure of a solid or liquid substance is the pressure exerted by its vapour under equilibrium conditions at a given temperature.
The current vapour pressure values, as used for the calculations of the exposure of the first series of compounds, are based on the same references as mentioned for solubility (section 2.1.2). Vapour pressure influences directly the partitioning of the compound over the three soil phases as the vapour pressure is used for the calculation of the Henry's law constant (section 2.1.4).
The value of the vapour pressure is substantially influenced by temperature. It is uncertain (for compounds of the first series) if all data on vapour pressure were corrected for soil temperature (10 °C).
Vapour pressure influences directly the SRC_{human} for volatile compounds (when exposure via inhalation is the dominant route). The vapour pressure value is found critical for the exposure routes inhalation indoor and inhalation outdoors.

2.1.4. Henry's law constant (H)

The dimensionless Henry's law constant (or the air-water partition coefficient) is the proportionality constant between the vapour pressure of a solute above an aqueous solution and the concentration in solution. Henry's law constant is in particular important for the more volatile compounds. Moreover Henry's law constant is used in the CSOIL model to calculate the exposure to compounds during showering. This exposure route however, is found negligible for all compounds of the first series.

According the current CSOIL concept, the Henry's law constant (H) is calculated from the vapour pressure and the solubility by:

$$H = Vp \ / \ (S*R*T)$$

H: Henry's Law constant (-)
Vp: vapour pressure (Pa)
S: water solubility ($mol.m^{-3}$)
R: gas constant (8.3144 Pa . m^3 mol^{-1}. K^{-1})
T: soil temperature (K)

As the calculation of the Henry constant from vapour pressure and solubility is maintained, a specific evaluation of this parameter is not appropriate.

2.1.5. Acid dissociation constant (Ka)

The acid dissociation constant (Ka) expresses the capacity of an organic compound to dissociate. As the pH changes the tendency to dissociate is influenced (Figure 2.1)
The non-dissociated fraction is calculated from the pKa.

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

fnd: non-dissociated (neutral) fraction (-)
pKa: dissociation coeffcient (pKa = -log Ka)
pH: soil pH ($-\log[H^+]$)

Negatively charged compounds are more mobile compared with their neutral parent. The current CSOIL model assumes that the dissociated form not sorbs to organic matter and totally present in the pore water phase (dissolved). Thus, for the calculation of the Kp value, the current CSOIL concept considers only the non-dissociated or neutral form. The Kp for dissociating compounds (e.g. chlorophenols) is calculated as follows:

$$Kp = Koc * foc * fnd$$

Kp: partition coefficient (dm^3/kg)
Koc: organic carbon normalised partition coefficient (dm^3/kg)
foc: fraction organic carbon (-)
fnd: non dissociated (neutral) fraction (-)

The formularies show that the Kp of dissociating organic contaminants depends on the selected pKa and the soil characteristics (pH and organic matter).

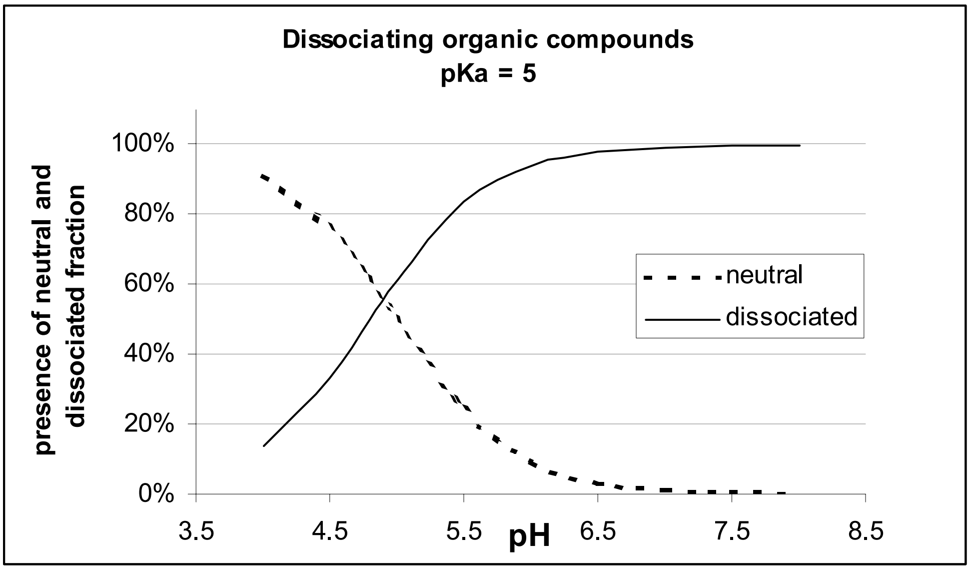


Figure 2.1: Presence of neutral and dissociated form at different pH for an organic compound with a pKa of 5.

Considering the effect of dissociation on the Kp value, the evaluation of pKa values for dissociating compounds is important.

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

The octanol-water partition coefficient expresses the hydrophobic character of a compound. The Kow is the unitless ratio of the concentration in the n-octanol phase to the concentration in the water phase.
The current Kow values for compounds of the first series Intervention Values were based on literature data of merely measured values. References were not always mentioned (Van den Berg, 1997). Because the lack of data on Kow values for some compounds, for sixteen compounds the Kow values were calculated from the solubility using the relation between Kow, and water solubility (according to Verschueren en Kolkhuis Tanke (1989) en Van den Berg (1997):

$$Kow = 10^{4.75} * S^{-0.67}$$

Kow: octanol-water partition coefficient (-)
S: water solubility (mg/dm^3)

Although the relation between calculated Kow and measured Kow was demonstrated by Van den Berg (1997), occasionally differences up till one log unit or more can be found.

The Kow is a key input parameter for the calculation of the human exposure from organic compounds according the current concept of CSOIL. The current concept implies that the organic matter normalised soil-water partition coefficient (Koc) and the bioconcentration factors (BCF) for the accumulation of compounds in crops are based on Kow values. Thus the Kow determines the human exposure via two important routes i.e. crop consumption and indoor air inhalation. The exposure from dermal uptake during bathing is directly controlled by the Kow value. This route however contributes not more than 5 % to total exposure.
If measured Koc values are used, the effect on the model output (human exposure) for Kow will become less. Only exposure via consumption of home-grown crops and via dermal uptake during bathing remains Kow dependent.
Because of the use of the Kow value for the calculation of BCF and possibly the Koc (measured) Kow values are searched and evaluated for all compounds.

2.1.7. Organic carbon normalised soil-water partition coefficient (Koc)

The soil water partition coefficient (K_p) determines the distribution of a compound over the soil and water phases. Generally it is defined as the ratio between the content of a compound adsorbed at the solid phase and its equilibrium pore water concentration.
The K_p can be calculated from the Koc under the assumption that organic carbon is the major sorption phase:

$$Kp = Koc * foc$$

Kp: partition coefficient (dm^3/kg)
Koc: organic carbon normalised soil-water partition coefficient (dm^3/kg)
foc: fraction organic carbon (-)

For most organic compounds an accurate estimate (e.g. an experimental value) of the Koc is not available. In the literature often Koc values generated with quantitative linear models, in

particular Kow-Koc relationships, are published. However, such relationships should be used with caution (Bockting et al., 1993).
According to the current CSOIL concept all the Koc values are calculated from the Kow using the equation of Karickhoff (Koc = 0.411 * Kow; Karickhoff, 1981).
The exposure routes influenced by the Koc value are the inhalation of indoor and outdoor air, the consumption of crop, and the less important routes via drinking water and showering and bathing.

2.1.8. Bioconcentration factor for crops (BCF)

The tendency for accumulation of compounds by crops is expressed by the bioconcentration factor (BCF). The BCF for metals is based on field or laboratory experiments, while the BCF for organic compounds is calculated from the octanol-water partition coefficient (Kow).

Metals

The BCF for metals is defined as the ratio of the metal content in crops (mg/kg dry weight) and soil (mg/kg dry weight). The CSOIL model uses different bioconcentration factors for root and leaf vegetables. The current BCFs are based on Bockting and Van den Berg (1992). The BCF, as used in the CSOIL model, are considered non-crop-specific or generic based on available bioconcentration factors from different crops (preferably vegetables *and* potatoes). In case no experimental data were available the BCF was calculated from the formula of Baes et al. (1984) giving the correlation between the BCF value and the soil-water partition coefficient (Kp):

$$\ln BCF = 2.67 - 1.12 * \ln Kp$$

BCF: bioconcentration factor ($mg.kg^{-1}$ dry weight / $mg.kg^{-1}$ dry weight)
Kp: partition coefficient (dm^3/kg)

Most BCF values currently used were based on data collected from field experiments. Bockting and Van den Berg stressed that the selected BCF values represent at best *indicative values* because of various reasons (Bockting et al., 1992 and Versluijs et al., in prep.):

- BCFs for cadmium, zinc, nickel, lead, chromium and copper are based on one data set only.
- BCFs are partly based on pot experiments. Application to field grown crops is limited.
- BCFs are based on a few different vegetables.
- Average vegetable consumption pattern is not taken into consideration (except for potatoes).
- For some metals the BCFs are based on vegetables or crops not frequently grown in home gardens.
- The BCFs have not been normalised on the basis of the standard soil (pH, clay and organic matter)
- The influence of total metal soil content on BCF values has not been considered
- For some metals the BCF is estimated based on other crops or metals
- Selection criteria are not always clear

Table 2.2 shows the current BCF values for root and leaf crops with the estimated BCF range between brackets. The second column shows the contribution (in %) via consumption of home-grown vegetables to the total exposure.

Table 2.2: BCF values for metals (Bockting and Van den Berg, 1992)

compound	relative contribution (%)	BCF roots (mg/kg dw)/(mg/kg)	BCF leafs (mg/kg dw)/(mg/kg)
Arsenic	51	0.015 (estimated from BCF leaf)	0.03 (0.001-0.1)
Barium	68	0.005 (estimated from BCF leaf)	0.1 (< 0.1-<0.1)
Cadmium	95	0.15 (0.01-0.75)	0.7 (0.34-1.34)
Chromium (III)	32	0.002 (0.001-0.004)	0.02 (0.017-0.017)
Chromium (VI)	32		
Cobalt	51	0.015 (estimated from BCF leaf)	0.03 (0.01-0.05)
Copper	83	0.1 (0.032-0.30)	0.1 (0.08-0.22)
Mercury	51	0.015 (estimated)	0.03 (0.001-0.04)
Lead	39	0.001 (0.0001-0.006)	0.03 (0.012-0.044)
Molybdenum	86	0.015 (estimated from BCF leaf)	0.3 (0.01-1)
Nickel	80	0.07 (0.011-0.678)	0.1 (estimated from BCF root)
Zinc	91	0.1 (0.02-0.61)	0.4 (0.26-0.65)

The exposure to metals via consumption of home-grown vegetables contributes significantly to the total exposure. Evaluation of the underlying data showed that the BCF-leaf is based on metal accumulation of vegetables while the BCF-root is based on metal accumulation of potatoes only.
The CSOIL equation for the calculation of the metal concentration in the crop is:

For leafy crops:
Cpl, leaf = BCF leaf * Cs + Cdp

For root crops:
Cpl, root = BCF root * Cs

Cpl: concentration in the plant, the leaf or root (mg/kg dry weight).
BCF bioconcentration factor (mg.kg^{-1} dry weight / mg.kg^{-1} dry weight).
Cs: total soil content (mg/kg dry weight).
Cdp: contribution due to metal deposition from soil particles originated from the same location (mg/kg dry weight).

The importance of the exposure path ‘crop consumption’ and the indicated large uncertainties in the current CSOIL BCF values gives the evaluation of metal accumulation by vegetables and potatoes a high priority. This evaluation is carried out in close relation with the project on ‘Accumulation in crops’. This project aims to develop a model for the estimation of site-specific accumulation of metals in consumed parts of vegetables and potatoes (Versluijs, 1998).

Organic compounds

In contrast with the BCF for metals, the BCF for organic compounds is on the basis of pore water concentration and based on statistical relations between crop content and octanol-water partition coefficient, developed by Briggs et al. (1982, 1983). The relation according Briggs is:

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

$$BCFl_{leaf,\ stem} = [10^{(0.95 * \log Kow - 2.05)} + 0.82] * [0.784 * 10^{(-0.434 * (\log Kow - 1.78)\hat{}2 / 2.44)}]$$

BCF: bioconcentration factor (mg/kg fresh weight) / (mg/dm^3)

The BCF value of organic compounds is evaluated within the subproject 'Evaluation of concepts' (Rikken et al., 2001). In this report no specific evaluation of the BCF for organic compounds will take place.

2.1.9. Soil-water partition coefficient for metals (Kp)

The soil water partition coefficient[1] (Kp) describes the partitioning of a compound over the two phases. The Kp is defined as:

$$Kp = Cs / Cpw$$

Kp:	soil-water partition coefficient (dm^3/kg)
Cs:	total metal content (mg/kg)
Cpw:	metal concentration pore water (mg/dm^3)

The current CSOIL concept calculates the exposure to a metal from the total soil concentration (e.g. accumulation of metal by plants). This means that the selected Kp does not affect the SRC_{human} levels. The Intervention Value for groundwater however is based on the calculated pore water concentration (by equilibrium partition) at Intervention Value level for soil.

The current Kp values are based on a study of Van den Berg en Roels (1991). The selected Kp is the geometric mean of the reported values after which some values were adjusted and rounded off. Soil characteristics as clay, organic matter content and pH were not taken into account. However, the selected values were considered applicable for standard soil but in fact a possible relation was not determined.

Table 2.3 shows the current Kp set and shows the estimated 10 and 90 percentiles.

An evaluation of the current Kp values is considered of utmost importance for the determination of the Intervention Values for groundwater.

---

[1] The definition of the partition concept depends on the objective and its use. Koops et al. (1998) gives an overview of possible definitions.

Table 2.3: Current CSOIL partition coefficients (Van den Berg and Roels, 1991).

metal	log Kp	Kp (dm^3 / kg)	estimated range 10 – 90 percentiles [1)]
As	2.99	980	200 – 5400
Ba	1.78	60	-
Cd	2.28	190	7 – 51000
Cr	4.16	14400 [2)]	20000 – 170000
Co	2.09	120	70 – 270
Cu	2.73	540	30 – 22000
Hg	3.46	3300	1200 – 89000
Pb	3.38	2380	280 – 260000
Mo	1.30	20 [2)]	26 – 90
Ni	2.75	560	40 – 300000
Zn	2.40	250	20 – 45000

1) A precise determination of the percentiles is not feasible because of the small set of underlying data
2) The selected Kp values for chromium and molybdenum are outside the 10 and 90 percentiles of the used data set for unknown reason.

2.1.10. Permeation coefficient (Pe)

The permeation coefficient (expressed in m^2 per day) is a measure of the affinity for transport of a compound through a membrane. It is used to calculate the concentration of soil contaminants in drinking water after permeation of the compound through the tube. The water tube is specified as a Low-Density Polyethylene (LDPE) tube, as permeation through this material is found higher than with other materials.

Current permeation coefficient values are based on reports of Vonk (1985) and Van der Heijden en Hofman (1987). Van den Berg (1997) gives an evaluation and description of the procedure.

The exposure pathways influenced by permeation coefficient are ‘consumption of drinking water’, ‘inhalation during showering and bathing’ and ‘dermal contact during showering and bathing’. These exposure pathways are found of minor importance.
An additional evaluation of the permeation coefficient is considered not necessary. The findings of Van den Berg (1997) are subscribed and revised values will be implemented.

2.1.11. Dermal sorption factor (Daw)

Exposure through dermal uptake during showering is a minor exposure route. The maximum contribution, in terms of percentage of total exposure, reaches only 4 (naphthalene and chlorobenzenes). The dermal sorption factor is calculated from the Kow. In section 2.1.5 the evaluation of all Kow values was decided, consequently no further considerations are required.

2.1.12. Relative absorption factor (fa)

The relative absorption factor (fa) is the fraction of a compound in soil (or crops, water, air etc.) absorbed in the body. Vissenberg en Swartjes (1996) identified the relative absorption factor as a parameter that contributes substantial to the uncertainty of the exposure. A separate project was initiated to evaluate the relative absorption factor (Lijzen et al., 2001).

The current CSOIL concept sets the relative absorption factor to 1.0 for all compounds, except for lead (Lijzen et al., 1999)

2.1.13. Summary

The current data set is tabulated in Appendix 1: Current CSOIL-1995 input parameter set. Table 2.4 gives an overview of all the physicochemical parameters and the effect on the exposure pathways. The ✔sign indicates a direct effect of the parameter on the exposure through the named exposure route. A ✔ sign between brackets indicates an indirect effect (e.g. limitation of the exposure in case of limited solubility).
Based on the findings as reported in this section it was decided that:

- *For metals*
  - *the evaluation of partition coefficients and BCF values do have a high priority.*
- *For organic compounds:*
  - *evaluation of Koc do have a high priority;*
  - *evaluation of Kow, S, Vp and pKa (only dissociating compounds) is considered important;*
  - *molecular weight (M) and Permeation coefficient (Pe) will be verified only;*
  - *the Henry' law coefficient (H) and the dermal sorption factor (Daw) are calculated from other parameters; consequently a further evaluation of data is not necessary.*

Table 2.4: Physicochemical parameters and the effect on the different exposure paths.

parameter	**soil**			**air**		**crop**	**drinking water**	**showering / bathing**	
	ingestion	dermal contact	inhalation	inhalation air indoor	inhalation air outdoor	consumption	consumption	inhalation	dermal contact
M (all)	✔	✔	✔	✔	✔	✔	✔	✔	✔
Kp (metals)						(✔)	✔		
BCF (metals)						✔			
S (organic compounds)				✔	✔	(✔)	(✔)		
Vp (organic compounds)				✔	✔				
H (organic compounds)								✔	
Kow (organic compounds)				✔	✔	✔	✔	✔	✔
Koc (organic compounds)				✔	✔	✔	✔	✔	✔
Ka (organic compounds)				✔	✔	✔			
Pe (organic compounds)							✔	✔	✔

2.2. Site and exposure parameters

2.2.1. Introduction

This section focuses on all site and exposure parameters. The following criteria are used to identify the most relevant parameters for evaluation:

- importance of the exposure route for the total human exposure to compounds;
- sensitivity and uncertainty of the input parameters in relation with the distribution of the calculated human exposure with CSOIL;

These criteria can be applied by using the results and conclusions from the sensitivity and uncertainty analysis by Vissenberg en Swartjes (1996) and two reports of Van den Berg (1995 and 1997). Based on the results of these studies the most critical site and exposure parameters for determining the SRC_{human} are selected.

Appendix 1: Current CSOIL-1995 input parameter set, gives an overview of all the parameters values used for the calculation of the SRC_{human}. It shows which parameters are classified as exposure and site parameters.

2.2.2. Importance of exposure routes

From the CSOIL report (Van den Berg, 1995) the exposure routes can be extracted that have a major contribution to the total human exposure. It depends on the characteristics of the compound, which of the routes play an important role in the exposure. Three exposure routes are responsible for at least 90% of the total exposure for almost all compounds. Because of the high contribution of the exposure to the total exposure the following routes are important in the evaluation:

- soil ingestion (max 90 %, benzo(ghi)perylene, maneb);
- inhalation of air (max. 100%, vinylchloride);
- crop consumption (max. 100%, inorganic compounds, e.g. cyanides).

A minor contribution is given by the exposure routes (for some compounds):

- dermal uptake via soil contact (max. 7%, benzo(ghi)perylene);
- drinking-water intake due to permeation through LDPE (max. 13%, cresol);
- dermal uptake during bathing (max. 5%, p-dichlorobenzene, styrene).

A negligible contribution is given by the exposure routes:

- inhalation of outdoor air (< 1 %);
- inhalation during bathing (max. 1%, monochlorobenzene, p-dichlorobenzene, styrene);
- inhalation of soil particles (max. 1%, some PCA, DDT, maneb).

The parameters determining the exposure routes: *soil ingestion*, *inhalation of air* and *crop consumption*, have a high priority in the evaluation. The parameters related to *dermal uptake via soil contact* (>1% for 19 compounds) and *drinking-water intake* (>1% for 30 compounds) have a lower priority. The relevant parameters for the exposure route *dermal uptake during bathing* are excluded from this evaluation.
No attention will be given to the parameters on the three exposure routes with a negligible contribution.

2.2.3. Selected parameters

Table 2.5 shows the selected parameters for the five considered exposure routes.

Inhalation of indoor air

The parameters relevant for the inhalation of indoor air are related to the composition of the soil (Va, Vw, foc) and characteristics of the location at the polluted site (Ev, dp, Vv, Bh, fbi).

Consumption of contaminated crops

Three parameters relevant for *crop consumption* are the organic carbon content (foc) and the fraction of the consumed crops (root or leaf) that are contaminated (exposure parameters Fvk and Fvb). Other selected parameters for evaluation and relevant for this major exposure route are the daily consumption of crops for adult and child (Qfv) and the ratio dry weight-fresh weight (fdw)

Ingestion of soil

For the *ingestion of soil* the only important parameter is the daily intake of soil by adults and by children (AIDa and AIDc).

Other exposure routes

Many parameters are important for the calculated exposure by *dermal uptake by soil contact*. For the *uptake of contaminated drinking water* because of the permeation of compounds through LDPE water-pipes, two soil parameters are relevant: the organic carbon content (foc) and the mass volume of dry soil (SD).

Table 2.5: CSOIL-parameters contributing to the uncertainty of the calculated human exposure by that exposure route (Vissenberg and Swartjes, 1996)

Parameter	**unit**	**Description**
inhalation of indoor air		
Va	$m^3.m^{-3}$	volume fraction air
Vw	$m^3.m^{-3}$	volume fraction water
foc	$kg.kg^{-1}$	fraction organic carbon
Ev	$dm^3.m^{-2}.d^{-1}$	flux of evaporating water
dp	m	mean depth of the contamination
Vv	h^{-1}	air-exchange rate
Bh	m	height of the crawl space
fbi	-	contribution of the crawl space air to indoor air (fraction)
crop consumption		
foc	$kg.kg^{-1}$	fraction organic carbon
Fv (k,b)	$kg.kg^{-1}$	fraction consumed contaminated root and leaf crops
Qfv (k,b)	kg $fw.d^{-1}$	average consumption of children and adults
fdw (r,s)	-	fraction dry weight vegetables and potatoes
soil ingestion		
AID (a,c)	$mg.d^{-1}$	daily intake of soil by children and adults
dermal uptake by soil contact		
fm	-	matrix factor,
frs (i,o)	-	fraction soil in dust indoor/outdoor
Aexp	m^2	exposed surface area adult indoor/outdoor
DAE	$g.m^{-2}$	degree of coverage indoor/outdoor (adults and children)
Tba (i, o)	h	time fraction exposure indoor/outdoor
DAR	h^{-1}	absorption velocity
uptake by polluted drinking water		
foc	kg/kg	fraction organic carbon
SD	$kg.dm^{-3}$	mass volume of dry soil (kg dry soil. dm-3 humid soil)

3 Retrieval and selection of compound-specific input parameters

3.1. Introduction

This section discusses briefly the approach to retrieve compound-specific parameter values and the selection of the parameter value used for the calculation of human exposure (the CSOIL value).
Data searches were focussed on the most critical parameters as mentioned in chapter 2. It was decided to minimise the work by using chemical databases for data collection (M, S, Vp, Ka, Kow and Koc). To prevent much time being spent on searches, an evaluation of 12 databases was carried out. Based on the evaluation the most promising databases were selected. Moreover the method for the temperature correction of vapour pressure and solubility was defined and the determination of the selected CSOIL parameter value was laid down. A detailed description of the evaluation and approach is given in Appendix 2: Evaluation of databases and selection of physicochemical parameter values. For a number of organic compounds, it was experienced that the retrieved data for Koc, originated from the selected databases, resulted in a poor data set. To improve the data set and to select a recognised value the selection of Koc values was carried out according a guideline which was determined in co-operation with other *'Koc users'* (Appendix 3: A guideline for the selection of the soil-water partition coefficients for organic compounds.

Below, for each (group of) parameters a summary of the used method is given.

- M, S, Vp, pKa and Kow:

First, the current CSOIL documentation on physicochemical parameter values was reviewed. Second, new data was collected from the selected databases (Table 3.1) and added. After data collection a further selection was made on the basis of completeness of the acquired data. Incomplete data (e.g. missing temperatures) were not considered. To compare the remaining data all variables were converted to the same units. Vapour pressure and solubility data were corrected for soil temperature (10 °C). In some cases evident outliers were removed after which the geometric mean (M, S, Vp) or average value (pKa and log Kow) was determined.

- Koc:

The selection of organic-carbon normalised soil-water partition coefficients (Koc) was carried out according to the Koc guideline (Appendix 3: A guideline for the selection of the soil-water partition coefficients for organic compounds). Data on soil-water partition coefficients reported by Bockting et al. (1993) and Van den Berg (1997) and data taken from the databases searched were taken. For some compounds other sources were considered. A derived Koc value (from the Kow) according to Sabljić et al. (1995) was added to the collection. In principle the final Koc value will be the geometric mean[2] of all experimental (measured) Koc's and one derived Koc according Sabljić. Note that a surplus value is assigned to the experimental Koc's by combining <u>ALL</u> experimental Koc's with <u>ONE</u> derived Koc.

- BCF metals:

The collection of data used to derive bioconcentration factors for metal accumulation in plants (Versluijs et al., in prep.) was part of the subproject 'metal accumulation in plants', in which soil-plant relations for metal accumulation were derived. These soil-plant relationships

---

[2] In case the Koc values are expressed as log, a normal average is calculated.

were used as the basis for the derivation of BCF values suitable for potential risk assessment. The derivation of BCF values, considerations and applicability is discussed in section 3.4.

- Kp metals:

The evaluation of the current Kp data set was based, for example, on the work of Koops at al. (1998) and Otte et al. (2000b). Criteria were formulated for the selection of Kp values suitable for the derivation of Intervention Values for groundwater and for the estimation of the risk of dispersion. Four data sets were assessed from which Kp values were derived.

- Permeation Coefficient:

The determination of permeation coefficients was not considered as a priority given the limited effect of the exposure route involved. The assessment was based on the evaluation of Van den Berg (1997).

Table 3.1 gives the databases searched and reviews used. An asterix (*) indicates the main databases used. Other databases were used only in the case of additional demands.

Table 3.1 Databases searched and (review) articles used for standard data searches. An asterix (*) indicates the main databases used.

	Name of database
	Merck database
	Chemiekaarten
	Merck Safety Data Sheet
*	International Chemical Safety Cards
*	Beilstein
*	Hazardous Substance Database
	Ohmstads
	Cheminfo
	CESARS: Chemical Evaluation Search and Retrieval System
	Pesticide manual 11 ed.
*	Medchem
*	ASTER
	Epiwin
	Review articles and reports
*	Van den Berg, R. (1997), Verantwoording van gegevens en procedures voor de eerste tranche interventiewaarden. RIVM report no. 715810012, RIVM, Bilthoven
*	Bockting et al. (1993), Soil-Water partition coëfficiënts for organic compounds. RIVM report no. 679101013, RIVM, Bilthoven
	Mackay database, CD-ROM (1999)
	Sabljić, A. et al. (1995), Qsar modelling of soil sorption. Improvement and systematics of log Koc vs. log Kow correlations. Chemosphere 31: 11-12; 4489-4514.

3.2. Retrieved M, S, Vp, H, Ka and Kow data

3.2.1. M, S, Vp, H and Ka data

The verification of all molecular weights indicated that adjustments would be necessary for seven compounds (Table 3.2). Moreover, given the reliability of molecular weight data it was proposed to express the molecular weight values to one decimal point accuracy.

Table 3.2: Adjustments for molecular weight values

Compounds	**current value Van den Berg (1995)**	**geomean g/mol**	**number of references**
Ethylbenzene	102	106.2	3
Toluene	90	92.1	4
m-Xylene	102	106.2	3
Naphthalene	130	128.2	3
Endrin	393	380.9	4
Heptane	98	100.2	2
Octane	110	114.2	3

For most compounds the revised solubility and vapour pressure is based on more references than the current CSOIL (1995) values. Table 3.3 gives the current (Van den Berg, 1995) and the revised data for solubility, vapour pressure and Henry's Law constant. The number of references from which the revised data was determined is also given.

The Henry's law constant is calculated from solubility, molecular weight and vapour pressure (see section 2.1.4). The calculation of the Henry's law constant is also used for the evaluation of substances (EUSES, 1997), for deriving environmental risks limits in the Netherlands (J. de Bruijn et al., 1999), and for the evaluation of the environmental aspects of pesticides (Mensink, 1995). It was considered to use measured Henry's law constants. However, because measured H constants are often not available it was decided to maintain the current CSOIL concept for the determination of Henry's law constant.
Van de Berg (1997) reported input errors for several compounds (e.g. 2,3,4-trichlorophenol, pyridine, carbaryl, carbofuran, tetrahydrofuran and tetrahydrothiophene). Table 3.3 gives the corrected data. The compounds marked with an asterix (*) were added at the end of the evaluation process. For these compounds only part of the evaluation process was completed. Six PAH congeners were added to the PAH group because the MPR values were determined for 17 PAH congeners. The non-ortho substituted (planar) PCBs were added because the risk of PCB-contaminated soil is particularly dependent on the presence of these planar isomers. Data are based on the report of Van Wezel et al. (1999) on the derivation of Maximum Permissible Concentrations for polychlorinated biphenyls. More phthalates were added in coherence with the selected phthalates for deriving SRC_{eco} values (Verbruggen, 2000), and thus the basis for the determination of the Intervention Value for total phthalates could be strengthened.

The selected pKa values are given in Table 3.4. The role of the pKa values estimating the Koc is described in section 2.1.5.

Table 3.3: Solubility, vapour pressure and Henry's law constant for all evaluated organic compounds. Both current data (Van den Berg, 1995) and revised data are given

Compound	**S (mg/dm3) vdBerg 95**	**S (mg/dm3)**	**number of refs.**	**Vp (Pa) vdBerg 95**	**Vp (Pa)**	**number of refs.**	**H (-) vdBerg 95**	**H (-)**
Aromatic compounds								
Benzene	1.78E+03	1.99E+03	17	1.01E+04	9.51E+03	3	1.88E-01	1.59E-01
Ethylbenzene	1.52E+02	1.59E+02	15	9.33E+02	9.53E+02	3	2.77E-01	2.70E-01
Phenol	8.20E+04	6.56E+04	7	2.67E+01	3.29E+01	4	1.30E-05	2.00E-05
p-Cresol	2.40E+04	2.86E+04	3	5.33E+00	1.88E+01	3	-	3.02E-05
o-Cresol	-	1.49E+04	3	-	2.35E+01	3	-	7.26E-05
m-Cresol	-	6.32E+03	3	5.33E+00	1.14E+01	3	-	8.25E-05
Toluene	5.15E+02	6.11E+02	11	2.94E+03	2.96E+03	3	2.23E-01	1.90E-01
o-Xylene	-	2.19E+02	6	-	6.76E+02	4	-	1.39E-01
p-Xylene	-	2.11E+02	9	-	8.60E+02	3	-	1.84E-01
m-Xylene	1.80E+02	1.97E+02	7	8.01E+02	8.05E+02	3	2.00E-01	1.84E-01
Catechol	4.51E+05	1.24E+05	3	1.33E+02	3.39E+00	3	1.38E-05	1.28E-06
Resorcinol	8.40E+05	2.42E+05	3	1.33E+02	8.03E-01	3	7.40E-06	1.55E-07
Hydroquinone	5.90E+04	3.92E+04	13	1.34E+02	3.86E-02	7	1.06E-04	4.61E-08
Styrene	3.00E+02	3.20E+02	13	6.67E+02	5.25E+02	11	9.83E-02	7.27E-02
PAH [1)]								
Naphthalene	3.00E+01	3.18E+01	6	2.27E+00	6.83E+00	5	4.11E-03	1.17E-02
Anthracene	7.50E-02	7.13E-02	7	1.30E-04	8.43E-04	3	1.31E-04	8.95E-04
Phenanthrene	1.60E+00	8.50E-01	11	2.41E-03	1.51E-02	3	1.14E-04	1.35E-03
Fluoranthene	2.65E-01	2.01E-01	4	2.31E-04	3.80E-03	4	7.48E-05	1.63E-03
Benzo(a)anthracene	1.00E-02	1.16E-02	6	5.51E-06	2.07E-07	3	5.34E-05	1.73E-06
Chrysene	1.50E-03	1.79E-03	7	2.60E-07	8.74E-08	3	1.68E-05	4.73E-06
Benzo(a)pyrene	3.00E-04	8.42E-04	4	1.31E-08	1.25E-07	3	4.68E-06	1.60E-05
Benzo(ghi)perylene	2.60E-04	1.86E-04	4	2.60E-09	5.04E-09	3	1.17E-06	3.18E-06
Benzo(k)fluoranthene	6.00E-04	4.84E-04	3	2.60E-09	1.24E-08	3	4.64E-07	2.76E-06
Indeno, 1,2,3-cd pyrene	1.00E-04	2.65E-04	3	2.60E-09	2.65E-09	2	3.05E-06	1.17E-06
Pyrene *)	-	1.06E-01	6	-	9.20E-05	4	-	7.49E-05
Acenaphthene *)	-	2.57E+00	1	-	4.22E-01	1	-	1.08E-02
Benzo(b)fluoranthene *)	-	1.68E-02	1	-	1.82E-06	1	-	1.16E-05
Benzo(j)fluoranthene *)	-	8.81E-03	1	-	1.82E-06	1	-	2.21E-05
Dibenz(a,h)anthracene *)	-	8.28E-04	1	-	2.67E-07	1	-	3.81E-05
9H-Fluorene *)	-	1.32E+00	1	-	1.16E-01	1	-	6.19E-03
Acenaphthylene *)	-	4.01E+00	2	-	1.79E-01	2	-	2.89E-02
Chlorinated hydrocarbons								
1,2-Dichloroethane	8.69E+03	1.02E+04	3	8.14E+03	7.39E+03	4	3.94E-02	3.05E-02
Dichloromethane	2.00E+04	1.80E+04	4	4.66E+04	4.30E+04	5	8.42E-02	8.61E-02
Tetrachloromethane	8.00E+02	9.38E+02	5	1.20E+04	9.49E+03	5	9.82E-01	6.61E-01
Tetrachloroethene	1.50E+02	1.19E+02	3	1.87E+03	1.57E+03	4	8.78E-01	9.29E-01
Trichloromethane(chloroform)	8.00E+03	9.39E+03	4	2.14E+04	2.01E+04	5	1.36E-01	1.09E-01
Trichloroethene	1.10E+03	1.16E+03	3	8.01E+03	5.81E+03	5	4.07E-01	2.78E-01
Vinylchloride	1.10E+03	4.28E+02	11	3.55E+05	2.98E+05	17	8.57E+00	1.85E+01
Monochlorobenzene	5.00E+02	5.07E+02	3	1.17E+03	1.19E+03	6	1.12E-01	1.13E-01
1,2-Dichlorobenzene	-	1.40E+02	6	-	1.30E+02	5	-	5.80E-02
1,3-Dichlorobenzene	-	1.13E+02	5	-	1.49E+02	3	-	8.28E-02
1,4-Dichlorobenzene	4.90E+01	6.05E+01	5	8.00E+01	9.06E+01	4	1.02E-01	9.35E-02
1,2,3-Trichlorobenzene	-	1.36E+01	4	-	2.47E+01	3	-	1.40E-01
1,2,4-Trichlorobenzene	1.90E+01	2.88E+01	6	1.87E+01	4.07E+01	3	7.59E-02	1.09E-01
1,3,5-Trichlorobenzene	-	4.71E+00	2	-	2.80E+02	2	-	4.58E+00
1,2,3,4-Tetrachlorobenzene	3.50E+00	3.40E+00	3	5.34E-01	6.78E-01	3	1.40E-02	1.83E-02
1,2,3,5-Tetrachlorobenzene	-	2.61E+00	3	-	1.29E+00	3	-	4.53E-02
1,2,4,5-Tetrachlorobenzene	-	6.82E-01	3	-	4.00E+00	3	-	5.37E-01
Pentachlorobenzene	2.40E-01	3.23E-01	8	1.33E-01	4.52E-01	4	5.90E-02	1.49E-01
Hexachlorobenzene	1.10E-01	1.17E-02	4	1.33E-03	6.13E-04	3	1.60E-03	6.36E-03
2-Chlorophenol	2.85E+04	8.71E+03	3	1.07E+02	2.25E+02	3	2.05E-04	1.41E-03
3-Chlorophenol	-	7.97E+03	3	-	1.93E+01	3	-	1.33E-04

Compound	**S (mg/dm3) vdBerg 95**	**S (mg/dm3)**	**number of refs.**	**Vp (Pa) vdBerg 95**	**Vp (Pa)**	**number of refs.**	**H (-) vdBerg 95**	**H (-)**
4-Chlorophenol	-	7.67E+03	3	-	1.13E+01	3	-	8.03E-05
2,3-Dichlorophenol	-	9.05E+02	2	-	1.27E+01	3	-	9.76E-04
2,4-Dichlorophenol	4.60E+03	1.91E+03	4	1.33E+01	4.09E+00	3	2.00E-04	1.48E-04
2,5-Dichlorophenol	-	4.21E+02	3	-	1.04E+01	3	-	1.71E-03
2,6-Dichlorophenol	-	5.34E+02	3	-	7.14E+00	3	-	9.26E-04
3,4-Dichlorophenol	-	3.02E+01	3	-	4.40E-01	2	-	1.01E-03
3,5-Dichlorophenol	-	3.99E+01	3	-	2.46E+00	3	-	4.26E-03
2,3,4-Trichlorophenol	1.00E+03	7.11E+01	2	1.07E+00	7.93E-01	2	8.96E-05	9.36E-04
2,3,5-Trichlorophenol	-	1.26E+02	-	-	2.02E-01	-	-	1.35E-04
2,3,6-Trichlorophenol	-	1.26E+02	3	-	2.02E-01	2	-	1.35E-04
2,4,5-Trichlorophenol	1.00E+03	3.80E+02	4	-	1.00E+00	3	-	2.22E-04
2,4,6-Trichlorophenol	-	2.43E+02	3	-	9.83E-01	3	-	3.40E-04
3,4,5-Trichlorophenol	-	3.46E+01	3	-	2.02E-01	2	-	4.89E-04
2,3,4,5-Tetrachlorophenol	1.25E+02	3.61E+00	3	1.33E-01	3.94E-02	3	1.05E-04	1.07E-03
2,3,4,6-Tetrachlorophenol	-	1.47E+01	3	-	6.03E-02	3	-	4.05E-04
2,3,5,6-Tetrachlorophenol	-	4.79E+00	3	-	3.94E-02	3	-	8.10E-04
Pentachlorophenol	1.40E+01	4.28E+00	10	1.47E-02	8.53E-03	9	1.19E-04	2.26E-04
1-Chloronaphatalene	2.24E+01	1.68E+01	4	5.25E+00	4.25E+00	6	1.62E-02	1.75E-02
2-Chloronaphatalene	-	9.71E+00	3	-	1.00E+00	4	-	7.14E-03
PCB 28	2.25E-01	1.21E-01	20	7.00E-04	1.60E-02	8	3.40E-04	1.44E-02
PCB 52	-	2.65E-02	23	-	6.07E-03	19	-	2.85E-02
PCB101	-	1.32E-02	3	-	9.27E-03	2	-	9.76E-02
PCB118	-	6.54E-03	4	-	2.96E-04	1	-	6.28E-03
PCB138	-	6.96E-04	3	-	4.30E-06	2	-	9.48E-04
PCB153	1.20E-02	2.74E-03	4	7.00E-04	1.75E-04	12	8.95E-03	9.79E-03
PCB180	-	7.69E-04	4	-	4.96E-05	6	-	1.08E-02
Dioxins (+PCDF, PCBs $^{2)}$)								
1-MCDD	4.20E-01	4.20E-01		1.61E-02	1.61E-02		3.57E-03	3.57E-03
2-MCDD	2.80E-01	2.80E-01		1.90E-02	1.90E-02		6.32E-03	6.32E-03
27-DCDD	3.75E-03	3.75E-03		1.20E-04	1.20E-04		3.44E-03	3.44E-03
28-DCDD	1.67E-02	1.67E-02		1.41E-04	1.41E-04		9.08E-04	9.08E-04
124-TrCDD	8.41E-03	8.41E-03		1.12E-04	1.12E-04		1.63E-03	1.63E-03
2,3,7,8-TCDD	3.00E-04	3.00E-04		1.40E-06	1.40E-06		6.39E-04	6.39E-04
1,3,6,8-TeCDD	3.20E-04	3.20E-04		7.06E-07	7.06E-07		3.02E-04	3.02E-04
PCDD	1.20E-04	1.20E-04		8.88E-08	8.88E-08		1.12E-04	1.12E-04
HxCDD	4.40E-06	4.40E-06		5.08E-08	5.08E-08		1.92E-03	1.92E-03
HpCDD	2.40E-06	2.40E-06		7.51E-10	7.51E-10		5.65E-05	5.65E-05
OCDD	4.00E-07	4.00E-07		5.93E-10	5.93E-10		2.90E-04	2.90E-04
PCB 77 *)	-	1.91E-03	4	-	5.09E-05	2	-	3.30E-03
PCB 105 *)	-	7.15E-03	2	-	1.55E-04	1	-	3.01E-03
PCB 126 *)	-	7.00E-03	1	-	1.55E-04	1	-	3.07E-03
PCB 156 *)	-	1.22E-03	1	-	4.05E-05	1	-	5.09E-03
PCB 157 *)	-	1.22E-03	1	-	4.05E-05	1	-	5.09E-03
PCB 169 *)	-	5.58E-04	3	-	1.26E-06	2	-	3.46E-04
TetraCDF	4.13E-04	4.13E-04		7.89E-06	7.89E-06		8.12E-06	8.12E-06
PentaCDF	2.36E-04	2.36E-04		2.17E-05	2.17E-05		3.91E-05	3.91E-05
HexaCDF	8.25E-06	8.25E-06		8.09E-06	8.09E-06		4.17E-04	4.17E-04
HeptaCDF	1.35E-06	1.35E-06		1.55E-06	1.55E-06		4.87E-04	4.87E-04
OctaCDF	2.15E-07	2.15E-07		2.91E-08	2.91E-08		5.75E-05	5.75E-05
Pesticides								
DDT	3.10E-03	6.48E-03	5	2.53E-05	1.22E-05	4	1.23E-03	2.84E-04
DDE	4.00E-02	4.09E-02	3	1.33E-05	4.29E-05	3	4.49E-05	1.42E-04
DDD	-	6.23E-02	4	-	1.93E-05	3	-	4.22E-05
Aldrin	1.00E-02	2.46E-02	3	3.07E-03	2.33E-03	4	4.76E-02	1.47E-02
Dieldrin	1.00E-01	2.99E-01	3	2.40E-05	2.94E-05	3	3.89E-05	1.60E-05
Endrin	2.00E-02	4.66E-01	3	2.67E-05	1.25E-05	3	2.16E-04	4.33E-06
α-HCH	1.63E+00	1.63E+00	3	3.33E-03	3.50E-02	3	2.53E-04	2.65E-03
β-HCH	2.40E-01	9.38E-01	9	3.73E-05	1.98E-02	13	1.92E-05	2.61E-03

Compound	**S (mg/dm3) vdBerg 95**	**S (mg/dm3)**	**number of refs.**	**Vp (Pa) vdBerg 95**	**Vp (Pa)**	**number of refs.**	**H (-) vdBerg 95**	**H (-)**
γ-HCH	7.80E+00	5.81E+00	6	2.13E-02	1.23E-03	5	3.38E-04	2.61E-05
δ-HCH	3.14E+01	1.01E+01	3	2.26E-03	3.06E-02	3	8.91E-06	3.75E-04
Carbaryl	1.20E+02	8.16E+01	3	6.67E-01	1.43E-01	3	4.75E-04	1.50E-04
Carbofuran	5.00E+02	3.76E+02	3	2.70E-03	2.03E-03	3	5.07E-07	5.07E-07
Maneb	1.00E-04	8.50E-05	2	1.00E-04	2.08E-06	2	1.13E-01	2.76E-03
Atrazine	7.00E+01	3.81E+01	6	4.00E-05	2.70E-05	3	5.23E-08	6.50E-08
Mineral oil 3)								
aliphatic >EC5-EC6	-	2.80E+01	-	-	5.07E+04	-	-	6.23E+01
aliphatic >EC6-EC8	-	4.20E+00	-	-	8.61E+03	-	-	8.71E+01
aliphatic >EC8-EC10	-	3.25E-01	-	-	8.21E+02	-	-	1.40E+02
aliphatic >EC10-EC12	-	2.61E-02	-	-	7.90E+01	-	-	2.06E+02
aliphatic >EC12-EC16	-	5.90E-04	-	-	3.55E+00	-	-	5.11E+02
aliphatic >EC16-EC21	-	9.99E-07	-	-	1.72E-01	-	-	1.98E+04
aromatic >EC5-EC7	-	2.20E+02	-	-	1.11E+04	-	-	1.67E+00
aromatic >EC7-EC8	-	1.30E+02	-	-	3.24E+03	-	-	9.77E-01
aromatic >EC8-EC10	-	6.50E+01	-	-	8.21E+02	-	-	6.44E-01
aromatic >EC10-EC12	-	2.48E+01	-	-	7.90E+01	-	-	1.76E-01
aromatic >EC12-EC16	-	5.81E+00	-	-	3.55E+00	-	-	3.90E-02
aromatic >EC16-EC21	-	5.43E-01	-	-	1.72E-01	-	-	2.56E-02
aromatic >EC21-EC35	-	6.60E-03	-	-	8.00E-04	-	-	1.24E-02
Other pollutants								
Cyclohexanone	2.30E+04	1.90E+04	6	5.33E+02	4.90E+02	9	9.65E-04	1.08E-03
Dimethyl phthalate (DMP) *) 4)	-	2.01E+03	1	-	3.87E+00	1	-	1.58E-04
Diethyl phthalate (DEP) *) 4)	-	2.87E+02	1	-	6.68E-01	1	-	2.20E-04
Dibuthyl phthalate (DBP) *) 4)	-	2.35E+00	1	-	3.40E-02	1	-	1.71E-03
Diisobutylphthalate (DIBP) *)	-	9.60E+00	6	-	1.37E-02	3	-	1.69E-04
Butylbenzylphthalate (BBP)	2.90E+00	4.22E+00	3	1.15E-03	6.53E-04	3	5.26E-05	2.06E-05
Dihexyl phthalate (DHP) *) 4)	-	1.15E-02	1	-	1.61E-03	1	-	1.99E-02
Di(2-ethylhexyl)phthalate (DEHP)	2.85E-01	4.57E-02	5	8.60E-04	2.72E-04	4	5.00E-04	9.88E-04
Pyridine	2.33E+05	6.65E+05	3	3.11E+03	2.02E+03	14	4.48E-04	1.02E-04
Tetrahydrofuran	2.18E+05	4.06E+05	3	2.21E+04	1.47E+04	3	3.11E-03	1.11E-03
Tetrahydrothiophene	1.06E+04	1.29E+04	2	2.41E+03	2.05E+03	2	8.50E-03	5.94E-03

1) The data on the added PAHs, marked with an asterix (*) represent, with exception of pyrene, values from EPIWIN.

2) The physicochemical parameters of dioxins (belonging to the second series of compounds) were not evaluated. The data are taken from Van den Berg (1994). The data of the added planar PCBs are based on Van Wezel et al. (1999). Mono-, di- and trichlorobiphenyls were left out because the MPR does not include these congeners.

3) The data on Total Petroleum Hydrocarbons are taken from Franken (1999).

4) The data on the added compound are values from EPIWIN and Staples et al. (1997).

*) Added compounds (explained in section 3.2.1)

Table 3.4: Acid dissociation constant (pKa) for dissociating organic compounds, with both current and revised data given

compound	PKa current [1]	pKa	number of refs.
dissociating compounds			
Phenol	-	10.0	22
p-Cresol	-	10.1	11
o-Cresol	-	10.2	10
m-Cresol	-	10.0	11
Catechol	-	10.6	13
Resorcinol	-	9.68	4
Hydroquinone	-	10.6	8
2-Chlorophenol	-	8.43	10
3-Chlorophenol	-	9.06	10
4-Chlorophenol	-	9.23	12
2,3-Dichlorophenol	-	7.66	3
2,4-Dichlorophenol	-	7.81	7
2,5-Dichlorophenol	-	7.54	3
2,6-Dichlorophenol	-	6.84	4
3,4-Dichlorophenol	-	8.60	4
3,5-Dichlorophenol	-	8.17	5
2,3,4-Trichlorophenol	7.04	7.01	2
2,3,5-Trichlorophenol [2]	7.04	6.79	-
2,3,6-Trichlorophenol	7.04	5.95	4
2,4,5-Trichlorophenol	7.04	7.07	6
2,4,6-Trichlorophenol	7.04	6.22	6
3,4,5-Trichlorophenol	7.04	7.46	7
2,3,4,5-Tetrachlorophenol	6.22	6.07	3
2,3,4,6-Tetrachlorophenol	6.22	5.29	6
2,3,5,6-Tetrachlorophenol	6.22	5.21	4
Pentachlorophenol	4.74	4.85	6

Remarks

1) Only pKa values for di-, tri- and tetrachlorophenols were reported (VROM, 1995).

2) No reliable pKa value for 2,3,5-trichlorophenol was found. The selected value is the average pKa of other trichlorophenols.

3.2.2. Octanol – water partition coefficient (Kow)

The octanol-water partition coefficient for all compounds was selected according to the procedure mentioned. The data obtained were compared with the LOGPSTAR Kow values, a reliable experimental Kow. Considering the status of LOGPSTAR data and the frequent use within related frames (e.g. the project 'Setting Integrated Environmental Quality Standards'), it was proposed to use the measured Kow data from the Medchem database (called LOGPSTAR or MLOGP data) for the modelling of human and ecotoxicological risk.
Table 3.5 gives the current CSOIL Kow data according Van den Berg (1995) in the second column. For some compounds the corrected values (Van den Berg, 1997) are given. The proposed LOGPSTAR data, CLOGP data and log Kow data, derived according the procedure mentioned, are tabulated. LOGPSTAR data were found for almost all compounds. If not, the calculated Kow data from the Medchem database (CLOGP value) were taken. Where there was doubt the CLOGP data was compared with the average Kow value of the retrieved data. A specific evaluation may be appropriate later. For maneb, which is a polymer, a separate evaluation will be necessary due to deviant behaviour.

Table 3.5: Log Kow values for all compounds evaluated

Compound	Van den Berg (1995)	LOGPSTAR (proposed)	CLOGP	geometric mean selected values	number of refs.
Aromatic compounds					
Benzene	2.13	2.13	2.14	2.11	9
Ethylbenzene	3.15	3.15	3.17	3.15	5
Phenol	1.46	1.47	1.47	1.46	7
o-Cresol	-	1.95	1.97	2.00	5
m-Cresol	-	1.96	1.97	1.97	5
p-Cresol	2.00	1.94	1.97	1.94	5
Toluene	2.69	2.73	2.64	2.71	6
o-Xylene	-	3.12	3.09	3.03	6
p-Xylene	-	3.15	3.14	3.15	6
m-Xylene	3.20	3.20	3.14	3.20	5
Catechol	0.88	0.88	0.88	0.91	6
Resorcinol	0.78	0.80	0.81	0.79	4
Hydroquinone	0.55	0.59	0.81	0.59	9
Styrene	3.09	2.95	2.87	2.98	11
PAH 1)					
Naphthalene	3.36	3.30	3.32	3.35	9
Anthracene	4.49	4.45	4.49	4.48	9
Phenanthrene	4.54	4.47	4.49	4.51	7
Fluoranthene	5.33	5.16	4.95	5.05	6
Benzo(a)anthracene	5.61	5.54	5.66	5.64	7
Chrysene	6.64	5.81	5.66	5.63	7
Benzo(a)pyrene	6.35	6.13	6.12	6.04	7
Benzo(ghi)perylene	6.00	6.22	-	6.74	7
Benzo(k)fluoranthene	6.84	6.11	6.12	6.20	5
Indeno, 1,2,3-cd pyrene	7.43	6.87	-	6.87	6
Pyrene *)	6.00	4.99	4.95	-	-
acenaphthene *)	-	3.92	-	-	-
Benzo(b)fluoranthene *)	-	5.78	-	-	-
Benzo(j)fluoranthene *)	-	6.11	-	-	-
Dibenz(a,h)anthracene *)	-	7.11	-	-	-
9H-Fluorene *)	-	4.18	-	-	-
Acenaphthylene *)	-	3.94	-	-	-
Chlorinated hydrocarbons					
1,2-Dichloroethane	1.45	1.47	1.46	1.47	5
Dichloromethane	1.87	1.25	1.25	1.34	6
Tetrachloromethane	2.64	2.83	2.88	2.76	7
Tetrachloroethene	2.60	3.40	3.48	2.89	8
Trichloromethane	1.97	1.97	1.95	1.96	7
Trichloroethene	2.71	2.61	2.63	2.48	9
Vinylchloride	2.71	1.52	1.52	1.32	10
Monochlorobenzene	2.81	2.89	2.86	2.85	5
1,2-Dichlorobenzene	-	3.43	3.45	3.43	8
1,3-Dichlorobenzene	-	3.53	3.57	3.51	7
1,4-Dichlorobenzene	3.40	3.44	3.57	3.48	7
1,2,3-Trichlorobenzene	-	4.14	4.04	4.01	4
1,2,4-Trichlorobenzene	4.06	4.05	4.16	4.11	7
1,3,5-Trichlorobenzene	-	4.19	4.28	4.24	2
1,2,3,4-Tetrachlorobenzene	4.70	4.64	4.63	-	-
1,2,3,5-Tetrachlorobenzene	-	4.66	4.75	4.57	3
1,2,4,5-Tetrachlorobenzene	-	4.60	4.75	4.62	5
Pentachlorobenzene	5.17	5.18	5.35	5.25	10
Hexachlorobenzene	5.34	5.73	6.06	5.61	8
2-Chlorophenol	2.39	2.15	2.15	2.16	6
3-Chlorophenol	-	2.50	2.48	2.49	5
4-Chlorophenol	-	2.39	2.48	2.45	6
2,3-Dichlorophenol	-	2.84	2.84	3.00	3
2,4-Dichlorophenol	3.15	3.06	2.96	2.96	5

Compound	**Van den Berg (1995)**	**LOGPSTAR (proposed)**	**CLOGP**	**geometric mean selected values**	**number of refs.**
2,5-Dichlorophenol	-	3.06	2.96	3.07	3
2,6-Dichlorophenol	-	2.75	2.63	2.73	3
3,4-Dichlorophenol	-	3.33	3.17	3.30	4
3,5-Dichlorophenol	-	3.52	3.29	3.44	4
2,3,4-Trichlorophenol	3.88	3.46	3.46	4.07	1
2,3,5-Trichlorophenol	-	3.58	3.58	-	-
2,3,6-Trichlorophenol	-	3.77	3.25	3.67	3
2,4,5-Trichlorophenol	-	3.72	3.58	3.61	6
2,4,6-Trichlorophenol	-	3.69	3.37	3.61	6
3,4,5-Trichlorophenol	-	4.01	3.79	4.06	3
2,3,4,5-Tetrachlorophenol	3.35	4.21	4.18	4.49	3
2,3,4,6-Tetrachlorophenol	-	4.12	3.97	4.18	4
2,3,5,6-Tetrachlorophenol	-	3.88	3.97	4.29	3
Pentachlorophenol	5.13	5.12	4.68	4.92	14
1-Chloronaphatalene	3.85	4.10	4.03	4.05	6
2-Chloronaphatalene	-	4.14	4.03	4.07	4
PCB 28	-	5.62	5.92	5.56	7
PCB 52	-	6.26	6.38	5.59	13
PCB101	-	6.85	6.97	5.89	5
PCB118	-	7.12	7.10	-	-
PCB138	-	7.45	7.45	6.68	3
PCB153	6.57	7.44	7.57	6.79	7
PCB180	-	8.16	8.16	7.21	2
Dioxins (+PCDF, PCBs 2))					
1-MCDD	4.75	4.75			
2-MCDD	5.00	5.00			
27-DCDD	5.75	5.75			
28-DCDD	5.60	5.60			
124-TrCDD	6.35	6.35			
2,3,7,8-TCDD	6.80	6.80			
1368-TeCDD	7.10	7.10			
PCDD	7.40	7.40			
HxCDD	7.80	7.80			
HpCDD	8.00	8.00			
OCDD	8.20	8.20			
PCB 77 *)	-	6.63	6.64	6.34	8
PCB 105 *)	-	6.98	6.98	-	-
PCB 126 *)	-	7.23	7.23	-	-
PCB 156 *)	-	7.70	7.70	-	-
PCB 157 *)	-	7.60	7.58	-	-
PCB 169 *)	-	7.41	7.83	7.54	7
TetraCDF	6.53	6.53			
PentaCDF	6.85	6.85			
HexaCDF	7.81	7.81			
HeptaCDF	7.92	7.92			
OctaCDF	8.28	8.28			
Pesticides					
DDT	6.18	6.91	6.76	6.47	8
DDE	5.73	6.96	6.74	6.23	6
DDD	-	6.22	6.06	5.94	5
Aldrin	7.40	6.50	5.41	5.62	8
Dieldrin	5.36	4.55	3.70	4.86	7
Endrin	4.95	4.55	3.70	4.34	8
α-HCH	3.72	3.72	3.75	3.81	6
β-HCH	3.72	3.72	3.75	3.83	17
γ-HCH	3.72	3.72	3.75	3.76	9
δ-HCH	3.72	3.72	3.75	3.70	5
Carbaryl	3.36	2.36	2.39	2.42	7
Carbofuran	2.94	1.63	2.47	2.16	6
Maneb 3)	7.43	-	-	-	-

Compound	Van den Berg (1995)	LOGPSTAR (proposed)	CLOGP	geometric mean selected values	number of refs.
Atrazine	2.18	2.61	2.50	2.62	8
Mineral oil					
aliphatic >EC5-EC6	-	3.52	-	-	-
aliphatic >EC6-EC8	-	3.60	-	-	-
aliphatic >EC8-EC10	-	3.69	-	-	-
aliphatic >EC10-EC12	-	3.76	-	-	-
aliphatic >EC12-EC16	-	3.85	-	-	-
aliphatic >EC16-EC21	-	3.97	-	-	-
aromatic >EC5-EC7	-	3.53	-	-	-
aromatic >EC7-EC8	-	3.54	-	-	-
aromatic >EC8-EC10	-	3.55	-	-	-
aromatic >EC10-EC12	-	3.58	-	-	-
aromatic >EC12-EC16	-	3.61	-	-	-
aromatic >EC16-EC21	-	3.66	-	-	-
aromatic >EC21-EC35	-	3.74	-	-	-
Other pollutants					
Cyclohexanone	1.83	0.81	0.86	0.81	8
Dimethyl phthalate (DMP) *)	-	1.56	1.56	-	-
Diethyl phthalate (DEP) *)	-	2.47	2.62	-	-
Dibuthyl phthalate (DBP) *)	-	4.72	4.73	-	-
Di-isobutylphthalate (DIBP) *)	-	4.46	-	-	-
Butylbenzylphthalate (BBP)	4.44	4.91	3.88	4.54	6
Dihexyl phthalate (DHP) *)	-	6.85	6.85	-	-
Di(2-ethylhexyl)phthalate (DEHP)	5.12	7.45	8.71	6.40	5
Pyridine	1.15	0.65	0.64	0.73	12
Tetrahydrofuran	1.17	0.47	0.53	0.42	3
Tetrahydrothiophene	2.05	1.61	1.45	1.51	3

1) The Kow data on the added PAHs, marked with an asterix (*) represent, with exception of pyrene, values from EPIWIN.
2) The physicochemical parameters of dioxins (belonging to the second series of compounds) were not evaluated. The data is taken from Van den Berg, 1994. The data of the added planar PCBs are based on Van Wezel et al. (1999). Mono-, di- and trichlorobiphenyls were left out because the MPR does not include these congeners.
3) No reliable Kow for Maneb was found.
*) Added compounds are explained in section 3.2.1.

3.3. Organic carbon normalised soil-water partition coefficients (Koc)

3.3.1. Koc for non-dissociating compounds

Organic-carbon normalised soil-water partition coefficients are, within the scope of potential risk assessment, considered to be independent of soil type. Ageing, the nature and type of organic matter (polarity C/N+O, aromaticity), and the process of so-called 'slow desorption' in situ (van Steenwijk et al., 1999), which can provoke additional variation, are not taken into account. These effects are site-specific and simply not predictable. As potential risk assessment considers the average situation, site-specific effects are outside the scope of this study.

De current SRC_{human} values of compounds for the first series were based on Kow derived Koc values according the relationship of Karickhoff (section 2.1.7). These values were found to show substantial differences when compared with measured Koc values or with other log Koc vs. log Kow correlations (Sabljić, 1995).

In general, we believe that experimental measured Koc values should be the basis of values suitable for potential risk assessment. The selection criteria agreed on by several ‘Koc users’ are given in Appendix 3. Moreover, it was agreed that both humantoxicological and ecotoxicological risk values (soils and sediments) will use the same Koc data set.

Table 3.6 gives the current CSOIL log Koc data (Van den Berg, 1995) and the revised log Koc data derived following the Koc guideline, together with the standard deviation (log) and the number of references.

Table 3.6: Current (Van den Berg, 1995) and revised log Koc values

compound	Van den Berg (1995) log Koc	revised log Koc	standard deviation 6)	number of references
Aromatic compounds				
Benzene	1.74	1.87	0.18	14
Ethylbenzene	2.76	2.53	0.40	4
Phenol	1.07	1.52	0.43	18
o-Cresol	-	1.59	1.30-2.14	3
m-Cresol	-	1.72	1.49-2.14	3
p-Cresol	1.61	1.64	0.20	9
Toluene	2.30	2.09	0.33	16
o-Xylene	-	2.18	1.76-2.60	2
p-Xylene	-	2.66	0.16	7
m-Xylene	2.81	2.41	0.20	4
Catechol	0.49	1.85	1.45-2.07	3
Resorcinol	0.39	1.14	0.98-1.41	3
Hydroquinone	0.16	1.95	1.27-2.64	2
Styrene	2.70	2.58	2.44-2.71	2
PAH 1)				
Naphthalene	2.97	2.98	0.27	13
Anthracene	4.10	4.30	0.25	9
Phenanthrene	4.15	4.23	0.27	7
Fluoranthene	4.94	5.18	0.76	9
Benzo(a)anthracene	5.22	5.79	0.64	5
Chrysene	6.25	5.72	0.90	5
Benzo(a)pyrene	5.96	5.82	0.90	5
Benzo(ghi)perylene	5.61	6.43	0.63	5
Benzo(k)fluoranthene	6.45	6.24	0.68	7
Indeno, 1,2,3-cd pyrene	7.04	6.02	5.66-6.20	3
Pyrene *)	5.61	4.83	0.25	40
1,2-dihydroacenaphthalene *)	-	3.53	3.28-3.79	2
Benzo(b)fluoranthene *)	-	5.34	4.78-5.91	2
Benzo(j)fluoranthene *)	-	5.48	5.05-5.91	2
Dibenz(a,h)anthracene *)	-	6.14	5.86-6.42	2
9H-Fluorene *)	-	3.77	3.49-4.05	2
Acenaphthylene *)	-	3.47	3.29-3.79	3
Chlorinated hydrocarbons				
1,2-Dichloroethane	1.06	1.49	0.21	8
Dichloromethane (methylenechloride)	1.48	1.22	0.33	5
Tetrachloromethane (carbontetrachloride)	2.25	1.75	0.44	11
Tetrachloroethene	2.21	2.42	0.23	17
Trichloromethane(chloroform)	1.58	1.66	0.17	7
Trichloroethene	2.32	2.06	0.11	19
Vinylchloride	2.32	1.56	0.24	4
Monochlorobenzene	2.42	2.34	0.22	14
1,2-Dichlorobenzene	-	2.60	0.24	11
1,3-Dichlorobenzene	-	2.69	0.34	6
1,4-Dichlorobenzene	3.01	2.82	0.26	16
1,2,3-Trichlorobenzene	-	3.23	0.28	7

compound	**Van den Berg (1995) log Koc**	**revised log Koc**	**standard deviation 6)**	**number of references**
1,2,4-Trichlorobenzene	3.67	3.28	0.32	15
1,3,5-Trichlorobenzene	-	3.98	3.26-5.10	3
1,2,3,4-Tetrachlorobenzene	4.31	3.91	0.13	4
1,2,3,5-Tetrachlorobenzene	-	3.57	0.29	5
1,2,4,5-Tetrachlorobenzene	-	3.77	0.31	11
Pentachlorobenzene	4.78	3.92	0.49	6
Hexachlorobenzene	4.95	4.06	0.51	13
2-Chlorophenol	2.00	1.97	0.44	5
3-Chlorophenol	-	2.56	0.49	18
4-Chlorophenol	-	1.93	0.27	5
2,3-Dichlorophenol	-	2.56	0.22	8
2,4-Dichlorophenol	2.76	2.54	0.29	13
2,5-Dichlorophenol	-	2.83	-	1
2,6-Dichlorophenol	-	2.63	-	1
3,4-Dichlorophenol 2)	-	2.90	0.42	17
3,5-Dichlorophenol	-	2.34	0.55	3
2,3,4-Trichlorophenol	3.49	3.08	-	1
2,3,5-Trichlorophenol	-	3.16	-	1
2,3,6-Trichlorophenol	-	3.28	-	1
2,4,5-Trichlorophenol 2)	-	3.36	0.32	17
2,4,6-Trichlorophenol 2)	-	3.47	0.89	14
3,4,5-Trichlorophenol	-	3.54	0.10	4
2,3,4,5-Tetrachlorophenol 2)	2.96	3.87	0.34	7
2,3,4,6-Tetrachlorophenol	-	3.10	0.26	13
2,3,5,6-Tetrachlorophenol	-	3.34	-	1
Pentachlorophenol 2)	4.74	3.20	0.54	84
1-Chloronaphatalene	3.46	3.42	3.36-3.48	2
2-Chloronaphatalene	-	3.42	3.36-3.47	2
PCB 28	5.18	4.61	0.62	5
PCB 52	-	4.70	1.08	6
PCB101	-	5.53	0.71	15
PCB118	-	6.35	0.42	8
PCB138	-	5.71	0.74	9
PCB153	6.18	5.87	0.70	62
PCB180	-	5.99	0.65	9
Dioxines and planar PCBs 3)				
1-MCDD	3.95	3.95	-	-
2-MCDD	4.15	4.15	-	-
27-DCDD	4.76	4.76	-	-
28-DCDD	4.64	4.64	-	-
124-TrCDD	5.24	5.24	-	-
2,3,7,8-TCDD	5.61	5.61	-	-
1368-TeCDD	5.85	5.85	-	-
PCDD	6.09	6.09	-	-
HxCDD	6.42	6.42	-	-
HpCDD	6.58	6.58	-	-
OCDD	6.74	6.74	-	-
PCB 77 *)	-	5.85	5.47-6.31	3
PCB 105 *)	-	6.13	0.33	7
PCB 126 *)	-	5.94	5.92-5.96	3
PCB 156 *)	-	6.34	-	1
PCB 157 *)	-	6.26	-	1
PCB 169 *)	-	6.01	5.92-6.10	2
TetraCDF	5.39	5.39		
PentaCDF	5.65	5.65		
HexaCDF	6.42	6.42		
HeptaCDF	6.52	6.52		
OctaCDF	6.80	6.80		

compound	Van den Berg (1995) log Koc	revised log Koc	standard deviation 6)	number of references
Pesticides				
DDT	5.79	5.58	0.56	39
DDE	5.34	5.35	0.83	5
DDD	-	5.18	0.48	4
Aldrin	7.01	3.94	1.04	12
Dieldrin	4.97	3.99	0.50	10
Endrin	4.56	3.95	0.80	3
α-HCH	3.33	3.33	0.22	19
β-HCH	3.33	3.37	0.16	20
γ-HCH	3.33	2.99	0.29	99
δ-HCH	3.33	3.14	-	1
Carbaryl	2.97	2.27	0.25	33
Carbofuran	2.55	1.64	0.39	63
Maneb 4)	7.04	-	-	-
Atrazine	1.79	2.20	0.13	228
Mineral oil 5)				
aliphatic >EC5-EC6	-	2.90	-	-
aliphatic >EC6-EC8	-	3.60	-	-
aliphatic >EC8-EC10	-	4.50	-	-
aliphatic >EC10-EC12	-	5.40	-	-
aliphatic >EC12-EC16	-	6.70	-	-
aliphatic >EC16-EC21	-	9.00	-	-
aromatic >EC5-EC7	-	3.00	-	-
aromatic >EC7-EC8	-	3.10	-	-
aromatic >EC8-EC10	-	3.20	-	-
aromatic >EC10-EC12	-	3.40	-	-
aromatic >EC12-EC16	-	3.70	-	-
aromatic >EC16-EC21	-	4.20	-	-
aromatic >EC21-EC35	-	5.10	-	-
Other compounds				
Cyclohexanone	1.44	0.99	0.80-1.18	2
Dimethyl phthalate (DMP) *)	-	2.25	0.31	6
Diethyl phthalate (DEP) *)	-	2.64	0.57	5
Diisobutylphthalate (DIBP) *)	-	4.46	0.55	4
Dibuthyl phthalate (DBP) *)	-	2.98	1.41-4.17	3
Butylbenzylphthalate (BBP)	4.05	3.91	0.51	5
Dihexyl phthalate (DHP) *)	-	4.65	0.17	4
Di(2-ethylhexyl)phthalate (DEHP)	4.73	5.37	0.47	6
Pyridine	0.76	1.93	0.96	4
Tetrahydrofuran	0.78	0.47	-	1
Tetrahydrothiophene	1.66	1.40	-	1

1) The Koc data on the added PAHs represent, with exception of pyrene, (calculated) values from EPIWIN. The value was averaged with a Kow derived Koc according Sabljić (1995).

2) The Koc value is corrected for dissociation and derived for soil pH 6 (see section 3.3.2.).

3) The physicochemical parameters of dioxins (belonging to the second series of compounds) were not evaluated. The data are taken from Van den Berg, 1994. The Koc values of the added planar PCBs are based on Van Wezel et al. (1999).

4) No reliable Koc was found for Maneb.

5) The Koc values for Total Petroleum Hydrocarbons were determined by the TPH working group (Franken, 1999).

6) The standard deviation of the log Kow. Where the number of references is less than four, the minimum and maximum values are given.

*) Added compounds are explained in 3.2.1.

3.3.2. Koc for dissociating compounds

The use of Koc values as derived in section 3.3.1 is not valid for dissociating organic compounds. Dissociating organic compounds exist in both neutral and ionised forms. The relative amounts of the ionised and neutral (fnd: fraction non-dissociated form) form represent a function of pH. Table 3.7 shows that the degree of dissociation is only of importance for some chlorophenols. The current CSOIL model (Van den Berg, 1995) accounts only for the sorption of the neutral form. However, if the amount of ionisation is substantial, ignoring the sorption of the ionised form can lead to an inaccurate estimation of the soil sorption.

Table 3.7: Degree of dissociation at different soil pH

		available neutral form in percentage (fnd)			
compound	**pKa**	**pH 5**	**pH 6**	**pH 7**	**pH 8**
Phenol	10	100%	100%	100%	99%
o-Cresol	10.1	100%	100%	100%	99%
m-Cresol	10.2	100%	100%	100%	99%
p-Cresol	10	100%	100%	100%	99%
Catechol	10.6	100%	100%	100%	100%
Resorcinol	9.68	100%	100%	100%	98%
Hydroquinone	10.6	100%	100%	100%	100%
2-Chlorophenol	8.43	100%	100%	96%	73%
3-Chlorophenol	9.06	100%	100%	99%	92%
4-Chlorophenol	6.23	94%	63%	15%	2%
2,3-Dichlorophenol	7.66	100%	98%	82%	31%
2,4-Dichlorophenol	7.84	100%	99%	87%	41%
2,5-Dichlorophenol	7.54	100%	97%	78%	26%
2,6-Dichlorophenol	6.84	99%	87%	41%	6%
3,4-Dichlorophenol	8.6	100%	100%	98%	80%
3,5-Dichlorophenol	8.17	100%	99%	94%	60%
2,3,4-Trichlorophenol	7.01	99%	91%	51%	9%
2,3,5-Trichlorophenol	6.79	98%	86%	38%	6%
2,3,6-Trichlorophenol	5.95	90%	47%	8%	1%
2,4,5-Trichlorophenol	7.07	99%	92%	54%	11%
2,4,6-Trichlorophenol	6.22	94%	62%	14%	2%
3,4,5-Trichlorophenol	7.46	100%	97%	74%	22%
2,3,4,5-Tetrachlorophenol	6.07	92%	54%	11%	1%
2,3,4,6-Tetrachlorophenol	5.29	66%	16%	2%	0%
2,3,5,6-Tetrachlorophenol	5.21	62%	14%	2%	0%
Pentachlorophenol	4.85	41%	7%	1%	0%

In addressing this problem, the derivation of Koc values for ionising organic compounds is somewhat different from the procedure applied for non-ionising compounds. The selection of Koc values takes place according to the guideline. However, for the derivation of the generic Koc valid for the standard soil, only those values determined at known soil pH may be considered. Lee et al. (1991) describes the prediction of the soil-water partition coefficient for ionising organic compounds. He defines the total sorption coefficient as the sum of the weighted individual sorption coefficients for the ionised and neutral species at a given pH.

$$\mathrm{Koc} = \mathrm{Koc}_{\mathrm{neutral}} * \mathrm{fnd} + \mathrm{Koc}_{\mathrm{ionised}} *(1 - \mathrm{fnd}) \quad (1)$$

where:

Koc:	soil organic carbon / water partition coefficient (dm^3/kg)
$\mathrm{Koc}_{\mathrm{neutral:}}$	partition coefficient for the neutral species (dm^3/kg)
fnd:	fraction of the neutral species present at given pH (-)
$\mathrm{Koc}_{\mathrm{ionised}}$:	partition coefficient for the ionised species (dm^3/kg)

The fraction of the neutral species can be calculated as follows:

$$\mathrm{fnd} = 1 / (1+10^{[\,\mathrm{pH} - \mathrm{pKa}\,]}) \quad (2)$$

where:

pKa: dissociation constant

FThe selected experimental Koc values are in fact the overall Koc as the weighted sum of the Koc for the neutral part and the Koc for the ionised part. Sorption coefficients for both neutral and ionised species are often not reported. The ratio of Koc-ionised to Koc-neutral could be calculated from published data (U.S. EPA, 1996) on the sorption of some chlorophenolic compounds (Table 3.8).

Table 3.8: Koc ratio for ionised and neutral forms

compound	**ratio Koc $_{\mathrm{ionised}}$ to Koc $_{\mathrm{neutral}}$**
2,4,5 –trichlorophenol	0.015
2,4,6 –trichlorophenol	0.1
2,3,4,5 – tetrachlorophenol	0.051
Pentachlorophenol	0.02
Other phenolic compounds	0.015
All chlorophenols	0.02 *(used for generic risk assessment)*

From:

- equations 1 and 2;
- the known ratio of the Koc values for the ionised and neutral species (given that the generic approach of risk assessment as a fixed ratio of 0.02 is used for all chlorophenols) and
- the selected Koc data (measured Koc values at known soil pH).

The overall generic Koc values (valid for standard soil at a given soil pH) are computed as follows:

First, the Koc $_{\mathrm{neutral}}$ and the Koc$_{\mathrm{ionised}}$ are computed from the selected measured Koc (at known soil pH):

$$\mathrm{Koc}_{\mathrm{neutral}} = \mathrm{Koc} / \{\mathrm{fnd} + [0.02 * (1\text{-}\mathrm{fnd})]\}$$
$$\mathrm{Koc}_{\mathrm{ionized}} = 0.02 * \mathrm{Koc}_{\mathrm{neutral}}$$

Second, the overall Koc at a soil pH of 6 (standard soil) is calculated according the relationship in equation (1). This was done for all selected experimental Koc values. Afterwards the geometric mean is considered as the best Koc value for potential risk analysis.

Table 3.7 gives the average of the retrieved pKa data and the calculated neutral fraction for different soil pH, proving that an adjustment of the measured Koc values is appropriate for penta-, tetra- and some trichlorophenols. Due to available Koc data only an adjustment for pentachlorophenol, 2,3,4,6-tetrachlorophenol, 2,4,6-trichlorophenol and 2,4,5-trichlorophenol could be realised (Table 3.9). For the missing tetra- and trichlorophenols the overall Koc was based on measured data.

Table 3.9: Log Koc for different chlorophenolic forms at soil pH 6

compound	**log Koc neutral**	**log Koc Ionized**	**log Koc overall at pH 5**	**log Koc overall at pH 6**	**log Koc overall at pH 8**
3,4-Dichlorophenol	2.9	1.2	2.90	2.90	2.80
2,4,5-Trichlorophenol	3.4	1.7	3.40	3.37	2.49
2,4,6-Trichlorophenol	3.67	1.97	3.65	3.47	2.23
2,3,4,6-Tetrachlorophenol	3.84	2.15	3.66	3.10	2.19
Pentachlorophenol	4.27	2.57	3.90	3.20	2.59

3.4. Bioconcentration factor metals

The BCF is defined as the ratio of the metal concentration in the edible part of the plant and the total metal concentration in the soil. Versluijs et al. derived relationhips of BCF to soil type and soil concentrations. The derivation of the bioconcentration factors is reported in detail by Versluijs et al. (in prep.).

The authors describe metal accumulation with a (*Freundlich type*) linearised model:

$$\log [C\text{-plant}] = \text{constant} + b*\log(Q) + c*pH + d*\log (\%OC) + e*\log (\%clay)$$

where:

C-plant:	metal concentration in the edible part of the plant in mg/kg dry matter
Q:	total metal concentration in the soil in mg/kg dry matter
pH:	$-{}^{10}\log [H^+]$
% clay:	clay content of the soil
% OC:	organic carbon content of the soil
b,c,d,e:	coefficients

For each metal and crop available the coefficients a, b, c, d, e were derived with linear regression. A generic BCF suitable for potential risk assessment was computed with the derived models. The generic BCF is a consumption-weighted average, based on the average consumption pattern in the Netherlands (Dooren-Flipsen et al., 1996). A generic BCF can be calculated for a given soil, e.g. the *CSOIL standard soil* at a certain total metal soil content, e.g. at the Intervention Value level.

Table 3.10 outlines the Bockting and Van den Berg approach compared with the proposed model (Versluijs et al., in prep). It gives a general sketch of the underlying assumptions, practicability and estimated uncertainty. Bockting and Van den Berg (1992) based BCF values on field data, laboratory experiments and estimations. Versluijs et al. (in prep.) extended the data set and restricted it exclusively to field data and to the consumed parts of the crops. The use of field data implies more variability in metal soil content, soil type and pollution sources but is more realistic. An improvement is the derivation of the soil type and metal content depending on the BCF for metals. As a result site-specific risk assessment is made feasible.

The data on metal accumulation for individual crops are summarised in Appendix 4, Tables 1 and 2. For potential risks, the assessment is geared to an average human with an average consumption pattern. BCF is consequently calculated as a weighted average of the amounts consumed in the Netherlands (see section 4.4.4.2). The BCF values are valid for standard soil and metal content around the Intervention Value. Appendix 4-Table 1 overviews the ranges and averages of the BCF values. This appendix does not distinguish the total metal concentrations in the soil and the soil types. Table 2 of Appendix 4 gives the parameter values for the derived crop-specific plant-soil models as a function of soil metal concentration and soil type.

Table 3.10: Fundamental comparison of approaches used, practicability and underlying assumptions

Approach	**Bockting and Van den Berg (1992)**	**Versluijs et al. (2000)**
general character	average or median BCF based on field data	plant-soil accumulation relation obtained by linear modelling of field data
total soil-metal content dependent	no	yes
soil type-dependent	no	yes, pH, clay and organic matter
Consumption pattern considered	no, only the consumption of potatoes is separately considered	yes, based on the average consumption pattern. Calculation for deviant patterns possible (within limits)
UNDERLYING DATA		
data sets	one data set completed with estimations and data from pot experiments	field data from different sources
Field data	dominant	exclusive
Home-grown vegetables	dominant	exclusive
Data from consumable parts	if available	exclusive
VALIDITY/ USE		
potential risk assessment	yes	yes
metal content range	probably around Target Value level	metal-content dependent. Range is determined
site-specific risk 1)	no	yes, within certain ranges for pH, clay and organic matter
actual risk 2)	no	limited
UNCERTAINTIES		
Determined BCF –ranges	**Global and based on estimation and expert judgement** min – average – max (estimation 3))	**Partly analyzed by Monte Carlo simulation** 5 – 50 - 95 percentile (dataset)
As	0.001 – 0.03 – 0.1	0.0014 - 0.025 - 0.15
Ba	0.02 – 0.05 – 0.08	Not determined
Cd	0.01 – 0.7 – 10	0.09 - 0.55 - 4.6
Cr	0.001 – 0.02 – 1	Not determined
Co	0.01 – 0.03 – 0.05	Not determined
Cu	0.01 – 0.1 – 10	0.09 - 0.29 - 0.80
Hg	0.001 – 0.03 – 0.02	0.02- -0.33 - 3
Pb	0.0001 – 0.03 – 0.5	0.002 - 0.015 - 0.083
Mo	0.01 – 0.3 – 1	Not determined
Ni	0.01 – 0.1 – 2	0.010 - 0.025 - 0.15
Zn	0.01 – 0.4 – 10	0.07 - 0.30 - 1.3

1) Site-specific risk: soil-type dependent risk (pH, %clay and %OC)

2) Actual risk: risk assessment for different soil types and deviant receptor characteristics (e.g. crop-specific approach)

3) The reported minimum and maximum values are from Bockting and Van den Berg (1992). Considering the data used, the given minimum and maximum values are concluded to show a limited image of the uncertainties.

The correlation coefficients of the derived soil-plant relationships (see Table 2, Appendix 4) are generally low. This is due to the fact that a number of effects are not included in the applied model. Season, root depth, chemical form of the metals, contaminant matrix, amounts of iron and aluminium in the soil, variety of crop and probably also variations in chemical analysis also influence the results. By agreement, these effects are not taken into account. Given this restriction and aiming for an ideal generic approach, the data set should mirror the average situation for parameters not included in the Freundlich model. Also in this ideal case many values will not be on the regression line; this line is only valid for an average situation and the correlation coefficient is not necessarily close to unity. The collection of more data (while conserving the average situation) does not necessarily lower the regression coefficient.

In the present situation, where data is lacking, the data set used cannot be expected to mirror an ideal average of all contamination situations. The regression line is also dependent on the distribution of effects not included in the Freundlich model. A high correlation coefficient (approach 1) may even be caused by data from a too limited number of contamination situations and may indicate an adverse situation. This effect makes it difficult to evaluate the predicting value of the collected data. It is recommended to collect more data to be able to describe the average situation. It could be advantageous to differentiate between contamination situations.

The predicting values of the soil-plant relationships are evaluated with an F-test (one-sided 5% exceeding probability). If the relationship for a particular crop fails in the test, the geometric mean of the BCF is used. If the predicting value of the relationship is acceptable, it is used to calculate the BCF value for the standard soil with a total soil concentration near the Intervention Value.
An associated problem is that the data sets cover only a restricted range of soil types and concentrations. Extrapolation outside the ranges of the field data sets used were found to possibly lead to unpredictable and unreliable results. Table 3.11 overviews the application range of the relationships for a metal in terms of the 5- and 95-percentiles of the relevant parameters.

Table 3.11: Application range of the derived metal accumulation models for generic risk assessment

	Q (mg/kg dm) (Q5 - Q95)	**pH**	**OC% [1)]**	**clay %**
As	1.4 - 24	5.1 - 7.5	0.8 - 3.7	2 – 45
Cd	0.12 - 3.2	5.4 - 7.5	0.9 - 13	3 – 33
Cu	21 - 45	5.2 - 8.4	1.6 - 3.5	12 – 16
Hg	0.01 - 0.2	5.1 - 7.5	0.8 - 3.7	2 – 45
Ni	19 - 44	6.8	2.9 - 3.7	12 – 16
Pb	10 - 359	5.0 - 7.5	0.9 - 13	1.7 – 33
Zn	57 - 748	5.2 - 8.4	0.5 - 2.9	6 – 16

1) OC: organic carbon (= 0.58 * % organic matter)

As a result, the following approach is proposed for determining BCF values for potential risk assessment:

- No extrapolation outside the ranges of the underlying field data sets. Only interpolations within the given ranges (Table 3.11).
- Outside the ranges indicated, the BCF values are fixed at the limit values (conservative estimation).

Table 3.12 gives an overview of the consumption average BCF values determined for potential risk assessment. The E column shows the revised BCF values for CSOIL standard soil and column F the revised BCF values for the alternative standard soil (see section 4.2). Columns A - D illustrate intermediate steps of the calculation. Column A contains consumption averages of the geometric means mentioned in Table 1, Appendix 4. Columns B and C are calculated with the model results of Table 2, Appendix 4 using the limiting conditions and consumption weight averaging for different metal soil content levels. The columns D, E and F are calculated using the limiting conditions, consumption weight averaging and the choice of geometric mean or model for a crop. It should be noted that for the new standard soil, the organic carbon and clay values are more in the experimental range than for the current standard soil. Column G is added to compare the current results with the results of Bockting and Van den Berg. The values in column G are calculated using consumption averaging as in Bockting and Van den Berg (1992).

For barium, chromium and cobalt the encountered field data on metal accumulation was limited and data on soil type and soil contamination level was often not given or incomplete. Consequently, it was impossible to derive the soil-plant relationships for these metals. Therefore the given BCF values for these metals are based on geometric mean of available BCF. No new suitable data was found for molybdenum. Details on metal accumulation for barium, chromium, cobalt and molybdenum are given in Appendix 5 of this report and by Versluijs et al. (in prep.).

Table 3.12: Derived BCF values for the generic risk assessment. The columns D, E and F are calculated using the limiting conditions, consumption weight averaging and the choice of geometric mean or model for a crop discussed.

	A	B	C	***D***	***E***	***F***	G
	Geometric mean only	Model only at Q50 and median soil type	Model only at IW/Q95 and median soil type	***Calculated for Q50 and median soil type***	***Calculated for IW/Q95 and current standard-soil***	***Calculated for IW/Q95 and new standard-soil***	Values from Bockting and Van den Berg
As	0.009	0.011	0.003	***0.006***	***0.009***	***0.009***	0.021
Ba	0.017						0.043
Cd	0.51	0.41	0.11	***0.48***	***0.31***	***0.35***	0.37
Cr	0.011						0.009
Co	0.58						0.02
Cu	0.32	0.47	0.37	***0.40***	***0.20***	***0.33***	0.10
Hg	0.15	0.17	0.06	***0.15***	***0.15***	***0.15***	0.02
Pb	0.009	0.026	0.013	***0.025***	***0.017***	***0.020***	0.013
Mo	0.13						0.13
Ni	0.025	0.031	0.029	***0.025***	***0.028***	***0.030***	0.082
Zn	0.22	0.21	0.07	***0.21***	***0.18***	***0.18***	0.22

The columns A, B and D are all calculated for the median values of Q, pH, % organic carbon and % clay as determined in the data set [3]. The differences in the calculated values show to which extent the three calculation methods agree. Column C compared with B shows that the effect of the concentration calculated from the model is significant for all metals except Ni. This effect is also seen in columns E and F, but here the correction for the soil type is also included. For Cu the amounts of organic carbon have a significant effect. (Some effects are dampened by the conservative estimation with respect to soil concentration and type levels).

---

[3] The median values of the data set for the soil type parameters differ for each metal. The average over all the metals is pH =7, organic carbon = 2.5%, clay =13%

The values of Bockting and Van den Berg are calculated similarly to values in column A. Differences originate in the selection of crops, inclusion of laboratory experiments and the calculation of the consumption average. Comparing column G with the columns E and F involves the correction for soil concentration and types.

It should be recognised that the values are given for the current Intervention Value and may change if the Intervention Value is changed. The calculation of new Intervention Values should, in principle, be made iterative, or with the help of relationships be included in the dependency of the generic BCF on the soil total concentration. The BCF values are estimated conservatively as constant values above the Q95 of the data set. Since Q95 usually <IV in practice the calculation is often straightforward. The dependency of the BCF on soil concentration can also play an important role in an uncertainty analysis.

3.5. Kp metals for soil

3.5.1. Introduction

The Kp in this section is primarily meant for the derivation of the risk limits for groundwater. As part of this derivation the concentration calculated in the groundwater is calculated that is in equilibrium with a total concentration in soil equal to the Intervention Value for soil (see 2.1.9). According to this standard the Kp should represent the fraction of contaminants in the pore water that is subject to transport, i.e. the total pore water concentration including organic and inorganic metal complexes. Because metal transport takes place in the unsaturated part of the soil before leaching into the groundwater takes place, the partition coefficients should preferentially represent this whole unsaturated soil layer. However, because information on partition in deeper soil layers is lacking, the variation of Kp values with depth is not considered in this study. Because in most cases samples are taken in the upper soil layer, where at least the organic matter content is relatively high (see 4.2), the Kp values which are derived in this study generally overestimate Kp values for the whole unsaturated soil profile. For practical reasons the total soil content is taken as the representative metal content in soil. As a consequence, the relevant Kp for deriving the Intervention Value for groundwater, the Kp-transport, is defined as:

$$\text{Kp-transport} = \text{total soil content} / \text{total pore water concentration}$$

A different pore water concentration (e.g. the readily bioavailable fraction) and hence a different Kp might be used when assessing bioavailability.

The derivation of Kp relationships for metals is affected by a variety of soil characteristics. Frequently mentioned factors are (Koops et al., 1998 and Otte et al. 2000b):

- pH, clay content and organic matter;
- redox potential, iron or aluminium oxide content;
- Cation Exchange Capacity;
- presence of inorganic and organic complexing agents;
- presence of other metal ions;
- soil moisture content;
- presence of the metal in reactive or inert pools (matrix effects).

The relationship between these factors and Kp values is difficult to quantify. The reason for this is the great number of factors involved; some of these factors are mutually dependent and the influence of some factors is not univocal. Besides, it is not feasible to consider all the factors mentioned above because of limitations in the available data sets. For the intended use of Kp values, i.e. the derivation of groundwater quality standards, there are roughly two methods for derivation of Kp values.

1. Kp value based directly on measured data (measured metal content in the soil and the measured metal concentration in the pore water).
2. Kp value based on sorption models, which describe the concentration in the pore water as a function of the soil characteristics and, in some cases, the total metal content in soil.

Both options will be discussed in the next sections.

3.5.2. Kp values based on measured data

Given the purpose of the Kp, preferentially Kp sets based on total metal content and total metal pore water concentration is considered. Furthermore, a choice has to be made on how to convert the measured data to a representative Kp, e.g. selecting the most relevant measured metal content in the soil and the most relevant measured metal concentration in the pore water, or calculating a geometric mean or the median value of (part of) the data set.
In this section four Kp data sets were evaluated:

1. The Van den Berg-Roels set (Van den Berg and Roels, 1991) is based on both measured and calculated Kp values. The calculated Kp values are, for example, estimated from empirical bioconcentration factors (Baes et al., 1984). Koops et al. (1998) gives a detailed survey of this data set. The resulting Kp values are the geometric means of the collected data and have been used for the derivation of the first series of Intervention Values for groundwater (Van den Berg and Roels, 1991).
2. The Bockting set (Bockting et al., 1992) has been used to derive the ecotoxicological Maximum Permissible Concentrations and Negligible Concentrations for metals (Crommentuijn et al., 1997). The set is based on batch experiments from Buchter et al. (1989) and King (1988). For some metals the Kp values were based on Kp values for other metals complemented with additional data. This accounts for barium (assumed similarity with Kp for calcium), cobalt (additional data) and tin (assumed similarity with Kp for lead).
3. The recently published Kp values of Sauvé (2000) are based on an extended literature review on partition coefficients. Over 70 different studies were considered for this study. The Kp values are compiled with a similar purpose, i.e. derivation of Kp values required for risk assessment models as well as the evaluation of the dependency of Kp values on metal content and soil characteristics. The study is based on total soil metal content and total metal pore water concentration of a wide geographical variety of in-situ contaminated soils. The reported Kp values are the medians.
4. The PGBO[4] data set was compiled on the basis of a field-based data set (Otte et al., 2000b). This data set is the combined set of the Van den Hoop data set (Van den Hoop, 1995), the Janssen data set (Janssen et al., 1996 and 1997) and the National Soil Monitoring Network (LMB) data set (Lagas et al., 1996) concerning data on metal sorption and soil characteristics. The given Kp values are the geometric means of the collected data, but only data from soils with a metal content higher than the Target Value were used.

---

[4] PGBO refers to the governmental programme Programme on Integrated Soil Management).

Table 3.13 tabulates the Kp values resulting from the four data sets.

Table 3.13: Kp values (l/kg) computed from four data sets (see text for references)

Metal	Van den Berg-Roels set (currently used)	Bockting set	Sauvé Kp values	PGBO set
As	980	191	1800	-
Ba	60	60	2500	-
Cd	190	200	390	3200
Cr	14400	110	4800	-
Co	120	40	-	-
Cu	540	977	2120	2400
Hg	3300	170	7500	-
Pb	2380	1905	102000	62700
Mo	20	871	40	-
Ni	560	120	2330	-
Zn	250	158	1730	6800

The differences between the four data sets reflect the wide variability of partition coefficients. In general, the Kp values from the Bockting set (except molybdenum) and from the Van den Berg-Roels set (except chromium and molybdenum) are considerably lower than the Kp values calculated from the PGBO set and the Kp values reported by Sauvé et al. (2000). Possible reasons are: (1) only the data of Sauvé and PGBO are exclusively field data on in-situ contaminated soils, (2) the data set of Bockting is derived from batch experiments and (3) the underlying data of Van den Berg-Roels comprise a mixture of experimental and calculated Kp values. Moreover, none of the a fore-mentioned soil characteristics are considered. This defect increases the differences between the four data sets, and a relationship of the computed Kp values (Table 3.13) with the standard soil (see section 4.2) does not exist.

3.5.3. Kp values based on sorption models

As mentioned in the introduction, Kp values are affected by several soil parameters. It is generally recognised that soil pH, clay content and organic matter content have a large effect on metal concentration in the pore water and hence on Kp values. Besides, these parameters are relatively easy to measure. For this reason, sorption models based on one or more of these parameters can be used to predict the metal content in soil and are suitable for application. To improve sorption models, other soil parameters like aluminium or iron oxide content could be added to the model. However, this might hamper practical application in the field. In this study only the models with 'the easy available' characteristics, i.e. soil pH, clay content and organic matter, are considered. As a consequence, the models of Elzinga et al. (1996), for example, are left out of the evaluation of sorption models, although these models (for Cd, Cu and Zn) are based on an enormous number of data and attention has been focused on total pore water concentration.

Two sorption models for calculating Kp values are considered in this section:

- Models which assume a relation between the Kp and soil parameters ('Kp models'):
  $\log Kp = a + b * pH + c \log [\%OM] + d \log [\%L]$
  %OM = percentage of organic matter
  %L = percentage of lutum
  The sorption models considered in this study are the combined Van den Hoop-Janssen models and the Kp models based on the PGBO data set.

- Models that describe the concentration in the pore water as a function of total content in the soil and soil characteristics. In this study Freundlich sorption models are considered (‘Freundlich models’).

Kp Models from Van den Hoop-Janssen

Table 3.14 tabulates the Kp models based on the combined Van den Hoop-Janssen set (Janssen et al., 1996). The Kp model for arsenic is missing, because this model is mainly based on the Fe(hydr)oxide content.

Table 3.14: Kp models based on Van den Hoop-Janssen set, R^2 and number of soils (N)

Metal	**Kp model**	**R^2**	**N**
Cd	Log Kp = -0.43 + 0.48 pH + 0.71 log (%OM)	0.70	31
Cr	log Kp = 2.64 + 0.21pH	0.54	19
Cu	log Kp = 0.38 + 0.36 pH	0.49	33
Ni	log Kp = 1.00 + 0.25 pH + 0.57 log (%L)	0.74	32
Pb	log Kp = 2.05 + 0.35 pH	0.60	32
Zn	Log Kp = -0.26 + 0.45 pH + 0.60 log (%L)	0.85	33

details of the used data set

pH:	pH after 0.01 M $CaCl_2$	(average = 5.35)
%L:	clay content (%)	(average = 16.1)
%OM:	organic matter content (%)	(average = 9.06)

Kp models based on the PGBO data set

A similar Kp model was fitted using the PGBO data set (Otte et al., 2000b), starting with elimination of the Kp data on total metal content below Target Value. The resulting Kp models are listed in Table 3.15.

Table 3.15: Kp models based on PGBO set, R^2 and number of soils (N)

	median concentration mg/kg	**Kp model**	**R^2**	**N**
Cd	6.8	log Kp = 0.30 + 0.36 pH + 0.41 log (%L) + 0.52 log %OC	0.60	41
Cu	104	log Kp = 0.62 + 0.31 pH + 0.73 log %OC	0.39	34
Pb	320	log Kp = 0.83 + 0.46 pH + 0.71 log (%L)	0.66	37
Zn	750	log Kp = -2.05 + 0.62 pH + 1.34 log (%L) – 0.18 log %OC	0.82	44

%OC: organic carbon (= 0.58 * % organic matter)

Freundlich sorption model

The Freundlich sorption model predicts the total concentration in the pore water as a function of pH, organic matter, clay and total metal content. As a consequence, Kp values can be derived for the optimal metal soil content and most relevant soil characteristics. Total pore water concentration has been derived with a model in the following form:

$$\log [C\text{-}pw] = a + b*\log(Q) + c*pH + d*\log (\%clay) + e*\log (\%OM)$$

log[C-pw]: metal concentration in pore water (mg/l)
log (Q): total metal content soil (mg/kg d.m.)

Models were derived for seven metals within the subproject ‘Metal accumulation in plants’ (Versluijs et al., in prep.). These are based on the Van den Hoop-Janssen data set. The relation with the total metal content facilitates the derivation of Kp values at the optimal contamination levels. The resulting models (‘Freundlich sorption models’) are given in Table 3.16. The use of such models is still under investigation.

Table 3.16: Freundlich sorption models and R^2

Metal	Derived model for the estimation of log (C-pore water)	R^2	N
As	= -2.29 + 0.16 log(Q) + 0.02 pH – 0.53 log (%clay) + 0.16 log (%OM)	0.22	20
Cd	= -1.18 + 0.61 log(Q) – 0.26 pH – 0.6 log (%clay) + 0.33 log (%OM)	0.79	31
Cr	= -2.4 + 0.14 log(Q) – 0.03 pH + 0.14 log (%clay) – 0.11 log (%OM)	0.30	19
Cu	= -1.53 + 0.12 log(Q) – 0.07 pH – 0.2 log (%clay) + 0.87 log (%OM)	0.57	33
Ni	= -1.59 + 0.71 log(Q) – 0.13 pH – 0.33 log (%clay) – 0.08 log (%OM)	0.45	32
Pb	= -2.9 + 1.26 log(Q) – 0.32 pH – 0.47 log (%clay) + 0.45 log (%OM)	0.66	32
Zn	= 0.372 + 82 log(Q) – 0.4 pH – 0.5 log (%clay) – 0.27 log (%OM)	0.72	33

Kp values computed from Kp models and sorption models

The Kp values were computed from the models for the current and proposed standard soil and have been calculated at Target Value level and Intervention Value level. Only the models with a R^2 higher than 0.6 were considered. Table 3.17 and Table 3.18 tabulate the Kp values for the different metals for the current and alternative standard soils (see section 4.2).

Table 3.17: Kp values (l/kg) for the current standard soil (pH=6, %OM=10, %L=25)

Metal	**Van den Hoop-Janssen Kp model**	**Kp model based on PGBO data**	**Freundlich sorption model**	
			Target Value	Intervention Value
As			*	*
Cd	1450	2560	1600	4700
Cr	*		*	*
Cu	*	*	*	*
Pb	14000	36000	34000	20800
Ni	2000		*	*
Zn	1900	2600	2400	3200

*: the model is rejected, because $R^2 < 0.6$

Table 3.18: Kp values (l/kg) for the alternative standard soil (pH=5, %OM=5, %L=15)

Metal	**Van den Hoop-Janssen Kp model**	**Kp model based on PGBO data**	**Freundlich sorption model**	
			Target Value	Intervention Value
As			*	*
Cd	300	720	980	2800
Cr	*		*	*
Cu	*	*	*	*
Pb	6300	11000	20000	12000
Ni	1000		*	*
Zn	590	520	710	960

*: the model is rejected, because $R^2 < 0.6$

3.5.4. Selection of Kp values

Koops et al. (1998) already evaluated the sets of Bockting and Van den Berg-Roels. Koops concluded that the Van den Berg-Roels Kp set demonstrated a high level of consistency with other Kp sets and was widely accepted. A demerit of the set is its vague fundament and the lack of relevancy for Dutch soils. The Kp set from Bockting et al. (1992) was not recommended because of the vague fundament, weak consistency with other sets and lack of relevancy for Dutch soils. The Van den Hoop-Janssen Kp sorption models are recommended by Koops et al. (1998) as an alternative for the present Kp values. The authors concluded the resulting Kp values to be thoroughly founded and consistent with other Kp values. The Kp set does not account for the degree of contamination. However, no strong variation of the Kp value with total metal content was registered.

The resulting Kp values are judged on the basis of the following criteria (in decreasing order of importance):

- Quality of the data set or sorption models, based on:
  i) the number of underlying data,
  ii) R^2 and
  iii) the type of data:
  Preferentially, the total metal content and total pore water concentration are taken into account (criteria *'type of data'*) and in the case of the R^2 of the sorption models being inferior to 0.6, the model is rejected.
- Metal content: the ideal data set would have been compiled with the metal content at a level at which application of Intervention Values takes place, i.e. around and above the Intervention Value.
- Compatibility with Dutch soils: preferentially, experiments on Dutch soils are taken into consideration. It is also advantageous if the partition coefficients are appropriate for the average soil characteristics (standard soil), which could be achieved if organic matter content, clay content, pH, etc. are variables as in the case of the Kp and sorption models.
- Experimental set-up: although under discussion, field data are preferred over laboratory experiments.
- Status: Kp values in use are preferred to alternative Kp values

Table 3.19 tabulates the scoring on the above-mentioned criteria. The resulting ranking (from best to worst options) is given in the outermost left column of the table. The scores (- = poor, 0 = average, + = good, ++ = very good) are based on the following analysis:

- Quality of the data set. The Sauvé set contrasts with the other options for the large number of soils and data that have been incorporated (++). The Van den Berg and Bockting set contrasts with the other sets because of the arbitrary selection of data (-).
- Metal content. Most options are based on metal content between Target and Intervention Values (+). The Bockting set is based on metal content that is substantially above, up to several orders of magnitudes, than the Intervention Value (-). No information is found on the metal content of the Van den Berg and Roels and the Sauvé sets.
- Compatibility with Dutch soils. Most options are based on samples taken from Dutch soils (+). Besides, for all Kp and sorption models the Kp can be made compatible with average Dutch soil characteristics (++). The Van den Berg-Roels, Bockting and Sauvé sets are based mainly on foreign soil types, but not on exotic soil types (0).
- Experimental set-up. Apart from the Van den Berg and Bockting set (-) the options are based on field experiments (+).

- Status. The Van den Berg and Roels data Kp values and the Bockting Kp values are used for the derivation of the Intervention Values for groundwater of the first series and for the derivation of the ecotoxicological Maximum Permissible Concentrations and Negligible Concentrations, respectively (+). The Freundlich sorption model has not yet been published (-).

Table 3.19: Criteria for judgement of Kp values (- = poor, 0 = average, + = good, ++ = very good) and ranking (1 = best option; 7 = worst option)

	Quality	**Metal content**	**Compatibility with Dutch soils**	**Experimental set-up**	**Status**	**Ranking**
Van den Berg-Roels set	-	?	0	-	+	6
Bockting set	-	-	0	-	+	7
Sauvé set	++	?	0	+	0	4
PGBO set	+	+	+	+	0	5
Van den Hoop-Janssen Kp	+	+	++	+	0	2
Kp model based on PGBO data	+	+	++	+	0	1
Van den Hoop-Janssen Freundlich model	+	+	++	+	-	3

Table 3.20 tabulates the revised Kp values for current standard soil (pH 6, OM 10% and clay 25%), the alternative standard soil (pH 5, OM 5% and clay 15%). Besides, the current Kp values are incorporated in the table. Although the scores of the PGBO and Van den Hoop-Janssen Kp models are equal, first priority is given to the Kp values based on the PGBO Kp model, because this model is of more recent date and more data have been taken into consideration. However, reliable models are only found for cadmium, lead en zinc. The Kp value for nickel is taken from the second option, i.e. Van den Hoop-Janssen Kp model. The remaining Kp values are taken from the fourth option (the third option, i.e. the Van den Hoop-Janssen Freundlich model, does not give reliable relations for the remaining metals), i.e. the Sauvé data set.

Table 3.20: Kp values (l/kg) and references

Metal	**Reference**	**revised Kp** (pH 6, OM 10%, clay 25%)	**revised Kp** (pH 5, OM 5%, clay 15%)	**current CSOIL Kp**
As	Sauvé et al., 2000	1800	1800	*980*
Ba	Sauvé et al., 2000	2500	2500	*60*
Cd	PGBO Kp model, this report	2560	720	*190*
Cr	Sauvé et al., 2000	4800	4800	*14400*
Co	Van den Berg and Roels, 1991	120	120	*120*
Cu	Sauvé et al., 2000	2120	2120	*540*
Hg	Sauvé et al., 2000	7500	7500	*3300*
Pb	PGBO Kp model, this report	36000	11000	*2380*
Mo	Sauvé et al., 2000	40	40	*20*
Ni	Van den Hoop-Janssen, 1996	2000	1000	*560*
Zn	PGBO Kp model, this report	2600	520	*250*

From Table 3.20 it can be concluded that, with the exception of the Kp values for chromium and cobalt, revised Kp values are generally higher than the current Kp values. This varies for the alternative standard soil from a factor of 2 for molybdenum up to a factor of 40 for barium. The Kp values for cadmium, lead, nickel and zinc are influenced by the choice of the standard soil.

3.6. Permeation coefficient (Pe)

Van den Berg (1997) gave a justification of the derived permeation coefficients based on reports of Vonk (1985) and van der Heijden and Hofman (1987), together with a detailed description of the interpretation of data. An additional evaluation of the permeation coefficient was not considered necessary (see 2.1.10) The selected values were accordingly reported by Van den Berg (1997). Based on this report, the permeation coefficients of phenol, tetrachloroethene, monochlorophenols, trichlorophenols and PCBs were adjusted. The Pe for aliphatic TPH fractions were estimated from the Pe values of hexane, heptane, octane and nonane while the Pe for aromatic TPH fractions were considered comparable with the Pe of benzene. The Pe values of dioxins were taken from Van den Berg, 1994. For chlorodibenzofurans, the Pe values of dioxins were selected.

4 The evaluation and revision of soil, site and exposure parameters

4.1 Current CSOIL data.

In Table 4.1 the selected parameters for evaluation (see section 2.2.3), mentioned together with the current values used in the CSOIL-model (Van den Berg, 1995) and the 50 percentile of the values used in the uncertainty analysis (Vissenberg and Swartjes, 1996) are given. Appendix 1 gives an overview of *all* the soil, site and exposure parameters used for the calculation of human exposure.

Table 4.1: Values of relevant parameters of the selected exposure routes in CSOIL and in the uncertainty analysis 1996

parameter	**code**	**kind of parameter**	**unit**	**current CSOIL (1995)**	**50-perc**
Inhalation of inside air					
volume fraction air	Va	soil	$m^3.m^{-3}$	0.2	0.14
volume fraction water	Vw	soil	$m^3.m^{-3}$	0.2	0.35
fraction organic carbon	foc	soil	$kg.kg^{-1}$	0.058	0.031
flux of evaporating water	Ev	site	$dm^3.m^{-2}.d^{-1}$	0.1	0.105
mean depth of the contamination	dp	site	m	1.25	1.5
air-exchange rate	Vv	site	h^{-1}	1.25	0.6
height of the crawl space	Bh	site	m	0.5	0.5
contribution of the crawl space air to indoor air (fraction)	fbi		-	0.1	0.15
Crop consumption					
fraction organic carbon	foc	soil	$kg.kg^{-1}$	0.058	0.031
fraction dry weight root crops	fdwr	site	-	0.202	n.a.
fraction dry weight leafy crops	fdws	site	-	0.117	n.a.
fraction contaminated root crops	Fvk	exposure	$kg.kg^{-1}$	0.1	0.022
fraction contaminated leafy crops	Fvb	exposure	$kg.kg^{-1}$	0.1	0.061
Soil ingestion					
daily intake of soil by child	AIDc	exposure	$mg.d^{-1}$	150	153
daily intake of soil by adult	AIDa	exposure	$mg.d^{-1}$	50	50
Dermal uptake by soil contact					
fraction soil in dust inside/	frsi	site	-	0.8	0.8
outside	frso	site	-	0.5	0.5
matrix factor	fm	exposure	-	0.15	0.3
exposed surface area adult indoor/	Aexpai,	exposure	m^2	0.09	0.22
outdoor	Aexpao,	exposure	m^2	0.17	0.54
exposed surface area child indoor	Aexpci,	exposure	m^2	0.05	0.08
degree of coverage indoor/	DAEai,	exposure	$g.m^{-2}$	0.56	n.a.
outdoor	DAEao,	exposure	$g.m^{-2}$	37.5	n.a.
time fraction exposure adult inside/	Tbai	exposure	h	14.86	12.3
outside	Tbao	exposure	h	1.14	1.7
absorption velocity adult	DARa	exposure	h^{-1}	0.005	0.007
Uptake by polluted drinking water					
fraction organic carbon	foc	soil	kg/kg	0.058	0.031
mass volume of dry soil	SD	soil	$kg.dm^{-3}$	1.5	1.27

n.a.: not analysed

Table 4.1 and Appendix 1: Current CSOIL-1995 input parameter set tabulates the values used for the standard scenario *residential garden*. The values of most of the parameters are supported by literature data. These data, together with new data, will be described in the next sections. The parameters are subdivided into soil parameters (section 4.2), site parameters (section 4.3), parameters describing the crop consumption (section 4.4), parameters describing soil ingestion (section 4.5) and parameters on the dermal exposure to soil route (section 4.6).

4.2 Soil parameters

4.2.1 Soil characteristics within the CSOIL model

Some soil characteristics have a direct effect on the Intervention Value for soil, because they are used in the calculation of human exposure using the CSOIL model and/or for the normalisation of ecotoxicological effect data. Besides, soil characteristics are used for correction of the Intervention Values for a standard soil for bioavailability when used in the practice of soil and groundwater quality assessment. At the moment this correction is performed on the basis of 'easy available' soil characteristics, i.e. organic matter content and clay.

To identify the soil characteristics two different approaches could be followed. In the first approach an average value for Dutch soils could be derived for each soil characteristic. As a result the combination of soil characteristics might represent a hypothetical, i.e. non-existent soil type. In the second approach the soil characteristics are extracted from a representative soil type in the Netherlands. This implies that in the first approach the soil characteristics are representative, and in the second approach the soil type is representative.

According to the second approach, two major soil types are found in the Netherlands, i.e. sandy soils (45%) and clay soils (42%)(see Table 4.1). Because it does not seem valid to ignore one of these major soil types, a combination of soil characteristics of sandy and clay soils could be arranged, as an alternative 'representative soil type', resulting in a hypothetical soil type. If this alternative version of the second approach is followed, the difference between the two approaches diminishes: in the first approach soil characteristics of all Dutch soil types are incorporated and in the second approach the contribution of peat soils (11%) and the loess soils (2%) is ignored. In this study the first approach is worked out, in which a surface-area weighted-average value for each soil characteristic is derived. The reason is that information on the whole area of application of Intervention Values (i.e. the Netherlands) is used and that there are no strong arguments against application of a hypothetical soil type. Besides, the result would be similar if the second approach was followed (a combination of sandy and clay soils), because the surface-area contribution of peat and loess soils is limited.

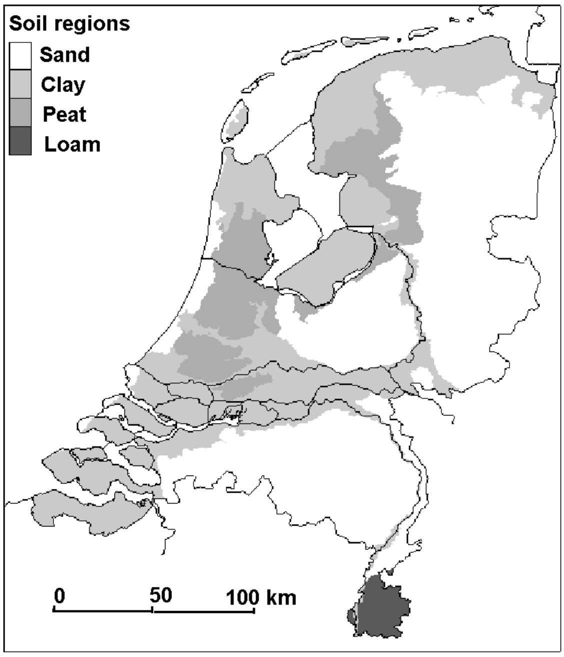


Figure 4.1 Soil types in the Netherlands.

4.2.2 Pore, pore water, and pore air fraction.

The pore water fraction and the pore air fraction are complementary and combined equally with the pore fraction. Is has been assumed that accumulation of compounds by crops and adverse effects on ecosystems are related to the concentration in the pore water rather than to the total content in soil. However, in the procedure used to derive the Intervention Value the distribution of compounds over the solid and the liquid phases is calculated on the basis of equilibrium, independent of the pore-water fraction. This implies that the pore-water fraction does not affect the concentration in the pore water and, as a consequence, does not affect exposure or acceptable ecotoxicological risk limits. For the same reason, the concentration in pore air is independent of the pore-air fraction. However, human exposure increases with a higher pore-air fraction because diffusion takes place over a larger surface area, and so is only relevant for volatile organic compounds.

Identification of a representative value for the different fractions is hampered by spatial variability due to climatic dynamics. The situation at pF = 3 is proposed as a representative state for soil moisture. Based on pore water fractions at pF = 3 of 0.05 for sand, 0.50 for clay and 0.40 for peat (Koorevaar et al., 1983) a surface- area-weighted average value of 0.29 can be calculated for the pore water fraction. Ranges for pore fractions for different soil types are also given in Koorevaar et al. (1983): 0.35-0.60 for sand, 0.30-0.70 for clay and 0.80-0.85 for peat soils. A surface-area-weighted average value of the pore fraction of 0.51 can be calculated on the basis of average values for the pore fractions for each soil type. A value of 0.22, resulting as the difference between representative pore fraction and pore-water fraction, can be assumed as the representative, i.e. surface-area-weighted average value of the pore-air fraction.

- *The representative surface-area-weighted average pore water fraction is determined at 0.3 and the corresponding pore air fraction at 0.2.*

4.2.3 Dry bulk density of the standard soil

On the basis of the fugacity theory (Mackay and Paterson, 1981), the mass fractions of the three soil phases are calculated using the density of the solid phase as one of the parameters. A higher density results in higher human exposure to organic compounds. However, the calculation of human exposure is not very sensitive to the density of the solid phase. Koorevaar et al., 1983 give the following dry bulk densities of the solid phase: for sand 1600 kg/m^3, for clay 1100 kg/m^3 and for peat 250 kg/m^3. A surface- area-weighted average representative dry bulk density of the solid phase of 1210 kg/m^3 can be calculated.

- *The representative value for dry bulk density is determined at 1210 kg/m^3 .*

4.2.4 Organic matter content

Organic matter is a well-known sorbing agent in soils for metals as well as for organic compounds. As a consequence, the available contaminant fraction in the pore water decreases with higher organic matter. And reduction of the available fraction implies reduced contaminant accumulation by crops (which means lesser exposure) and, in general, a decrease in adverse ecological effects. It should be noted that some organisms are (also) exposed through consumption of contaminated particles in soils, in which case adverse effects are independent of the available fraction. Because contaminant concentration in pore air is correlated to contaminant concentration in pore water, indoor air concentration (and exposure due to inhalation of contaminated air) also decreases with increasing organic matter content. Calculation of human exposure and determination of adverse ecological risk limits have proven to be very sensitive to the organic matter content.

A practical problem is that the influence of organic matter on the available metal fraction is dependent on the type of organic matter and other soil characteristics. Herms and Bruemmer (1980, 1984), for instance, observe an increase of the available fraction of copper and lead in the pore water with increasing organic matter content, particularly with high pH and under reduced redox conditions. In this case the organic matter is available as Dissolved Organic Carbon (DOC), which tends to form soluble metal-organic ligands. This mobilising influence of organic matter is difficult to quantify and can at best be assessed in the stage when the actual i.e. site-specific risks, are determined.

In CSOIL, the organic matter content is used to determine the partition coefficient for organic compounds (=Koc * fraction organic matter, see section 2.1.6.), which controls the distribution of these organic compounds over the solid and the pore water phases. Besides, ecotoxicological effect data for organic compounds are normalised on the basis of the organic matter content.

The organic matter content varies from almost 0 for some sandy soils up to 90% for peat soils. A value of 4.5 % is proposed as being representative for the organic matter content. This is the average value for 39 soil samples from five different soil types in the Netherlands, taken in a depth range of 0-15 cm under arable land, grassland and forest (De Vries, 1994). Figure 4.2 (page 62) gives the cumulative frequency distribution of the organic matter content. Note that the organic matter content generally greatly decreases with depth, which means that these values overestimate the organic matter content for deeper soil layers.

- *An organic matter content of 4.5 % (organic carbon 2.61 %) is determined as being a representative value for Dutch soil.*

4.2.5 Clay content

Clay particles also act as strong sorbing agents in soil for metals. Sorption of organic compounds, however, is hardly influenced by the presence of clay particles. The clay content does not influence calculated exposure, because this parameter is not incorporated in the CSOIL model. However, the clay content is used for normalising ecotoxicological effect data and for the bioavailability correction of the Intervention Value for metals. As a result the Intervention Value of metals is quite sensitive to the clay content.

The clay content shows huge geographical variation and is, of course, strongly dependent on soil type. In the Soil Map of the Netherlands (De Vries, 1994) values of 2% (sandy soil) and 50% (clay soil) are given as the extreme average values for the different soil units. From this soil map the following average clay contents could be derived for the different soil types: 27% for clay soils (150 sea clay soils and 100 river clay soils); 5,4% for sandy soils (175 observations) and 35% for peat soils (58 observations). From these data a surface-area-weighted average representative value for the clay content of 16% is calculated. Figure 4.2 gives the cumulative frequency distribution of the clay content.

- *Clay content of 16% is determined as a surface- area-weighted average representative value for Dutch soil.*

4.2.6 pH (KCl)

Because hydrogen ions act as competitors for the available sorption sites, the metal concentration in the pore water increases with lower pH values. As a consequence, accumulation of metals by crops (and hence: human exposure through crop consumption) and adverse effects on ecosystems due to metal accumulation also increase with lower pH values. The pH is generally recognised as a very influential parameter for availability of metals.

The pH is used in the current CSOIL model, but only for calculating the dissociated fraction. The pore-water concentration of metals is calculated on the basis of a constant, i.e. independent of pH value or partition coefficient. However, the pH could be used for normalising ecotoxicological effect data and for the bioavailability correction of the Intervention Value for metals. In this case the Intervention Value of metals could be very sensitive to the pH. Attention should be paid to the fact that soil pH is currently (see sections 3.4 and 3.5) considered for the derivation of bioconcentration factor for metal accumulation by crops and for the derivation of soil-water partition coefficients for metals.

The pH is determined by the soil material, soil use and anthropogenic activities. The average pH values for the different soil units varies from 3.2 for sandy soils under forest up to 7.4 for clay soil under arable land (De Vries, 1994). Compared with other soil characteristics the pH in the soil is relatively dynamic. As representative value for the pH (KCl) a value of 5.2 is proposed. This is the average value for 39 soil samples from five different soil types in the Netherlands, taken in a depth range of 0-15 cm under arable land, grassland and forest (De Vries, 1994). Figure 4.2 gives the cumulative frequency distribution of the pH (KCl). Note that the majority of the soil types considered concern agricultural soils, which implies that these soils are influenced by agricultural activity (liming). If only undisturbed forest soils had been considered an average pH of 4.0 would result. However, forest soils are not representative for most contaminated sites in the Netherlands.

- *A soil pH of 5.2 is determined as a representative value for Dutch soil.*

4.2.7 Résumé

The soil characteristics that have a direct effect on the Intervention Value for soil are pore, pore-water and pore-air fractions, density of the solid phase and organic matter content. They are used in the calculation of human exposure and/or for the normalisation of ecotoxicological effect data.

The organic matter and clay content are used for the soil-type correction of the Intervention Values (derived for standard soil). At the moment the use of the soil pH for site-specific assessment is under discussion.

In Table 4.2 the representative values of the soil characteristics have been summarised. The current values (Van den Berg, 1995), the ranges of the soil characteristics on the basis of ‘frequently found soils in the Netherlands’ and proposed values are given (in **bold**).

*Table 4.2: Soil characteristics: present values, range on the basis of 'frequently found soils in the Netherlands', representative values and proposed value (**bold**)*

Soil characteristic	Present value	Range	Representative value	**Proposed value**
Pore fraction (-)	0.4	0.35 (sand) - 0.85 (peat)	0.51	**0.5**
Pore-water fraction (-)	0.2	0.05 (sand) - 0.50 (clay)	0.29	**0.3**
Pore-air fraction (-)	0.2	-	0.22	**0.2**
Density soil phase (kg/m^3)	1500	250 (peat) – 1600 (sand)	1210	**1200**
Organic matter content (%)	10	0 (sand/clay) – 90 (peat)	4.5	**5**
Clay content (%)	25	2 (sand) - 50 (clay)	16	**15**
pH (KCl)	6	3.2 (sand/forest)- 7.4 (clay/arable)	5.2	**5**

- *From Table 4.2 it is proposed to revise the CSOIL standard soil by:*
  - *increasing the pore water fraction from 0.2 to 0.3 (and the pore fraction from 0.4 to 0.5);*
  - *decreasing the organic matter content from 10% to 5%;*
  - *decreasing the dry bulk density from 1500 (kg/m^3) to 1200 (kg/m^3);*
  - *decreasing the pH (KCl) from 6 to 5;*
  - *decreasing the clay content from 25 % to 15 %;*

Furthermore, it is proposed to maintain the value of the pore air fraction (0.2).

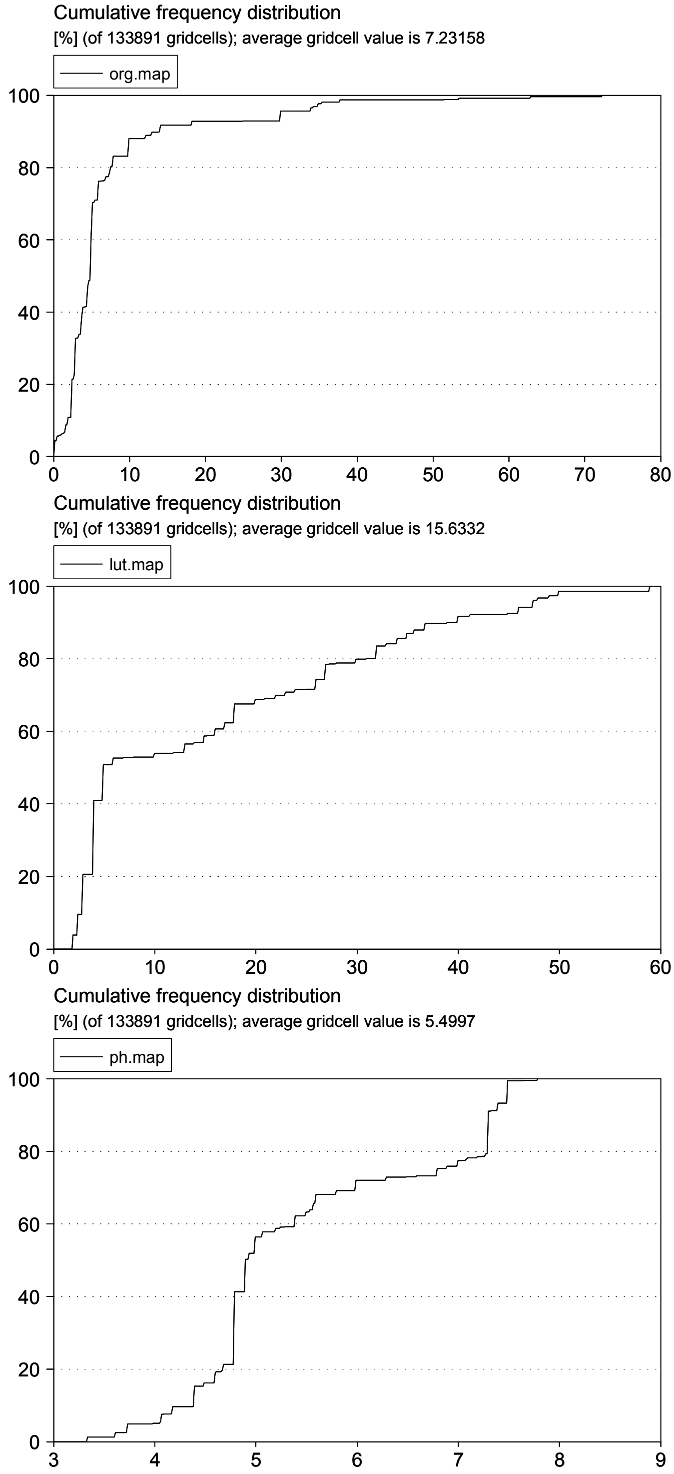


Figure 4.2 Cumulative frequency distribution of the organic matter content (%), clay content (%) and pH (KCl), derived from the 1:50,000 digitised soil map (De Vries, 1994),

4.3 Site parameters

The most important site parameters used for the assessment of human exposure, and selected for evaluation, are given in Table 4.1. For a complete statement refer to Appendix 1. This section describes the evaluation of the most important parameters. Besides, two new parameters are introduced for the estimation of the convective flow, contributing to the concentration of volatile compounds in indoor air: the pressure difference between soil and crawl space (ΔP) and the permeability of the soil (κ). The data and the selection of the value to be used in the calculation are described in Rikken et al. (2001).

4.3.1 The flux of the evaporating water (Ev)

In the evaluation of the model concept it is proposed to exclude the evaporation flux in the calculation of the indoor air concentration (Rikken et al., 2001). Therefore this parameter has not been evaluated. In the uncertainty analysis (Vissenberg and Swartjes, 1996) this parameter has a log- distribution between 0.05 and 0.25 (50-perc. 0.105 dm^3/m^2 per day).

- *It is proposed to remove the evaporation flux from the CSOIL model.*

4.3.2 Mean depth of the contamination (dp)

In the evaluation of the model concepts it is proposed to relate the mean depth of the (volatile) compound to the depth of the groundwater table. The compound may be present in the unsaturated zone of the soil or in the groundwater. For both situations it is proposed to use the depth of the groundwater table (dg) combined with the height of the (almost) saturated zone, the capillary transition boundary (z) to estimate de depth of the compound (dp= dg+z) (Rikken et al., 2001). The current *mean depth of the contamination* in CSOIL is 1.25 m below land surface. A range of 0.5m to 5 m demonstrated a large influence on the calculated exposure (Vissenberg and Swartjes, 1996).

The data from the National Groundwater Monitoring Network (LMG) from 1990 till 1998 were analysed to get an impression of the distribution of the groundwater depth in the Netherlands. The average height of rise for all observations is 2.09 m below land surface (STD=2.15). The 50-, 75-, and 90-percentiles of the observations are 1.60, 1.09 and 0.73 m, respectively, below land surface (see Figure 4.3).
For the risk assessment it is important to know the situation in built-up areas, which comprises 11% of the available observations (n=1418). These data show an average groundwater level of 2.45 below land surface (STD=1.82). The 50-, 75-, and 90-percentiles of the observations are 1.82, 1.32 and 1.0 m, respectively, below land surface (see Figure 4.3). It can be concluded that the groundwater level, in general, in built-up areas is lower than for all locations. Reasons for this difference can be that the ground level is raised, or that the groundwater level was lowered or that construction is taking place on higher ground.

Besides the LMG database there is a database for monitoring the effects of the policy on nutrients. All data originate from agricultural areas, mostly in sandy regions. The average rise at these locations is 1.39 m below land surface (STD=0.59) and 50-, 75-, and 90-percentiles of 1.28, 0.99 and 0.8 m, respectively, below land surface (see Figure 4.3).

A third database is the OLGA database used in the National Groundwater Model (LGM) in which the average height of rise of the groundwater in the upper aquifer is monitored. The average height of rise at these locations is 2.82 m below land surface. The 50-, 75-, and 90-percentiles are 1.52, 1.02 and 0.5 m, respectively, below land surface (see Figure 4.3).

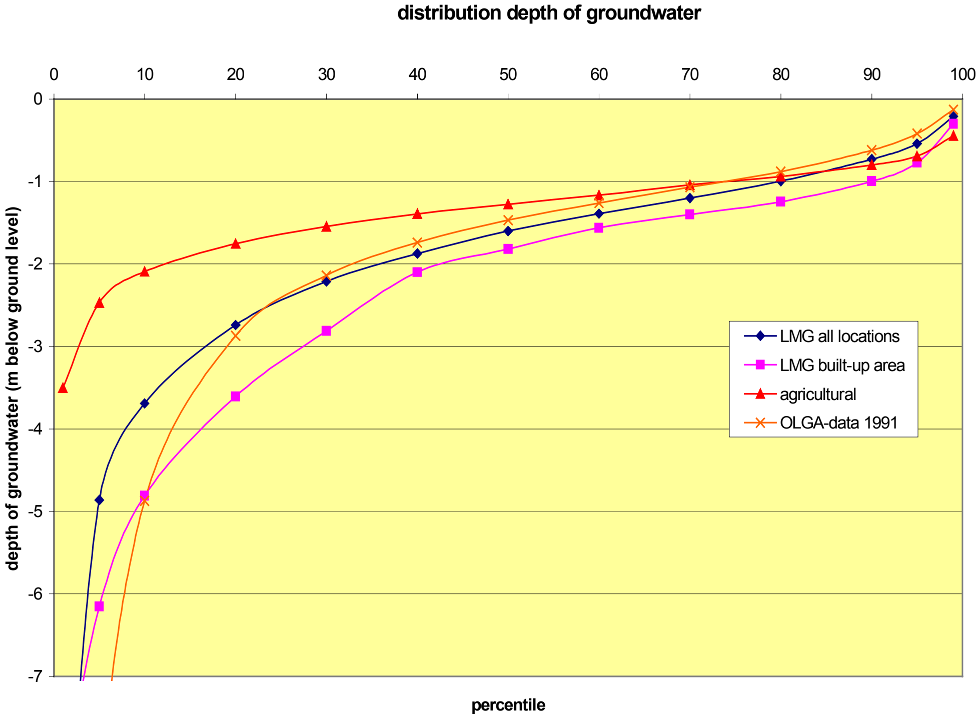


Figure 4.3 Distribution of the depth of the groundwater based on 3 databases.

The height of the capillary transition boundary (CTB) above the groundwater table determines the height above the groundwater table below which the blocking of the water-filled pores becomes relevant for diffusion (and the convective flow). For the 18 soils of the Staring series (Wösten et al., 1994) the height is calculated at between 12 and 84 cm (Waitz et al., 1996). The arithmetic mean of all soils (47 cm) is almost the same as that of sand: 50 cm. It is proposed to use this generic value of 0.5 m.

- *It is proposed to use the median groundwater depth. Based on the LMG database and because mostly built-up areas are referred to here, it is proposed to set the generic depth of the groundwater level (dg) at -1.75 m (below land surface). Combining this value with the height of the capillary transition boundary (z) leads to a proposal for the depth of the contaminant (dp) of -1.25 m. This means there is no need to change the current value.*

4.3.3 Height of the crawl space (Bh)

The *height of the crawl space* in CSOIL is set at 0.5 m. The depth can be very low, but will normally not exceed 1.0 m. Therefore in the uncertainty analysis the range is set at 0.1 m to 0.9 m (Vissenberg en Swartjes, 1996). A lower crawl space will lead to a smaller crawl space volume and to a longer soil column over which transport takes place. The effect of both changes (crawl space volume and soil column) on the SRC$_{human}$ is in opposite directions. The conclusion is that the height of the crawl space is a moderate sensitive parameter for volatile compounds.

- *The current height of the crawl space is a good estimate of the average crawl space height. There is no reason to revise the current value.*

4.3.4 Air exchange rate of the crawl space (Vv)

The current *air exchange rate of the crawl space* in CSOIL is 1.25 h^{-1}, based on Fast et al. (1987). In the uncertainty analysis this parameter has a large range, which is set between 0.03 and 7.4 with a lognormal distribution 50-percentile of 0.6 (Vissenberg en Swartjes, 1996). From the data of Fast et al. (1987) it has become clear that this value will vary with time and location. The ventilation rate depends on weather conditions (e.g. wind, temperature) and properties of the house.

The mean air exchange rate of the crawl space in 77 houses is 1.25 h^{-1}, with a median value of 1.0 h^{-1} (Fast et al., 1987; Kliest et al., 1989). The average ventilation rate of the crawlspace of about 700 houses in a study on radon was 1.1 h^{-1} (STD=1.2), corresponding with 41.5 m^3/h. For the living room a ventilation rate of 0.9 h^{-1} (STD=0.7) was found (Stoop et al., 1998).

- *It is proposed to use an average ventilation rate of 1.1* h^{-1} *in the model as the air exchange rate of the crawlspace (Vv), based on both studies mentioned.*

4.3.5 Contribution of the crawlspace air to indoor air (fbi)

The *contribution of the crawl space air to indoor air* is currently 0.1, based on Fast et al. (1987). In that study the concentration of the crawlspace air to the indoor air in 77 houses was measured with a tracer gas. The average contribution of the crawlspace air to the indoor air was 10.6% with a substantial spread; the median value is 15.3 % and the 95-percentile 39 %. In the houses with a wooden and a concrete ground floor the average contribution was 19.3% and 9.6%, respectively (Fast et al., 1987). In a study on about 700 new built houses with a concrete floor, the contribution of the crawlspace air to the indoor air was measured with tracer gas. The average contribution of the airflow from the crawlspace to the living room to the total airflow in the living room was 7% (6 out of 85 m^3/h)(Stoop et al., 1998).

- *It is proposed to maintain the current value for the contribution of crawlspace air to indoor air (fbi) at 0.10, based on the measured average contribution in above- mentioned references and the fact that the latter reference concerns new houses with ground floors of concrete.*

4.3.6 Parameters for the description of the convective flow

Three new parameters are introduced for the estimation of the convective flow contributing to the concentration of volatile compounds in indoor air. The pressure difference between soil and crawl space (ΔP), the permeability of the soil (κ) and the viscosity of the air parameter were determined. The parameter η is a physical parameter of air, which is 18E-6 N/m^2 s (Pa.s) or 5E-9 Pa.h (Chang, 1981; CRC, 1998). The data and the selection of the values to be used in the calculation are described in Rikken et al. (2001).

- *The air permeability of soil (κ) is set at* 10^{-11} m^2 *.*
- *The pressure difference between soil and crawl space (ΔP) is set at 1 Pa.*
- *Viscosity of air (η or ETA) in Pa.h is set at 5 E-09.*

4.3.7 Parameters for the description of soil resuspension

Soil and dust parts can be deposited on the plant by wind or rain. This process is called soil resuspension or rainsplash. The contribution of soil resuspension to the concentration of soil contaminants in the plant is difficult to estimate and depends on many factors (e.g. the geometry of the plant). Nevertheless, the contribution via this route is considered important in the case of contaminated soils.

For organic compounds and for the aboveground plant parts, it is proposed to add a factor to account for soil particle resuspension. The contribution of this exposure route is provisionally set at 1% dry soil per dry plant (Rikken et al., 2001). For metals the contribution of soil resuspension is considered to be incorporated in the Bioconcentration Factors derived.

- *For organic compounds the contribution of soil resuspension to the aboveground parts of the plant is set at 1 % of the total soil concentration (in dry soil per dry plant).*
- *For metals the contribution of soil resuspension is not considered separately but incorporated in the selected Bioconcentration Factors.*

4.4 Crop consumption

4.4.1 Average consumption pattern

The proposed bioconcentration factors for metals are calculated from plant-soil relations (section 3.4). The model developed accounts for the average consumption pattern of vegetables and potatoes. Frequently consumed vegetables contribute more to the generic (consumption-weighted average) plant-soil metal accumulation relationship than occasionally consumed vegetables. The report of Versluijs and Otte (2000) gives full details about the derivation of the plant-soil metal accumulation relationship. Section 3.4 of this report gives the details on the derivation of the proposed bioconcentration factors.

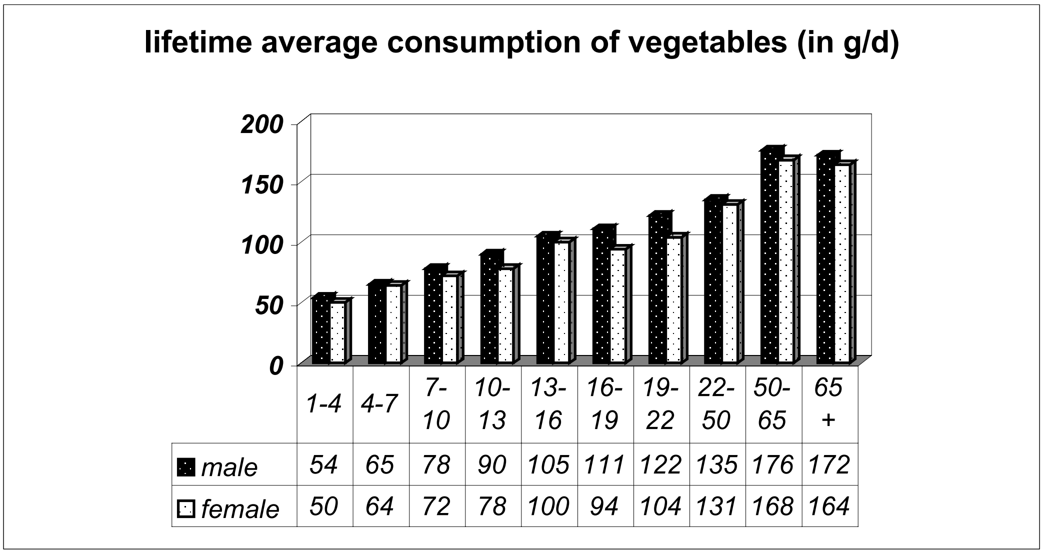
For the derivation of plant-soil accumulation models 31 vegetables and potatoes were considered. Table 4.3 gives the consumption pattern as used for the derivation of the *generic* plant-soil relationship. The crops and their respective consumption amounts are taken from Dooren-Flipsen et al. (1996, Theoretical maximum daily intake of pesticide residues in the Netherlands – A model for risk assessment). The consumption pattern, expressed in gram fresh product per day, is converted to the consumption pattern in gram dry weight per day. The figures expressed on dry weight were used for the derivation of the generic Bioconcentration Factors.

Table 4.3: Average consumption pattern (source: Dooren-Flipsen et al., 1996)

no	group	crop	consumption g fresh per day	water content g/100 g product	average consumption in g dry weight per day
0	potatoes	potatoes	179.7	83.3	30.0
1	other plants	beetroot	5.2	87.3	0.65
		carrots	13.4	87.8	1.64
		celeriac	0.8	88.0	0.09
		turnip	0.8	91.9	0.07
		radish	0.4	94.8	0.02
		winter carrot	0.2	87.8	0.02
2	bulbous plants	onions	17.0	90.8	1.56
		leek	12.9	83.0	2.19
3	fruits	tomatoes	26.1	94.0	1.56
		cucumber	8.0	96.1	0.31
		melon	2.2	89.7	0.23
		maize	1.4	76.0	0.34
4	cabbages	cauliflower	16.0	92.3	1.23
		brussels sprouts	4.7	86.0	0.65
		white cabbage	7.0	95.3	0.33
		red cabbage	5.1	91.6	0.43
		oxheart cabbage	2.0	95.3	0.10
		curly kale	4.9	84.5	0.76
		broccoli	2.0	90.7	0.18
5	leaf vegetables (greens)	lettuce (head)	8.5	95.4	0.39
		endive	7.4	93.8	0.46
		spinach	10.4	91.6	0.88
		chicory	9.2	95.3	0.43
6	legumes (peas and beans)	green bean	11.7	90.3	1.13
		string/bush bean	3.1	90.3	0.30
		broad/horse/fava bean	2.5	88.9	0.28
		garden pea	14.8	88.9	1.64
7	beans	haricot bean	0.9	77.1	0.20
		kidney bean	1.8	77.1	0.40
8	stem and stalk vegetables	rhubarb	0.7	93.6	0.05
		asparagus	1.7	92.3	0.13

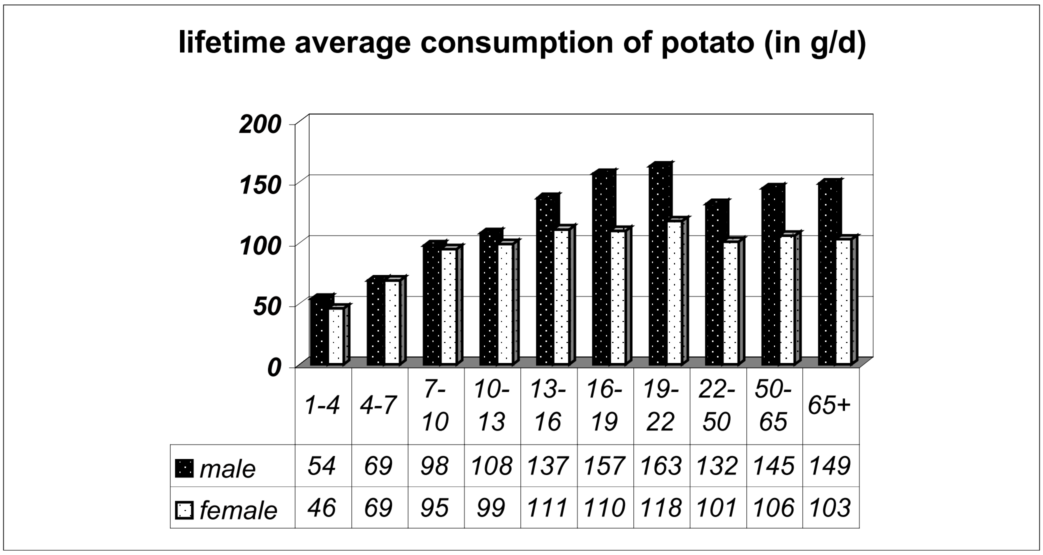
4.4.2 Average consumption (Qfvk, Qfvb)

The average consumption of vegetables and potatoes is based on the most recent Dutch National Food Consumption Survey of 1998 (Voedingscentrum, 1998). This survey shows the average vegetable and potato consumption for each phase of life (Figure 4.4 and Figure 4.5). Based on this survey the (weighted) average lifetime consumption of vegetables was found at 139 g per day fresh vegetables for adults and schoolgoing children (age 7-70) and at 58.3 g per day fresh vegetables for babies and pre-schoolers (age 1-6). For potatoes the average lifetime consumption was found at 122 g per day for adults and schoolgoing children and 59.5 g per day for pre-schoolers (1-6 year) (see Table 4.4).



	1-4	4-7	7-10	10-13	13-16	16-19	19-22	22-50	50-65	65 +
■ male	54	65	78	90	105	111	122	135	176	172
□ female	50	64	72	78	100	94	104	131	168	164

Figure 4.4 Average consumption of vegetables (g wet weight).



	1-4	4-7	7-10	10-13	13-16	16-19	19-22	22-50	50-65	65+
■ male	54	69	98	108	137	157	163	132	145	149
□ female	46	69	95	99	111	110	118	101	106	103

Figure 4.5 Average consumption of potatoes (in g wet weight).

Comparing the surveys (Dooren-Flipsen, 1996, with DNFCS, 1998) we observe differences in the total amounts of consumed potatoes and vegetables. These differences are understandable because the Dutch food consumption survey records in terms of prepared (cooked) actual amounts of foods eaten, with composite products included. The consumption pattern (Table 4.3), being the basis for the generic plant-soil relationships, is based on the fresh product (at harvesting), shrink and waste to be included.

Considering that the point of departure for potential risk assessment is the calculation of the average lifetime exposure, the determination of the consumption for vegetables and potatoes should be according to the Dutch National Food Consumption Survey of 1998 (Voedingscentrum, 1998)

As the modelling of metal content in vegetables and potatoes is based on the fresh product (at harvesting), this should be determined according the food consumption pattern as presented in Table 4.3.

- *Table 4.4 presents the proposed average lifetime consumption for vegetables and potatoes for the CSOIL exposure model.*

Table 4.4: The proposed average lifetime consumption[*)] *for vegetables and potatoes (source: DNFCS 1998, Voedingscentrum, 1998)*

Group	time span	consumption of vegetables g fw per day current(95)	consumption of potatoes g fw per day current (95)	**consumption of vegetables g fw per day proposed**	**consumption of potatoes g fw per day proposed**
babies and pre-schoolers	0-6 year	76.1	74.8	**58.3**	**59.5**
adults and schoolgoing children[5]	7-70 year	157.8	136.7	**139**	**122**

[*)] consumption in g fresh weight per day

4.4.3 Fraction dry weight of vegetables and potatoes (fdws, fdwr)

The dry matter content of vegetables and potatoes is used to express the crop metal content in mg/kg dry weight. Table 4.3 gives the water content of most vegetables according to the EPA Exposure Factor Handbook (1997).

- *The consumption pattern in weighted average dry weight is calculated at 13.5 g /100g fresh product (Table 4.5).*

Table 4.5: Water content of vegetables, potatoes and average of all relevant crops

	current CSOIL value (Bockting and Van den Berg, 1992)		**revised CSOIL values**	
data source method	Ng et al.1982 mean of available data		**EPA, 1997** **weighted average**	
	water content g/ 100g	dry weight (fdw) g/ 100g	**water content g/ 100g**	**dry weight (fdw) g/ 100g**
potatoes	79.8	20.2	**83.3**	**16.7**
vegetables [*)]	88.3	11.7	**90.2**	**9.8**
weighted average	-		**86.5**	**13.5**

[*)] fruits were not taken into account

4.4.4 Fraction contaminated crops (Fvk, Fvb)

The *fraction contaminated root crops (Fvk)* and *leafy crops (Fvb)* in CSOIL are currently both 0.1 for the standard scenario (residential with garden), based on Linders (1990). In the standard scenario vegetables and potatoes are grown in residential gardens. Many people living in houses with a garden do not grow consumption crops; on the other hand, there are people growing crops for home consumption. Besides, it is difficult to differentiate between an allotment garden and kitchen gardens.

According to Van de Ven-Breken (1990) the consumption from kitchen gardens in several European countries is 15 to 30 % of the national vegetable consumption. On the basis of the number of people owning a kitchen garden or allotment garden (Hulshof, 1988), it is estimated that about 18% (2.6 million people) of the Dutch population could eat crops from allotment gardens.

---

[5] About 6 % of the consumed amounts of vegetables and about 9 % of the consumed amount of potatoes are obtained outdoors. These amounts are not taken into account.

In a study using 154 households with kitchen gardens (Hulshof, 1988) the average consumption of vegetables and potatoes is 93 and 54 kg, respectively, per person per year (or 255 and 148 g per day, respectively). This is more than the average consumption of the whole Dutch population, as given in Table 4.4. Based on the study of Hulshof (1988), the respective average consumption from one's own garden was 51 kg and 7 kg per person per year. For all crops this comes to 58 kg per person per year. The average consumption per person per day and the percentage consumed vegetables and potatoes from one's own garden is given in Table 4.6.

Taking into account that about 18% of the whole population eats 54.8 % vegetables and 13 % potatoes from their own gardens and 88 % do not eat from their own gardens, the average consumption of home-grown vegetables (from kitchen gardens and all others) is around 10% and for potatoes around 2.3% (Table 4.6).

Table 4.6: Consumption of home-grown crops (source Hulshof, 1988; Van de Ven-Breken, 1990)

	Total consumption		**Home-grown consumption**			
	Kitchen gardeners		**Kitchen gardeners**			**All people**
	kg.yr^{-1}	g.pp^{-1}.d^{-1}	kg.yr^{-1}	g.pp^{-1}.d^{-1}	%	%
vegetables	93	254.8	51	139.7	54.8	9.9
potatoes	54	147.9	7	19.2	13.0	2.3
Total	147	402.7	58	158.9	39.5	7.1

Crop consumption in the Netherlands compared with other countries

To give an impression of the differences in total crop consumption and the fraction contaminated crops in other countries, the crop intake values for adults are compared with values used in models in the UK, Germany and the USA. More detailed information can be found in Rikken et al. (2001). In UMS (Germany) only the total vegetables and fruits consumption are defined. Besides, it must also be noted that potatoes are not considered as root vegetables in UMS. The differences between the different models are fairly large, especially for the amounts of consumed crops from one's own garden. The difference between the lowest and highest home-grown intake rate is a factor 13 for root crops and a factor 30 for leafy crops.

Table 4.7: Freshweight consumption of root crops and leafy crops

Model	**Consumption of home- grown root crops (g per day)**	**Consumption of home- grown leafy crops (g per day)**	**Total consumption of root crops (g per day)**	**Total consumption of leafy crops (g per day)**
CLEA [1)]	9.2	2.4	171	23.2
CalTOX[2)]	126	72	301	84
UMS [3)]	Vegetables: 195		Vegetables: 475	
CSOIL [4)]	13.7	15.8	136.7	157.8

[1)] The separate intakes of different vegetables are added to obtain the total values. The home-grown consumption rate is based on the difference between the average consumption and the average purchases.

[2)] The EFH values are used (US-EPA, 1997). The intake rates actually used in CalTOX are unknown.

[3)] Only the total vegetable values are presented, because root crops and leafy crops are not defined in UMS. The values do not take into account the correction factor of 0.5 for food preparation.

[4)] The current intake of home-grown crops is 10% of the total vegetable intake.

The consumption of home-grown crops compared to the total vegetable consumption vary from 5.4% to 42% for root crops and 10% to 86% for leafy crops (Table 4.8).

Table 4.8: Consumed crops from own garden in % of the total consumption

Model	**root crops from own garden (%)**	**leafy crops from own garden (%)**
CLEA	5.4	10.3
CalTOX	42	86
UMS	all vegetables: 41	
CSOIL	10	10

Discussion and Conclusion

Information on the growth of crops in kitchen gardens and allotment gardens is limited, especially for the Netherlands. Based on the available information it can be concluded that the average consumption of home-grown crops by the Dutch population is maximally 10 %. This is not at all equally distributed over the population, because 82% never eats home-grown crops, but about 3% of the population consume a large fraction (up to 50%) from their own gardens (and 15% small fractions).

The fraction of home-grown vegetables in Germany and the USA seems higher than in the Netherlands. In the UK this fraction is comparable.

The value to be chosen is highly determined by the policy of what individuals (and their behaviour) and which situations should be protected. Assuming a contaminated fraction of about 50% would protect the average consumption from allotment gardens, but is too high for general purposes in a ‘resident with garden’ scenario. A percentage of 0 would underestimate the potential exposure by soil contamination. About 18% of the people may be eating from their own kitchen garden.

- *It is proposed to maintain the current value for fraction-contaminated crops at 10%. Based on the available data it is expected that for all situations, except for allotment gardens, this will cover the exposure because of consumption of contaminated crops.*

4.4.5 Deposition constant

In Rikken et al. (2001) it was concluded that the *rainsplash concept (or resuspension of soil particles)* should be added to CSOIL, because soil and dust particles can deposit on the different plant parts by rainsplash. In the UK, the human exposure model CLEA 30 g dry soil per kg dry plant (= 3%) for soil attached to crops is used; this is based on a mean estimated soil load on plants as in Sheppard and Evenden (1992). Trapp and Matthies (1995) suggests a less conservative value of 1% dry soil per dry plant. Provisionally, the contribution of this route has been set at 1% dry soil per kg dry plant to add to the estimated uptake of organic compounds by plants. The empirical BCF data for metal accumulation in plants is supposed to include deposition by rainsplash.

4.5 Soil ingestion: daily intake of soil (AID)

4.5.1 Introduction

Important parameters for the exposure by soil ingestion are the *daily intake of soil by children (AIDc)* and the *daily intake of soil by adults (AIDa*, which are currently set (Van den Berg, 1995) at 150 and 50 mg/d, respectively. These values are mainly based on the data of Hawley (1985), Linders (1990) and van Wijnen et al. (1990). In Hawley the exposure of young children is estimated on 150 mg per day, based on an outside ingestion of 250 mg during 130 days a year, and inside ingestion of 100 mg per day in winter (182 d) and 50 mg per day in summer (182 d). Linders estimates a soil ingestion of 200 mg per day during 3 days a week (0.43 x 200= 86 mg per day).
First, the soil ingestion by children (1 to 6) and, second, the soil ingestion by older children and adults are discussed. The ingestion by older children (>7 yr.) and adults will be much less than for children.

4.5.2 Soil ingestion by children

For soil ingestion by children a difference should be made between:

A. intentional (incidental) soil ingestion (in fact to be compared with data about acute toxicity) and
B. inadvertent soil ingestion during a longer period of time.

For deriving Intervention Values we focus on children aged 1 to 6; especially the younger children aged 1 to 3 can have higher soil ingestion. The deliberate soil ingestion is not taken into account in this evaluation.

Several studies have been done to estimate the ‘normal’ soil ingestion by children aged 1 to 6 (Binder et al., 1986; Clausing et al., 1987; Calabrese et al., 1989; van Wijnen et al., 1990; Davis et al., 1990; Stanek and Calabrese 1995a and Stanek and Calabrese, 1995b). All these studies have in common that tracers have been used to estimate the amount of soil that is ingested. These tracers are natural compounds occurring in soil and are analysed from the faeces of children.

The amount of these tracers found is compared with their concentration in the soil and in house dust. The concentration found can originate from soil and dust, but for some tracers food can also be an important source. Therefore the most reliable tracers had to be identified. According to Calabrese (1989) and Stanek (1995) Aluminium and Silicon (and Yttrium) are the most reliable tracers. Beside these, the limited tracer method (LTM) is used, in which for every sample the lowest of all tracers are used (Binder et al., 1986; Clausing et al., 1987; van Wijnen et al., 1990).

Stanek and Calabrese (1995a; 1995b) give new interpretations of two earlier studies (Davis et al., 1990 and Calabrese et al., 1989) and claim to have a better interpretation of these experimental data. Clausing (1987) and van Wijnen et al. (1990) are the only Dutch studies and should therefore be of more importance to the Dutch situation, although large differences between countries are not expected. Most studies were done in the summer period, a time when the soil contact probably will be more frequent than other periods of the year.
There are some differences between the studies in correction for other routes of intake of tracers than soil ingestion. Van Wijnen (1990) and Clausing (1987) used measurements of a non-exposed group of children, others (Calabrese et al., 1989; Davis et al., 1990; Stanek and Calabrese, 1995a en 1995b) used measurements of the tracer content of food to make a mass balance for these elements. Binder (1986) did not make corrections and seems therefore less accurate.

Soil ingestion by young children can differ in time, and between children; it has a log normal distribution (Calabrese, 1989). Deliberate soil ingestion (known as ‘pica’) occurs within a substantial part of the children aged 1 to 3 at 1 or 2 days a year with an amount of more than 1 g per day or even 10 g per day (Calabrese, 1997). Although it seems possible that for some compounds toxicological effects could occur, this incidental exposure is not taken into account in this evaluation.

The data of the eight above-mentioned references are stated in Table 4.8. When available in de reference the (arithmetic) mean, the median (50-percentile), the geometric mean, the 90- and 95-percentiles of the data are given. These data show a large difference between mean and median value. The reason for this difference is the probably log normal distribution of the daily soil ingestion by children. The data show also that there is already a large spread in time of the soil ingestion, between different children and per child.

The (estimated) average daily soil ingestion of all references is between 61 and 179 mg per day, taking into account the background exposure. The mean of all these values is 102 mg per day. The median values are between 26 and 88, with a mean value of 42 mg per day (see Table 4.8) The 90-percentile of the several data sets is roughly between 150 and 200 mg per day, whereas the 95-percentile of the soil ingestion is around 200 mg per day.

Besides the tracer studies there are references in which the exposure of children (and adults) due to soil ingestion are estimated. In (US-EPA, 1997) an overview of these data is given. One of these references is the estimate according to Hawley (1985), on which the current estimate in CSOIL is mainly based. Some of these articles are based on the evaluation of seven earlier mentioned studies and others on the measured soil and dust on the skin of hands, and the hand-mouth behaviour of children. These studies are considered to be a supplementary to the quantitative data in the other references. Simon (1998) gives a fairly complete overview of the data on soil ingestion, but no conclusions are given on the best data.

Table 4.9: Daily soil ingestion by children in 8 references

Reference	n (number of children)	Tracer	mean	SD of mean	95% conf. limit of mean	median (50-perc.)	min.	max.	90-perc. (logn. distr.)	95-perc. (logn. distr.)	geometric mean	GSD (geom. st. deviation)
Binder et al, 1986	59	Al	181	203		121	25	1324		584	128	
		Si	184	175		136	31	799		578	130	
		LTM	**108**	121		**88**	4	708		**386**	**65**	
Clausing et al., 1987	18	Al	232	263		93	23	979	579	707	136	
		AIR	129	69		108	48	362	174	264	117	
		LTM	**105**	67		**82**			**162**	**201**	**90**	
background (hospital)			***49***	*22*		***48***			*75*	*79*	*45*	
Calabrese et al., 1989	64	Al	153	852		29		6837		223		
Soil		Si	154	693		40		5549		276		
		Y	85	890		9		6736		106		
		mean Al, Si, Y	**131**			**26**				**202**		
Davis et al,1990	101	Al	39	14		25	-297					
		Si	82	12		59	-404					
		mean Al, Si	**61**			**42**						
van Wijnen e.a., 1990												
all data daycare 1	292	LTM	232			124					145	2.24
daycare 2	187	LTM	106			90					92	1.69
daycare 1+2	166	LTM	**162**	286		**114**					**111**	1.6
Campground	78	LTM	213			160					174	1.73
Background (hospital)	*15*	*LTM*	***93***	*46*	*67-119*	*110*		*149*			***74***	*2.34*
selected daycare 1	22	LTM							**265**		162	
data daycare 2	15	LTM							**172**		104	
Campground	32	LTM							258		163	
Stanek&Calabrese, 1995 a	64	Al	122			29		4692	131	254		
(interpretation of		Si	139			32		4975	206	224		
Calebrese, 1989)		total	**179**			**45**		7703	**186**	**208**		
Stanek&Calabrese, 1995 b	229	median Al,Si,Ti	**113**			37		11874	**194**	**249**		
(interpretation of Davis, 1990;		median best 4 tracers	**104**			**37**		11415	**156**	**217**		
Calebrase, 1989)												
Calabrese et al, 1997.	64	median best 4 tracers	7	75		1	-101	380	73	160		
Average of all references [1)]			***102***			***42***			***150***	***230***	***49***	

[1)] Bold data are used in calculations (1 value per reference)

Uncertainties

Although the data give a good impression of the soil ingested, there are several uncertainties, which should be mentioned. First, we are concerned here with short studies, which means that the data do not have to represent long exposure. Second there is experimental uncertainty in the measurement of the soil ingestion by children, for example, by only partial sampling of the food and faeces or transit time differences. Third, there are uncertainties in the uptake of tracers by the human body. Also there is an uncertainty in the homogeneity of the soil samples (US-EPA, 1997).

4.5.3 Soil ingestion by adults and older children

Only four studies are available for making an estimation of the soil ingestion of adults. In Hawley (1985) estimates are based on soil and dust on hands and hand-to-mouth transfer. A soil ingestion of 480 mg per day was estimated for adults in outdoor activities and for indoor activities soil ingestion between 0.56 and 110 mg per day was estimated. In US-EPA (1997) an estimate of 10 mg per day is also mentioned, based on arsenic levels in urine, hand-to-mouth transfer and activity patterns. Because of the lack of direct measurements these data have a low reliability.

Calabrese et al. (1990) and Stanek et al. (1997) quantified soil ingestion in two tracer studies with adults. Although part of a childhood soil ingestion study (Calabrese et al., 1990) on the most reliable tracers (Al, Si, Y and Zr) yielded respective mean soil ingestion values of 77, 5, 53 and 22 mg per day (see Table 4.9), from which a average of 39 mg per day can be calculated. Stanek et al.(1997) also formed a part of a larger study involving 10 adults. The tracers used for estimating soil ingestion are Al, Si, Ti, Y and Zr. Based on the 'best tracer method' (BTM) the average daily soil ingestion (10 persons over 4 weeks) was 6 mg per day. The data also provide information on the distribution of soil ingestion. Based on these results, the average ingestion by adults is concluded to be 10 mg per day. Taking into account the results of the separate weeks (see Table 4.10), it can be concluded that this relatively low average is a result of the low values in week 4. The mean of the first three weeks is 53 mg per day. Although there are still a lot of uncertainties involved, as mentioned before, these studies give the best quantitative estimates currently available.

Table 4.10: Soil ingestion by adults

Reference	**n (number of adults)**	**tracer**	**mean**	**SD of mean**	**min.**	**median (50-perc.)**	**75-perc.**	**90-perc.**	**95-perc.**	**max**
Calabrese et al., 1990	6	Al	77	65		57				
		Si	5	55		1				
		Y	53	51		65				
		Zr	22	141		-4				
		median of Al, Si, Y, Zr	**38**			**29**				
		average of Al, Si, Y, Zr	**39**			**30**				
Stanek et al., 1997	10	*median of 4 best tracers*								
		4 weeks	**6**	**165**	**-400**	**-11**	**34**	**201**	**331**	**620**
		week 1	67	202	-39	-14	37	384	620	620
		week 2	44	120	-52	18	37	210	376	376
		week 3	49	127	-84	-5	120	269	285	285
		week 4	-137	126	-400	-143	-93	21	100	100

4.5.4 Soil ingestion data used in other countries

In addition to the data on soil ingestion in the literature, the data used in risk assessment tools in the UK, USA and Germany are summarised. More details can be found in Rikken et al. (2001).

In all models an age-adjusted soil ingestion factor is used because inadvertent soil ingestion is different for children and adults. The age categories used and corresponding soil ingestion rates are not the same for all models. On the basis of the yearly averaged soil ingestion rates it can be concluded that the present value for children in CSOIL of 150 mg per day is higher than the ingestion rates of the other models (see Table 4.11). For the relevant scenarios of the other models the yearly averaged soil ingestion rates for children are 123 mg per day and 74 mg per day for UMS, 114 mg per day for the CLEA and 60 mg per day for CalTOX. For adults the ingestion rate of the UK is comparable with the CSOIL value of 50 mg per day. The ingestion rate of UMS (Germany) is 16 mg per day and in CalTOX 10 mg per day. Further it must be noted that only the CLEA model accounts for an additional deliberate soil ingestion rate in the second year of life.
In Denmark an average daily intake of 200 mg per day is used for children, being a 90-95 percentile of a group of children. The Soil Quality Criteria is based on this figure only. For adults they assume an intake of 25 mg soil per day (pers. comm. Larsen).

Table 4.11: Soil ingestion rates and use of deliberate soil ingestion for the compared models

Model	Yearly average soil ingestion rate for adults (mg per day)	Yearly average soil ingestion rate for children (mg per day)	Use of deliberate soil ingestion for children	Absorption or resorption rate[3)]
CLEA	60	80 / 114 [1)]	Yes [2)]	No
CalTOX	10	60	No	No
UMS	16 [3)]	123 (1-3 year) 74 (4-8 year) [4)]	No	Yes (default 1)
CSOIL	50	150	No	Yes (default 1)

1) Without deliberate soil ingestion: 80 mg/kg. With deliberate soil ingestion: 114 mg/kg
2) 5000 mg per day for a maximum of 30 days in the second year of life
3) The uptake in the human body, based on a soil ingestion of 30 mg per day and an exposure duration of 190 d/y
4) Based on a soil ingestion of 250 mg per day (1-3) and 150 mg per day (4-8) and an exposure duration of 180 d/y

4.5.5 Discussion and conclusion

The quantitative data on soil ingestion from the 7 references for children and 2 references for adults, together with the background information in other countries will be the main bases for a proposal on daily soil ingestion by children and by adults. To decide on the soil ingestion to be used, it is important to decide what part of the behaviour of people should be protected. This is important because there is a distribution of exposure in time en between different persons. In the CSOIL exposure model the starting point is the average human lifetime exposure within the exposure scenario ‘residential with garden’. Therefore it is proposed to use the average exposure, but depending on de function of the risk assessment it could be decided to use an upper percentile (90 or 95 percentile). All studies are comparable with the scenario ‘residential with garden) except from a study on a campsite (worst case). Because of the spread of the soil ingestion between children and the spread of the ingestion in time, the average can be seen as a (yearly averaged) daily soil ingestion by children. Using the median value of soil ingestion would lead to an underestimation of the yearly soil ingestion.

Soil ingestion by children

Based on the literature data and the data used in other countries it can be concluded that the current value of 150 mg per day as an estimate of the average daily soil ingestion by children is relatively high. There also appears to be a large spread in the data: the estimate of the average soil ingestion in the studies lies between 56 and 179 mg.d-1. The most recent data from the risk assessment in the UK, Germany and US for the average daily soil ingestion are 114, 100 and 123, respectively.

- *Based on the evaluated and assessed data a good estimate of the average daily soil ingestion through children for the scenario 'residential home with garden' is 100 mg.d-1. It is proposed to use this value in the risk assessment.*
- *When the spread between the studies is considered also the upper limit of the 90-percent confidence interval of the mean, 125 mg per day could be used. For a realistic worst case a 90-percentile or 95-percentile of the soil ingestion of children could be chosen, being about 150 and 200 mg per day, respectively.*

Soil ingestion by adults

Based on the 2 references on soil ingestion by adults it can be concluded that the current value of 50 mg per day is well within the range found for the average soil ingestion. The most recent data from the risk assessment in the UK, Germany and US for the average daily soil ingestion are 60, 50 and 16, respectively. Although the most recent study suggests an average soil ingestion of 10 mg per day, because of the strongly differing results of week 4, a yearly average soil ingestion of 40 or 50 mg per day will be proposed as a good estimate. A 90-percentile of 200 mg per day can be estimated with substantial uncertainty.

- *It is proposed to maintain the current value of 50 mg per day soil ingestion by adults.*

4.6 Input parameters on the dermal exposure to soil route

Dermal exposure via soil contact is a less important exposure route compared with the three major exposure routes: soil ingestion, inhalation of indoor air and crop consumption.
In section 2.2.3 it was decided to give no priority to the evaluation of the input parameters involved with this route. In agreement with the priority setting it was also decided not to evaluate the current concept of this exposure route (Rikken et al., 2001).
Concerning the dermal exposure via sediment, other considerations have been made. The SRC_{human} for sediments is determined with the exposure model SEDISOIL and the standard use of sediments (inclusive the banks of rivers, lakes et cetera) is described with the scenario 'the possibility of recreation and recreational fishery'. Recreational activities imply a more intensive dermal contact with sediment than activities as defined for the standard CSOIL scenario 'residential use with garden'. Exploratory calculations with the SEDISOIL model showed that for certain compounds (e.g. PAH), the contribution of the exposure route dermal uptake via soil contact could be relevant (Otte et al., 2000a). Therefore it is recommended to evaluate in future this exposure route.

The following input parameters are used to calculate the dermal exposure to soil route.

- *Matrix factor (fm)*

The *matrix factor* in CSOIL is set at 0.15. It represents the fraction of the soil that is in contact with the skin and is based on observations of Hawley (1985). In the uncertainty analysis a uniform distribution is assumed to be between 0.1 and 0.5.

- *Exposed surface area adult indoor and outdoor (Aexpai/Aexpao)*

The *exposed surface area* for adults in CSOIL is set at 0.09 and 0.17 m^2, respectively. In the uncertainty analysis a normal distribution is assumed to be between 0.09-0.34 m^2 (inside) and between 0.09 and 0.98 (outside), based on data of Hawley (1985). For children a normal distribution is assumed to be between 0.04 and 0.125 m^2 (inside).

- *Degree of coverage indoor and outdoor (DAEai/DAEao)*

The *degree of coverage indoor* in CSOIL is set at 0.00056 and the *degree of coverage outdoor* for adults and children 0.0375 and 0.0051 kg soil per m^2, respectively.

- *Exposure period (Tb)*

The exposure period of an adult indoor and outdoor (Tbai/Tbao) in CSOIL is set at 14.86 and 1.14 h per day, respectively. The exposure time is related to the exposure by inhalation of inside air. In the uncertainty analysis a normal distribution of the exposure time is assumed to be between 6.7 and 16 h (inside) and 0.1 and 5 h (outside), based on data of Silvers et al. (1994). The exposure period for children indoor and outdoor (Tbci and Tbco) in CSOIL is set at 9.14 and 2.86 h per day, respectively).

- *Fraction soil in dust inside (frs)*

In CSOIL the fraction soil in dust is set at 0.8.

- *Absorption velocity for adults (DARa)*

In CSOIL the *absorption velocity* for an adult is set at 0.005 per h. Although the velocity is also substance-dependent, in the uncertainty analysis it is set at between 0.004 and 0.01 per h, based on data of McKone and Bogen (1990).

- *In agreement with the priority setting (section 2.2.4.) it was decided not to evaluate or revise the input parameters used for the calculation of dermal exposure to soil.*
- *It is recommended to evaluate the model concept jointly with the relevant input parameters in future.*

5 Discussion and recommendations

5.1. Physicochemical parameters

5.1.1. Introduction

All the relevant physicochemical parameters were evaluated, resulting in a revised data set. Data were completed for all the chlorophenols and the PAHs; PCBs and phthalates were extended with more congeners. This enhanced the base for deriving SRC values for groups of compounds. The physicochemical data of the dioxins (belonging to the second series of compounds) were not evaluated and maintained (Van den Berg et al., 1994).
The physicochemical data for petroleum hydrocarbons have been reviewed recently in a study supervised by the Mineral Oil Working Group (Franken et al., 1999). The physicochemical data as proposed by the Total Petroleum Hydrocarbon Criteria Working Group were evaluated and completed. The proposals reported by Franken et al. (1999) were adopted. The complete revised physicochemical data set is given in Appendix 7. The underlying individual data will be compiled and made available later. We propose to use the data set (chapter 3) for the assessment of potential human risks and for the evaluation of the current Intervention Values for Soil and Groundwater.
The most important details of the revised data set will be outlined in the sections below, followed by a comparison of the revised data with the current data (Van den Berg, 1995). Substantial differences are emphasised and the effect of the revised parameter (or parameters) on the calculated risk level examined.

5.1.2. Molecular weight, solubility, vapour pressure, Henry's law constant and acid dissociation constant

As the molecular weight (M) is a well-known parameter an evaluation was not necessary. Only the correction of the molecular weight for seven compounds due to earlier reported input errors (Van den Berg, 1997) was carried out.
The revised solubility (S) and vapour pressure (Vp) data is based on the geometric mean of the selected data. Contrary to the current data, the revised data is corrected for a standard soil temperature of 10^{o} C. According to the current CSOIL formulary Henry's law constant is calculated from the vapour pressure and solubility data. We considered using experimental Henry's law constants when available, however, it is not certain if measured Henry's law constants give better descriptions of the air-water partition in situ. Moreover, reliable experimental Henry's law constants for many compounds are often not available. The current practice was continued to maintain a consistent methodology.
The acid dissociation constant (pKa) only has effect on the determination of the Koc for some dissociating compounds. The effect on the Koc (and the calculated level of SRC_{human}) depends on the pKa value and the defined pH of the CSOIL standard soil (see section 2.1.7).

Table 5.1 overviews the compounds for which the differences between current and revised data exceed a factor of 3 (solubility) or 5 (vapour pressure and H constant). These factors are chosen on the basis of the estimated standard deviation for solubility and vapour pressure (Jager et al., 1997). In a broad sense, when the current solubility or vapour pressure differs more then respectively a factor 3 or 5 it indicates that the current value is outside the estimated 20th and 80th percentiles.

It is difficult to estimate if the proposed new solubility and vapour pressure data will lead to a substantially(> factor 2) different SRC_{human} value. This also depends on other revised compound-specific parameters as well as soil, exposure and site parameter adjustments. However, when only the revision of solubility (S), vapour pressure (Vp) and Henry's law constant (H calculated from S and Vp) is considered separately, a substantial effect on the SRC_{human} is found for four compounds (Table 5.1).

*Table 5.1: Differences between current and revised data (> a factor of 3 or 5) and the effect on the SRC_{human} (> a factor of 2 as difference) because of these differences (*in italics*)*

Solubility **Δ > factor 3**	**Vapour pressure** **Δ > factor 5**	**H constant** **Δ > factor 5**	**Effect on SRC human** **Δ > factor 2**
Catechol	Catechol	Catechol	Resorcinol
Resorcinol	*Resorcinol*	*Resorcinol*	Hydroquinone
Hexachlorobenzene	*Hydroquinone*	*Hydroquinone*	α-HCH
2-Chlorophenol	Anthracene	Anthracene	Di(2-ethylhexyl)phthalate
2,3,4-Trichlorophenol	Benzo(a)anthracene	Benzo(a)anthracene	
2,3,4,5-tetrachlorophenol	Benzo(a)pyrene	Fluoranthene	
Pentachlorophenol	Fluoranthene	Phenanthrene	
PCB153	Phenanthrene	Benzo(k)fluoranthene	
Endrin	PCB 28	2-Chlorophenol	
β-HCH	*α-HCH*	2,3,4-Trichlorophenol	
δ-HCH	β-HCH	2,3,4,5-Tetrachlorophenol	
Di(2-ethylhexyl)phthalate	γ-HCH	PCB 28	
	δ-HCH	*α-HCH*	
	Maneb	β-HCH	
		γ-HCH	
		δ-HCH	
		Endrin	
		Maneb	

The following remarks can be made on the revised solubility data. Van de Berg (1997) reported input errors for 2,3,4-trichlorophenol, pyridine, carbaryl, carbofuran, tetrahydrofuran and tetrahydrothiophene. The input data for these compounds were corrected before the evaluation process. When the current solubility data (Van den Berg, 1995 and 1997) are compared with the revised data, substantial differences (> factor 3) were found for 12 compounds. However, the use of the revised solubility data only have a substantial effect (> factor 2) on the SRC_{human} level for di(2-ethylhexyl)phthalate. The revised solubility value for di(2-ethylhexyl)phthalate (from 0.285 to 0.0457 mg/l) permits a lower maximum pore water concentration and consequently a lower plant uptake.

In the revision of vapour pressure data, substantial differences (> factor 5) were found for 14 compounds, mainly those with a low volatility (< 1 Pa); consequently, the effect on human exposure is small. The current vapour pressure values for hydroquinone, resorcinol and catechol were arbitrarily set at 133 Pa (Van den Berg, 1997) because data for these compounds were not available. The revised vapour pressure data were significantly lower, resulting in higher BCF values for leafy crops and, consequently, a higher plant uptake. For hydroquinone and resorcinol this implies lower SRC_{human} levels. The revised vapour pressure for α-HCH (from 3.33E-03 to 3.50E-02 Pa) resulted in a small increase in the human exposure via inhalation of indoor air. This resulted in a significant lower SRC level due to the low TCA (compared with the TDI) for α-HCH.

5.1.3. Octanol-water partition coefficient (Kow)

After ample discussion it was decided to use the LOGPSTAR Kow data from the Medchem database when available (section 3.2.2). If the LOGPSTAR value is not available the CLOGP value is selected. In general, the average Kow values based on own Kow collection (data collect from the selected databases) are similar to the LOGPSTAR of CLOGP value. Substantial differences between LOGPSTAR values and the average log Kow values based on own set were encountered for tetrachloroethene, vinylchloride, some PCBs and aldrin (Table 3.5). In Table 5.2, the compounds for which substantial differences in log Kow data were encountered are tabulated.

Table 5.2: Substantial differences between LOGPSTAR Kow and the average log Kow values based on own Kow set

Compound	**LOGPSTAR Kow**	**Average Kow (based on own Kow set)**
Tetrachloroethene	3.40	2.89
Vinylchloride	1.52	1.32
PCB 52	6.26	5.59
PCB 101	6.85	5.89
PCB 138	7.45	6.68
PCB 153	7.44	6.79
PCB 180	8.16	7.21
Aldrin	6.50	5.62

Differences in the selected log Kow values with the present CSOIL Kow data (Van den Berg, 1995) are more frequent. Table 5.3 gives the compounds for which substantial differences were encountered (Δ > standard deviation). Compounds with low, medium and high Kow values are listed when the difference exceeds 0.2 log unit 0.5 log unit and 0.7 log units, respectively. The standard deviations for low, medium and high log Kow values are based on Jager et al. (1997). The compounds showing a substantial effect on the SRC_{human} are given in the outermost left column.

Table 5.3: Differences between current and revised log Kow (> 0.2, 0.5 and 0.7 log unit) and the effect (> a factor 2) of the revision of the Kow on the SRC_{human}.

log Kow < 4 **Δ > 0.2 log unit**	**log Kow 4-5.5** **Δ > 0.5 log unit**	**log Kow > 5.5** **Δ > 0.7 log unit**	**Effect on SRC_{human}** **Δ > factor 2**
Dichloromethane	2,3,4,5-Tetrachlorophenol	Chrysene	2,3,4,5-Tetrachlorophenol
Tetrachloroethene	Dieldrin	Benzo(k)fluoranthene	PCB 153
Vinylchloride		PCB 153	DDE
o-Monochlorophenol		DDE	DDT
2,3,4-Trichlorophenol		DDT	Dieldrin
Atrazine		Aldrin	Carbaryl
Carbofuran		Di(2-ethylhexyl)phthalate	Carbofuran
Carbaryl			Pyridine
Cyclohexanone			Tetrahydrofuran
Tetrahydrofuran			Di(2-ethylhexyl)phthalate
Tetrahydrothiophene			
Pyridine			

The differences between current and revised Kow data for carbaryl, carbofuran, pyridine, tetrahydrofuran and tetrahydrothiophene were due to the Kow being calculated from incorrect solubility data (see section 5.1.2). After correction of the solubility (Van den Berg, 1997), the calculated Kow data continue to be different from LOGPSTAR data. Other solubility-based Kow data were used for vinylchloride, cyclohexanone, dichloromethane, 2,3,4,5-tetrachlorophenol, di(2-ethylhexyl)phthalate, benzo(ghi)perylene, indeno(1,2,3-cd)pyrene, trichloroethene, pentachlorobenzene, chloronaphthalene, maneb and butylbenzylphthalate (Van den Berg, 1997). Substantial differences were frequent between solubility-based Kow and the LOGPSTAR Kow data. Other substantial differences were noticed for tetrachloroethene, atrazine, 2,3,4-trichlorophenol, 2,3,4,5-tetrachlorophenol, dieldrin, di(2-ethylhexyl)phthalate, DDE, aldrin, PCB 153, DDT and benzo(k)fluoranthene.

Whether these differences provoke substantial alterations in the level of the SRC_{human} also depends on the chosen concept for deriving Koc values. Van den Berg (1995) derived Koc values from the Kow according to Karickhoff (1981). This implies that with an alteration of the Kow value the calculated Koc also changes. In section 3.3.1 it was decided to use experimentally based Koc values, resulting in a different (smaller) effect of Kow alterations than with the current 1995 approach for Koc derivation. Table 5.3 gives the effect on the SRC_{human} of the revision of Kow only (means that the Koc within the model is independent of Kow).

5.1.4. Organic carbon normalised soil–water partition coefficients (Koc)

The current Koc values in Van den Berg (1995) were based on Kow values (Karickhoff, 1981). In contrast with the CSOIL 1995 log Koc data, the revised Koc data is based mainly on experimental data. Databases and reviews used are given in Table 3.1.
For dissociating contaminants the **overall Koc** for a standard soil is computed, taking into account both neutral and negatively charged forms (Koc for dissociating compounds3.3.2). The CSOIL 1995 log Koc data (Van den Berg, 1995) considered only the sorption of the neutral form.
The current Koc data set (Van den Berg, 1995) is compared with the revised Koc data (see Table 3.6). The compounds for which substantial differences were encountered are tabulated in Table 5.4. Compounds are listed when the log Koc differs more than 0.3 log, 0.5 log and 0.7 log unit for compounds with low, medium and high Kow values, respectively. This criterion is based on the estimated standard deviation calculated from the collected Koc values.
The revision of the log Koc influences the calculated exposure and the SRC_{human} for soil substantially (> factor 2) for 27 compounds (Table 5.4 right column).

Part of the encountered differences were caused by the fact that some Koc values were based on weakly founded (calculated from solubility) Kow values. This applies to carbofuran, carbaryl, tetrahydrofuran, 2,3,4,5-tetrachlorophenol, pentachlorobenzene, vinylchloride and cyclohexanone). For some of the other compounds the use of the Kow-Koc model (Karickhoff, 1981) is doubtful (e.g. hydroquinone, catechol, resorcinol and chlorophenols), as such models are mainly class-specific (e.g. predominantly hydrophobic). The revised log Koc values of aldrin, dieldrin and endrin are lower than the current log Koc values.

Table 5.4: Comparison of current and revised log Koc data and the effect of the Koc revision on the SRC human

log Koc < 3.5 $\Delta > 0.3$	**log Koc 3.5-4.5 $\Delta > 0.5$**	**log Koc > 4.5 $\Delta > 0.7$**	**Effect on SRC human $\Delta >$ factor 2**
Phenol M-Xylene Catechol Resorcinol Hydroquinone 1,2-Dichloroethane Tetrachloromethane Vinylchloride 1,2,4-Trichlorobenzene 2,3,4-Trichlorophenol Pentachlorophenol γ-HCH Atrazine Carbofuran Carbaryl Cyclohexanone Pyridine Tetrahydrofuran	Pentachlorobenzene Hexachlorobenzene 2,3,4,5-Tetrachlorophenol Aldrin Dieldrin Endrin	Benzo(ghi)perylene Indeno, 1,2,3-cd pyrene Maneb	Phenol M-Xylene Catechol Resorcinol Hydroquinone 1,2-Dichloroethane Tetrachloromethane Vinylchloride 1,2,4-Trichlorobenzene 1,2,3,4-Tetrachlorobenzene Pentachlorobenzene Hexachlorobenzene 2,3,4-Trichlorophenol 2,3,4,5-Tetrachlorophenol Pentachlorophenol PCB 28 Aldrin Dieldrin Endrin γ-HCH Atrazine Carbofuran Carbaryl Cyclohexanone Pyridine Tetrahydrofuran

5.1.5. Bioconcentration factor for metal accumulation in crops

The current BCF values for metals (Bockting et al., 1992) were evaluated and revised (section 3.4). In contrast to the CSOIL 1995 BCF data, the revised BCF values are solely based on field data. The revision improved the description of the real situation, being the average vegetable garden in the Netherlands. The most important metal accumulation factors were taken into account for the derivation of BCF values. These factors are:

- Selection of crops;
- The degree of soil contamination;
- The soil type (organic carbon and clay content), and pH.

Taking these factors into account permits the derivation of generic BCF values representing the average consumption pattern of home-grown vegetables. Furthermore, the BCFs are normalised on a known contamination level and according to standard soil type.

Despite the fact that the revised BCF values are based on a large field database, the available information did not allow accounting for several accumulation factors known to be of importance. These accumulation factors are:

- matrix effects (contamination source);
- seasonal effects;
- effect of crop variety;
- calcium, iron and alumina soil content;
- ageing;

- harvesting period;
- farm management and use of fertilisers;
- root zone in relation with the spatial variability of the pollution;
- effect of aerial deposition.

The use of data from different sources is expected to cause suppression of the effects of these accumulation factors thus providing a good picture of the average situation.
The underlying plant–soil relationships can be improved when more field data sets become available. However, at the moment it is clear that with the proposed BCF data-set risk assessment due to consumption of home-grown crops has been improved.

5.1.6. Kp for metals

When the current CSOIL Kp set was evaluated and compared with three other Kp sets (section 3.5), the current CSOIL Kp set was shown to be considerably lower Kp than the sets of Sauvé (2000) and PGBO (Otte et al., 2000b). Based on five criteria the data sets and derived Kp values or Kp models were compared.
The presented Kp values (Table 3.13, Table 3.17 and Table 3.18) are estimated average values applicable to soils in the Netherlands. The Kp values show a wide variability - several orders of magnitude - due to differences in:

- soil characteristics;
- soil moisture content;
- metal content;
- speciation of the metal.

There are also several questions under discussion including:

- How can the fraction of metals in the groundwater that is subject to transport (total concentration in pore water) be assessed?
- Which results are more reliable: sorption coefficients that are based on laboratory or field experiments?
- Under which conditions should (field and or laboratory) experiments be performed?
- How must we deal with changes in metal pore water concentration in time due to changes in soil moisture content?

The derivation of the bioavailable fraction, i.e. that part of the metals in the pore water that adversely affects soil organisms, is even more complex than the derivation of the fraction of metals in the groundwater subject to transport (Otte et al., 2000b).

At the moment there is no ideal set of Kp values available. However, the revised values are an improvement thanks to the better basis. Furthermore the revised Kp values are related to the significant fraction in the pore water. The revised Kp values are considered to be more appropriate for Dutch soils in the most relevant concentration range and, as they are average values, more appropriate for potential risk assessment.

Kp values are used for the calculation of pore water concentration in CSOIL, applying the equilibrium-partitioning concept. The derived pore water concentration is used for the derivation of SRC levels for groundwater. The revision of the procedure, including the effect of the revised Kp set, is described in Lijzen et al. (2001). Verbruggen et al. (2001) used Kp values to derive soil concentrations (risk limits) from aquatic toxicological data.

5.1.7. The overall effect of the revision of physicochemical data on calculated human exposure

Metals

The BCF is the only compound-specific parameter that influences the human exposure to metals. The revision of the BCF values cause a substantial increase (> factor 2) of the SRC_{human} level for cobalt (BCF from 0.02 to 0.58) and mercury (BCF from 0.02 to 0.15). The effect of the revision of the BCF for the other metals is smaller.

Organic compounds

The exposure to aromatic compounds is mainly via three exposure routes: the inhalation of indoor air, consumption of crops and ingestion of soil. The last mentioned exposure route is independent of selected physicochemical parameters (not sensitive to compound-specific parameters). Thus the effects of the revised physicochemical data set on the calculated exposure of compounds like polyaromatic hydrocarbons is limited. The two other exposure routes are sensitive to the selected S and Vp (by H constant, inhalation of indoor air), Kow (crop consumption) and Koc (both routes).

Differences between the current physicochemical data set (Van den Berg, 1995) and the revised data prevail. They are caused by differences in derivation and or selection methods. This accounts in particular for the Koc values. In contrast with the current Koc values (calculated from the Kow, section 2.1.6) the revised Koc values are based merely on measured data. Differences are also caused by the use of new data and the fact that vapour pressure and solubility are corrected for soil temperature. The use of solubility based Kow values (see section 2.1.2) and the use of estimated values for vapour pressure (Van den Berg, 1997) could be avoided.

The effect of the revised data on the SRC_{human} level was evaluated for each parameter separately in the preceding sections (5.1.2 - 5.1.4). The total effect on the SRC_{human} level of the revision of the physicochemical data (the combined effects of S, Vp, Kow and Koc revisions) for each compound can provide a substantially different picture. It is most likely that some alterations work contrarily.

For 39 compounds, the revision of the physicochemical data did not change the calculated human exposure significantly (more than a factor 2).

For 24 compounds, the revision of the physicochemical data leads to a higher exposure and lower SRC_{human} levels (Table 5.5). In general, the revision of the Koc has the largest effect and in many cases the exposure via the consumption of home-grown crops is the dominant route involved. Both Kow (plant uptake) and the Koc (concentration in pore water) largely affect this exposure route.

For nine compounds, the revision of physicochemical data leads to a lower exposure and to higher SRC_{human} levels.

In all cases, this concerns only the effect of the revision of the physicochemical data set. All the calculations were performed with the revised CSOIL model concept, the revised MPR values and the revised soil, site and exposure parameters.

Table 5.5: Effect of the revised physicochemical data on the SRC$_{human}$ level compared with the current data set (arranged in order of effect)

Compound	**Lower** 1) **SRC$_{human}$** 2) ***(higher exposure)***	**Main cause is the revision of:**	**Dominant exposure route**
Aldrin	<<<	Koc	crop consumption
Carbofuran	<<<	Kow/Koc	crop consumption
Tetrahydrofuran	<<<	Kow	perm. drinking water
Di(2-ethylhexyl)phthalate	<<<	Koc	crop consumption
Hexachlorobenzene	<<<	Koc	crop consumption
Carbaryl	<<<	Kow	crop consumption
Pentachlorobenzene	<<	Koc	inhalation inside
DDE	<<	Koc	crop consumption
PCB153	<<	Kow/Koc	crop consumption
Vinylchloride	<<	S,Vp (H)	inhalation inside
DDT	<	Koc/Kow	crop consumption
Cobalt	<	BCF	crop consumption
Mercury	<	BCF	crop consumption
α-HCH	<	S, Vp (H)	crop consumption
Dichloromethane	<	Koc/Kow	inhalation inside
PCB 28	<	Koc	crop consumption
γ-HCH	<	Koc	crop consumption
Cyclohexanone	<	Koc	crop consumption
m-Xylene	<	Koc	inhalation inside
1,2,3,4-Tetrachlorobenzene	<	Koc	crop consumption
Pentachlorophenol	<	Koc	crop consumption
Dieldrin	<	Kow/Koc	crop consumption
Endrin	<	Koc	crop consumption
Tetrachloromethane	<	Koc	inhalation inside

Compound	**Higher** 1) **SRC$_{human}$** 3) ***(lower exposure)***	**Main cause is the revision of:**	**Dominant exposure route**
p-Cresol	>>	Koc	crop consumption
Catechol	>>	Koc	crop consumption
2,3,4,5-Tetrachlorophenol	>	Koc	crop consumption
1,2-Dichloroethane	>	Koc	inhalation inside
1,2,4-Trichlorobenzene	>	Koc	inhalation inside
Tetrahydrothiophene	>	Koc	inhalation inside
Atrazine	>	Koc	crop consumption
Hydroquinone	>	Koc	crop consumption
Phenol	>	Koc	crop consumption

1) A higher exposure leads to a *potential* lower SRC$_{human}$ level. The effect of other revisions such as MPR$_{human}$, model concepts and the revision of soil, site and exposure parameters can change the picture. The same remark is made in the case of a *potential* higher SRC$_{human}$ level caused by a lower exposure.

2) <<<: the decrease of the SRC$_{human}$ is more than a factor 10
<< : the decrease of the SRC$_{human}$ is between a factor 5 and 10
< : the decrease of the SRC$_{human}$ is between a factor 2 and 5

3) >> : the increase of the SRC$_{human}$ is between a factor 5 and 10
> : the increase of the SRChuman is between a factor 2 and 5

5.1.8. Comparison with other data used for risk assessment

Appendix 6 gives the data as presented in 'Environmental Risk Limits in the Netherlands' (De Bruijn et al., 1999), the so-called INS data. It tabulates the data on vapour pressure, Henry's law constant, log Kow and log Koc for the compounds present in the revised CSOIL data set. By way of comparison, the revised data are also tabulated. The revised data are compared with the INS data (De Bruijn et al., 1999), using the same method and criteria as for the comparison of current and revised data (see sections 5.1.2 - 5.1.7).

Table 5.6 tabulates the compounds for which significant differences were encountered. Although differences are encountered, the two data sets are concluded to be, in the main, comparable. Comparing calculations with the INS data showed only significant differences on derived SRC$_{\text{human}}$ levels for nine compounds (outermost left column, with name of compound printed in **bold**).

Table 5.6: Comparison of revised physicochemical data with physicochemical INS data

Vapour pressure and /or H constant Δ > factor 5	**log Kow < 3.5: $\Delta > 0.3$ log Kow 3.5-4.5: $\Delta > 0.5$ log Kow > 4.5: $\Delta > 0.7$**	**log Koc < 3.5: $\Delta > 0.3$ log Koc 3.5-4.5: $\Delta > 0.5$ log Koc > 4.5: $\Delta > 0.7$**	**OVERALL effect on SRC human Δ > factor 2**
Benzo(a)anthracene	Carbofuran	**Aldrin**	Aldrin
Benzo(a)pyrene	2,3-Dichlorophenol	4-Chlorophenol	2,4-dichlorophenol
Benzo(k)fluoranthene	3,4-Dichlorophenol	**2,4-Dichlorophenol**	2,3,4-trichlorophenol
1,3,5-Trichlorobenzene	**2,3,4-Trichlorophenol**	**2,3,4-Trichlorophenol**	2,3,4,5-tetrachlorophenol
1,2,3,4-Tetrachlorobenzene	2,3,5-Trichlorophenol	2,4,6-Trichlorophenol	Dieldrin
1,2,3,5-Tetrachlorobenzene	**2,3,4,5-Tetrachlorophenol**	3,4,5-Trichlorophenol	γ-HCH
1,2,4,5-Tetrachlorobenzene	2,3,5,6-Tetrachlorophenol	**2,3,4,5-Tetrachlorophenol**	Tetrachloromethane
Pentachlorobenzene	**Dieldrin**	Dichloromethane	Pentachlorobenzene
Vinylchloride	Endrin	**Dieldrin**	Vinylchloride
		γ-HCH	
		Naphthalene	
		Styrene	
		Tetrachloromethane	
		o-Xylene	

Next, the observed differences will be briefly discussed.

Vapour pressure and Henry's law constant

Differences are found between the vapour pressure data of some PAHs. However, given the low volatility of PAHs (<< 1 Pa), these differences will not provoke alterations in calculated exposure.

Other differences in selected vapour pressure data concerns the tri- and tetrachlorobenzenes. The small set of underlying data can be the cause. The aggregation of the data for individual chlorobenzenes to one average value for di-, tri- and tetrachlorobenzenes is a possible solution. Appendix 6 also gives the values for ALL di-, tri- and tetrachlorobenzenes. The encountered differences have no serious effects on the calculated risk levels.

The INS vapour pressure value for pentachlorobenzene (2.2 Pa) is higher than the revised CSOIL value (0.452 Pa) and the current CSOIL value (0.133 Pa). The Henry's law constant selected by INS (experimental value) is lower than the revised Henry's law constant, which is calculated from vapour pressure and solubility (0.033 vs. 0.15, respectively). Calculations with the INS data lead to a higher (factor 2) SRC$_{\text{human}}$ level.

The vapour pressure for vinylchloride differs considerably from the INS value (33700 Pa). The revised CSOIL value is based on 17 values ranged from 181,000 to 341,000 Pa. The selected geometric mean is 298,000 Pa. The resulting Henry's law constant (18.5) also differs from the INS value (0.646). The INS value is a measured value. However, Van de Plassche and Bockting (1993) observed considerable differences between measured values (range 0.646 to 50). Because the Henry's law constant for the human risk assessment is critical (see outermost right column of Table 5.6:), it is recommended to determine the Henry's law constant and or the vapour pressure values for vinylchloride according to state-of-the-art quality standards.

Kow and Koc

The INS-log Koc selected for aldrin (5.11) differs by one log unit from the revised log Koc for aldrin (4; standard deviation 1, N=12), and two log units from the current Koc (7.01) according Van den Berg (1995). The LOGPSTAR value for aldrin (also used by INS) seems high compared with the CLOGP value and the average value from selected values (see Table 3.5: Log Kow values for all compounds). The INS Koc is a Kow-based partition coefficient according to Gerstl (1990). Because the Koc is a critical parameter it is recommended to evaluate the observed differences, if necessary completed with additional measurements. Also for other drins differences between INS log Kow and log Koc values and revised log Kow and log Koc values are observed. The revised set seems more consistent.
The INS log Koc selected for tetrachloromethane (2.83) differs from the revised log Koc (1.75). The INS log Koc is derived from the Kow value according to the empirical regression equation *Koc = Kow* (Van de Plassche and Bockting, 1993). The revised log Koc is based on 11 values (Table 3.6) ranging from 1.1 – 2.1.
The INS log Koc selected for carbofuran (1.63) matches well with the revised log Koc (1.64). The INS-log Kow (Bockting et al., 1993) is somewhat higher (2.32 against 1.63) which implies a higher plant uptake. The INS log Koc values for ethylbenzene, naphthalene, styrene, o-xylene and dichloromethane are somewhat higher (0.3 log unit) than the revised log Koc values. The effects of these differences are less than a factor 2 on the SRC_{human} level. Other differences are observed for some chlorophenols. The small set of underlying data may be the cause. The aggregation of the data for individual chlorophenols to one average value for di-, tri- and tetrachlorophenols is a possible solution. Appendix 6 gives the values for ALL di-, tri- and tetrachlorophenols. Calculations with the physicochemical data for ALL di-, tri- and tetrachlorophenols lead to comparable risk levels.

Summarising, it may be said that the two sets are comparable, taking into account the nature and expected uncertainty of physicochemical data (e.g. Koc values, see section 3.3). The differences found for aldrin and dieldrin remain unclear. Another matter for attention is the uncertainty of the derived data for vinylchloride (Vp and H) and, consequently. the uncertainty of the derived SCR_{human} for this compound.

5.2. The soil, site and exposure parameters

Table 5.7 gives an overview of all the parameters describing the CSOIL standard soil, the site and the exposure parameters for adults and children (also called the receptor characteristics). The site and exposure parameters are based on the user scenario 'residential with garden'. In chapter 2 it was explained that only the most critical parameters were selected for evaluation. For al the evaluated parameters, a current 1995 and a revised value are given; changes are given in bold. The revised parameters will be shortly discussed below. The relevant section for each evaluated parameter is given in the outermost right column.

Table 5.7: Current and revised soil, site and exposure parameters and constants

Parameters	**code**	**unit**	**current value (1995)**	**revised value (2000)**	**evaluated in section**
Soil parameters					
soil temperature	T	[K]	283		
volume fraction air	Va	[-]	0.2	0.2	4.2.2
volume fraction water	Vw	[-]	0.2	**0.3**	4.2.2
volume fraction soil	Vs	[-]	0.6	**0.5**	4.2.2
fraction organic carbon	foc	[-]	0.058	0.058[*1]	4.2.4
percentage clay	L	[%]	25	25[*1]	4.2.5
dry bulk density	SD	[kg/dm3]	1.5	**1.2**	4.2.3
pH	pH	[-]	6	6[*1]	4.2.6
Constants and site parameters					
gas constant	R	[Pa.m3/mol.K]	8.3144		
thickness boundary layer	d	[m]	0.005	**removed**	Rikken et al., 2001
flux of evaporating water	Ev	[m3/m2.d]	0.0001	**removed**	4.3.1
viscosity of air	ETA	[Pa.h)	-	**5 E-09**	4.3.6
mean depth of contamination	dp	[m]	1.25	1.25	4.3.2
air permeability of soil	KAPPA	[m2]	-	**1 E-11**	4.3.6
air-exchange rate	Vv	[1/h]	1.25	**1.1**	4.3.4
height of crawl space	Bh	[m]	0.5	0.5	4.3.3
depth of groundwater table	dg	[m]	-	**1.75**	4.3.2
height of the capillary transition boundary	z	[m]	-	**0.5**	4.3.2
air pressure difference crawl space and room	DELTAPCS	[Pa]	-	**1**	4.3.6
contribution of the crawl space air to indoor air	fbi	[-]	0.1	0.1	4.3.5
diameter contaminated area	Lp	[m]	100		
fraction dry matter root crops	fdwr	[-]	0.202	**0.167**	4.4.3
fraction dry matter leafy crops	fdws	[-]	0.117	**0.098**	4.4.3
deposition constant	dpconst	[kg/kg]	1.09E-03	**0.01**	Rikken et al., 2001
fraction soil in dust inside	frsi	[-]	0.8		
fraction soil in dust outside	frso	[-]	0.5		
dillution factor pore water-ground water	fdil	[-]	0.1	**removed**	Lijzen et al., 2001
temperature bath water	Tsh	[K]	313		
drinking water constant	dwconst	[-]	45.6		
Exposure parameters					
fraction exposed skin showering	fexp	[-]	0.4		
retention factor soil particles in lungs	fr	[-]	0.75		
relative sorption factor	Fa	[-]	1		
relative sorption factor soil ingestion	Fag	[-]	-	1 [*2]	Lijzen et al., 2001
matrix factor dermal uptake	fm	[-]	0.15		
showering period	tdc	[h per day]	0.25		
bathing period	td	[h]	0.5		
fraction contaminated root crops	Fvk	[-]	0.1	0.1	
fraction contaminated leafy crops	Fvb	[-]	0.1	0.1	

Table 5.7 continued

Exposure parameters	code	unit	children 1995	adults 1995	children 2000	adults 2000	evaluated section
body weight	BWc,a	[kg]	15	70			
daily intake soil	AIDc,a	[kg per day]	1.50E-04	5.00E-05	**1.00E-04**	5.00E-05	4.5.
consumption of root crops	Qk'c,a	[kg fw per day]	0.0748	0.1367	**0.0595**	**0.1220**	4.4.2.
consumption of leafy crops	Qb'c,a	[kg fw per day]	0.0761	0.1578	**0.0583**	**0.1390**	4.4.2.
consumption of drinking water	Qdw,c,a	[dm3 per day]	1	2			
dermal sorption coefficient	DACc,a	[kg per day]	6.43E-06	5.92E-06			
inhalation of soil particles	ITSPc,a	[kg per day]	3.13E-07	8.33E-07			
inhalation period indoors	Tiic,a	[h]	21.14	22.86			
inhalation period outdoors	Tioc,a	[h]	2.86	1.14			
air volume	Avc,a	[m3/h]	0.32	0.83			
body surface	Atotc,a	[m2]	0.95	1.8			
exposed surface skin indoors	Aexpc,a i	[m2]	0.05	0.09			
exposed surface skin outdoors	Aexpc,a o	[m2]	0.28	0.17			
degree of coverage skin indoors	DAEc,a i	[kg/m2]	5.6E-04	5.6E-04			
degree of coverage outdoors	DAEc,a o	[kg/m2]	5.1E-03	3.8E-02			
dermal absorption velocity	DARc,a	[1/h]	0.01	0.005			
period exposure through contact soil indoors	Tbci,a	[h per day]	9.14	14.86			
period exposure through contact soil outdoors	Tbco,a	[h per day]	2.86	1.14			
dillution velocity	Vfc,a	[m/h]	161.3	324.6			

*1 These values differ from the recommended values in Table 4.2: foc= 0.029, %clay= 15, pH= 5.2 (see text)
*2 Only for lead were enough data available to provisionally lower this Relative Absorption Factor to 0.6 (Lijzen et al., 2001).

Soil parameters

The soil parameters describe the standard soil as used in the CSOIL model. The SRC levels (both ecotoxicological as humantoxicological risk concentrations) are based on this *standard soil*. Two approaches for the determination of the standard soil were considered. In the evaluation (section 4.2) it was proposed to base the standard soil characteristics on a combination of two major Dutch soil types, which resulted in hypothetical representative soil characteristics. By mutual agreement it was decided to revise only a part of the recommended parameter values (see footnote Table 5.7). The implementation of the recommended standard soil characteristics in the procedure so as to derive ecotoxicological risk limits was one of the main constrains. Implementing all revised values in the future is recommended.
The impact of the revised values on the SRC_{human} is small. If the recommended value for foc were to be implemented, the SRC_{human} for most compounds would be halved. Changing the percentage of clay and pH would have an impact on the BCF and Kp for metals.

Constants and site parameters

The evaluation of the model concept for calculating the indoor air concentration led to removal of the thickness boundary layer (d) and the evaporation flux of water (Ev). The air-exchange rate of the crawl space (Vv) was based on more data, slightly changed. The evaluation of model concepts also led to the introduction of the constant viscosity of air (ETA) and the parameters air permeability of soil (KAPPA, κ), pressure difference between crawl space and soil air (DELTAPCS, ΔPcs), depth of the groundwater table (dg) and the capillary transition boundary (z). The revised parameters are described in section 4.3. Further details are given in Rikken et al. (2001). The impact of the changed model concept on the SRC_{human} is given in Lijzen et al. (2001). The impact of only the changed data (Vv) is small. A minor change is the revision of the fraction dry matter of vegetables and potatoes, leading to a slightly lower estimated accumulation of metals in crops. Another change for organic compounds is the higher value for deposition (better called 'soil resuspension'), of which the impact on the risk limit also depends on the change in the model concept for uptake by plants. The dillution factor of pore water to groundwater has been removed from the procedure. The main reason for this modification of the proposed derivation of SRC levels for groundwater is the lack of scientific backing for including this factor in the model, as described in Lijzen et al. (2001).

Exposure parameters
The daily intake of soil by children has been revised from 150 to 100 mg per day. This value is uncertain for specific children or situations but is based on a statistical interpretation of the reported yearly average soil ingestion rate of eight references (see section 4.5.2.). The impact of this change is small for most compounds, because a lifetime-averaged exposure is used. Only for lead, for which exposure to children is used, this change led to a higher human risk limit for soil. The daily intake of soil refers only to inadvertent soil ingestion. Pica behaviour, which can provoke acute toxicity effects (Calabrese et al., 1997), is considered to be outside the scope of potential risk assessment, but could be considered in the future. The daily soil ingestion rate by adults is maintained at 50 mg per day.
The fraction of contaminated crops is maintained at 0.1, although it can be argued that it does not describe the average situation in the Netherlands (section 4.4.4). The intake of root crops and leafy crops is revised for children and adults and leads to a lower exposure of about 10% for the exposure pathway of crop consumption. The relative sorption factor (Fag) for soil ingestion is maintained at one for all compounds except lead. Metals present in the soil matrix are considered less available for the human body than metals present in food (Sips et al., in prep.).

5.3. Recommendations

Evaluation and revision of the CSOIL parameters have resulted in a well-founded, state-of-the-art data set. The use of the revised data contributes to the improved derivation of SRC_{human} levels for soil, sediment and groundwater.
For vinylchloride uncertainty remains about the selected values for vapour pressure and Henry's law constant. Because both parameters are critical for the derived SRC_{human}, an additional study is recommended. This also applies to the Kow and Koc values selected for aldrin and dieldrin. Deviation of the selected values might be arguable, also for other compounds. However, it must be realised that the selected parameter values are meant for generic purposes (potential risk assessment) and moreover, the encountered uncertainties of physicochemical data must be balanced against the uncertainties of other parameters, model concepts and human toxicological risk levels (MTR).

In conclusion, the evaluation has broadened the information on the uncertainty and variation of the input parameters; it is recommended using this information to deal quantitatively with uncertainties in the risk assessment.
The revised data is also used (in part) for deriving ecotoxicological risk levels (SRC_{eco}). A further harmonisation with other related activities is desirable although it is realised that differences in objectives, starting points and selection criteria could constitute a possible obstacle.

References

Baars AJ, Theelen RMC, Janssen PJCM, Hesse JM, Van Apeldoorn ME, Meijerink MCM, Verdam, L; Zeilmaker MJ (2001): Re-evaluation of human-toxicological Maximum Permissible Risk levels. RIVM, Bilthoven. RIVM report 711701025.

Baes, C.F. Sharp, R.D., Sjoreen, A.L., and Shor, R.W. (1984) A review and analysis of parameters for assessing transport of environmentally released radionuclides. Compound data for organic solvents. Values used for further calculations through agriculture. Oak Ridge National Laboratory, USA. ORNL Report No. 5786. Available from National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Road, Springfield, Virginia 22161.

BEVER (1999). Van Trechter naar Zeef. UPR BEVER/Sdu , The Hague, October (in Dutch).

Binder, S.M.D. D.M.D. Sokal, D.M.A. Maughan, 1986. Estimating soil ingestion: the use of tracer elements in estimating the amount of soil ingested by young children. Archives of Environmental health, Vol 41, No 6, 341-345.

Bockting, G.J.M.; Van den Berg, R. (1992) The accumulation of trace metals in crops grown on contaminated soils. A literature study. RIVM, Bilthoven. RIVM report 725201009 (in Dutch).

Bockting, G.J.M., Van de Plassche, E.J., Struijs, J.; Canton, J.H. (1992) Soil-water partition coefficients for trace elements. RIVM, Bilthoven. RIVM report 679101003.

Bockting, G.J.M., Van de Plassche, E.J., Struijs, J.; Canton, J.H. (1993) Soil-water partition coefficients for organic compounds. RIVM, Bilthoven. RIVM report 679101013.

Bockting, G.J.M., J.G.M. Koolenbrander; F.A. Swartjes. (1996) SEDISOIL: Model for the calculation of human exposure due to contaminated sediments. RIVM, Bilthoven. RIVM report 715810011 (in Dutch).

Boerngen, J.H. and H.T. Shacklette (1980). Chemical analysis of fruits, vegetables and their associate soils from ares of commercial production in the conterminous United States. Geological survey, U.S.A open file report 80-84. United States.

Briggs, G.G., R.H. Bromilow, and A.A. Evans (1982) Relationship between lipophilicity and root uptake and translocation of non-ionised chemicals by barely. Pestic.Science, 13: 495-504.

Briggs, G.G., R.H. Bromilow, A.A. Evans, and M. Williams, (1983) Relationship between lipophilicity and distribution of non-ionised chemicals in barely shoots following uptake in roots. Pestic.Science, 14: 492-500.

Buchter, B., B. Davidoff, M.c. Amacher, C. Hinz, I.K. Iskander and H.M. Selim. 1989. Correlation of freundlich Kd and n retention parameters with soils and elements. Soil Science vol. 48: 370-379.

Chang, R.1981. Physical chemistry with applications to biological systems ; 2nd ed New York ; MacMilland.

Calabrese, E.J., R. Barnes, E.J. Stanek III, H. Pastides, C.E. Gilbert, P. Veneman, X. Wang, A. Lasztity, P. Kostecki, (1989) How much soil do young children ingest; an epidemiologic study. Regulatory Toxicology and Pharmacology, Vol 10, 123-137.

Calabrese, E.J., E.J. Stanek III, C.E. Gilbert and R.M. Barnes, 1990. Preliminary Adult Soil ingestion Estimates: Results of a pilot study. Regulatory toxicology and pharmacology 12, 88-95 (1990)

Calabrese, J., E.J. Stanek, R.C. James and S.M. Roberts. (1997) Soil ingestion: a concern for acute toxicity in Children. Environmental Health Perspectives 105.

Chang, R., 1990. Physical chemistry with applications to biological systems. Macmillan Publ. Co., New York (NY), USA.

Clausing, P, B. Brunekreef, J.H. van Wijnen, 1987. A method for estimating soil ingestion by children. Int. Arch. Occup. Environm. Health, Vol 59, 73-82

Crommentuijn, T., M.D. Polder and E.J. van de Plassche (1997). Maximum Permissable Concentrations and Negligable Concentrations for metals, taken background concentrations into account. RIVM, Bilthoven. RIVM report 679101019.

CRC Handbook of chemistry and physics, 79th edition, 1998.

Davis, S., P. Waller, R. Buschom, J. Ballou, and P. White (1990) Quantative estimates of soil ingestion in normal children between the ages 2 and 7: population based estimates using Al, Si and Ti as soil tracer elements. Archives of Environmental Health 45, 112-122.

De Bruijn, J., Crommentuijn, T., Van Leeuwen, K., Van der Plassche, E., Sijm, D. and Van der Weiden, M. (1999) Environmental Risk Limits in The Netherlands. RIVM, Bilthoven. RIVM report 601640 001.

Elzinga, E.J., B. van den Berg, J.J.M. van Grisven en F.A. Swartjes. 1997. Freundlich adsorptievergelijkingen voor cadmium, koper en zink in de bodem op basis van literatuurgegevens. RIVM, Bilthoven. RIVM report 711501001.

EUSES (1997) EUSES; the European Union System for the evaluation of substances; EUSES1.00 User Manual. TSA Group Delft BV, The Netherlands.

Fast, T., J. Kliest, H. van de Wiel, 1987. De bijdrage van verontreiniging van de lucht in woningen. Report no. 6 in de publicatiereeks Milieubeheer. VROM, Leidschendam, The Netherlands.

Franken, R.O.G., A.J. Baars, G.H. Crommentuijn and P.F. Otte (1999). Proposal for revised Intervention Values for petroleum hydrocarbons (‘minerale olie’) on base of fractions of petroleum hydrocarbons. RIVM, Bilthoven. RIVM report 7117015.

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

Hawley, J.K. (1985). Assessment of health risk from exposure to contaminated soil. Risk Analysis, Vol. 5, no. 4.

Herms, U. und G. Brümmer, (1980). Einfluss der Bodenreaktion au Löslichkeit und tolerierbare Gesamtgehalte an Nickel, Kupfer, Zink, Cadmium und Blei in Böden und kompostierten Siedlungsabfällen. landw. Forsch. 33(4): 408-423.

Hulshof, P.J.M., (1988). De groentenconsumptie van volkstuinders. Staatstoezicht op de Volksgezondheid, Rijswijk.

Jager, D.T., M.G.J. Rikken and P. van der Poel (1997). Uncertainty analysis of EUSES: Improving risk management by probabilistic risk assessment. RIVM, Bilthoven. report 679102039.

Janssen, R.P.T., P.J. Pretorius, W.G.J.M. Peijnenburg, M.A.G.T. van den Hoop (1996). Determination of field-based partition coefficients for heavy metals in Dutch soils and the realtionships of these coefficients sith soil characteristics. RIVM Bilthoven. RIVM report 719101023.

Janssen, R.P.T.; Peijnenburg, W.J.G.M.; Posthuma, L.; Van den Hoop, M.A.G.T. (1997) Equilibrium partitioning of heavy metals in Dutch field soils. I. Relationship between metal partition coefficients and soil characteristics. Environ. Toxicol. Chem. 16: 2470-2478.

Karickhoff, S.W., Brown, D.S. and Scott, T.A. (1979). Sorption of hydrophobic pollutants on natural sediments. Water Res. 13: 241-248.

Karickhoff, S.W. (1981). Semi-empirical estimation of sorption of hydrophobic pollutants on natural sediments and soils. Chemosphere 10(8): 833-846.

King, L.D. (1988). Retention of metals by several soils of the Southeastern United States. Journal of Environmental Quality, 17(2): 239-250.

Kliest, J.J.G. (1991). Vaststelling van de potentiële en actuele inhalatoire blootstelling als gevolg van bodemverontreiniging. RIVM, Bilthoven. Report 725201004.

Koops, R., J.J.M. van Grinsven, T. Crommentuijn, M.A.G.T. van den Hoop, F.A. Swartjes, P.R.G. Kramer and W.J.G.M. Peijnenburg (1998). Evaluatie van door het RIVM gehanteerde partitiecoëfficiënten voor metalen. RIVM, Bilthoven. RIVM report 711401005.

Koorevaar , P, G. Menelik, C. Dirksen (1983). Elemenst of Soil Physics. Developments in Soil Science 13. Elsevier, Amsterdam.

Köster , H.W. (2001). Risk assessment of historical soil contamination with cyanides; origin, potential human exposure and evaluation of Intervention Values. RIVM, Bilthoven. RIVM report 711701019.

Kreule, P.; Swartjes, F.A. (1998) Proposals for Intervention Values for soil and groundwater, including the calculation of the human-toxicological serious soil contamination concentrations: fourth series of compounds. RIVM report 711701005.

Lagas, P. and Groot, M.S.M. (1996). Bodemkwaliteitskartering van de nederlandse landbouwgronden. RIVM, Bilthoven. RIVM report 714801003.

Lee, L.S., P.S.C. Rao, and M.L. Brusseau (1991). Nonequilibrium sorption and transport of neutral and ionized compounds. Environ. Sci. Tech., 25: 722-729.

Linders, J.B.H.L. (1990). Risicobeoordeling voor de mens bij blootstelling aan stoffen. Uitgangspunten en veronderstellingen. RIVM, Bilthoven. RIVM report 725201003.

Lijzen, J.P.A.; Baars, A.J.; Crommentuijn, G.H.; Otte, P.F.; Plassche, E. van de; Rikken, M.G.J. ; Rompelberg, C.J.M.; Sips, A.J.A.M.; Swartjes, F.A. (1999). Revision of the Intervention value for lead; evaluation of the Intervention Values derived for soil/sediment and groundwater. RIVM, Bilthoven. RIVM report 711701013 (in Dutch).

J.P.A. Lijzen, A.J. Baars, P.F. Otte, M. Rikken, F.A. Swartjes, E.M.J. Verbruggen and A.P. van Wezel (2001). Technical evaluation of the Intervention Values for Soil/sediment and Groundwater. Human and ecotoxicological risk assessment and derivation of risk limits for soil, sediment and groundwater. RIVM, Bilthoven. report 711701 023.

Mackay D., S. Paterson, B. Cheung, W. Brock Neely (1985). Evaluating the environmetal behaviour of chemicals with a level III fugacity moel. Chemosphere 14: 335-374.

McKone T.E. and K.T. Bogen (1990). Uncertainty in exposure and health risk assessment: An integrated approach. Livermore, Lawrence Livermore National Laboratory, 90-186.2.

Medchem (1996). Database and calculation method for Kow values (developed at Pomona College, Claremont, California, and described by Leo et al., 1971).

Mensink, B.J.W.G. M. Montforts, L. Wijkhuizen-Máslankiewics, H. Tibosch and J.B.H.J. Linders. (1995). Manual for summarising and evaluating the environmental aspects of pesticides. RIVM, Bilthoven. RIVM report 679101022.

Ng, Y.C.., Cosher, Y.C., and Thompson, S.E. (1982). Soil-to-plant concentration factors for radiological assessments. Washington, Lawrence Livermore National laboratory. Reportnumber, NUREG/CR-2975 UCID-19463.

Otte, P.F, M. van Elswijk, M. Bleijenberg, F. Swartjes en C. van de Guchte (2000a). Calculation of human risk limits voor sediments; Discussion report RIZA-werkdocument 2000.084x (in Dutch). Bilthoven/Lelystad, mei 2000.

Otte, J.G., P.F.A.M. Römkens, A. Tiktak and W. de Vries (2000b). Partitie relaties voor zware metalen (Cd, Cu, Pb, Zn) voor diffuus verontreinigde Nederlandse bodems (in Dutch). PGBO, Wageningen. Reports PGBO, deel 30, 44pp.

Rikken, M.G.J, J.P.A. Lijzen and A.A. Cornelese (2001). Evaluation of model concepts on human exposure; proposals for updating of the most relevant exposure routes of CSOIL. RIVM, Bilthoven. RIVM 711701022.

Sauerbeck, D. (1989) Der Transfer von Schwermetallen in die Pflanze: Die Beurteilung von Schwermetallkontaminationen im Bodem. DECHEMA, Frankfurt am Main, ISBN 3-926959-06-1.

Sabljić, A., Güsten, H., Verhaar, H. and Hermens, J. (1995). Qsar modelling of soil sorption. Improvement and systematics of log Koc vs. log Kow correlations. Chemosphere 31 (11-12); 4489-4514.

Sauvé, S.; Henderschot, W.; Allen, H.E. (2000). Solid-solution partitioning of metals in contaminated soils: dependence on pH, total metal burden and organic matter. Environ. Sci. Technol. 34:1125-1131.

Sheppard, S.C., W.G. Evenden (1992). Contaminant enrichment of sparingly soluble contaminants (U, Th and Pb) by erosion and by soil adhesion to plants and skin. Environmental Geochemistry and Health 14 121-131

Silvers, A., B.T. Florence, D.L. Rourke, R.J. Lorimor (1994). How children spend their time: A sample survey for use in exposure and risk assessment. Risk Analysis, Vol. 14, No. 6: 931-944

Simon, S.L. (1998). Soil ingestion by humans: a review of history, data and etiology with application to risk assessment of radioactively contaminated soil. Health Physics, Volume 74, No 6, pp 647-672.

Sips AJAM, Bruil MA, Dobbe CJG, van de Kamp E, Pereboom DPKH, Rompelberg CJM, Zeilmaker MJ. (in preparation). Bioaccessibility of contaminants from ingested soil in humans assessed in an in vitrodigestion model. - I. a) Project definition, b) optimisation and c) results for lead and benzo[a]pyrene. RIVM, Bilthoven. RIVM report 711701 012.

Stanek III, E.J. and E.J. Calabrese (1995a). Daily estimates of soil ingestion in children. Environmental health perspectives 103, no 3, pp 276-285.

Stanek III, E.J. and E.J. Calabrese (1995b). Soil ingestion estimates for use in site evaluations based on the best tracer method. Hum. Ecol. Risk Assess. Vol 1, No 2, pp 133-156.

Staples. C.A., D.R. Peterson, T.F. Parkerton and W.J. Adams (1997). The environmenta fate of phthalate esters: A literature review. Chemosphere 35 (4): 667-749.

Steenwijk, J.M. van, G. Cornelissen, Th.E.M. Ten Hulscher (1999). Omgaan met verdelingscoëfficiënten voor organische verbindingen. RIZA rapport 99.023, Lelystad.

Stoop, P., P. Glastra, Y. Hiemstra, L. de Vries and J. Lembregts (1998). Results of the second Dutch national survey on radon in dwellings. RIVM, Bilthoven. RIVM report 610058006).

Swartjes, F.A. (1999). Risk-based assessment of soil and groundwater quality in the Netherlands: Standards and remediation urgency. Risk Anal. 19:1235-1249.

Trapp, S. and M. Matthies (1995). Generic one-compartment model for uptake of organic chemicals by foliar vegetation. Environmental Science and Technology, vol. 29, no.9, 2333-2338.

United States Environmental Protection Agency (1997). Exposure Factors Handbook Volume I – General Factors. EPA/600/P-95/002Fa. Update to Exposure Factors Handbook. EPA/600/8-89/043.

United States Environmental Protection Agency (1996). Soil Screening Guidance: Technical Background Document. Publication 9355.4-17A.

Van den Berg, R. and Roels, J.M. (1991). Assessment of risks to man and the environment in case of exposure to soil contamination. Integration of the results of the preceding studies. RIVM, Bilthoven. RIVM report 725201013.

Van den Berg, R. (1995). Exposure of man to soil contamination. A qualitative and quantitative analysis, resulting in proposals for human-toxicological C values. RIVM, Bilthoven, Revised version of RIVM report 725201011.

Van den Berg, R. (1997). Verantwoording van gegevens en procedures voor de 1e tranche interventiewaarden: van RIM-rapporten naar de Notitie interventiewaarden bodemsanering. RIVM, Bilthoven. RIVM report 715810012.

Van de Plassche, E.J., and G.J.M. Bockting (1993). Towards integrated environmental quality objectives for several volatile compounds. RIVM, Bilthoven, RIVM report 679101011.

Van der Heyden and Hofman (1987). Bemonstering van drinkwater op plaatsen van bodemverontreiniging. SBD-36104. Gemeentelijke Drinkwaterleiding Rotterdam.

Van den Hoop, M.A.G.T. (1995). Metal speciation in Dutch soils: Field based partition coefficients for heavy metals at background levels. RIVM, Bilthoven. RIVM report 719191913.

Van de Ven-Breken, T.J., J. Brenot, S. Bonnefous, H. Noordijk, H.P. Leenhouts (1990). Consumption of food in EC countries, CEC research programme Post Chernobyl, Action 5: Underlying data for derived emergency reference levels. RIVM, Bilthoven. RIVM report 243402002.

Van Gestel, C.A.M., E.M. Dirven-van Breemen. J.W. Kamerman (1992). Beoordeling van gereinigde grond IV. Toepassing van bioassays met planten en regenwormen op referentiegronden. RIVM, Bilthoven. RIVM report 216402004.

Van Wezel, A.P. Van Vlaardingen, P.; Posthumus, R.; Crommentuijn, G.H.; Sijm, D.T.H.M. (2000) Environmental risk limits for two phthalates, with special emphasis on endocrine disruptive properties. Ecotoxicol. Environ. Saf. 46:305-321.

Van Wijnen, J.H., P. Clausing, B. Brunekreef (1990). Estimated soil ingestion by children. Environmental Research, Vol 51, 147-162.

Verbruggen, E.M.J., R. Posthumus and A.P. van Wezel, (2001) Ecotoxicological Serious Risk Concentrations for soil, sediment and water: updated proposals for first series of compounds. RIVM, Bilthoven. RIVM report 711701020.

Verschueren, K. en R. Kolkhuis Tanke (1989). Risicoindexen voor bodem- en grondwaterbedreigende stoffen. Micon milieuconsultants, 1989, rapportnr. 050153-4.

Versluijs, C.W., R. Koops, P. Kreule and M.F.W. Waitz (1998). The accumulation of soil contaminants in crops, location-specific calculation based on the CSOIL module. RIVM, Bilthoven. RIVM report 711701008.

Versluijs, C.W., and P.F. Otte (in preparation). Accumulation of metals in plants as function of soil type. RIVM, Bilthoven. RIVM report 711701024 (in Dutch).

Vissenberg, H.A., and F.A. Swartjes (1996). Evaluatie van de met CSOIL berekende blootstelling, middels een op Monte Carlo-technieken gebaseerde gevoeligheids- en onzekerheidsanalyse. RIVM, Bilthoven. RIVM rapport 715810018.

Voedingscentrum, Den Haag (1998). Zo eet Nederland. Resultaten van de voedselconsumptiepeiling 1997-1998.

Vonk, M.W. (1985). Permeation of organic chemicals through piping materials. Mededelingen no. 85, KIWA, Nieuwegein, The Netherlands (in Dutch), also in: H2O, 18: 529-538 (in Dutch).

Vries, F. de (1994). Een fysisch-chemische karakterisering van de bodemeenheden van de Bodemkaart van Nederland, schaal 1:50,000, met onderscheid naar grondgebruik. Rapport 286. DLO-Staring Centrum, Wageningen, 1994.

VROM (1988). Premises for risk management (annex to the Dutch Environmental Policy Plan). Lower House, session 1988-1989, 21 137, no. 5.

VROM, Ministry of, (1994). Ministerial Circular on second phase remediation paragraph, Soil Protection. Act. Reference DBO/16d94001.

VROM, Ministry of, (1995). Urgentie van bodemsanering; de handleiding. SDU, Den Haag , 1995 (ISBN 9012082218).

VROM, Ministry of, (1999). Governmental view on the soil use specific and cost-effective approach of soil contamination (in Dutch). Tweede Kamer 1999-2000, 25411, no 7.

Waitz, M.F.W., J.I. Freijer, P. Kreule and F.A. Swartjes (1996). The Volasoil risk assessment model based on CSOIL for soils contaminated with volatile compounds. RIVM, Bilthoven, RIVM report 715810014.

Wösten, J.H.M., G.J. Veerman, J. Stolte (1994). Waterretentie- en doorlatendheidkarakteristieken van boven- en ondergronden in Nederland: De Staringreeks. New edition 1994. DLO-Staring centrum, Wageningen, The Netherlands. Technische Document 18.

Mailing List

1- 6	DGM/BWL-directeur, Drs. J.A. Suurland
7	Plv. Directeur-Generaal Milieubeheer, VROM, Dr.ir. B.C.J. Zoeteman
8	Directoraat-Generaal Milieubeheer, Directie Bodem, Water en Landelijk gebied, Afdeling Landelijk gebied en Bodembeheer, Dr. J.M. Roels
9	Hoofdinspectie van de Volksgezondheid voor de Milieuhygiëne, Mr. G.J.R. Wolters
10-14	Regionale Inspecties van de Volksgezondheid voor de Milieuhygiëne
15	Mr. drs. A. Gravesteijn (DGM/BWL)
16	Drs. N.H.S.M. de Wit (DGM/BWL)
17	Dr. ir. A.E. Boekhold (DGM/BWL)
18	Dr. T. Crommentuijn (DGM/BWL)
19	Mr. A.B. Holtkamp (DGM/LMV)
20	Dr. J.A. van Zorge (DGM/SAS)
21	Dr. M.E.J. van der Weiden (DGM/SAS)
22-44	Onderzoeksbegeleidingsgroep ECO, via dr. D.T.H.M. Sijm (RIVM-CSR)
45-61	Onderzoeksbegeleidingsgroep HUMAAN, via ir. J.P.A. Lijzen (RIVM-LBG)
62-70	Leden Werkgroep UI, via Dr. T. Crommentuijn (DGM/BWL)
71	VNG/WEB, via J. Verburg (VNG, Den Haag)
72	IPO/ABO, via F. Kok (Prov. Zuid-Holland, Den Haag)
73	NARIP, via Dr. H. Leenaers (NITG-TNO, Delft)
74	ONRI-werkgroep bodem, via Drs. M.F.X. Veul (Witteveen en Bos, Deventer)
75	CLARINET, via Mr. H. Kasamas (CLARINET office, Vienna, Austria)
76	Dr. N. Earl (University of Nottingham, UK)
77	Ir. C. Cornelis (VITO, Belgium)
78	Dr. D. Müller (Umweltbundesamt, Vienna ,Austria)
79	Dr. R. Bonnart (INERIS, Verneuil-en-Halatte, France)
80	Dr. J. Brogan (EPA, Dublin, Ireland)
81	Dr. F. Quercia (ANPA, Rome, Italy)
82	Dr. C. Jorge (LNEC, Lissabon, Portugal)
83	Dr. J. Sovari (Finish Environment Institute, Helsinki, Finland)
84	Dr. J. Vegter (TCB, Den Haag)
85	Ir. T.M. Lexmond (WUR, Wageningen)
86	Drs. J. Wezenbeek (Grontmij, Houten)
87	Ing. P.J. Smit (Van Hall Instituut, Groningen)
88	Dr. ir. P. Römkens (Alterra, Wageningen)
89	Dr. ir. W. de Vries (Alterra, Wageningen)
90	Dr. B. Bosveld (Alterra, Wageningen)
91	Dr. N. Earl (University of Nottingham)
92	Drs. P. Kreule (TAUW)
93	Drs. M.F.W. Waitz (TAUW)
94	Drs. C. diMauro (TNO-MEP)
95	Dr. A. Sinke (TNO-MEP)
96	Drs. J. Tuinstra (IWACO)
97	Dr. I. Canter-Cremers (IWACO)
98	Drs. E. van der Plassche (Haskoning)
99	Dr. V. Dries (OVAM)
100	Dr. J. Vink (RIZA)
101	Drs. M. van Elswijk (RIZA)
102	Ir. A.B. Roeloffzen (Gemeentewerken Rotterdam)
103	Depot Nederlandse Publikaties en Nederlandse Bibliografie
104	Directie van het Rijksinstituut voor Volksgezondheid en Milieu

105 Prof.ir. N.D.van Egmond (dir. Milieu)
106 Ir. F. Langeweg (dir. Sector Milieuonderzoek)
107 Dr. ir. G. de Mik (dir. Sector Stoffen en Risico's)
108 Dr. W.H. Könemann (hCSR)
109 Ir. R. van den Berg (hLBG)
110 Ir. J.J.G. Kliest (hIEM)
111 Dr. R.C.G.M. Smetsers (hLSO)
112 Ir. A.H.M. Bresser (hLWD)
113 Dr. A. Opperhuizen (hLEO)
114 Drs. J.H. Canton (hECO)
115 Dr. A.P. van Wezel (CSR)
116 Prof.dr. C.J. van Leeuwen (CSR)
117 Dr. D.T.H.M. Sijm (CSR)
118 Drs. T.G. Vermeire (CSR)
119 Ing. P. Janssen (CSR)
120 Drs. M.G.J. Rikken (CSR)
121 Dr. E.M.J. Verbruggen (CSR)
122 Dr. A.J. Baars (CSR)
123 Dr. T. Traas (CSR)
124 Drs. D.T. Jager (ECO)
125 Dr. W. Peijnenburg (ECO)
126 Dr. L. Posthuma (ECO)
127 Dr. M. Rutgers (ECO)
128 Dr. A.J.A.M. Sips (LBM)
129 Dr. M.P.M. Janssen (LSO)
130 Drs. B.J. de Haan (LBG)
131 Dr. H.W. Köster (LBG)
132 Ir. R.O.G. Franken (LBG)
133- 137 Auteurs
138 SBD/Voorlichting and Public Relations
139 Bureau Rapportenregistratie
140 Bibliotheek RIVM
141 Bibliotheek RIVM, depot LBG
142 Bibliotheek CSR
143-170 Bureau Rapportenbeheer
171-180 Reserve exemplaren

Appendix 1: Current CSOIL-1995 input parameter set

Physicochemical parameters **Metals**	**M** **[g.mol-1]**	**BCF-metal root crop** **[-]**	**BCF-metal leafy crop** **[-]**	**BCF-metaal overall** **[-]**	**Kp** **[dm3/kg]**
Arsenic	74.9	0.015	0.030	0.021	980
Barium	137.3	0.005	0.100	0.043	60
Cadmium	112.4	0.150	0.700	0.370	190
Chromium (III)	52.0	0.002	0.020	0.009	14400
Cobalt	58.9	0.015	0.030	0.021	120
Copper	63.5	0.100	0.100	0.100	540
Mercury	200.6	0.015	0.030	0.021	3300
Lead	207.2	0.001	0.030	0.013	2400
Molybdenum	95.9	0.015	0.300	0.129	20
Nickel	58.7	0.070	0.100	0.082	560
Zinc	65.4	0.100	0.400	0.220	250

Physicochemical parameters **Aromatic compounds**	**M** **g.mol-1**	**S** **mg/dm3**	**Vp** **Pa**	**H** **[-]**	**log Kow** **[-]**	**Koc** **[-]**	**Dpe** **m2 per day**	**pKa** **[-]**
Benzene	78	1.78E+03	1.01E+04	1.88E-01	2.13	1.74	1.40E-06	
Ethylbenzene	102	1.52E+02	9.33E+02	2.66E-01	3.15	2.76	2.10E-06	
Phenol	94	8.20E+04	2.67E+01	1.30E-05	1.46	1.07	8.50E-09	
p-Cresol	108	2.40E+04	5.33E+00	1.02E-05	2.00	1.61	1.00E-06	
Toluene	90	5.15E+02	2.94E+03	2.18E-01	2.69	2.30	1.20E-06	
m-Xylene	102	1.80E+02	8.01E+02	1.93E-01	3.20	2.81	1.60E-06	
Catechol	110	4.51E+05	1.33E+02	1.38E-05	0.88	0.49	1.00E-07	
Resorcinol	110	8.40E+05	1.33E+02	7.40E-06	0.78	0.39	1.00E-07	
Hydroquinone	110	5.90E+04	1.34E+02	1.06E-04	0.55	0.16	1.00E-07	
PAH								
Naphthalene	130	3.00E+01	2.27E+00	4.18E-03	3.36	2.97	5.00E-07	
Anthracene	178	7.50E-02	1.30E-04	1.31E-04	4.49	4.10	5.00E-07	
Phenanthrene	178	1.60E+00	2.41E-03	1.14E-04	4.54	4.15	5.00E-07	
Fluoranthene	202	2.65E-01	2.31E-04	7.48E-05	5.33	4.94	2.00E-07	
Benzo(a)anthracene	228	1.00E-02	5.51E-06	5.34E-05	5.61	5.22	2.00E-07	
Chrysene *)	228	1.50E-03	2.60E-07	1.68E-05	6.64	6.25	2.00E-07	
Benzo(a)pyrene	252	3.00E-04	1.31E-08	4.68E-06	6.35	5.96	2.00E-07	
Benzo(ghi)perylene	276	2.60E-04	2.60E-09	1.17E-06	6.00	5.61	2.00E-07	
Benzo(k)fluoranthene	252	6.00E-04	2.60E-09	4.64E-07	6.84	6.45	2.00E-07	
Indeno, 1,2,3-cd pyrene	276	1.00E-04	2.60E-09	3.05E-06	7.43	7.04	2.00E-07	
Chlorinated hydrocarbons								
1,2-dichloroethane	99	8.69E+03	8.14E+03	3.94E-02	1.45	1.06	3.00E-07	
Dichloromethane	85	2.00E+04	4.66E+04	8.42E-02	1.87	1.48	5.00E-07	
Tetrachloromethane	154	8.00E+02	1.20E+04	9.82E-01	2.64	2.25	8.00E-07	
Tetrachloroethene	166	1.50E+02	1.87E+03	8.78E-01	2.60	2.21	7.70E-07	
Trichloromethane	120	8.00E+03	2.14E+04	1.36E-01	1.97	1.58	1.00E-06	

Physicochemical parameters	M	S	Vp	H	log Kow	Koc	Dpe	pKa
Aromatic compounds	g.mol-1	mg/dm3	Pa	[-]	[-]	[-]	m2 per day	[-]
Trichloroethene	132	1.10E+03	8.01E+03	4.07E-01	2.71	2.32	1.60E-06	
Vinylchloride	63	1.10E+03	3.55E+05	8.57E+00	2.71	2.32	1.00E-06	
Monochlorobenzene	113	5.00E+02	1.17E+03	1.12E-01	2.81	2.42	3.50E-06	
1,4-Dichlorobenzene	147	4.90E+01	8.00E+01	1.02E-01	3.40	3.01	2.00E-06	
1,2,4-Trichlorobenzene	182	1.90E+01	1.87E+01	7.59E-02	4.06	3.67	1.00E-06	
1,2,3,4-Tetrachlorobenzene	216	3.50E+00	5.34E-01	1.40E-02	4.70	4.31	1.00E-06	
Pentachlorobenzene	251	2.40E-01	1.33E-01	5.90E-02	5.17	4.78	1.00E-06	
Hexachlorobenzene	285	1.10E-01	1.33E-03	1.46E-03	5.34	4.95	1.00E-06	
2-Chlorophenol	129	2.85E+04	1.07E+02	2.05E-04	2.39	2.00	4.80E-09	8.43
2,4-Dichlorophenol	163	4.60E+03	1.33E+01	2.00E-04	3.15	2.76	1.00E-07	7.81
2,3,4-Trichlorophenol	198	1.19E+03	1.07E+00	7.55E-05	3.88	3.49	5.40E-07	7.01
2,3,4,5-Tetrachlorophenol	232	1.25E+02	1.33E-01	1.05E-04	3.35	2.96	1.00E-06	6.07
Pentachlorophenol	267	1.40E+01	1.47E-02	1.19E-04	5.13	4.74	2.24E-06	4.85
1-Chloronaphatalene	163	2.24E+01	5.25E+00	1.62E-02	3.85	3.46	5.00E-07	
2,5,2'-Trichlorobiphenyl (PCB 18)	258	2.25E-01	7.00E-04	3.40E-04	5.60	5.21	5.00E-07	
Hexachlorobiphenyl	361	1.20E-02	7.00E-04	8.95E-03	6.57	6.18	2.00E-07	
Pesticides								
DDT	355	3.10E-03	2.53E-05	1.23E-03	6.18	5.79	5.00E-07	
DDE	318	4.00E-02	1.33E-05	4.49E-05	5.73	5.34	5.00E-07	
Aldrin	365	1.00E-02	3.07E-03	4.76E-02	7.40	7.01	5.00E-07	
Dieldrin	381	1.00E-01	2.40E-05	3.89E-05	5.36	4.97	5.00E-07	
Endrin	393	2.00E-02	2.67E-05	2.23E-04	4.95	4.56	5.00E-07	
α-HCH	291	1.63E+00	3.33E-03	2.53E-04	3.72	3.33	5.00E-07	
β-HCH	291	2.40E-01	3.73E-05	1.92E-05	3.72	3.33	5.00E-07	
γ-HCH	291	7.80E+00	2.13E-02	3.38E-04	3.72	3.33	5.00E-07	
δ-HCH	291	3.14E+01	2.26E-03	8.90E-06	3.72	3.33	5.00E-07	
Carbaryl *)	201	1.20E-01	6.67E-01	4.75E-01	5.37	4.98	2.00E-07	
Carbofuran *)	221	5.00E-01	2.70E-03	5.07E-04	4.95	4.56	2.00E-07	
Maneb	265	1.00E-04	1.00E-04	1.13E-01	7.43	7.04	2.00E-07	
Atrazine	216	7.00E+01	4.00E-05	5.23E-08	2.18	1.79	2.00E-07	
Others								
Cyclohexanone *)	98	2.30E+04	5.33E+02	9.65E-04	1.83	1.44	1.00E-07	
Butylbenzylphthalate	312	2.90E+00	1.15E-03	5.26E-05	4.44	4.05	2.00E-06	
Di(2-ethylhexyl)phthalate	390	2.85E-01	8.60E-04	5.00E-04	5.12	4.73	2.00E-06	
Pyridine *)	79	2.33E+02	3.11E+03	4.48E-01	3.16	2.77	2.00E-06	
Styrene	104	3.00E+02	6.67E+02	9.83E-02	3.09	2.70	2.00E-06	
Tetrahydrofuran *)	72	2.18E+02	1.02E+05	1.43E+01	3.18	2.79	2.00E-06	
Tetrahydrothiophene *)	88	1.06E+01	2.41E+03	8.52-00	4.06	3.67	2.00E-06	

*) For compounds marked with a star the physicochemical parameters were changed in 1998 as recommended by Van den Berg (1997). In the above table the values are according Van den Berg (1995).

Soil parameters	**unit**	**code**	**current value (1995)**
soil temperature	[K]	T	283
volume fraction air	[-]	Va	0.2
volume fraction water	[-]	Vw	0.2
volume fraction soil	[-]	Vs	0.6
fraction organic carbon	[-]	foc	0.058
percentage clay	[%]	L	25
dry bulk density	[kg/dm3]	SD	1.5
pH	[-]	pH	6
constants			
gas constant	[Pa.m3/mol.K]	R	8.3144
thickness boundary layer	[m]	d	0.005
flux of evaporating water	[m3/m2.d]	Ev	0.0001
viscosity of air	[Pa.h)	ETA	-
mean depth of contamination	[m]	dp	1.25
air permeability of soil	[m]	KAPPA	-
air-exchange rate	[1/h]	Vv	1.25
height of crawl space	[m]	Bh	0.5
air pressure difference crawl space and room	[Pa]	DELTAPCS	-
contribution of the crawl space air to indoor air	[-]	fbi	0.1
diameter contaminated area	[m]	Lp	100
fraction dry matter root crops	[-]	fdwr	0.202
fraction dry matter leafy crops	[-]	fdws	0.117
deposition constant	[-]	dpconst	1.09E-03
fraction soil in dust inside	[-]	frsi	0.8
fraction soil in dust outside	[-]	frso	0.5
dillution factor pore water-ground water	[-]	fdil	0.1
temperature bath water	[K]	Tsh	313
drinking water constant	[-]	dwconst	45.6
exposure parameters			
fraction exposed skin showering	[-]	fexp	0.4
retention factor soil particles in lungs	[-]	fr	0.75
relative sorption factor	[-]	Fa	1
relative sorption factor soil ingestion	[-]	Fag	-
matrix factor dermal uptake	[-]	fm	0.15
showering period	[h per day]	tdc	0.25
bathing period	[h]	td	0.5
fraction contaminated root crops	[-]	Fvk	0.1
fraction contaminated leafy crops	[-]	Fvb	0.1

exposure parameters for adults and children	**code**	**unit**	**children** **1995**	**adults** **1995**
body weight	BWc,a	[kg]	15	70
daily intake soil	AIDc,a	[kg dm per day]	1.50E-04	5.00E-05
consumption of root crops	Qk'c,a	[kg fw per day]	0.0748	0.1367
consumption of leafy crops	Qb'c,a	[kg fw per day]	0.0761	0.1578
consumption of drinkwater	Qdw,c,a	[dm3 per day]	1	2
dermal sorption coefficient	DACc,a	[kg per day]	6.43E-06	5.92E-06
inhalation of soil particles	ITSPc,a	[kg per day]	3.13E-07	8.33E-07
inhalation period indoors	Tiic,a	[h]	21.14	22.86
inhalation period outdoors	Tioc,a	[h]	2.86	1.14
air volume	Avc,a	[m3/h]	0.32	0.83
body surface	Atotc,a	[m2]	0.95	1.8
exposed surface skin indoors	Aexpc,a i	[m2]	0.05	0.09
exposed surface skin outdoors	Aexpc,a o	[m2]	0.28	0.17
degree of coverage skin indoors	DAEc,a i	[kg/m2]	5.6E-04	5.6E-04
degree of coverage outdoors	DAEc,a o	[kg/m2]	5.1E-03	3.8E-02
dermal absorption velocity	DARc,a	[1/h]	0.01	0.005
period exposure through contact soil indoors	Tbci,a	[h per day]	9.14	14.86
period exposure through contact soil outdoors	Tbco,a	[h per day]	2.86	1.14
dillution velocity	Vfc,a	[m/h]	161.3	324.6

Appendix 2: Evaluation of databases and selection of physicochemical parameter values.

1. Database analysis

Chemical databases can be used for extracting values for a number of CSOIL input parameters. Values for the following input parameters, indispensable for the calculation of human exposure, can be found in these databases:

- molecular weight;
- solubility;
- vapour pressure;
- dissociation exponent;
- octanol-water partition coefficient (K_{ow});
- organic carbon normalised soil-water partition coefficient (K_{oc}).

To prevent that much time will be spent on searching, it is recommended to restrict the number of databases that will be searched for. To evaluate which databases contain the most and the most reliable values for of the above mentioned physicochemical properties, the following databases were examined:

- Merck
- Chemiekaarten;
- Merck Safety Data Sheet;
- International Chemical Safety Cards;
- Beilstein;
- HSDB: Hazardous Substance Data Bank;
- Ohmtads;
- Cheminfo;
- CESARS: Chemical Evaluation Search and Retrieval System;
- Pesticide Manual 11th edition.
- Medchem;
- ASTER;

The database ‘Epiwin’, which in fact is a computer program which calculates values for parameters for organic compounds, is not used for this database analysis.

The 11 organic compounds, for which the databases are searched, are:

- Hydroquinone;
- Vinyl Chloride;
- Pyridine;
- Pentachlorobenzene;
- Pentachlorophenol;
- 1-Chloronaphtalene;
- 2-Chloronaphtalene;
- Beta-hexachlorocyclohexane (β-HCH);

- Cyclohexanone;
- Styrene.

2. Selection of retrieved values

Not all the available values in the databases are used for the examination of the databases. On the condition that three or more values are available for a certain compound, in the following cases values are not used:
When the temperature belonging to the value of the solubility, the vapour pressure or the dissociation exponent is beyond the temperature range 0 - 25°C;
When the temperature belonging to the value of the solubility, the vapour pressure or the dissociation exponent is lacking. When less than three values are given a temperature of 20°C is supposed;
In case a value of a variable is expressed as a ‘smaller than’-value;
When the solubility is described, for example as ‘not soluble’, these descriptions are not used.
In case a relatively small range of solubility or vapour pressure is given at one temperature, the mean value of solubility or vapour pressure is used. When a vapour pressure range and a corresponding temperature range are given, the minimum value of the vapour pressure is supposed to belong to the minimum value of the temperature and the maximum value of the vapour pressure to the maximum value of the temperature.

To compare the values of the various variables it is necessary that the variables be expressed in the same units. Therefore the values for the solubility and the vapour pressure are recalculated to the same units. For solubility the unit ‘mg/l’ is used and for vapour pressure the unit ‘Pascal’ is used. In case the solubility is expressed as a percentage, the unit is interpreted as weight solute per weight solvent when the compound is a solid at soil temperature (10 °C). When the compound is a fluid at soil temperature (10 °C) the unit is interpreted as volume solute per volume solvent. The formulas to convert the unit ‘percentage’ in these two cases are nevertheless identical. All the occurring units and the way of conversion are presented in table 1.

Table 1: Units and way of conversion (M = molecular weight; SW = specific weight)

Parameter	**Conversion**	**Formula**
Solubility	$mol/m^3 \Rightarrow mg/l$	$mg/l = mol/m^3 * M$
	$mol/l \Rightarrow mg/l$	$mg/l = mol/l * 1000 * M$
	$ppm \Rightarrow mg/l$	$mg/l = ppm$
	$\% (m^3/ m^3) \Rightarrow mg/l$	$mg/l = \% * SW$
	$\% (g/g) \Rightarrow mg/l$	$mg/l = \% * SW$
Vapour pressure	$mmHg \Rightarrow Pa$	$Pa = mmHg * 133.33$
	$bar \Rightarrow Pa$	$Pa = bar * 10^5$
	$torr \Rightarrow Pa$	$Pa = torr * 133.33$
	$atm \Rightarrow Pa$	$Pa = atm* 1.01325*10^5$
pKa	$pKb \Rightarrow pKa$	$pKa = 14 - pKb$

3. Temperature correction of vapour pressure (Vp) and solubility (S)

Vapour pressure and solubility are physicochemical properties correlated with each other via the Henry constant. Both vapour pressure and solubility are highly temperature dependent (Waitz et al., 1996). The values of these input parameters given in the chemical databases are measured or calculated at several temperatures. To use these values for the calculation of geometric means and the distribution, the values are recalculated to soil temperature (10 °C) by applying temperature corrections.

The vapour pressure at a given temperature will be recalculated to a vapour pressure at 10 °C (283 K) by using the Clausius-Clapeyron equation (Chang, 1990).

$$Vp_2 = Vp_1 e^{\frac{(T_2 - T_1) H_{vap}}{T_1 \times T_2 \times R}} \qquad [1]$$

Vp_1 = vapour pressure at T_1 [Pa]
Vp_2 = vapour pressure at T_2 [Pa]
R = molar gas constant [8.3144 $J.mol^{-1}.K^{-1}$]
H_{vap} = enthalpy of vaporisation at 298 K [$J.mol^{-1}$]
T_1 = temperature at known vapour pressure (e.g. 293 K) [K]
T_2 = temperature at unknown vapour pressure (e.g. 283 K) [K]

The value of the enthalpy of vaporisation at 298 K (25 °C) is 104.8089 Joules per gram. This value can be recalculated for each compound by multiplication by the molecular weight of the compound (Weast et al.,1974).

Because solubility and vapour pressure are correlated to each other, temperature correction for solubility will be realised using a temperature correction for the Henry constant (Waitz et al.,1996):

$$H_1 = \frac{Vp_1}{S_1} \qquad [2]$$

H_1 = Henry constant at T_1 [$Pa.m^3.mol^{-1}$]
Vp_1 = vapour pressure at T_1 [Pa]
S_1 = solubility at T_1 [$mol.m^{-3}$]

To obtain the value of the vapour pressure at T_1 in the above mentioned equation, first the geometric mean of all the calculated values per compound at 10 °C are calculated with the exception of outliers. Then the values of the vapour pressure at T_1 are calculated by using a temperature correction for the vapour pressure (formula [1]). The Henry constant at 10 °C (H_2) can be calculated by the following temperature correction:

$$H_2 = H_1 e^{\left(0.024(T_2 - T_1)\right)} \qquad [3]$$

H_2 = Henry constant at T_2 [$Pa.m^3.mol^{-1}$]
H_1 = Henry constant at T_1 [$Pa.m^3.mol^{-1}$]
T_1 = temperature at known Henry constant (e.g. 293 K) [K]
T_2 = temperature at unknown Henry constant (e.g. 283 K) [K]

This temperature correction is an empirical expression of the Arrhenius equation, which is based on the assumption that in a closed container the number of collisions between gas molecules increases with higher temperatures (Waitz et al., 1996).

By using the vapour pressure at 10 °C (T_2)(calculated with the temperature correction for vapour pressure, equation [1]) and the Henry constant at 10 °C (T_2) (calculated with equation [3]), the unknown solubility (S_2) at 10°C (T_2) can be calculated (Waitz et al., 1996):

$$S_2 = \frac{Vp_2}{H_2} \qquad [4]$$

S_2 = solubility at T_2 [$mol.m^{-3}$]
Vp_2 = vapour pressure at T_2 [Pa]
H_2 = Henry constant at T_2 [$Pa.m^3.mol^{-1}$]

4. Determination of geometric means and the spread of values

To express the uncertainty of a calculated geometric mean, the spread of the values is calculated by the following equation:

$$\frac{(X_{\max} - X_{\min})}{geometric\_mean} \times 100\% \qquad [5]$$

It is considered to exclude outliers on the basis of a Z-test and to express the uncertainty as the standard deviation, but for application of the Z-test and the standard deviation a normal distribution of the data is required. In the data sets too few values are available to assume a normal distribution.

On the other hand, the use of the relative spread as an indicator for the quality of the calculated value is disrupted in case of low values, log expressed values (Kow, Koc and pKa) and in case of clear-cut outliers. It is concluded that a univocal parameter to indicate the quality of a data set is not easily found. In this report (chapter 2) an indication is given to input values that are considered critical to the model output. The stigma is based on the results of the sensitivity analysis.

5. Results of the database analysis

In table 2 the findings are resumed to obtain an overview of databases that yield the most values. To produce this overview the number of compounds is considered for a certain database for which one or more values are available.

Table 2: Overview of databases that yield the most values

Input parameter	**Order of databases that yield the most values (from left tot right)**				
Molecular weight	12	4	2	1	8
Solubility	12	5, 6	7	9	
Vapour pressure	12	6	2,4,5		
Log K_{ow}	11,12	6	4	9	
pKa	5	12	6	1	
Log K_{oc}					

Number database:
1 Merck
2 Chemiekaarten
3 Merck Safety Data Sheet
4 International Chemical Saftey Cards
5 Beilstein
6 HSDB
7 Ohmtads
8 Cheminfo
9 CESARS
10 Pesticide Manual 11^{ed}
11 Medchem
12 ASTER

It appears that the databases ‘ASTER’ and ‘International Chemical Safety Cards’ yield the most values for the input parameter molecular weight. The databases ‘ASTER’, ‘Beilstein’ and ‘HSDB’ yield the most values for solubility. ‘HSDB’ and ‘Chemiekaarten’ yield the most values for vapour pressure. Further yield ‘Medchem’, ‘ASTER’ and ‘HSDB’ the most values for the octanol-water partition coefficient (K_{ow}). ‘Beilstein’ and ‘HSDB’ yield the most values for the dissociation coefficient (pKa).

6. Conclusion and recommendation

The quality judgement of the geometric mean of each data set strongly depends on the accuracy of the measuring method and on the number of values that are available.
The databases that produce the most values on the whole and which can be searched best are:
ASTER;
HSDB;
Beilstein;
The databases, which can be searched second best, are:
Medchem;
Chemiekaarten;
International Safety Cards.

The databases that yield the most values for each input parameter are considered. In table 3 an overview is presented of databases that are advised to search for each parameter.

Table 3: Overview of databases that are advised to search for each parameter

	ASTER	**HSDB**	**Beilstein**	**Medchem**	**Chemie-kaarten**	**ICSC**
Molecular weight	X					X
Solubility	X	X	X			
Vapour pressure		X			X	
Log K_{ow}	X	X		X		
pKa		X	X			

Based on these findings it was decided that:

- *Data on molecular weight , solubility, vapour pressure, pKa and log Kow will be retrieved from the three best* [6] *databases (standard procedure).*
- *Occasionally it will be necessary to complete the data set with data from other sources.*
- *Conversion of data according to table 1*
- *Temperature correction of Vp and S according to the method of this appendix*
- *Determination of the parameter value according to 1.3.*

Given the poor results of retrieved Koc data a different approach for this parameter will be followed (see Appendix 3).

---

[6] With the earmark *'best'* we willnot suggest a quality judgment in the general sense of speaking. The judging of databases must be seen in the frame of the objectives of this study.

Appendix 3: A guideline for the selection of the soil-water partition coefficients for organic compounds

For a number of organic compounds, it is experienced that the retrieved data for Koc, originated from the selected databases, results in a poor data set. To improve the data set and to select a recognised value a guideline for selecting Koc values for risk assessment was determined in co-operation with others.
Appendix 2 gives a guideline for extracting values for a number of CSOIL input parameters. For the selection of a Koc value however, this elementary guideline will, for most compounds, results in unsatisfactory number of values.
It is understood by researchers that, because of the complexity of the selection of Koc's, a closer look is always required. This results in a current practice were different researchers applies different approaches resulting in a number of Koc values.
This problem was put to several *'Koc users'* within the RIVM and RIZA. Simultaneous with this question a stepwise guideline was formulated as a first move to establish some kind of guideline and finally achieve a recognised set of Koc values.

Explanation

About harmonisation
To some extent, harmonisation of Koc values (within the RIVM) is seen as a useful activity. The proposed steps seem to fit with the current practice within INS scope. The proposed use of the Sabljić models has common consent.

About experimental Koc values
Generally speaking, the feeling exist that experimental measured values should be the basis of a recognised Koc value. Although the Koc is normalised on organic matter, it is said that each measured Koc is in fact a site-specific Koc (Van Steenwijk et al. 1999). Nature and type of organic matter (polarity C/N+O, aromaticity) can influence the Koc value up till a factor 10. Moreover, the process of so-called 'slow desorption' in situ can provoke variation up till a factor 100. This effect is site-specific and simply not predictable. For potential risk assessment however these site-specific effects are considered outside the scope of this study. The general feeling is that a Koc based on a set of good experimental determined values (in situ) will meet the requirements to asses potential risks.

'Kow derived' Koc values
If a reliable set of measured Koc values is not available the Koc can be derived from the Kow. All consulted Koc users prefer the models of Sabljić (1995). Sabljić defined QSAR models for 20 compound groups. He reported the application range (log Kow range) and indicated the reliability ($\pm 2\sigma$ range). A diagram for the selection of the proper QSAR model is available. In case the derivation according to Sabljić is problematic it is recommended to use the Syracuse Program EPIWIN. This program calculates as well the Kow as the Koc. The calculation of the Koc is based on first order molecular connectivity indices. The program is more easy than the application of the Sabljić models because it is not necessary to select the appropriate model.

Koc values for sediments
Some Koc users mentioned the lack of (experimental) data on sediments. Therefor the application of the soil Koc's for sediments is recommended. In case of actual (site-specific) risk assessment of sediments, additional measurements are recommended.

Guideline

The guideline is based on the suggestions and experiences of the consulted 'Koc users' and should be seen in relation with the overall objective: 'a recognised Koc value for the potential risk assessment'.
A time consuming activity like literature study is not explicitly included. Of course there are arguments to carry out additional literature study, but this should be judged from case to case.

The selection of a Koc value for potential risk assessment follows the next steps:

Step 1
The retrieval of measured Koc's from the recommended databases and surveys

Step 2
A derived Koc value from the Kow (the Kow value from the CSOIL data set) according to Sabljić et al. The log Kow – log Koc relationships, based on QSAR modelling are developed for 19 chemical domains (table 1). The selection of the most appropriate QSAR sorption model should be according the guidelines of Sabljić et al. (1995).

Step 3
In principle the final Koc value will be the geometric mean[7] of:

- all experimental (measured) Koc's
- one derived Koc according Sabljić.

Remarks
Erratic Koc values should be judged separately. If there is report of unsatisfactory quality or deviant methods the Koc value should be eliminated from the data set.
The applied Sabljić model can be disputable. If the derived Koc deviates from the set of measured Koc's it should be considered to remove this value from the data set.
Note that a surplus value is assigned to the experimental Koc's by combining ALL experimental Koc's with ONE derived Koc.

---

[7] In case the Koc values are expressed as log, a normal average is calculated.

Table 1: Derived log Kow-log Koc relationships for 19 chemical domains (Sabljić et al., 1995).

No.	Chemical domain	Equation
1	Predominantly hydrophobic	log Koc = 0.10 + 0.81 log Kow
2	Nonhydrophobic	log Koc = 1.02 + 0.52 log Kow
3	Phenols, anilines, benzonitriles, nitrobenzenes	log Koc = 0.90 + 0.63 log Kow
4	Acetanilines, carbamates, esters, phenylureas, phophates, triazines, triazoles, uracils	log Koc = 1.09 + 0.47 log Kow
5	Alcohols, organic acids	log Koc = 0.50 + 0.47 log Kow
6	Acetanilides	log Koc = 1.12 + 0.40 log Kow
7	Alcohols	log Koc = 0.50 + 0.39 log Kow
8	Amides	log Koc = 1.25 + 0.33 log Kow
9	Anilines	log Koc = 0.85 + 0.62 log Kow
10	Carbamates	log Koc = 1.14 + 0.365 log Kow
11	Dinitroanilines	log Koc = 1.92 + 0.38 log Kow
12	Esters	log Koc = 1.05 + 0.49 log Kow
13	Nitrobenzenes	log Koc = 0.55 + 0.77 log Kow
14	Organic acids	log Koc = 0.32 + 0.60 log Kow
15	Phenols and benzonitriles	log Koc = 1.08 + 0.57 log Kow
16	Phenylureas	log Koc = 1.05 + 0.49 log Kow
17	Phosphates	log Koc = 1.17 + 0.49 log Kow
18	Triazines	log Koc = 1.50 + 0.30 log Kow
19	Triazoles	log Koc = 1.405 + 0.47 log Kow

The selection of soil-water partition coefficients for dissociating organic compounds

The use of fixed Koc values, as derived according the guideline is not valid for ionising organic compounds. Several of the organic compounds ionise in the soil environment existing in both neutral and ionised forms. The relative amounts of the ionised and neutral species are a function of pH.
To address this problem, the derivation of Koc values for ionising organic compounds is partly different from the guideline.

The retrieval of Koc values can take place according the guideline. However, for the derivation of the generic Koc valid for the standard soil, only those values determined at known soil pH will be considered. The derivation of a Koc normalised for known soil pH is described in chapter 3.

Appendix 4: Crop specific data on metal accumulation.

Table 1. Overview of averages and ranges of BCF values

	Crop	Range (5 percentile-95 percentile)	Median	Geometric mean	Average of log BCF	Standard error of log BCF
As	all	0.001- 0.15	0.025	0.019	-1.73	0.65
	potatoes	0.001- 0.015	0.003	0.003	-2.48	0.40
	carrots	0.04- 0.21	0.066	0.026	-1.59	0.32
	spinach	0.01- 0.08	0.024	0.067	-1.17	0.30
Cd	all	0.09- 4.6	0.55	0.55	-0.26	0.54
	potatoes	0.07- 0.93	0.27	0.28	-0.56	0.40
	beetroot	0.10- 0.82	0.32	0.31	-0.51	0.28
	carrots	0.33- 6.6	1.3	1.3	0.12	0.38
	radish	0.50- 0.77	0.71	0.66	-0.18	0.07
	leek	0.04- 0.27	0.13	0.12	-0.92	0.27
	tomatoes	0.15- 43	10	3.0	0.48	1.14
	cabbage	0.04- 25	0.19	0.29	-0.54	1.08
	curly kale	0.08- 0.42	0.23	0.22	-0.66	0.23
	lettuce	0.24- 2.0	0.73	0.74	-0.13	0.38
	endive	0.17- 2.4	0.63	0.68	-0.17	0.34
	spinach	0.7- 7	2.2	2.27	0.36	0.34
	beans	0.07- 18	0.24	0.42	-0.37	0.55
Cu	all	0.09- 0.80	0.29	0.28	-0.56	0.29
	potatoes	0.16- 0.56	0.37	0.33	-0.48	0.24
	carrots	0.14- 0.39	0.23	0.23	-0.64	0.17
	tomatoes	0.44- 0.80	0.55	0.59	-0.23	0.11
	cabbage	0.07- 0.16	0.09	0.01	-1.00	0.13
	cauliflower	-	0.12	-	-	-
	lettuce	0.30- 0.48	0.33	0.35	-0.46	0.09
	beans	0.16- 0.90	0.24	0.32	-0.50	0.26
Hg	all	0.02- 3	0.33	0.28	-0.55	0.62
	potatoes	0.01- 0.5	0.11	0.10	-0.99	0.59
	carrots	0.1- 1.4	0.45	0.53	-0.28	0.64
	spinach	0.08- 4	0.40	0.43	-0.37	0.34
Ni	all	0.010- 0.15	0.025	0.029	-1.54	0.38
	potatoes	0.009- 0.024	0.015	0.015	-1.84	0.17
	carrots	0.013- 0.10	0.021	0.030	-1.53	0.39
	tomatoes	0.017- 0.08	0.029	0.033	-1.48	0.28
	cabbage	0.009- 0.037	0.021	0.019	-1.72	0.25
	cauliflower	-	0.06	-	-	-
	lettuce	0.020- 0.043	0.035	0.031	-1.50	0.15
	beans	0.030- 0.34	0.19	0.11	-0.96	0.57
Pb	all	0.002- 0.08	0.015	0.015	-1.83	0.55
	potatoes	0.002- 0.01	0.005	0.005	-2.28	0.30
	beetroot	0.0011- 0.01	0.003	0.004	-2.45	0.33
	carrots	0.008- 0.08	0.030	0.028	-1.55	0.34
	radish	0.01- 2.6	0.12	0.14	-0.9	0.91
	onions	0.006- 0.016	0.0095	0.009	-2.03	0.16
	leek	0.002- 0.012	0.0048	0.005	-2.31	0.24
	tomatoes	0.0010- 0.07	0.015	0.010	-2.02	0.85
	cabbage	0.0024- 0.02	0.012	0.009	-2.07	0.36
	curly kale	0.010- 0.06	0.030	0.027	-1.58	0.26
	lettuce	0.005- 0.11	0.018	0.020	-1.69	0.46
	endive	0.007- 0.04	0.018	0.016	-1.78	0.26
	spinach	0.013- 0.10	0.038	0.37	-1.44	0.29
	beans	0.0015- 0.05	0.012	0.009	-2.05	0.61

	Crop	**Range (5 percentile-95 percentile)**	**Median**	**Geometric mean**	**Average of log BCF**	**Standard error of log BCF**
	cauliflower	-	0.008	-	-2.10	-
Zn	all	0.07- 1.3	0.30	0.30	-0.52	0.51
	potatoes	0.018- 0.61	0.10	0.11	-0.97	0.48
	carrots	0.09- 0.46	0.19	0.18	-0.73	0.30
	tomatoes	0.22- 13	0.55	0.86	-0.07	0.70
	cabbage	0.12- 0.31	0.20	0.19	-0.73	0.18
	cauliflower	-	0.49	-	-	-
	lettuce	0.22- 1.1	0.37	0.41	-0.39	0.28
	beans	0.28- 1.3	0.80	0.68	-0.17	0.27

Table 2. *Crop specific derived soil-plant relations*

log [C-plant] = a + b*log(Q) + c*pH + d*log (%OC) + e*log (%clay)

	used in generic model	constant (a)	Q-soil (b)	pH (c)	OC% (d)	clay % (e)	R^2 [-]	n	F-test	Expl. variance [%]
Arsenic										
potatoes	no	-1.1	-0.0	0.01	-0.4	-0.13	0.07	90	0	3
carrot	yes	-0.93	0.32	0.01	-0.11	-0.11	0.30	100	1	26
spinach	no	-0.84	0.17	-0.00	0.11	-0.11	0.10	80	0	5
Barium	no workable field data available									
Cadmium										
potatoes	yes	-0.86	0.36	0.06	-0.13	-0.27	0.35	103	1	90
lettuce	yes	1.0	0.28	-0.18	-0.19	0.16	0.30	125	1	99
carrot	yes	0.74	0.45	-0.16	0.2	0.09	0.50	112	1	99
radish	yes	0.0	0.12	-0.32	-	-	0.22	8	1	100
leak	yes	0.7	0.31	-0.20	-0.29	0.0	0.36	68	1	99
curly kale	yes	1.0	0.39	-0.14	-0.5	-0.4	0.58	58	1	99.8
endive	yes	0.0	0.42	-0.1	0.1	0.3	0.28	93	1	99
spinach	yes	1.3	0.28	-0.22	-0.64	0.37	0.34	86	1	99
beetroot	yes	1.9	0.37	-0.18	-0.3	-0.8	0.34	67	1	99.7
tomato	no	2	0.1	-0.3	-	-	0.22	6	0	97
French beans	yes	10	0.13	-0.13	-0.1	-9	0.85	13	1	99.9
white cabbage	no	12	0.6	-0.6	17	-	0.11	7	0	98
Chromium	no workable field data available									
Cobalt	no workable field data available									
Copper										
potatoes	yes	2.8	0.2	0.00	-4.2	-	0.93	7	1	85
tomato	no	1.0	0.2	-0.01	-	-	0.16	6	0	-37
lettuce	no	0.1	0.9	-0.05	-	-	0.52	6	0	19
carrot	no	0.6	1.3	-0.2	-	-	0.29	6	0	-18
white beans	no	6.6	0.0	-0.06	0.05	-4.5	0.98	13	0	96
white cabbage	no	1	0.7	-0.07	-2	-	0.24	6	0	-52
Mercury										
potatoes	no	-0.8	0.07	-0.18	-0.3	0.1	0.03	91	0	-2
carrot	no	-1.67	0.13	0.03	0.02	-0.10	0.16	97	1	0
spinach	no	-2.1	0.10	0.05	0.5	0.3	0.12	83	1	9
Lead										
potatoes	yes	-2.0	0.67	0.12	-0.02	-0.50	0.67	113	1	66
beetroot	yes	0.5	0.75	-0.08	-0.64	-1.2	0.47	75	1	44
lettuce	yes	-0.60	0.90	-0.07	-0.34	-0.19	0.36	156	1	
carrot	yes	0.64	0.56	-0.04	-0.16	-0.03	0.40	124	1	38
radish	no	1.8	0.25	-0.27	-0.3	-0.50	0.28	33	0	18

	used in generic model	constant (a)	Q-soil (b)	pH (c)	OC% (d)	clay % (e)	R^2 [-]	n	F-test	Expl. variance [%]
leak	yes	0.8	0.5	-0.12	-0.61	0.57	0.41	68	1	37
curly kale	yes	2.0	0.29	-0.11	-0.62	-0.65	0.48	59	1	44
endive	yes	1.9	0.52	-0.17	-0.68	-0.8	0.42	89	1	39
spinach	yes	-0.12	0.36	-0.03	0.25	-0.23	0.34	80	1	39
onions	no	-1	0.4	0.1	-	-	0.12	9	0	-16
tomato	no	-2	-1.2	-0.4	-	-	0.51	6	0	18
white beans	yes	3.2	-0.1	-0.2	-5.3	-	0.83	8	1	71
white cabbage	yes	7	0.6	-0.3	-3.1	-5	0.93	14	1	89
Molybdenum	no workable field data available									
Nickel										
potatoes	no	-1.7	-0.0.	-	2.9	-	0.38	7	0	7
lettuce	no	-1.1	0.7	-	-	-	0.17	6	0	-4
white beans	no	6.1	-4.0	-	-	-	0.80	4	0	70
white cabbage	yes	-2.7	3.3	-	-5	-	0.81	7	1	71
tomato	no	-2.5	1.7	-	-	-	0.26	6	0	8
carrot	yes	-5.9	4.2	-	-	-	0.70	6	1	63
Zinc										
potatoes	yes	3.0	0.33	-0.04	0.5	-2.1	0.96	12	1	94
white beans	no	2.2	0.19	-0.13	0.3	-	0.10	13	0	29
tomato	no	3	5	1.2	-	-	0.19	6	0	-36
lettuce	no	2.0	0.9	-0.3	-	-	0.11	6	0	-48
white cabbage	no	1.1	0.1	0.02	0	-	0.29	7	0	-39
carrot	no	1.9	0.2	-0.1	-	-	0.08	6	0	-54

Appendix 5: Bioconcentration factors for barium, chromium, cobalt and molybdenum

Barium

For barium two references on accumulation were encountered with data for individual crops (table 1). The default BCF values as recommended by Ng (1982) are based on field data of Boerngen (1980). Other (default) BCF values were determined by Baes (1984) and Sauerbeck (1989). Mentioned compiled BCF values were used by Bockting and Van den Berg (1992) for estimation a BCF for root and leafy vegetables

Table 1 BCF values for barium

crop	**BCF (geomean)**	**std. dev.**	**N**	**reference**
cabbage	0.021	0.00096	unknown	Boerngen, 1980
lettuce	0.096	0.0056	unknown	Boerngen, 1980
beans	0.023	0.006	unknown	Boerngen, 1980
tomato	0.010	0.0006	unknown	Boerngen, 1980
carrots	0.024	0.0027	unknown	Boerngen, 1980
onion	0.021	0.0097	unknown	Boerngen, 1980
potato	0.0047	0.00064	unknown	Boerngen, 1980
sweet corn	0.00062	0.00018	unknown	Boerngen, 1980
radish	1.13	4.07	19	Van Gestel, 1992
lettuce	0.273	1.3	16	Van Gestel, 1992
default BCF	0.05			Ng, 1982
default BCF leaf	0.15			Baes, 1984
default BCF root	0.015			Baes, 1984
BCF leaf	0.01-0.1			Sauerbeck, 1989
BCF leaf	0.1			Bockting and Van den Berg, 1992
BCF root	0.005			

From the figures of Boerngen (1980) and Van Gestel (1992) it is possible to compute a BCF which accounts for the average consumption pattern of home-grown vegetables. Table 2 shows clearly that the average BCF is dominated by the high BCF values of radish. As radish is consumed in low quantities the use of the consumption pattern weighted BCF is recommended.

Table 2 Computed BCF values for barium

	BCF value
average	0.177
geometric mean	0.035
minimum value	0.0047
maximum value	1.13
number of crops	8
BCF reflecting average consumption pattern	0.0167

The proposed BCF for barium is 0.017

Due to limited available data on barium accumulation it is stressed that, amongst others, the following important accumulation factors could not be taken into account:

- influence of soil type
- contamination grade
- Dutch soil and climate

Chromium

BCF data for chromium was retrieved by Versluijs et al. (in prep.). Table 3 gives an overview of the used references for the computation of a generic BCF values for potential risk assessment

Table 3 Overview of BCF values for chromium

crop	BCF (geometric mean)	Standard deviation	reference (see Versluijs et al., in prep.)
radish	0.184		Van Gestel, 1992
lettuce	0.308	1.058	Van Gestel, 1992
pea	0.003		Sauerbeck, 1991
carrot	0.006		Sauerbeck, 1991
leak	0.007		Sauerbeck, 1991
spinach	0.013	0.025	Sauerbeck, 1991
sellery	0.014		Sauerbeck, 1991
lettuce	0.018		Sauerbeck, 1991
field lettuce	0.021	0.002	Sauerbeck, 1991
radish	0.044	0.006	Sauerbeck, 1991
spinach	0.0002		Smilde, 1981
lettuce	0.010	0.069	Smilde, 1981

An average consumption weigthed BCF of **0.011 is proposed.**
The proposed BCF is comparable with other published BCF values for chromium.

Cobalt

Table 4 gives details of the computation of a BCF for potential risk assessment. Data was retrieved from different sources by Versluijs et al. (in prep.). The table shows the different possibilities (selection criteria) for selection of an appropriate BCF.

Table 4 BCF values for cobalt

selection criteria	number of data (N)	BCF (geomean)	standard dev.	Co soil content. (mg/kg d.m.)
1. non	128	0.062	7.21	
2. field data only	105	0.055	7.95	
3. home-grown crops only	26	0.58	15.3	
4. contaminated sites only	74	0.026	0.063	min 91 max 3865 geomean 484
5. combination of criteria 2 and 3	18	0.77	17.9	**) min 0.1 max 11.7 geomean 0.9
6. individual crops				
• lettuce	7	8.75	24.2	
• potato	3	0.066	0.045	
• radish	6	0.290	0.516	
• carrot	1	0.180	-	
• tomato	1	0.070	-	

The selection on crops results in a dataset dominated by BCF data of Van Gestel for lettuce. The data of Van Gestel was obtained on non contaminated soil and the BCF for lettuce was determined on 8.75. Compared with other crops this BCF seems high.
To prevail domination of a single crop a consumption average weigthed BCF was computed.

It is proposed to use the average consumption pattern weighted BCF. This was determined on 0.58 and equal to the geometric mean of data on home-grown crops only.

Molybdenum

No new suitable data on molybdenum accumulation was found. Thus only the references used by Bockting and Van den Berg (1992) were reviewed and evaluated.
Bockting and Van den Berg (1992) based the BCF on data of Ng (1982) and Baes (1984). The given values of Ng (1982) and Baes (1984) were both based on data sources from (public) literature and (statistical) analysis and interpretation of the retrieved data. Baes stresses that acceptance or rejection of data on metal accumulation in plants was subjective depending on a variety of considerations.
Given above considerations and the fact that no additional data on molybdenum accumulation was found it is proposed to maintain the current CSOIL BCF values.

Integrating the current seperate BCF values for root (0.015) and leafy crops (0.3) to one generic **BCF a value of 0.12 is determined.**

Appendix 6: Comparison of revised and INS physicochemical data

	Vp revised	Vp INS	H revised	H INS	log Kow revised	log Kow INS	log Koc revised	log Koc INS
Aromatic compounds								
Benzene	9.51E+03	1.27E+04	1.59E-01	1.42E-01	2.13	2.19	1.87	1.90
Ethylbenzene	9.53E+02	9.33E+02	2.70E-01	1.40E-01	3.15	3.15	2.53	2.22
Toluene	2.96E+03	2.93E+03	1.90E-01	1.64E-01	2.73	2.79	2.09	2.06
o-Xylene	6.76E+02	6.67E+02	1.39E-01	1.23E-01	3.12	3.12	2.18	3.12
m-Xylene	8.05E+02	8.00E+02	1.84E-01	1.77E-01	3.20	3.20	2.41	2.51
p-Xylene	8.60E+02	8.67E+02	1.84E-01	1.81E-01	3.15	3.15	2.66	2.72
Styrene	5.25E+02	6.00E+02	7.27E-02	1.77E-01	2.95	2.95	2.58	2.95
PAH								
Naphthalene	6.83E+00	1.04E+01	1.17E-02		3.30	3.30	2.99	3.37
Anthracene	9.31E-04	1.00E-03	9.89E-04		4.45	4.45	4.29	4.52
Phenanthrene	1.51E-02	2.00E-02	1.35E-03		4.47	4.46	4.24	4.53
Fluoranthene	3.80E-03	1.20E-03	1.63E-03		5.16	5.16	5.16	5.23
Benzo(a)anthracene	2.07E-07	2.80E-05	1.73E-06		5.54	5.79	5.92	5.86
Benzo(a)pyrene	1.25E-07	7.00E-07	1.60E-05		6.13	5.97	5.82	6.04
Benzo(k)fluoranthene	1.24E-08	5.20E-08	2.76E-06		6.11	6.00	6.25	6.07
Chlorinated hydrocarbons								
1,2-Dichloroethane	7.39E+03	8.53E+03	3.05E-02	5.00E-02	1.47	1.48	1.49	1.62
Dichloromethane	4.30E+04	4.65E+04	8.61E-02	3.90E-02	1.25	1.25	1.22	1.56
Tetrachloromethane	9.49E+03	1.19E+04	6.61E-01	6.37E-01	2.83	2.83	1.75	2.83
Tetrachloroethene	1.57E+03	1.87E+03	9.29E-01	3.64E-01	3.40	3.40	2.42	2.38
Trichloromethane	2.01E+04	2.13E+04	1.09E-01	7.40E-02	1.97	1.97	1.66	1.81
Trichloroethene	5.81E+03	7.71E+03	2.78E-01	1.49E-01	2.61	2.42	2.06	2.04
Vinylchloride	2.98E+05	3.37E+04	1.85E+01	6.46E-01	1.52	1.52	1.56	1.53
Monochlorobenzene	1.19E+03	1.58E+03	1.13E-01	1.05E-01	2.89	2.90	2.34	2.34
1,2-Dichlorobenzene	1.30E+02	1.96E+02	5.80E-02	7.00E-02	3.43	3.43	2.60	2.64
1,3-Dichlorobenzene	1.49E+02	3.07E+02	8.28E-02	9.50E-02	3.53	3.53	2.69	2.64
1,4-Dichlorobenzene	9.06E+01	9.00E+01	9.35E-02	9.10E-02	3.44	3.44	2.82	2.64
ALL dichlorobenzenes	1.19E+02		7.38E-02		3.46		2.70	
1,2,3-Trichlorobenzene	2.47E+01	2.80E+01	1.40E-01	5.60E-02	4.14	4.14	3.23	3.30
1,2,4-Trichlorobenzene	4.07E+01	6.10E+01	1.09E-01	5.60E-02	4.05	4.05	3.28	3.30
1,3,5-Trichlorobenzene	2.80E+02	2.80E+01	4.58E+00	5.60E-02	4.19	4.19	3.98	3.30
ALL trichlorobenzenes	5.47E+01		2.54E-01		4.13		3.34	
1,2,3,4-Tetrachlorobenzene	6.78E-01	5.00E+00	1.83E-02	1.30E-02	4.64	4.64	3.91	3.78
1,2,3,5-Tetrachlorobenzene	1.29E+00	1.00E+01	4.53E-02	2.10E-02	4.66	4.66	3.57	3.78
1,2,4,5-Tetrachlorobenzene	4.00E+00	7.00E-01	5.37E-01	1.70E-02	4.60	4.60	3.77	3.78
ALL tetrachlorobenzenes	1.52E+00		7.66E-02		4.63		3.72	
Pentachlorobenzene	4.52E-01	2.20E+00	1.49E-01	1.30E-02	5.18	5.18	3.92	3.90
Hexachlorobenzene	6.13E-04		6.36E-03		5.73	5.73	4.06	4.04
2-Chlorophenol	2.25E+02		1.41E-03		2.15	2.20	1.97	2.26
3-Chlorophenol	1.93E+01		1.33E-04		2.50	2.50	2.56	2.26
4-Chlorophenol	1.13E+01		8.03E-05		2.39	2.60	1.93	2.26
ALL monochlorophenols	3.66E+01		2.47E-04		2.35		2.34	
2,3-Dichlorophenol	1.27E+01		9.76E-04		2.84	3.19	2.56	2.64
2,4-Dichlorophenol	4.09E+00		1.48E-04		3.06	2.75	2.54	3.94
2,5-Dichlorophenol	1.04E+01		1.71E-03		3.06	3.20	2.83	2.64
2,6-Dichlorophenol	7.14E+00		9.26E-04		2.75	2.80	2.63	2.60
3,4-Dichlorophenol	4.40E-01		1.01E-03		3.33	3.37	2.90	2.64
3,5-Dichlorophenol	2.46E+00		4.26E-03		3.52	3.52	2.34	2.64
ALL dichlorophenols	3.67E+00		1.01E-03		3.09	3.14	2.69	2.64
2,3,4-Trichlorophenol	7.93E-01		9.36E-04		3.46	4.07	3.08	2.90
2,3,5-Trichlorophenol	2.02E-01		1.11E-04		3.58	4.21	3.16	2.90
2,3,6-Trichlorophenol	2.02E-01		1.35E-04		3.77	3.88	3.28	2.90
2,4,5-Trichlorophenol	1.00E+00		2.22E-04		3.72	3.72	3.36	3.08

	Vp revised	Vp INS	H revised	H INS	log Kow revised	log Kow INS	log Koc revised	log Koc INS
2,4,6-Trichlorophenol	9.83E-01		3.40E-04		3.69	3.69	3.47	2.48
3,4,5-Trichlorophenol	2.02E-01		4.89E-04		4.01	4.39	3.54	2.68
ALL trichlorophenols	5.62E-01		3.42E-04		3.71	3.99	3.32	2.90
2,3,4,5-Tetrachlorophenol	3.94E-02		1.07E-03		4.21	4.95	3.87	3.24
2,3,4,6-Tetrachlorophenol	6.03E-02		4.05E-04		4.12	4.10	3.10	3.08
2,3,5,6-Tetrachlorophenol	3.94E-02		8.10E-04		3.88	4.90	3.34	3.45
ALL tetrachlorophenols	4.54E-02		7.07E-04		4.07	4.65	3.44	3.24
Pentachlorophenol	8.53E-03		2.26E-04		5.12	4.74	3.20	3.24
Pesticides								
DDT	1.22E-05		2.84E-04		6.91	6.91	5.58	5.63
DDE	4.29E-05		1.42E-04		6.96	6.50	5.35	4.82
DDD	1.93E-05		4.22E-05		6.22	6.22	5.18	4.91
Aldrin	2.33E-03		1.47E-02		6.50	6.50	3.94	5.11
Dieldrin	2.94E-05		1.60E-05		4.55	6.20	3.99	5.87
Endrin	1.25E-05		4.33E-06		4.55	5.20	3.95	4.29
α-HCH	3.50E-02		2.65E-03		3.72	3.78	3.33	3.25
β-HCH	1.98E-02		2.61E-03		3.72	3.84	3.37	3.36
γ-HCH	1.23E-03		2.61E-05		3.72	3.69	2.99	3.70
Carbofuran	2.03E-03		5.07E-07		1.63	2.32	1.64	1.63

Appendix 7: Revised CSOIL 2000 dataset

Physicochemical data

	CASnr.	M	Kp	BCF
		[g/mol]	[dm3/kg]	[kg/kg]
Metals and trace elements				
arsenic	7440-38-2	74.9	1800	0.009
barium	7440-39-3	137.3	2500	0.017
cadmium	7440-43-9	112.4	2560	0.310
chromium (III)	7440-47-3	52.0	4800	0.011
chromium (VI)	18450-29-9	52.0	4800	0.011
cobalt	7440-48-4	58.9	120	0.580
copper	7440-50-8	63.5	2120	0.200
mercury	7439-97-6	200.6	7500	0.150
lead	7439-92-1	207.2	36000	0.017
molybdenum	7439-98-7	95.9	40	0.120
nickel	7440-02-0	58.7	2000	0.028
zinc	7440-66-6	65.4	2600	0.180

	CASnr.	M	S	Vp	log Kow	log Koc	pKa	Dpe
		[g/mol]	[mg/dm3]	[Pa]	[-]	[dm3/kg]	[-]	[m2 per day]
Aromatic compounds								
Benzene	71-43-2	78.1	1.99E+03	9.51E+03	2.13	1.87		1.40E-06
Ethylbenzene	100-41-4	106.2	1.59E+02	9.53E+02	3.15	2.53		2.10E-06
Phenol	108-95-2	94.1	6.56E+04	3.29E+01	1.47	1.52	10.00	8.40E-09
o-Cresol	95-48-7	108.1	1.49E+04	2.35E+01	1.95	1.59	10.20	1.00E-06
m-Cresol	108-39-4	108.1	6.32E+03	1.14E+01	1.96	1.72	10.00	1.00E-06
p-Cresol	106-44-5	108.1	2.86E+04	1.88E+01	1.94	1.64	10.10	1.00E-06
Toluene	108-88-3	92.1	6.11E+02	2.96E+03	2.73	2.09		1.20E-06
o-Xylene	95-47-6	106.2	2.19E+02	6.76E+02	3.12	2.18		1.60E-06
p-Xylene	106-42-3	106.2	2.11E+02	8.60E+02	3.15	2.66		1.60E-06
m-Xylene	108-38-3	106.2	1.97E+02	8.05E+02	3.20	2.41		1.60E-06
Catechol	120-80-9	110.1	1.24E+05	3.39E+00	0.88	1.85	10.60	1.00E-07
Resorcinol	108-46-3	110.1	2.42E+05	8.03E-01	0.80	1.14	9.70	1.00E-07
Hydroquinone	123-31-9	110.1	3.92E+04	3.86E-02	0.59	1.95	10.60	1.00E-07
Styrene	100-42-5	104.1	3.20E+02	5.25E+02	2.95	2.58		2.00E-06
Polyciclic aromatic hydrocarbons								
Naphthalene	91-20-3	128.2	3.18E+01	6.83E+00	3.30	2.98		5.00E-07
Anthracene	120-12-7	178.2	7.13E-02	9.31E-04	4.45	4.30		5.00E-07
Phenanthrene	85-01-8	178.2	8.50E-01	1.51E-02	4.47	4.23		5.00E-07
Fluoranthene	206-44-0	202.4	2.01E-01	3.80E-03	5.16	5.18		2.00E-07
Benzo(a)anthracene	56-55-3	228.3	1.16E-02	2.07E-07	5.54	5.79		2.00E-07
Chrysene	218-01-9	228.3	1.79E-03	8.74E-08	5.81	5.72		2.00E-07
Benzo(a)pyrene	50-32-8	252.3	8.42E-04	1.25E-07	6.13	5.82		2.00E-07
Benzo(ghi)perylene	191-24-2	276.3	1.86E-04	5.04E-09	6.22	6.43		2.00E-07
Benzo(k)fluoranthene	207-06-9	252.3	4.84E-04	1.24E-08	6.11	6.24		2.00E-07
Indeno, 1,2,3-cd pyrene	193-39-5	276.3	2.65E-04	2.65E-09	6.87	6.02		2.00E-07
Pyrene	129-00-0	202.3	1.06E-01	9.20E-05	4.99	4.83		2.00E-07
Acenaphthene	83-32-9	154.2	2.57E+00	4.22E-01	3.92	3.53		5.00E-07
Acenaphthylene	208-96-8	152.2	4.01E+00	1.79E-01	3.94	3.47		5.00E-07
Benzo(b)fluoranthene	205-99-2	252.3	1.68E-02	1.82E-06	5.78	5.34		5.00E-07
Benzo(j)fluoranthene	205-82-3	252.3	8.81E-03	1.82E-06	6.11	5.48		5.00E-07
Dibenz(a,h)anthracene	53-70-3	278.4	8.28E-04	2.67E-07	7.11	6.14		5.00E-07
9H-Fluorene	86-73-7	166.2	1.32E+00	1.16E-01	4.18	3.77		5.00E-07

	CASnr.	M	S	Vp	log Kow	log Koc	pKa	Dpe
		[g/mol]	[mg/dm3]	[Pa]	[-]	[dm3/kg]	[-]	[m2 per day]
Chlorinated hydrocarbons								
1,2-Dichloroethane	107-06-2	99.0	1.02E+04	7.39E+03	1.47	1.49		3.00E-07
Dichloromethane	75-09-2	84.9	1.80E+04	4.30E+04	1.25	1.22		5.00E-07
Tetrachloromethane	56-23-5	153.7	9.38E+02	9.49E+03	2.83	1.75		8.00E-07
Tetrachloroethene	127-18-4	165.8	1.19E+02	1.57E+03	3.40	2.42		8.00E-07
Trichloromethane	67-66-3	119.4	9.39E+03	2.01E+04	1.97	1.66		1.00E-06
Trichloroethene	79-01-6	131.4	1.16E+03	5.81E+03	2.61	2.06		1.60E-06
Vinylchloride	75-01-4	62.5	4.28E+02	2.98E+05	1.52	1.56		1.00E-06
Chlorobenzenes								
Monochlorobenzene	108-90-7	112.6	5.07E+02	1.19E+03	2.89	2.34		3.50E-06
1,2-Dichlorobenzene	95-50-1	147.0	1.40E+02	1.30E+02	3.43	2.60		2.00E-06
1,3-Dichlorobenzene	541-73-1	147.0	1.13E+02	1.49E+02	3.53	2.69		2.00E-06
1,4-Dichlorobenzene	106-46-7	147.0	6.05E+01	9.06E+01	3.44	2.82		2.00E-06
1,2,3-Trichlorobenzene	87-61-6	181.4	1.36E+01	2.47E+01	4.14	3.23		1.00E-06
1,2,4-Trichlorobenzene	120-82-1	181.4	2.88E+01	4.07E+01	4.05	3.28		1.00E-06
1,3,5-Trichlorobenzene	108-70-3	181.4	4.71E+00	2.80E+02	4.19	3.98		1.00E-06
1,2,3,4-Tetrachlorobenzene	634-66-2	215.9	3.40E+00	6.78E-01	4.64	3.91		1.00E-06
1,2,3,5-Tetrachlorobenzene	634-90-2	215.9	2.61E+00	1.29E+00	4.66	3.57		1.00E-06
1,2,4,5-Tetrachlorobenzene	95-94-3	215.9	6.82E-01	4.00E+00	4.60	3.77		1.00E-06
Pentachlorobenzene	608-93-5	250.1	3.23E-01	4.52E-01	5.18	3.92		1.00E-06
Hexachlorobenzene	118-74-1	284.8	1.17E-02	6.13E-04	5.73	4.06		1.00E-06
Chlorophenols								
2-Chlorophenol	95-57-8	128.6	8.71E+03	2.25E+02	2.15	1.97	8.43	5.00E-09
3-Chlorophenol	108-43-0	128.6	7.97E+03	1.93E+01	2.50	2.56	9.06	5.00E-09
4-Chlorophenol	106-48-9	128.6	7.67E+03	1.13E+01	2.39	1.93	9.23	5.00E-09
2,3-Dichlorophenol	576-24-9	163.0	9.05E+02	1.27E+01	2.84	2.56	7.66	1.00E-07
2,4-Dichlorophenol	120-83-2	163.0	1.91E+03	4.09E+00	3.06	2.54	7.81	1.00E-07
2,5-Dichlorophenol	583-78-8	163.0	4.21E+02	1.04E+01	3.06	2.83	7.54	1.00E-07
2,6-Dichlorophenol	87-65-0	163.0	5.34E+02	7.14E+00	2.75	2.63	6.84	1.00E-07
3,4-Dichlorophenol	95-77-2	163.0	3.02E+01	4.40E-01	3.33	2.90	8.60	1.00E-07
3,5-Dichlorophenol	591-35-5	163.0	3.99E+01	2.46E+00	3.52	2.34	8.17	1.00E-07
2,3,4-Trichlorophenol	15950-66-0	197.5	7.11E+01	7.93E-01	3.46	3.08	7.01	5.00E-07
2,3,5-Trichlorophenol	933-78-8	197.5	1.26E+02	2.02E-01	3.58	3.16		5.00E-07
2,3,6-Trichlorophenol	933-75-5	197.4	1.26E+02	2.02E-01	3.77	3.28	5.95	5.00E-07
2,4,5-Trichlorophenol	95-95-4	197.5	3.80E+02	1.00E+00	3.72	3.36	7.07	5.00E-07
2,4,6-Trichlorophenol	88-06-2	197.5	2.43E+02	9.83E-01	3.69	3.47	6.22	5.00E-07
3,4,5-Trichlorophenol	609-19-8	197.5	3.46E+01	2.02E-01	4.01	3.54	7.46	5.00E-07
2,3,4,5-Tetrachlorophenol	4901-51-3	231.9	3.61E+00	3.94E-02	4.21	3.87	6.07	1.00E-06
2,3,4,6-Tetrachlorophenol	58-90-2	231.9	1.47E+01	6.03E-02	4.12	3.10	5.29	1.00E-06
2,3,5,6-Tetrachlorophenol	935-95-5	231.9	4.79E+00	3.94E-02	3.88	3.34	5.21	1.00E-06
Pentachlorophenol	87-86-5	266.3	4.28E+00	8.53E-03	5.12	3.20	4.85	2.24E-06
Chloronaphthalenes								
1-Chloronaphatalene	90-13-1	162.6	1.68E+01	4.25E+00	4.10	3.42		5.00E-07
2-Chloronaphatalene	91-58-7	162.6	9.71E+00	1.00E+00	4.14	3.42		5.00E-07
Polychlorobiphenyls								
PCB 28	7012-37-5	257.5	1.21E-01	1.60E-02	5.62	4.61		2.00E-07
PCB 52	35693-99-3	292.0	2.65E-02	6.07E-03	6.26	4.70		2.00E-07
PCB101	37680-72-3	326.4	1.32E-02	9.27E-03	6.85	5.53		2.00E-07
PCB118	31508-00-6	326.4	6.54E-03	2.96E-04	7.12	6.35		2.00E-07
PCB138	35065-28-2	360.9	6.96E-04	4.30E-06	7.45	5.71		5.00E-07
PCB153	35065-27-1	360.9	2.74E-03	1.75E-04	7.44	5.87		5.00E-07
PCB180	35065-29-3	395.3	7.69E-04	4.96E-05	8.16	5.99		5.00E-07
Dioxins (+PCDF and PCB)								
2,3,7,8-TCDD	1746-01-6	322.0	3.00E-04	1.40E-06	6.80	5.61		1.00E-07
PCDD	36088-22-9	356.0	1.20E-04	8.88E-08	7.40	6.09		1.00E-07
HxCDD	34465-46-8	391.0	4.40E-06	5.08E-08	7.80	6.42		1.00E-07
HpCDD	37871-00-4	425.0	2.40E-06	7.51E-10	8.00	6.58		1.00E-07
OCDD	3268-87-9	460.0	4.00E-07	5.93E-10	8.20	6.74		1.00E-07

	CASnr.	M [g/mol]	S [mg/dm3]	Vp [Pa]	log Kow [-]	log Koc [dm3/kg]	pKa [-]	Dpe [m2 per day]
PCB 77	32598-13-3	292.0	1.91E-03	5.09E-05	6.63	5.85		2.00E-07
PCB 105	32598-14-4	326.4	7.15E-03	1.55E-04	6.98	6.13		2.00E-07
PCB 126	57465-28-8	326.4	7.00E-03	1.55E-04	7.23	5.94		2.00E-07
PCB 156	38380-08-4	360.9	1.22E-03	4.05E-05	7.70	6.34		5.00E-07
PCB 157	69782-09-7	360.9	1.22E-03	4.05E-05	7.60	6.26		5.00E-07
PCB 169	32774-16-6	360.9	5.58E-04	1.26E-06	7.41	6.01		5.00E-07
TetraCDF	51207-31-9	306.0	4.13E-04	7.89E-06	6.53	5.39		1.00E-07
PentaCDF	-	340.4	2.36E-04	2.17E-05	6.85	5.65		1.00E-07
HexaCDF	-	374.9	8.25E-06	8.09E-06	7.81	6.42		1.00E-07
HeptaCDF	-	409.3	1.35E-06	1.55E-06	7.92	6.52		1.00E-07
OctaCDF	39001-02-0	443.8	2.15E-07	2.91E-08	8.28	6.80		1.00E-07
Pesticides								
DDT	50-29-3	354.5	6.48E-03	1.22E-05	6.91	5.58		5.00E-07
DDE	72-55-9	318.0	4.09E-02	4.29E-05	6.96	5.35		5.00E-07
DDD	72-54-8	320.0	6.23E-02	1.93E-05	6.22	5.18		5.00E-07
Aldrin	309-00-2	365.1	2.46E-02	2.33E-03	6.50	3.94		5.00E-07
Dieldrin	60-57-1	380.9	2.99E-01	2.94E-05	4.55	3.99		5.00E-07
Endrin	72-20-8	380.9	4.66E-01	1.25E-05	4.55	3.95		5.00E-07
α-HCH	319-84-6	290.8	1.63E+00	3.50E-02	3.72	3.33		5.00E-07
β-HCH	319-85-7	290.8	9.38E-01	1.98E-02	3.72	3.37		5.00E-07
γ-HCH	58-89-9	290.8	5.81E+00	1.23E-03	3.72	2.99		5.00E-07
δ-HCH	319-86-8	290.8	1.01E+01	3.06E-02	3.72	3.14		5.00E-07
Carbaryl	63-25-2	201.2	8.16E+01	1.43E-01	2.36	2.27		2.00E-07
Carbofuran	1563-66-2	221.3	3.76E+02	2.03E-03	1.63	1.64		2.00E-07
Maneb	12427-38-2	265.3	8.50E-05	2.08E-06	8.00	8.00		2.00E-07
Atrazine	1912-24-9	215.7	3.81E+01	2.70E-05	2.61	2.20		2.00E-07
Mineral oil								
aliphatic >EC5-EC6	-	81.0	2.80E+01	5.07E+04	3.52	2.90		4.00E-06
aliphatic >EC6-EC8	-	100.0	4.20E+00	8.61E+03	3.60	3.60		4.00E-06
aliphatic >EC8-EC10	-	130.0	3.25E-01	8.21E+02	3.69	4.50		4.00E-06
aliphatic >EC10-EC12	-	160.0	2.61E-02	7.90E+01	3.76	5.40		4.00E-06
aliphatic >EC12-EC16	-	200.0	5.90E-04	3.55E+00	3.85	6.70		4.00E-06
aliphatic >EC16-EC21	-	270.0	9.99E-07	1.72E-01	3.97	9.00		4.00E-06
aromatic >EC5-EC7	-	78.0	2.20E+02	1.11E+04	3.53	3.00		1.40E-06
aromatic >EC7-EC8	-	92.0	1.30E+02	3.24E+03	3.54	3.10		1.40E-06
aromatic >EC8-EC10	-	120.0	6.50E+01	8.21E+02	3.55	3.20		1.40E-06
aromatic >EC10-EC12	-	130.0	2.48E+01	7.90E+01	3.58	3.40		1.40E-06
aromatic >EC12-EC16	-	150.0	5.81E+00	3.55E+00	3.61	3.70		1.40E-06
aromatic >EC16-EC21	-	190.0	5.43E-01	1.72E-01	3.66	4.20		1.40E-06
aromatic >EC21-EC35	-	240.0	6.60E-03	8.00E-04	3.74	5.10		1.40E-06
Phthalates								
Dimethyl phthalate (DMP)	131-11-3	194.2	2.01E+03	3.87E+00	1.56	2.25		2.00E-06
Diethyl phthalate (DEP)	84-66-2	222.2	2.87E+02	6.68E-01	2.47	2.64		2.00E-06
Diisobutylphthalate (DIBP)	84-69-5	278.4	9.60E+00	1.37E-02	4.46	3.24		2.00E-06
Dibuthyl phthalate (DBP)	84-74-2	278.4	2.35E+00	3.40E-02	4.72	2.98		2.00E-06
Butylbenzylphthalate (BBP)	85-68-7	312.4	4.22E+00	6.53E-04	4.91	3.91		2.00E-06
Dihexyl phthalate (DHP)	84-75-3	334.5	1.15E-02	1.61E-03	6.85	4.65		2.00E-06
Di(2-ethylhexyl)phthalate (DEHP)	117-81-7	390.6	4.57E-02	2.72E-04	7.45	5.37		2.00E-06
Others								
Cyclohexanone	108-94-1	98.1	1.90E+04	4.90E+02	0.81	0.99		1.00E-07
Pyridine	110-86-1	79.1	6.65E+05	2.02E+03	0.65	1.93		2.00E-06
Tetrahydrofuran	109-99-9	72.1	4.06E+05	1.47E+04	0.47	0.47		2.00E-06
Tetrahydrothiophene	110-01-0	88.2	1.29E+04	2.05E+03	1.61	1.40		2.00E-06

Soil, site and exposure parameters (*'residential with garden'*)

Values in ***'bold'*** are revised.

parameters	code	unit	value (2000)
Soil parameters			
soil temperature	T	[K]	283
volume fraction air	Va	[-]	0.2
volume fraction water	Vw	[-]	**0.3**
volume fraction soil	Vs	[-]	**0.5**
fraction organic carbon	foc	[-]	0.058^{*1}
percentage clay	L	[%]	25^{*1}
dry bulk density	SD	[kg/dm3]	**1.2**
pH	pH	[-]	6^{*1}
Constants and site parameters			
gas constant	R	[Pa.m3/mol.K]	8.3144
viscosity of air	ETA	[Pa.h)	**5 E-09**
mean depth of contamination	dp	[m]	1.25
air permeability of soil	KAPPA	[m]	**1 E-11**
air-exchange rate	Vv	[1/h]	**1.1**
height of crawl space	Bh	[m]	0.5
depth of groundwater table	dg	[m]	**1.75**
height of the capillary transition boundary	z	[m]	**0.5**
air pressure difference crawl space and room	DELTAPCS	[Pa]	**1**
contribution of the crawl space air to indoor air	fbi	[-]	0.1
diameter contaminated area	Lp	[m]	100
fraction dry matter root crops	fdwr	[-]	**0.167**
fraction dry matter leafy crops	fdws	[-]	**0.098**
deposition constant	dpconst	[-]	**0.01**
fraction soil in dust inside	frsi	[-]	0.8
fraction soil in dust outside	frso	[-]	0.5
temperature bath water	Tsh	[K]	313
drinking water constant	dwconst	[-]	45.6
Exposure parameters			
fraction exposed skin showering	fexp	[-]	0.4
retention factor soil particles in lungs	fr	[-]	0.75
relative sorption factor	Fa	[-]	1
relative sorption factor soil ingestion	Fag	[-]	1 ^{*2}
matrix factor dermal uptake	fm	[-]	0.15
showering period	tdc	[h per day]	0.25
bathing period	td	[h]	0.5
fraction contaminated root crops	Fvk	[-]	0.1
fraction contaminated leafy crops	Fvb	[-]	0.1

continued

Exposure parameters	code	unit	children value (2000)	adults value (2000)
body weight	BWc,a	[kg]	15	70
daily intake soil	AIDc,a	[kg per day]	**1.00E-04**	5.00E-05
consumption of root crops	Qk'c,a	[kg fw per day]	**0.0595**	**0.1220**
consumption of leafy crops	Qb'c,a	[kg fw per day]	**0.0583**	**0.1390**
consumption of drinking water	Qdw,c,a	[dm3 per day]	1	2
dermal sorption coefficient	DACc,a	[kg per day]	6.43E-06	5.92E-06
inhalation of soil particles	ITSPc,a	[kg per day]	3.13E-07	8.33E-07
inhalation period indoors	Tiic,a	[h]	21.14	22.86
inhalation period outdoors	Tioc,a	[h]	2.86	1.14
air volume	Avc,a	[m3/h]	0.32	0.83
body surface	Atotc,a	[m2]	0.95	1.8
exposed surface skin indoors	Aexpc,a i	[m2]	0.05	0.09
exposed surface skin outdoors	Aexpc,a o	[m2]	0.28	0.17
degree of coverage skin indoors	DAEc,a i	[kg/m2]	5.6E-04	5.6E-04
degree of coverage outdoors	DAEc,a o	[kg/m2]	5.1E-03	3.8E-02
dermal absorption velocity	DARc,a	[1/h]	0.01	0.005
period exposure through contact soil indoors	Tbci,a	[h per day]	9.14	14.86
period exposure through contact soil outdoors	Tbco,a	[h per day]	2.86	1.14
dillution velocity	Vfc,a	[m/h]	161.3	324.6

*1 These values differ from the recommended values (see Lijzen et al., 2001).

*2 Only for lead enough data are available to provisionally lower this Relative Absorption Factor to 0.6 (Lijzen et al., 2001)