

RIVM report 711701 022

**Evaluation of model concepts on human
exposure**

Proposals for updating the most relevant exposure
routes of CSOIL

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Abstract

Since 1991 the human exposure model CSOIL has been used in the Netherlands for deriving proposals for Intervention Values. The main purpose of the evaluation of model concepts is to obtain adjusted systematic methods for deriving Intervention Values according to the most recent views on the human exposure assessment to soil contaminants. The research is limited to the concepts of the most relevant routes of CSOIL, i.e. the ingestion of contaminated soil particles, the inhalation of volatile compounds in indoor air and the consumption of contaminated crops. Here, concepts of other human exposure models have been selected (including three foreign models), which might be useful for the improvement of CSOIL.

The soil ingestion route of CSOIL is identical to the concepts of the models that are used abroad. For this route it is proposed to implement deliberate soil ingestion for children and the introduction of a separate exposure duration combined with a daily intake rate. Further, a distinction between the oral and inhalative absorption should be made.

In CSOIL the concept for the inhalation of volatile compounds in indoor air does not always correspond with other models. For a more accurate description of the flux from soil air to indoor air, inclusion of a convective flux into the volatilisation module of CSOIL has been proposed, along with the removal of the evaporation flux and boundary flux from CSOIL. There is a recommendation to discuss the use of the respirable fraction for the inhalative route.

For the consumption of contaminated crops a distinction has been made between metals and organic compounds for roots and aboveground plant parts. Except for incorporating the influence of the soil pH, no further adjustments of CSOIL are proposed for the uptake of metals in roots and aboveground plant parts. For the uptake of organic compounds in roots and aboveground plant parts, the use of the model concepts of Trapp and Matthies is proposed, instead of the current relations of Briggs. Soil and dust particles can deposit on the different plant parts by rainsplash. For organic compounds, the proposal is to add the concept of 'soil resuspension' to CSOIL.

Preface

To be able to provide an up-to-date scientific basis for parts of the Dutch Soil Protection Act the Directorate General of Environment commissioned the National Institute of Public Health and the Environment (RIVM) to carry out the project ‘Evaluation of Intervention Values Soil’. This report presents the result of evaluating the most relevant model concepts related to human exposure. Other reports covering the results of this project concern:

- The accumulation of soil contaminants in crops, location-specific calculations based on the CSOIL module. Part I Evaluation and suggestions for model development (RIVM Report 711701008);
- Evaluation and revision of the CSOIL parameter set (RIVM Report 7117021);
- Evaluation of the ecotoxicological Serious Risk Concentrations for soil, sediment and (ground)water (RIVM Report 711701020);
- Risk assessment of historical soil contamination with cyanides; origin, potential human exposure and evaluation of Intervention Value (RIVM Report 711701019);
- Proposal for revised Intervention Values for petroleum hydrocarbons on the basis of fractions of petroleum hydrocarbons (RIVM Report 7117015);
- Integration report with a technical evaluation of the Intervention Values for soil/sediment and groundwater and proposals for Intervention Values on soil/sediment and groundwater of all compounds of the first series of Intervention Values (RIVM Report 711701023).

Also related to this project is a report on the re-evaluation of the human-toxicological Maximum Permissible Risk levels (Baars et al., 2001).

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Samenvatting

Het Directoraat-Generaal Milieubeheer heeft het RIVM de opdracht gegeven voor het uitvoeren van het project 'Evaluatie Interventiewaarden Bodemsanering'. Het doel van dit project is om een bijgewerkte wetenschappelijke basis te verkrijgen voor de onderbouwing van de Nederlandse Interventiewaarden (IW) voor bodem en grondwater. Het belangrijkste doel van de evaluatie van modelconcepten is om een systematiek te verkrijgen die overeenkomt met de meest recente inzichten betreffende het bepalen van de humane blootstelling aan bodemverontreinigingen. Sinds 1991 wordt het humane blootstellingsmodel CSOIL gebruikt voor het berekenen van de IW voor bodemsanering. Deze IW zijn gebaseerd op potentiële blootstellingsrisico's. In deze evaluatie zijn de concepten van andere modellen geselecteerd (waaronder drie buitenlandse), die bruikbaar kunnen zijn voor het verbeteren van het CSOIL. Het onderzoek is beperkt tot de concepten van de meest relevante routes van CSOIL. Deze concepten zijn de ingestie van verontreinigde grond, de inhalatie van vluchtige verbindingen in binnenlucht en de consumptie van verontreinigde gewassen

De grondingestie route van CSOIL is over het algemeen identiek aan de concepten van de modellen die in het buitenland worden gebruikt. Het verschil wordt vooral veroorzaakt door het gebruik van verschillende waarden voor de inname van grond (zie § 3.3.5).

Voor de grondingestie route wordt voorgesteld om het concept van de opzettelijke ingestie door kinderen alleen te implementeren als in nader onderzoek de volharding of duur van deze gewoonte is gekwantificeerd. Een relatief korte periode van opzettelijk eten van grond is wijdverspreid en kan een significante invloed hebben op de blootstelling van kinderen. Deze route is vooral van belang als de blootstelling van kinderen wordt gescheiden van volwassenen. Verder wordt voorgesteld om CSOIL zo aan te passen dat een aparte blootstellingsduur gecombineerd kan worden met een dagelijkse inname, zodat CSOIL flexibel worden gebruikt om de huidige (jaar)gemiddelde ingestie aan te passen voor de verschillende scenario's t.b.v. actuele risicobeoordeling. Voor potentiële risico's zal deze aanpassing de CSOIL berekeningen niet beïnvloeden.

Tot slot wordt voorgesteld om een onderscheid te maken tussen de orale en inhalatieve absorptie, omdat deze in werkelijkheid ook verschillend zijn. Voor het bepalen van de potentiële blootstelling zal voor beide routes een defaultwaarde van 1 worden gebruikt, maar voor enkele stoffen is het mogelijk dat de absorptie via bodemingestie wordt bijgesteld.

Voor de inhalatie van vluchtige stoffen in binnenlucht blijkt dat, naast CSOIL, het CLEA model (UK) ook rekening kan houden met een kruipruimte onder de woning. Net als in CSOIL wordt in het UMS model (Duitsland) aangenomen dat de concentratie in binnenlucht alleen gerelateerd is aan de concentratie in bodemlucht. De diffuse fluxen van bodemlucht naar de lucht in de kruipruimte zijn identiek in CSOIL en VOLASOIL en wellicht ook in CLEA. CLEA en VOLASOIL gebruiken expliciet een convectieve flux naast de genoemde diffuse fluxen. CalTOX en UMS houden impliciet rekening met een convectieve flux.

Voorgesteld wordt om voor de inhalatie van vluchtige stoffen in binnenlucht de convectieve flux toe te voegen aan CSOIL, omdat naast de huidige diffusie ook het convectieve transport van belang is. Voor de implementatie van deze route in CSOIL zijn voorstellen gemaakt voor de nieuwe invoergegevens (zie hoofdstuk 4.6). Voor binnen- en buitenlucht wordt de evaporatieflux niet meer meegenomen in de vervluchtigingsmodule, omdat de bijdrage laag is en neerslag over het algemeen de evaporatie overschrijdt. De grenslaagflux leidt in CSOIL niet tot het begrenzen van de totale flux en wordt daarom ook weggelaten. Meer informatie betreffende de genoemde fluxen is te vinden in de hoofdstukken 4.2 en 4.3.

Voor de overzichtelijkheid van CSOIL wordt voor de humane blootstelling de twee afzonderlijke parameters voor inhalatie tijd binnen en buiten geïntegreerd tot een tijdparameter.

Aanbevolen wordt om het gebruik van de respirabele fractie te overwegen. De respirabele fractie is het deel van de totale geïnhalede hoeveelheid dat werkelijk de longen bereikt. In het huidige model is alleen de absorptie gedefinieerd. Er zijn geen voorstellen gemaakt om CSOIL te verbeteren betreffende een afzonderlijke correctiefactor voor absorptie en de respirabele fractie. De voornaamste reden is dat dit voorstel alleen van toepassing is op locatiespecifieke beoordelingen en daarom buiten deze evaluatie valt.

Voor de consumptie van gecontamineerde gewassen is een onderscheid gemaakt tussen metalen en organische verbindingen voor wortels en bovengrondse plantendelen.

Er wordt geen aanpassing van CSOIL voorgesteld voor de *opname van metalen door wortels en bovengrondse plantendelen*. Voor het schatten van de concentratie van metalen in wortel en blad wordt over het algemeen op BCF gebaseerde modellen gebruikt. Het CLEA model neemt de invloed van de bodem pH mee. Het gebruik van de bodem pH wordt ook voorgesteld in de herziene methode voor het afleiden van een BCF op basis van veldmetingen (Otte et al., 2001). In deze methode wordt na de selectie van alle gegevens per plantensoort een gewogen gemiddelde BCF waarde afgeleid, die gerelateerd is aan pH, organisch stof gehalte en klei. Voor de *opname van organische stoffen in wortels* zijn de concepten van de verschillende modellen voor een groot deel vergelijkbaar, waarbij de BCF gerelateerd is aan de logKow. Als de resultaten van de verschillende modellen worden vergeleken met BCF waarden die zijn gebaseerd op literatuurgegevens, dan blijkt dat de blootstelling volgens Briggs (1982, 1983) en Trapp en Matthies (1995) wordt overschat bij hogere waarden van de logKow. Voor de opname van organische stoffen in de wortels wordt voorgesteld om het concept van Trapp en Matthies te gebruiken met een aangepaste waarde voor het vetgehalte en de exponent die corrigeert voor de verschillen tussen plantenvet en octanol. Verder wordt aanbevolen om de opname in wortelgewassen nader te onderzoeken, omdat voor stoffen met een hoge logKow de blootstelling voornamelijk wordt bepaald door de opname in wortels. Vanwege de hoge BCF waarden is in absolute zin de blootstelling via wortelgewassen belangrijker dan via bovengrondse plantendelen.

Voor de opname van *organische stoffen in bovengrondse plantendelen* wordt voorgesteld om het modelconcept van Trapp en Matthies (1995) te gebruiken in plaats van de relatie van Briggs (1982, 1983). In Trapp en Matthies wordt in overeenstemming met andere risicobeoordelings-modellen de relevante processen en de gebruikte parameters beter beschreven. Als de schattingen volgens Trapp en Matthies en Briggs worden vergeleken met BCF waarden die zijn gebaseerd op literatuurgegevens, dan worden de BCF waarden voor beide methoden onderschat. Een mogelijke verklaring hiervoor is dat de bijdrage vanuit de lucht niet door deze modellen is meegenomen. Het wordt aanbevolen om de geldigheid van de Trapp en Matthies benadering nader te onderzoeken in vergelijking met meer experimentele gegevens en met betrekking tot verschillende plantensoorten.

Door regen kunnen opgespatte bodemdeeltjes terechtkomen op de verschillende bovengrondse plantendelen. De BCF waarden voor metalen zijn gebaseerd op veldgegevens, waarbij impliciet het opspatten van bodemdeeltjes al is meegenomen. Deze route is daarom alleen van toepassing op organische stoffen en wordt gebruikt door de modellen CLEA en CalTOX.

Nadere gegevens ontbreken over het opspatten van bodemdeeltjes in CalTOX. CLEA houdt rekening met 3% droge bodem per droge plant als representatieve waarde voor de hoeveelheid bodem op planten die niet verwijderd kan worden bij normale voedselbereiding. Trapp and Matthies stellen een minder conservatieve waarde voor van 1%. Voorgesteld wordt om het opspatten van bodemdeeltjes mee te nemen in CSOIL. Voor de bijdrage van deze route kan een voorlopige waarde worden aangenomen van 1% droge bodem per droge plant.

Summary

The Directorate General of Environment commissioned the RIVM to carry out the project, 'Evaluation of Soil Intervention Values'. The objective was to obtain an up-to-date scientific base for the Intervention Values (IV) for soil and groundwater. The model concepts were to be evaluated mainly to obtain an adjusted systematic methods for deriving Intervention Values, which are based on potential risks, according to the most recent views on assessment of human exposure to soil contaminants. The CSOIL human exposure model has been used in the Netherlands to calculate IV since 1991. In this evaluation concepts of other models (including three foreign ones) are selected that might be useful for improvement of CSOIL. The research is limited to the concepts pertaining to the following relevant routes of CSOIL:

1. ingestion of contaminated soil particles;
2. inhalation of volatile compounds in indoor air;
3. consumption of contaminated crops.

In general, the CSOIL soil ingestion route is identical to the model concepts used abroad. Specifically, the difference has been caused by using different values for the soil intake rate (see section 3.3.5).

For the soil ingestion route, it has been proposed only to implement the concept of deliberate soil ingestion by children if, in further research, the persistence or duration of this habit is quantified in more detail. Relatively short-term soil-eating is widespread among children and can have a significant impact on childhood contaminant exposure. For the CSOIL model the deliberate soil ingestion is especially important when the exposure for children is separated from the exposure for adults.

The proposal is to adjust the CSOIL model slightly by introducing a separate exposure duration combined with a daily intake rate. In this way, CSOIL can be used more flexibly to adjust the current (yearly) average ingestion rate for the different scenarios. For potential risks this adjustment will not affect the outcome of the CSOIL calculations. A (yearly) average daily soil ingestion rate is proposed for CSOIL (Otte et al., 2001), but no suggestions are made for combining an intake rate with an exposure of less than 365 days per year.

Further, it has been proposed to make a distinction between the oral and inhalative absorption, because the actual oral and inhalative uptake is different. For calculating the potential exposure for both routes, a default value of 1 will be used, but for some contaminants the absorption for the ingestion of soil may have to be adjusted.

Besides CSOIL, the CLEA model (UK) accounts for a crawl space under the dwelling for calculating the inhalation of volatile compounds in indoor air. Just as in CSOIL, the UMS model (Germany) assumes that the concentration in indoor air is solely related to the concentration in soil air. The diffusion fluxes from soil air to crawl-space air in CSOIL, VOLASOIL and, probably CLEA, are identical. In CalTOX and UMS the indoor air concentrations are based on molecular diffusion from soil air to indoor air. CLEA and VOLASOIL make explicit use of convective flux (pressure driven air flux), besides the diffusive fluxes mentioned, while CalTOX and UMS take convective flux implicitly into account.

Because a convective flux and diffusion contributes to the indoor air concentrations, it has been proposed to include a convective flux in the volatilisation module of CSOIL. Proposals for new input parameters have been made for the implementation in CSOIL (see section 4.6). For indoor and outdoor air it was decided to exclude the evaporation flux from the volatilisation module. The contribution of this flux appeared to be low and precipitation, in general,

exceeded evaporation. The boundary flux in CSOIL does not lead to limitations of the total flux and will also be left out. More information on the fluxes mentioned is included in sections 4.2 and 4.3.

For convenience of comparison the two separate time parameters (t_i and t_{fi}) for the indoor and outdoor inhalation will be integrated into one exposure time parameter (T_i). The use of the respirable fraction for the inhalative route should be put to discussion. The respirable fraction is the part of the total inhaled contaminated quantity, which actually reaches the lungs or alveoli. In the current CSOIL model only absorption is defined. No proposals for an update of CSOIL has been made where a separate correction factor for the absorption rate and the respirable fraction are concerned, the main reason being that possible adjustments are only applicable to site-specific assessments, which are not a subject of this evaluation.

For the consumption of contaminated crops a distinction is made between metals and organic compounds for roots and aboveground plant parts. This evaluation did not lead to a proposal for adjustments of CSOIL for the uptake of *metals in roots and aboveground plant parts*. BCF correlation models are generally used for this route to estimate the concentration of metals in roots and leaf. The CLEA model also incorporates the influence of the soil pH. Use of soil pH was also proposed according to the revised method for deriving a BCF from field measurements (Otte et al., 2001). This method is based on a selection of data per plant species, after which a weighted average BCF value is calculated with relation to pH, organic matter and clay.

For the uptake of *organic compounds in roots* the concepts used in the different models are to a large extent comparable; here, the BCF is related to the logKow. In the comparison of the model results with BCF values based on literature data, there seems to be an overestimation of the exposure at higher logKow values according to Briggs (1982, 1983) and Trapp and Matthies (1995). The use of the concept of Trapp and Matthies was proposed with adjusted values for the lipid content and the correction exponent for differences between plant fat and octanol. It is recommended to further investigate the uptake by root crops. Research is especially recommended because the exposure is mainly determined by the uptake in roots for contaminants with a high logKow. Based on high BCF values, the exposure via root crops is, in an absolute sense, more important than via aboveground plant parts.

For the uptake of *organic compounds in aboveground plant parts*, the more acceptable model concept of Trapp and Matthies (1995) is proposed in preference to the current relationship of Briggs (1982, 1983). In conformance with other risk assessment models, the Trapp and Matthies approach better describes the relevant processes and parameters. Comparing the estimations with BCF values based on literature data, the BCF values for both approaches seem to be underestimated. A possible explanation for this difference is that these models do not account for the contribution from air. Investigating the validity of the Trapp and Matthies approach compared to more experimental data and in relation to different plant species is therefore recommended.

Soil and dust particles can be deposited on the different plant parts through *rainsplash*. The rainsplash route is implicitly included in the BCF values for metals, since these BCF values are based on field data, making the rainsplash route only applicable to organic compounds. The exposure models, CLEA and CalTOX, use the rainsplash route. Details are lacking on the rainsplash coefficient used in CalTOX. CLEA accounts for 3% dry soil per dry plant for soil attached to crops, which cannot be removed by normal food preparation. Trapp and Matthies suggest a less conservative value of 1%. The rainsplash concept should be added to CSOIL. The contribution of this route can be provisionally set at 1% dry soil per dry plant.

1. Introduction

1.1 Background and objective

In 1991 proposals were derived for the first series of Intervention Values for about 70 (groups of) compounds. Since the formalisation of these first series of Intervention Values for serious contaminated soils in 1994 (VROM, 1994) and the formalisation of the second and third series of compounds in 1997, more data, exposure models and calculation methods have become available. Besides, useful responses came from the large group of users of the Intervention Values for specific (groups of) compounds. To realise an up-to-date scientific basis for the Intervention Values soil and groundwater, as used in the Dutch Soil Protection Act, the Directorate General for Environmental Protection commissioned the RIVM to carry out the project 'Evaluation of Soil Intervention Values'. The evaluation of model concepts on human exposure is part of this project. The evaluation of model concepts focuses on the most relevant model concepts used in relation to potential human exposure¹. Therefore model concepts and recommendations on the actual site-specific human exposure are not considered. The main purpose of evaluating the concepts and comparing them with other models is to obtain adjusted systematic methods for deriving Intervention Values according to the most recent views on the exposure assessment to soil contaminants. For this reason, concepts of other human exposure models were selected that might be useful for CSOIL improvement.

This study will evaluate the major concepts of human exposure models, aiming at:

1. Acquiring insight into the possible concepts for calculating the exposure via the three major exposure routes;
2. Reviewing the concepts used in relevant (parts of) models for calculating the exposure.
3. Evaluating differences between the (parts of) models for each exposure route on the basis of differences in model concepts and input parameters.

The results and conclusions of this report will be used, along with revised data and calculation methods as presented in other reports, for making adjustments in the calculation of the human exposure. For example, the evaluation of the input parameters is taken up in a report on the evaluation of input parameters (Otte et al., 2001). The derivation of revised proposals based on these results can be found in an integration report of the RIVM (Lijzen et al, 2001).

1.2 Model concepts to be evaluated

The human exposure model CSOIL is used in the Netherlands to derive Intervention Values for soil and groundwater (Swartjes, 1999). CSOIL was developed for calculating the potential human exposure to contaminated terrestrial soils. The exposure is calculated using a standardised scenario, based on all possible exposure pathways for a residential situation. The exposure routes, described in CSOIL, are presented in Figure 1.1. The calculated exposure is compared with the human toxicologically based Maximum Permissible Risk (MPR). The human toxicologically based Intervention Value is defined as the soil concentration at which the exposure equals the MPR level. CSOIL back-calculates the Intervention Value for soil when the total exposure equals the MPR value. The distribution over the mobile soil phases (pore water and soil gas) is calculated according to the fugacity theory of Mackay and Paterson (1981).

¹ Potential exposure: exposure representing a standardised situation, assuming a standard scenario for a type of soil use (i.e. residential, industrial); all possible exposure pathways are included and the exposure can be seen as the average exposure for a large number of sites with that type of soil use.

This report discusses the concepts of the most relevant exposure routes of the CSOIL model in the framework of an extensive evaluation of the Intervention Values for soil/sediment and groundwater. The following three model concepts cover at least 90% of the total exposure for almost all substances (Van den Berg, 1995; Vissenberg, 1996):

1. the human exposure via the ingestion of contaminated soil particles
2. the human exposure to volatile compounds in indoor air
3. the human exposure via the consumption of contaminated crops

The following exposure routes make a minor contribution to the total exposure:

- Dermal uptake via soil contact (1-7% for 18 compounds);
- Drinking-water intake due to permeation through LDPE (1-13% for 29 compounds);
- Dermal uptake during bathing (1-5% for 20 compounds).

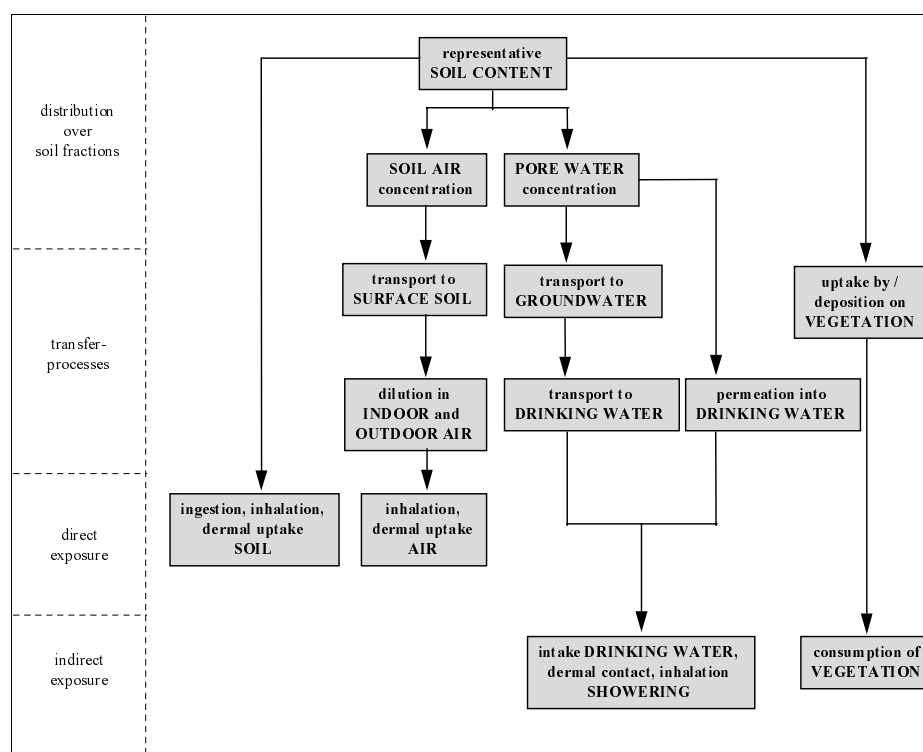


Figure 1.1 Exposure routes in CSOIL.

1.3 Readers' guide to the report

The next chapter will compare the corresponding model concepts of CSOIL and the European Union System for the Evaluation of Substances (EUSES). In chapter 3 CSOIL is compared with the international human exposure models, Contaminated Land Exposure Assessment model (CLEA, UK), 'Umweltmedizinische Beurteilung der Exposition des Menschen durch altlastbedingte Schadstoffe' (UMS, Germany) and the California Environmental Protection Agency, Department of Toxic Substances Control (CalTOX, US-EPA). Chapter 4 focuses on the human exposure to volatile compounds in indoor air in CSOIL, including a comparison with VOLASOIL. Chapter 5 describes and evaluates the current module in CSOIL for the uptake of organic substances in plants. The evaluation of metal uptake by plants forms part of the report on the evaluation of input parameters (Otte et al., 2001). The general conclusions and recommendation on possible adjustments of the CSOIL model concepts are presented in chapter 6.

2. Comparison of model concepts of CSOIL with EUSES

2.1 Introduction

In this chapter corresponding model concepts of CSOIL and the European Union System for the Evaluation of Substances (EUSES) are compared with each other by investigating the differences and similarities. For more specific information about EUSES the reader is referred to EC (1996).

The CSOIL model is developed to calculate (reverse-calculation) the serious soil contamination concentration (SCC) at which a human toxicological maximum permissible risk (MPR) is exceeded. The model is used to quantify the human exposure to soil pollutants for a residential situation at a local scale.

EUSES was developed for a quantitative assessment of the risks to man and environment at a local, regional and continental scale. For estimating the exposure levels and human intakes EUSES starts with emission rates which are distributed over different environmental compartments from which concentrations are calculated.

CSOIL and EUSES calculate a soil concentration starting from a different point. Within CSOIL there is no emission input, but only a partitioning concept is used for the three soil compartments soil solids, pore water and soil air. A soil concentration is calculated at a level where the exposure is equal to the MPR. Without a human-toxicological risk level CSOIL can not calculate a serious soil concentration contamination (SCC).

Within EUSES the soil compartment is receiving input by the application of sludge and deposition from air, after which a soil and pore water concentration is calculated. In contrast with CSOIL, EUSES can calculate a concentration in soil without a human-toxicological risk level. For humans a direct and indirect exposure via the environment is calculated, including the soil compartment. A risk characterisation is executed by using a human-toxicological risk level. Then the calculated human exposure is compared with the predicted no effect levels determined in the effect assessment.

2.2 Comparison of the human exposure routes of CSOIL and EUSES

In CSOIL for the determination of the human exposure the following direct and indirect exposure routes are taken into account:

1. ingestion of contaminated soil particles;
2. dermal contact with soil contaminants (indoor);
3. dermal contact with soil contaminants (outdoor);
4. inhalation of contaminated soil particles;
5. inhalation of vapours of contaminants via crawl space (indoor);
6. inhalation of vapours of contaminants (outdoor);
7. ingestion of contaminants via consumption of locally grown crops;
8. ingestion of soil contaminants via drinking water;
9. inhalation of vapours of contaminants in the drinking water during showering;
10. dermal contact with contaminants in the drinking water during showering.

For the determination of the human toxicological serious soil contamination concentrations (HUMTOX SCC) with CSOIL some direct (particularly via surface water) and indirect (via fish, meat and other animal derived products) routes are not taken into account. For an “actual” exposure analysis these routes can possibly be relevant. Therefore in CSOIL the indirect routes via meat and milk routes are quantified, but not taken into account for the determination of the HUMTOX SCC.

In EUSES the indirect exposure of humans to chemicals originates from several sources (see Figure 2.1). The inhalation of (outdoor) air is the only direct exposure route.

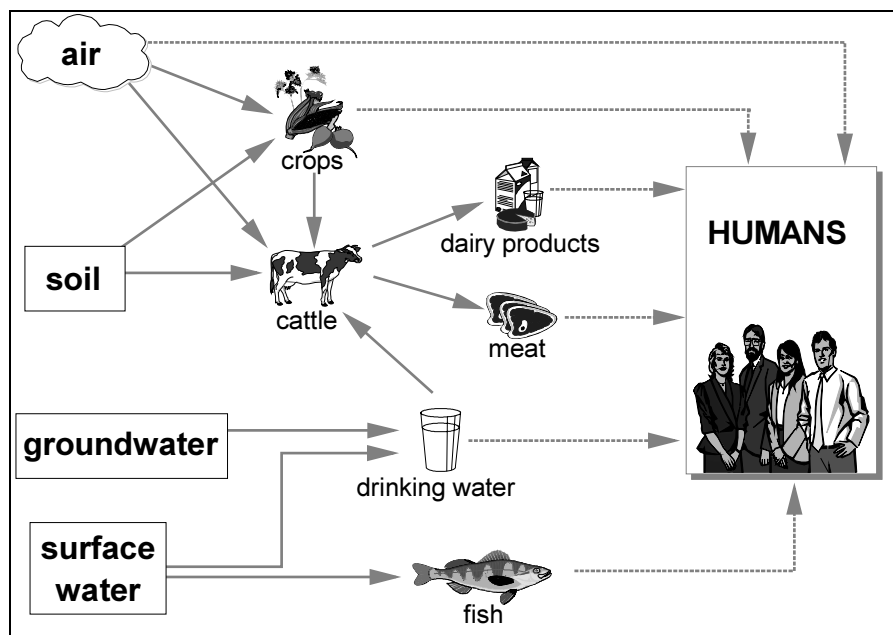


Figure 2.1 EUSES: exposure routes for humans through the environment.
Solid lines indicate (bio)transfer; broken lines indicate human intake.

For the determination of the indirect and direct exposure through the environment the following six pathways are taken into account within EUSES:

1. ingestion of soil contaminants via drinking water;
2. ingestion of contaminants via consumption of root and leaf crops;
3. ingestion of contaminants via consumption of fish;
4. ingestion of contaminants via consumption of milk;
5. ingestion of contaminants via consumption of meat;
6. outdoor inhalation of vapours (air).

Within CSOIL intake via consumption of animal products (number 3 to 5) is not an element in the exposure assessment for local soil contamination scenarios, because it is assumed that fish, dairy products and meat are purchased elsewhere. The exposure routes considered in CSOIL which are not used in EUSES are:

1. ingestion of soil particles;
2. inhalation of soil particles;
3. dermal uptake of soil particles;
4. inhalation of vapours during showering and bathing;
5. dermal uptake during showering.

2.3 Comparison of corresponding exposure routes of CSOIL and EUSES

For the 10 CSOIL exposure routes only the following three routes are taken into account within EUSES:

1. outdoor inhalation of vapours of contaminants;
2. ingestion of contaminants via drinking water;
3. ingestion of contaminants via consumption of crops.

In the next sections the concepts of these three exposure routes of EUSES and CSOIL are compared with each other. Additionally, the partitioning concepts of the soil compartments of both models are investigated.

2.3.1 The concepts for calculating outdoor inhalation of vapours

For calculating the inhalative exposure with EUSES only outdoor inhalation of vapours is considered. The indoor inhalation of air is assumed to be equal to the outdoor inhalation. The indoor inhalation of contaminants migrated from soil to the crawl space under the dwelling and subsequently indoor air is not considered in EUSES.

EUSES

The outdoor concentration in air is based on local industrial emissions to air. The air compartment receives its input from direct emissions to air and volatilisation from the sewage treatment plant (STP), see Figure 2.2.

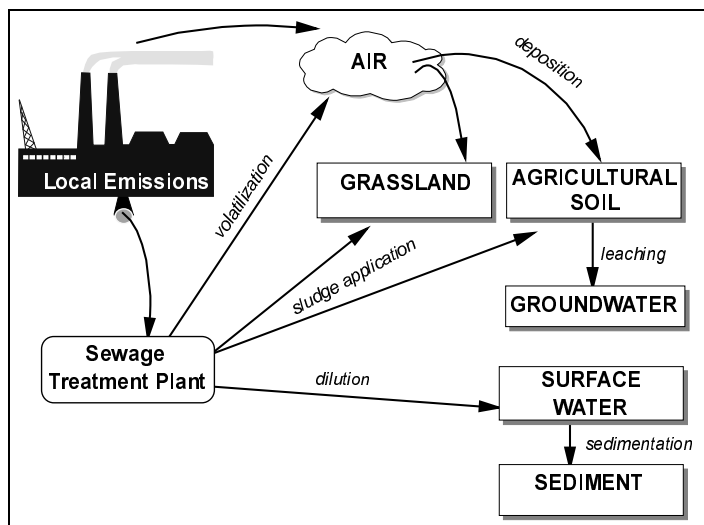


Figure 2.2 Local emission and distribution routes

The Gaussian plume model OPS (Van Jaarsveld, 1990) is applied in EUSES, using the standard parameters given by Toet and de Leeuw (1992). The OPS result is used in EUSES as the standard concentration ($C_{std,air}$) at a default source strength of 1 kg/d. The concentration of the chemical is calculated at distance of 100 meters from the point source and the STP. Further, the concentration in air is calculated from the largest emission to air for the direct emission and the indirect emission from STP:

$$C_{air} = \max(EMISSION_{direct,air}, EMISSION_{STP,air}) \cdot C_{std,air}$$

$$C_{air,annual} = C_{air} \cdot \frac{T_{emission}}{365}$$

EMISSION _{direct,air} :	local direct emission rate to air during emission period	[kg/d]
EMISSION _{STP,air} :	local indirect emission rate to air from STP during emission period	[kg/d]
Cstd _{air} :	concentration in air at source strength of 1 kg/d	[2.78.10 ⁻¹⁰ kg/m ³]
T _{emission}	number of days per year that emission occurs	[d/year]
C _{air}	local concentration in air during emission episode, 100m from source	[kg/m ³]
C _{air,annual}	annual average concentration in air, 100m from source	[kg/m ³]

For indirect exposure of humans via inhalation the dose (total daily intake) is based on the concentration in air multiplied with the inhalation volume both divided by the body weight. The dose is corrected for the respirable fraction of the chemical. The respirable fraction is the part of the total inhaled quantity of a substance, which actually reach the lungs or alveoli. The default for the respirable fraction of the inhaled substance is 1 within EUSES.

For several compounds the actual respirable fraction is lower than 1. For gaseous substances the respirable fraction depends on the water solubility. For insoluble gaseous compounds the respirable fraction is 0. For soluble compounds the absorption via inhalation is linear related to the water solubility with a range of 0-1. For aerosols the respirable fraction depends on the particle size. For sizes of 0.1 µm to 5 µm the respirable fraction varies from 0.2 to 0.6. For particles of 5 µm to 10 µm the respirable fraction decreases to a value of 0 (T. Vermeire pers. comm.).

In EUSES the daily dose via intake of air is further corrected for the bioavailability of the chemical (inhalation/oral). The bioavailability for inhalation and for oral uptake depends on compound properties. The bioavailability for inhalation is the part of total quantity of a substance in the lungs, which is absorbed by the human body. This correction is necessary because in EUSES the internal dose via inhalation must first be converted to an external dose, before it can be added to the external doses of the other oral routes (see Figure 2.1). Via the other oral routes a substance is taken up via the gastro-intestinal tract and not via the lungs. In EUSES the default fraction for the bioavailability for inhalation is set on an estimated value of 0.75 (and not 1), because it is assumed that via exhalation almost no substance can be completely absorbed.

The actual bioavailability for inhalation can be different. Considering all compounds the oral and inhalative uptake can range from 0.5 to 1 and from 0.05 to 1, respectively. (T. Vermeire pers. comm).

$$DOSE_{air} = \frac{F_{resp} \cdot C_{air} \cdot IH_{air}}{BW} \cdot \frac{BIO_{inh}}{BIO_{oral}}$$

DOSE _{air}	daily dose via intake of air	[kg/kg _{bw} .d]
F _{resp} :	respirable fraction of inhaled substance	[1.0]
IH _{air} :	daily inhalation rate	[20 m ³ /d]
BW:	body weight of adult	[70 kg]
BIO _{inh} :	bioavailability for inhalation	[0.75]
BIO _{oral} :	bioavailability for oral intake	[1.0]

CSOIL

The concentration in outdoor air is based on three fluxes (J2-J4), from which a total soil flux to outdoor air (Jo) is calculated:

$$J2 = \frac{Da \cdot Csa}{d}$$

$$J3 = \frac{C_{pw} \cdot Ev}{24}$$

$$J4 = \frac{Du \cdot Cs \cdot SD}{dp} \quad \text{where:} \quad Du = \frac{Pa \cdot Dsa}{Va} + \frac{Pw \cdot Dsw}{Vw}$$

if $J3 + J4 < J2$ then $Jo = J3 + J4$

if $J3 + J4 \geq J2$ then $Jo = J2$

Finally, the concentration in outdoor air is calculated according:

$$Coa = \frac{Jo}{Vfa}$$

Du:	diffusion coefficient in soil		[m ² /h]
J2	border-layer flux		[g/m ² .h]
J3	water-evaporation flux		[g/m ² .h]
J4	diffusion flux water-soil to soil surface		[g/m ² .h]
Jo	total soil flux to outdoor air		[g/m ² .h]
Pa:	weight fraction in soil air		[-]
Pw:	weight fraction in soil pore water		[-]
Da:	diffusion coefficient in (free) air		[m ² /h]
Dsa:	diffusion coefficient in soil air		[m ² /h]
Dsw:	diffusion coefficient in soil pore water		[m ² /h]
Va:	volume fraction air in soil	EUSES: Fair _{soil}	[0.2]
Vw:	volume fraction water in soil	EUSES: Fwater _{soil}	[0.2]
Csa:	concentration in soil air		[mol/dm ³ or g/m ³]
Cpw:	concentration pore water	EUSES: C _{soil,porew}	[mol/dm ³ or g/m ³]
Cs:	initial soil concentration	EUSES: C _{soil}	[mol/kg _{dwt}]
d	thickness border-layer		[0.005 m]
Ev	flux of evaporating water		[0.0001 m ³ /m ² .d]
SD	dry bulkdensity of soil	EUSES: RHO _{soil}	[1.5 kg _{dwt} /dm ³]
dp	mean depth of the contamination		[1.25 m]
Coa	concentration outdoor air (for an adult, at 1.5 m)	EUSES: PEC _{air,annual}	[g/m ³]
Vfa	dilution velocity for an adult		[m/h]

The inhaled dose in CSOIL is based on the concentration in air (indoor and outdoor) multiplied with the inhalation volume, both divided by the body weight. A correction is applied for the relative absorption in the human body (fa) and the relative time spent indoors and outdoors.

$$IV = \frac{fa \cdot (AV \cdot Coa \cdot tfo \cdot to + AV \cdot Cia \cdot tfi \cdot ti) \cdot 1000}{BW}$$

IV:	uptake of contaminations via vapours	EUSES: DOSE _{air}	[mg/kg.d]
fa:	relative absorption factor	EUSES: BIO _{inh}	[1.0]
AV:	daily inhalation rate	EUSES: IH _{air}	[20 m ³ /d]
W:	body weight of adult	EUSES: BW	[70 kg]
tfo:	timefraction for residence outdoor (mean for one year)		[-]
tfi:	timefraction for residence indoor (mean for one year)		[-]
to:	daily duration of exposure outdoors		[h]
ti:	daily duration of exposure indoors		[h]

Comparison:

The concept for calculating the outdoor concentration in air is completely different. Within EUSES it is based on the local industrial emissions to air and within CSOIL it is based on a diffusion flux (emission) from the soil compartment to air. Within EUSES the soil compartment is essentially free of contaminants and can only be contaminated via the deposition from air or via the application of sewage sludge. Within CSOIL a contaminated soil and the diffusion to the atmosphere is the starting point for calculating the outdoor air concentration.

The concept for calculating the inhaled dose is partly identical for EUSES and CSOIL. For both models the concentration in air is multiplied with the inhalation volume which is divided by the body weight. The relative absorption factor (f_a) of CSOIL can be compared with the bioavailability for inhalation (BIO_{inh}) of EUSES. The default values for the absorption factor (f_a) and the bioavailability for inhalation (BIO_{inh}) are different with a figure of 1.0 and 0.75, respectively. In EUSES is assumed that because of exhalation actually no substance can be totally absorbed. Another difference is that only in EUSES a correction is applied for the respirable fraction of inhaled substance and only within CSOIL indoor and outdoor air concentrations are weighted for the time spent indoors and outdoors. Indoor concentrations are not calculated in EUSES.

The (default) values for the daily inhalation rate ($20 \text{ m}^3/\text{d}$) and the body weight of an adult (70 kg) are the same for both models.

2.3.2 Ingestion of contaminants via drinking waterComparison

Within CSOIL the contamination of drinking water only occurs at the site of the contamination. It is assumed that drinking water can only be contaminated by the permeation of substances through the water mains. Within CSOIL drinking water leaving the purification plant is essentially free of contaminants. This is a different approach compared to EUSES. In EUSES drinking water can be contaminated via the intake of contaminated surface water or ground water. Then it is assumed that not all contaminants are removed during purification. Another route is the direct use of groundwater for drinking water, where the concentration in drinking water is assumed to be equal to the concentration in groundwater. From these two possible drinking-water concentrations the highest value is selected.

Exposure by the direct consumption of groundwater is not included in the CSOIL calculations, but is always investigated for the determination of the Intervention Value (IV) for groundwater. The pore water IV is used for the determination of a groundwater IV. The IV for groundwater is calculated using the calculated pore water concentration based on the equilibrium theory. For organic compounds the IV for groundwater is derived by decreasing the calculated pore water equilibrium concentration with a factor 10 (Van den Berg and Roels, 1991). For adults an intake rate of 2 l/d is assumed for calculating the daily intake of drinking water through direct consumption of groundwater. For the direct consumption of groundwater in EUSES the concentration in drinking water is assumed to be equal to the concentration in groundwater of agricultural soils. In EUSES the default intake rate of drinking water is 2 l/d. Further, in EUSES the groundwater concentration is equal to the porewater concentration. In EUSES the pore water concentration is calculated from the agricultural soil concentration by applying the soil-water partition coefficient according to:

$$PEC_{agr.soil,porewater} = \frac{PEC_{agr.soil} \cdot RHO_{soil}}{K_{soil-water}}$$

$PEC_{agr.soil,porewater}$:	predicted environmental concentration in porewater of agr. soil	[kg/m ³]
$PEC_{agr.soil}$:	predicted environmental concentration in agricultural soil	[kg/kg _{wwt}]
RHO_{soil} :	bulk density of wet soil	[kg _{wwt} /m ³]
$K_{soil-water}$:	soil-water partition coefficient	[m ³ /m ³]

The concepts for calculating the pore water concentration are identical in CSOIL and EUSES. For more information about the calculation of the pore water concentrations the reader is referred to section 2.3.4 and Appendix 5.2.

2.3.3 The concepts for calculating the concentrations in plants

A more thorough evaluation of the plant uptake module of CSOIL with other concepts are subject of section 3.5 and chapter 5. In this section only the concept of CSOIL is compared with EUSES.

EUSES

The modelling approach proposed by Trapp and Matthies (1995) is used to estimate levels in plants due to uptake from pore water and due to gaseous uptake from air (Figure 2.3).

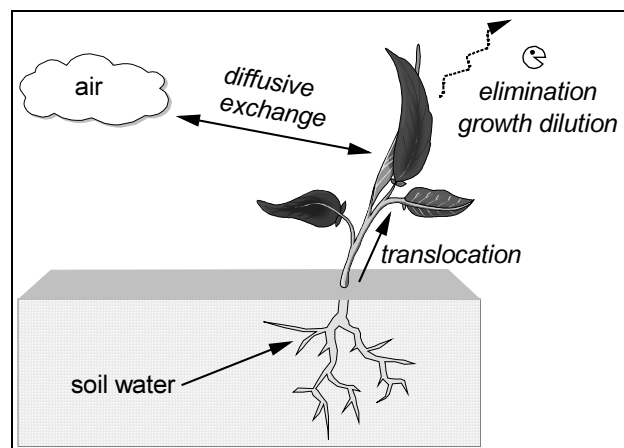


Figure 2.3 Fate processes accounted for in the plant uptake model of EUSES.

The general partitioning between water and plant tissue is assumed to be based on hydrophobic sorption to plant lipids:

$$K_{plant-water} = F_{water_{plant}} + F_{lipid_{plant}} \cdot Kow^b$$

$K_{plant-water}$:	partition coefficient between plant tissue and water	[m ³ /m ³]
$F_{water_{plant}}$:	volume fraction of water in plant tissue	[0.65 m ³ /m ³]
$F_{lipid_{plant}}$:	volume fraction of lipids in plant tissue	[0.01 m ³ /m ³]
b :	correction for differences between plant lipids and octanol	[0.95]

In the previous equation the Kow is slightly corrected for the differences between plant lipids and octanol.

The concentration in root tissue is governed mainly by physical sorption and is calculated according:

$$C_{root} = \frac{K_{plant-water} \cdot C_{soil,porewater}}{RHO_{plant}}$$

C_{root} :	concentration in root tissue	[kg/kg _{wwt}]
RHO_{plant} :	bulk density of plant tissue (wet weight)	[700 kg _{wwt} /m ³]

The steady state concentration in leaf tissue is calculated accounting for two source terms and three sink terms. The source terms are the uptake and translocation from soil and the gaseous uptake from air. The sink terms are formed by diffusive transfer from leaf to air, elimination in the plant tissue and dilution by growth. For the equations of all terms the reader is referred to appendix 5.1. In this appendix it is mentioned that the domain of the used transpiration stream concentration factor (TSCF) of Briggs et al. (1982) is log Kow -0.5 to 4.5. Outside this range the minimum or maximum Kow is used. Aerosol deposition is not considered in this model. The model is not suitable for inorganic substances.

The dose (total daily intake) is based on the calculated concentration in leaves and roots of plants multiplied with the intake of leaf crops (1.20 kg_{wwt}/d, crops including fruit and cereals) and root crops (0.384 kg_{wwt}/d, potatoes) divided by the body weight. The default consumption rates for each food product, used in EUSES, represents the highest country-average intake across all EU Member States for each food product. The maximum average food consumption in the EU and the average food consumption in The Netherlands is presented in Table 2.1 (ECETOC, 1994).

Table 2.1 Maximum average food consumption in the EU and average food consumption in The Netherlands (ECETOC, 1994)

Intake of	Maximum value for the EU (country) (g/d)	The Netherlands (g/d)
Fruit & crops	760 (Italy)	667
Cereals	440 (Italy)	203
Potatoes	384 (Ireland)	238

EUSES calculates different doses for the daily consumption of leaf and root crops.

$$DOSE_{root} = \frac{C_{root} \cdot IH_{root}}{BW}$$

$$DOSE_{leaf} = \frac{C_{leaf} \cdot IH_{leaf}}{BW}$$

$C_{root/leaf}$:	concentration in roots or leaves of crops	[kg/kg _{wwt}]
IH_{root} :	daily intake of root crops	[0.384 kg _{wwt} /d]
IH_{leaf} :	daily intake of leaf crops (incl. fruit and cereal)	[1.20 kg _{wwt} /d]

CSOIL

Within CSOIL there are different calculations available for the determination of the crop content for organic substances, metals and other inorganic substances. For (in)organic substances, other than metals, the concentrations in root crops and leafy crops are calculated with the uptake from pore water (BCF value) and by aerosol deposition. For metals the concentrations in crops are calculated with the uptake from soil and by aerosol deposition. For a comparison with EUSES, only the equations for organic substances are presented here:

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

$$Cpr' = BCFr' \cdot Cpw$$

$$BCFs' = (10^{(0.95 \log Kow - 2.05)} + 0.82) \cdot (0.784 \cdot 10^{\frac{-0.434(\log Kow - 1.78)^2}{2.44}})$$

$$Cps' = BCFs' \cdot Cpw + Cdp \cdot fdws$$

BCFr':	bioconcentration factor root crops		[mg/kg _{wwt} / mg/m ³]
BCFs':	bioconcentration factor tuber		[mg/kg _{wwt} / mg/m ³]
Cpr':	concentration in root crops	EUSES: C _{root}	[mg/kg _{dwt}]
Cps':	concentration in leaf crops	EUSES: C _{leaf}	[mg/kg _{dwt}]
Cpw	concentration pore water	EUSES: C _{soil,porew}	[mol/dm ³ or g/m ³]
Cdp:	concentration in crops consequent on deposition		[mg/kg _{dwt}]
fdws:	ratio between dryweight and freshweight of leaf crops		[0.117 kg _{dwt} /kg _{wwt}]

The dose is based on the added concentration in leaves and roots multiplied with the daily consumption and both divided by the body weight (adult, child).

$$VI = \frac{(Qfvk' \cdot Cpr' + Qfvb' \cdot Cps') \cdot fa \cdot fv}{W}$$

Cpr'/Cps':	concentration in roots or leaves of crops	EUSES: C _{root} /C _{leaf}	[mg/kg _{wwt}]
Qfvk':	daily intake of root crops (adult)	EUSES: IH _{root}	[0.1367 kg _{wwt} /d]
Qfvb':	daily intake of leaf crops (adult)	EUSES: IH _{leaf}	[0.1578 kg _{wwt} /d]
fa:	relative absorption factor		[1.0]
fv:	fraction contaminated food (fraction of own garden)		[0.1]

A correction is applied for the relative contribution of the daily consumption of leafy and root crops. Further a fraction of 0.1 is assumed for the use of home-grown crops (fv). CSOIL calculates one dose for the daily consumption of leafy and root crops. The daily consumption of leafy and root crops is different for metals (adults: 0.02761 and 0.01843 kg_{dwt}/d) and other (in)organic compounds (adults: 0.1367 and 0.1578 kg_{wwt}/d). The content of leafy and root crops is expressed on a dryweight basis and for (in)organic substances on a wetweight (freshweight) basis.

Comparison:

The EUSES approach for calculating the concentration of organic compounds in root crops and leafy crops is more advanced, because it accounts for uptake via pore water and air for elimination by metabolism, photolysis, growth and diffusive transfer to air. However, it must be noted that the default value for elimination by metabolism and photolysis within EUSES is 0. If these rate constants are known they can be added. CSOIL is only based on measured or calculated BCF values with a different approach for metals/inorganic substances and organic substances. The main disadvantage of the EUSES approach is that the model is not suitable for inorganic substances and that it does not account for aerosol deposition.

The concept for calculating the dose is identical for EUSES and CSOIL. The only exception is that the dose calculated with CSOIL is multiplied with a factor 0.1 to correct for the use of home-grown crops. In EUSES it is assumed that all consumed crops originate from agricultural soils. Therefore the dose is not corrected in EUSES.

The daily consumption of leafy and root crops is different. The main reason for the difference of the daily consumption of leafy crops is that EUSES, in contrast with CSOIL, is accounting for the intake of fruit and cereals. The daily consumption of root crops is more than a factor 2

higher within EUSES compared to CSOIL, with values of 0.384 kg_{wwt}/d and 0.1578 kg_{wwt}/d respectively. The daily consumption values for The Netherlands are lower than those chosen for EUSES (see Table 2.1). The EUSES values are based on the highest country average intake across the EU.

2.3.4 The partitioning concept of the soil compartment

EUSES

Within EUSES the topsoil layer is modelled as a single compartment, receiving input through a single application of sludge per year and a continuous deposition from air. The output of the soil compartment is formed by the processes leaching, volatilisation and biodegradation. The substance is divided over soil solids, pore water and air, which is described by the soil-water and air-water partition coefficients. See Figure 2.4.

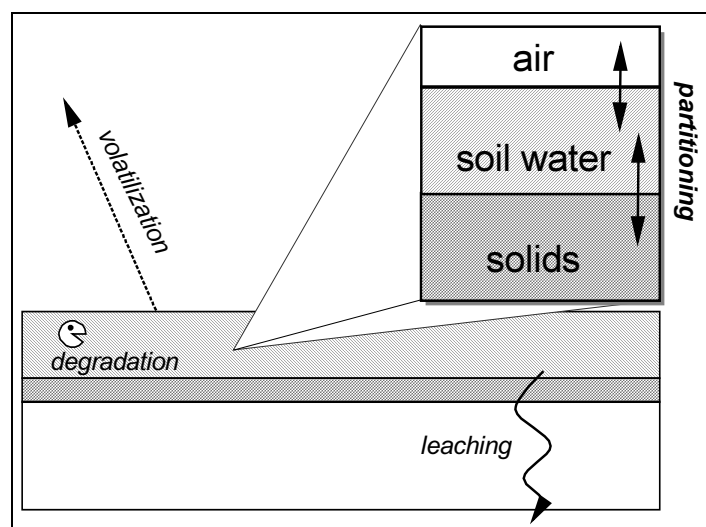


Figure 2.4 Possible fate processes in the soil compartment of EUSES.

The leaching from the soil compartment is calculated with default values for the amount of rain and infiltration into soil, the soil-water partition coefficient and the mixing depth of the soil type. See appendix 5.2 B for the equations.

The diffusive transfer from soil to air is estimated using a two-film resistance model. The soil side of the interface is treated as a pair of parallel resistances, that is the air phase and the water phase of the soil (Mackay et al., 1992). The rate constant for volatilisation is dependent on the air-water and soil-water partition coefficient, the mixing depth of the soil type and default values for partial mass-transfer coefficients at the air-soil interface.

The rate constant for biodegradation is based on standardised biodegradation tests. The rate constant is further estimated from the partition coefficient of the substance (see Table 2.2), because it is assumed that no biodegradation takes place in the bound phase.

Table 2.2 *Half-lives for soil, based on results from standardised biodegradation tests*

Partition coefficient soil: $K_{p_{soil}}$ [m ³ /kg]	Half life for soil: DT50 _{bio,soil}		
	Readily biodegradable	Readily biodegradable, failing 10-d window	Inherently biodegradable
≤ 0.1	30	90	300
> 0.1, ≤ 1.0	300	900	3000
> 1.0, ≤ 10	3000	9000	30000
etc.	etc.	etc.	etc.

CSOIL

Within CSOIL from the concentration in soil a concentration in pore water and a concentration in soil air is calculated, with the assumption that there is an equilibrium between the three soil phases. The concentrations in the three soil phases are calculated on the basis of equilibrium partitioning and stationary transport equations (Appendix 5.2 A). When the calculated concentration in pore water is higher than the water solubility, then the concentration in pore water is set equal to the water solubility. The concentrations in the three soil phases are calculated according the equations of the fugacity theory of Mackay et al. (1985). In CSOIL biological degradation and leaching are not taken into account. More about the volatilisation module of CSOIL is described in another part of the project “Evaluation of Intervention Values”.

Comparison

In the introduction of chapter 2.1 the conceptual differences of EUSES and CSOIL are already mentioned. Because of these differences, the routes for calculating a soil concentration can not be compared with each other. Only the partitioning concept can be compared for the part where a pore water concentration is calculated. A soil-air concentration is not calculated in EUSES and therefore can not be compared with the result of CSOIL.

As mentioned only the calculations of the concentrations in pore water of CSOIL and EUSES can be used for a comparison of the partitioning concepts in soil. With CSOIL the concentrations in the three soil phases are calculated according the fugacity theory of Mackay et al. (1985). The equations of the fugacity capacity constants for water, air and soil are presented in Appendix 5.2 A. With EUSES a concentration in pore water is mainly based on an air-water partition coefficient ($K_{air-water}$) and a solids-water partition coefficient in soil ($K_{soil-water}$), see equations in Appendix 5.2 B.

For some defaults a different value is chosen. For the soil temperature (TEMP) a value of 283 K is used in CSOIL. The default soil temperature in EUSES is 285 K. Further, the weight fraction organic carbon in soil solids ($F_{solid,soils}$) is different in CSOIL and EUSES with values of 0.058 kg/kg 0.02 kg/kg, respectively. The used relation for calculating an organic carbon-water partition coefficient (K_{oc}) with an octanol-water partition coefficient (K_{ow}) is different in CSOIL (Karickhof, 1981) and EUSES (Sabljić, 1995).

CSOIL:	$K_{oc} = 0.411 \cdot K_{ow}$	(Karickhof, 1981)
EUSES:	$K_{oc} = 1.26 \cdot K_{ow}^{0.81}$	(Sabljić et al., 1995)

The partitioning concepts of CSOIL and EUSES are compared with each other, using the same values for the soil temperature and the weight fraction organic carbon in soil solids. Also the water solubility in EUSES is adapted for a unit in mol/m³ instead of a unit of kg/m³ and the same Koc is used in both models. With these adaptations an identical pore water concentration is calculated for both models. Concluding it can be said that the partitioning concept for soil-pore water is identical in CSOIL and EUSES.

2.3.5 Additional concept: the concepts for calculating the exposure to fish

With CSOIL a mean lifetime exposure is calculated for soil contaminations in a residential situation. For this standard scenario the exposure to contaminated sediments is not accounted for, because this exposure route has a small contribution to the total potential exposure (Van den Berg, 1991). For the determination of actual risk this exposure route can be evaluated with the model SEDISOIL (Bockting et al., 1996). SEDISOIL is not a part of the project "Evaluation of Intervention Values". Nevertheless in this section a short description is given for the exposure route via fish of EUSES and SEDISOIL.

EUSES

The concentration in fish for human indirect exposure is given by:

$$C_{fish} = BCF_{fish} \cdot C_{water}$$

where:

$$\text{if } \log Kow \leq 6 \text{ then: } \log BCF_{fish} = 0.85 \cdot \log Kow - 0.70 - 3$$

$$\text{if } \log Kow > 6 \text{ then: } \log BCF_{fish} = -0.20 \cdot (\log Kow)^2 + 2.74 \cdot \log Kow - 4.72 - 3$$

C_{fish} :	concentration in fish (freshweight)	[kg/kg _{wwt}]
BCF_{fish} :	bioconcentration factor for fish-surface water (freshweight)	[m ³ /kg _{wwt}]
C_{water} :	concentration in surface water	[kg/m ³]

The dose (total daily intake) is based on the calculated concentration in fish multiplied with the intake of fish, divided by the body weight:

$$DOSE_{fish} = \frac{C_{fish} \cdot IH_{fish}}{BW}$$

C_{fish} :	concentration in fish (freshweight)	[kg/kg _{wwt}]
IH_{root} :	daily intake of fish	[0.115 kg _{wwt} /d]
BW :	body weight of (adult) human	[70 kg]

SEDISOIL

The concentration in fish is also calculated with the concentration in surface water and a contaminant specific BCF value:

$$C_{fi} = BCF_{fi} \cdot C_{sw}$$

where:

$$\text{if } \log Kow \leq 6 \text{ then: } BCF_{fi} = Kow \cdot Ff_{fi}$$

if $\log K_{ow} > 6$ then: $BCF_{fi} = 1 \cdot 10^6 \cdot Ff_{fi}$

C_{fi} :	concentration in fish (freshweight)	[kg/kg _{fw}]
BCF_{fi} :	bioconcentration factor for fish-surface water (freshweight)	[mg/kg _{fw} / mg/l]
C_{sw} :	concentration surface water	[mg/l]
Ff_{fi} :	fat fraction fish	[0.05 kg _{fat} /kg _{fw}]

$$FI = \frac{Q_{fi} \cdot FV_{fi} \cdot fa \cdot C_{fi}}{W}$$

FI:	daily intake of contamination via fish (angler)	[mg/kg.d]
Q_{fi} :	fish consumption angler (adult) [fish water:0.055 kg _{fw} /d] [not specific fish water:0.0011 kg _{fw} /d]	
FV_{fi} :	fraction contaminated fish	[0.5]
fa:	relative absorption factor	[1.0]

Comparison

Both models are similar for the part where the concentration in fish is calculated and for the concept of calculating the intake via fish. Different is the approach for calculating the BCF for fish and for the values assumed for the daily intake of fish.

2.4 Conclusions

In this section concepts of EUSES are selected that might be useful for improvement of CSOIL. For some recommendations additional research is necessary to get more insight in the exact use of the model concepts. The following two possible improvements are a subject of this project 'Evaluation of Intervention Values':

1. the use of the modelling approach for calculating the concentrations in plants proposed by Trapp and Matthies (sections 5.3 and 5.5);
2. the input-parameters for soil temperature and the weight fraction organic carbon (Otte, 2001).

Inhalation of vapours of contaminants

The respirable fraction of the inhaled substance:

For calculating the inhaled dose in CSOIL no correction is applied for the respirable fraction. The standard default for the respirable fraction of the inhaled substance is 1 within EUSES. For gaseous substances the respirable fraction depends on the water solubility. For aerosols the respirable fraction depends on the particle size. Based on this model comparison it should be considered to implement the respirable fraction in CSOIL, mainly for site specific assessments not necessarily for calculating potential risks.

Use of absorption rates:

A possible improvement can be the absorption factor or bioavailability for inhalation, which is 0.75 in EUSES (BIOinhalation) and 1.0 in CSOIL (fa). The default value of EUSES is lower than default value in CSOIL, because it is assumed that actually no substance is totally absorbed in the human body via exhalation. Discussion of the default value of 1, which is used for the absorption via the inhalative route, is recommended. For the time being, maintaining the default value of 1 in CSOIL is proposed.

The default value of 1 for the absorption factor or bioavailability for oral uptake is equal in EUSES (BIOoral) and CSOIL (fa). In CSOIL the oral and inhalative absorption is described by the same parameter. In EUSES both routes are described by different parameters and

their default value is different. A distinction must be made between oral and inhalative absorption and therefore a different parameter for each route should be included in CSOIL.

Ingestion of contaminants via consumption of crops

Plant uptake of organic substances:

The EUSES approach for calculating the concentrations in root tissue and leaf tissue is different from CSOIL. The only similarity is the use of the transpiration stream concentration factor (TSCF) of Briggs et al (1982). In EUSES the domain for using the transpiration stream concentration factor (TSCF) of Briggs et al. (1982) is log K_{ow} -0.5 to 4.5. For substances with log K_{ow} values of more than 4.5 the maximum K_{ow} of 4.5 is used. In EUSES Trapp and Matthies (1994) is used to account for the plant uptake of organic chemicals via pore water and the exchange via air. A possible improvement of CSOIL can be the use of the Trapp and Matthies approach, including the gaseous uptake from air.

Consumption rates of crops:

It appeared that the diverging values for the daily consumption of crops are difficult to evaluate. It can be useful to evaluate the importance of the values for the Netherlands presented in Table 2.1, which are proposed by ECETOC (1994).

The partitioning concept of the soil compartment

Relation for calculating an organic carbon-water partition coefficient (K_{oc}) with an octanol-water partition coefficient (K_{ow}):

It appeared that, instead of using the equation of Karickhof (1981) for calculating an organic carbon-water partition coefficient (K_{oc}) with an octanol-water partition coefficient (K_{ow}) the importance of the relation of Sabljic (1995) is usefull further to investigate. This because in the EU Sabljic is more accepted and the equations are based on more experimental data than those of Karickhof. The K_{oc} and K_{ow} are extensively evaluated in the report 'Evaluation and revision of the CSOIL parameter set' of Otte et al. (2001).

Other model concepts

Exposure to fish:

For the determination of actual risks the exposure via fish can be evaluated with the model SEDISOIL. SEDISOIL and EUSES are similar for the calculation of the concentration in fish and for the concept of calculating the intake via fish. Different is the approach for calculating the BCF for fish and the values assumed for the daily intake of fish. SEDISOIL is not a part of the project "Evaluation of Intervention Values". Therefore no further research is carried out to determine whether SEDISOIL can possibly be improved for calculating the BCF for fish.

3. Comparison of model concepts of CSOIL with international human exposure models

3.1 Introduction

In this chapter CSOIL will be compared with international human exposure models by investigating the differences and similarities of corresponding model concepts. For the international models a necessary condition is that (formalised) soil and groundwater quality standards are based or will be based on the model results. The models of Belgium, Germany, Norway, Sweden, the UK and the USA are conform this condition. A complete overview of the available international models is presented in Appendix 2. The models of the UK, Germany, and the USA are selected for a comparison with CSOIL, because many articles are written about the model concepts and the applications. They are also well documented and are developed separate and independent of each other. Further, the contact persons took part in this project. The selected international models are:

1. the Contaminated Land Exposure Assessment model. (CLEA) from the UK;
2. the Umweltmedizinische Beurteilung der Exposition des Menschen durch altlastbedingte Schadstoffe (UMS) from Germany;
3. the California Environmental Protection Agency, Department of Toxic Substances Control (CalTOX) from the US-EPA.

Still in progress is a project focussing on comparison of the calculated human exposure with several European exposure models (Swartjes et al., in prep). Aims of that project are to 1. gain insight into the variation in calculated human exposure and 2. gain insight into (differences in) default values for input parameters used in these models.

In the next section a short description is given of the three selected international human exposure models. In the following sections the concepts of the three relevant exposure routes of the international models and CSOIL are described separately, after which the international models are compared with CSOIL. In the last section recommendations are made for the improvement or refinement of CSOIL.

3.2 Short descriptions of the used international models

3.2.1 CLEA

In the UK CLEA is developed for deriving guideline values, but CLEA can also be used for site-specific risk assessments. The relative contribution of pathways varies according to site use. Where guideline values are exceeded, the intention is that either a further phase of risk assessment or remedial action is triggered. Guidelines on methodologies are being developed for estimating the degree of soil clean-up required for protecting groundwater. The CLEA model is designed to evaluate the average daily intake of a contaminant for a given (initial) contaminant concentration in soil for a particular site uses (forward sub-module). The model can not calculate a soil concentration from the relating average daily intake. This because in CLEA the contaminant concentration in soil is not a constant value but varies in time, because removal processes are included in the model. An approximation for this calculation is coded, but disabled, in the inverse sub-model of CLEA. The plant uptake module is capable of handling organic contaminants and metal contaminants.

Exposure is calculated as a function of time, including natural degradation and dispersion processes. Removal processes include photolysis, chemical reaction, volatilisation, biodegradation, run-off, erosion, leaching and crop harvesting. For organic contaminants the single first order approach of Jury (1983) is used for the determination of the natural degradation. It appeared that the actual use of the degradation in CLEA is not clear. CLEA uses 18 age intervals. The first 16 intervals correspond to the first 16 years of life. The last two intervals are the working life from 16 to 59 years and the interval from 60 to 70 years.

The possible exposure scenarios and exposure pathways of the CLEA model are presented below. The italic scenarios and pathways are used further in this document for the model comparison.

The exposure scenarios:

1. *residential with gardens;*
2. *residential without gardens;*
3. *allotments;*
4. parks, playing fields and open space;
5. commercial / industrial.

The exposure pathways:

1. *ingestion of soil (outdoor);*
2. ingestion of dust (indoor);
3. *ingestion of contaminants via home-grown crops;*
4. *ingestion of soil attached to crops;*
5. outdoor skin contact with soil contaminants;
6. indoor skin contact with dust;
7. outdoor inhalation of fugitive dust;
8. indoor inhalation of fugitive dust;
9. outdoor inhalation of soil vapour;
10. *indoor inhalation of soil vapour;*
11. ingestion of drinking water from main supply *);
12. skin contact with mains water during showering and bathing, etc. *);
13. inhalation of vapours during showering and bathing, and from ambient vapours otherwise derived from mains water *);

*) Not computed when an estimate of average daily intake from background sources (non-soil) is available.

3.2.2 UMS

For the detailed assessment of abandoned contaminated sites the UMS-system was developed to calculate the kind and extent of exposure for human health and ground water targets. Based on physical chemical and toxicological data, site specific characteristics and the behaviour of the population, the UMS-system quantifies the actual or potential exposure relevant for human health. For this UMS describes the release and the distribution of organic and metal contaminants in the environment as well as the exposure frequency, intake rates, absorption and bioavailability of contaminants for the different exposure groups. Only the transport of contaminants in groundwater is calculated as a function of time, including dispersion processes (SISIM module). Removal processes, like photolysis, chemical reaction, volatilisation or biodegradation, are not used in the UMS model.

The UMS model uses a stepwise procedure consisting of the following five modules:

1. Area module: discovers the relevant pathways of each exposure group (see Table 3.1)
2. Transfer module: simulates the transfer of pollutants from:
 - a) soil air to indoor and outdoor air;
 - b) soil to dust;
 - c) soil into plants;
 - d) soil to percolating pore water and groundwater;
 - e) groundwater to well.

The three soil types are sandy soil, loamy soil and clay soil.
3. SISIM calculates the transport of contaminants in the unsaturated zone based on equilibrium states (partition coefficients). It describes the movement of contaminants within and between the three different phases in soil:
 - a) as a solute dissolved in water;
 - b) as a gas in the vapour phase;
 - c) as an adsorbed compound in the solid phase.
4. Exposure module: calculates the actual, latent, and potential hazards of the exposure groups living or working on contaminated sites. The nine possible exposure scenarios are children playground, fallow, public green, garden, residential home, commercial buildings, sport field, industrial area and well.
5. Result module: gives a general view of the calculated total risk (tables/graphics) in comparison with the background dependent risk as the background exceeding rate.

Table 3.1 The exposure groups and age categories of the UMS model

Exposure group	Age (years)
Infant	<1
Little child	1-3
Child	4-8
Juvenile	9-16
Adult	>16
Lifetime	0-46

The possible exposure scenarios and exposure pathways of the UMS model are presented below. The italic scenarios and pathways are used in this document for the model comparison.

The italic scenarios and pathways are used further in this document for the model comparison. The potential exposure scenarios of the UMS models are:

1. children playground;
2. public green;
3. *garden*;
4. *residential home*;
5. fallow;
6. industrial area.

The following exposure pathways can be used in UMS:

Oral:

1. *outdoor ingestion of soil particles*;
2. indoor ingestion of dust;
3. ingestion of drinking water;
4. ingestion of bathing water;
5. *consumption of plants*;
6. ingestion of fish.

Inhalation:

7. *indoor inhalation of vapours (gas);*
8. indoor and outdoor inhalation of dust;

Dermal

9. outdoor dermal contact with soil contaminants;
10. dermal contact via bathing water.

3.2.3 CalTOX

The CalTOX model consists of a set of spreadsheet models and spreadsheet data sets that relates the concentration of a chemical in soil to the risk of an adverse health effect for a person living or working on or near the contaminated soil (CalTOX, 1993). It computes site-specific health-based soil clean-up concentrations given target risk levels, or human health risks given soil concentrations at the site. The risk-based soil screening levels for contaminants in soil for direct ingestion are based on a methodology that backcalculates a soil concentration level from a target risk (for carcinogens) or hazard quotient (for noncarcinogens).

The CalTOX model, in descending order of reliability, is capable of handling nonionic organic chemicals, radionuclides, fully dissociating organic and inorganic chemicals, and solid-phase metal species. With careful attention to inputs, the model can be used for partially dissociated organic and inorganic species. An adjusted distribution coefficient, K_d , for the soil/water partitioning is used in CalTOX for dissociated species. This issue introduces a significant amount of uncertainty to the exposure estimates for species that dissociate. However, because CalTOX can be used to carry out formal uncertainty analyses using Monte Carlo methods, these types of uncertainties can be explicitly represented. CalTOX is not designed to work with surfactants, inorganic chemical species with high vapour pressure to solubility ratios, and volatile metals such as mercury.

CalTOX contains a multimedia transport and a transformation model that uses equations based on conservation of mass and chemical equilibrium. Contaminant sources can be introduced to the compartments air, ground-surface soil, root-zone soil, vadose zone soil and surface water. The model assumes that soil is the primary environmental medium contaminated at a hazardous waste site. CalTOX predicts the time-dependent concentrations of a chemical in the eight environmental compartments at a site:

1. air;
2. three soil layers (ground-surface soil, rooting-zone soil, vadose-zone soil);
3. groundwater;
4. plants;
5. surface water;
6. sediment.

Quantities or concentrations within compartments are described by a set of linear, coupled, first-order differential equations. Contaminants are moved among and lost from each compartment through a series of transport and transformation processes that can be represented mathematically as first-order losses. The movement of a toxic substance is described by the partitioning of chemical species among the mentioned environmental compartments. CalTOX simulates decay and transformation processes as first-order irreversible removals. Decay and transformation are modelled in CalTOX as first-order or pseudo-first order irreversible losses. To each environmental medium a transformation rate is assigned that applies to the inventory in that compartment.

CalTOX is used either to:

1. calculate the long-term cumulative intake of chemical initially placed in one of the soil layers;
2. calculate the steady state source-to-dose relationship from a continuous emission of a chemical to air, surface soil, rooting soil, deep soil, surface water, and/or sediments.

For each of these calculation options, the rate of transformation used directly affects the estimated source-to-dose ratio that is used in the risk assessment. The transformation processes are photolysis, hydrolysis, oxidation and reduction and microbial transformation.

In CalTOX the following exposure pathway scenarios are used. The italic scenarios and pathways are used further in this document for the model comparison.

Ingestion:

1. *human soil ingestion;*
2. ingestion of tap water;
3. drinking water while bathing;
4. *consumption of fruits, crops and grains (atmospheric deposition to plants, soil and irrigation water);*
5. meat, milk and eggs (air and soil to plants to animals; air and soil and water to animals);
6. ingestion of fish and sea foods;
7. mother's milk (via air, soil, water);
8. ingestion of surface water during bathing or other water recreation;

Inhalation:

9. gases and particles in outdoor air;
10. gases and particles transferred from outdoor air to indoor air;
11. *inhalation of soil vapours and particles migrated or transferred to indoor air;*
12. indoor inhalation of contaminants transferred from tap water;

Dermal:

13. dermal contact with soil;
14. dermal contact in baths and showers;
15. dermal contact while bathing.

The multiple pathways exposure model requires either measured concentrations or calculated values of the transport and transformation model. CalTOX determines the chemical concentration in the following exposure media:

1. breathing air;
2. drinking water;
3. food;
4. soil that people inhale;
5. soil that people ingest;
6. dermal contact.

The input distributions in CalTOX are developed for three age categories, children (ages 1 to 15), adults (ages 16 to 70), and a lifetime equivalent (ages 1 to 70).

CalTOX uses the equations found in the U.S. Environmental Protection Agency Risk Assessment Guidance for Superfund (US-EPA RAGS) to estimate exposure and risk. Many of the issues described in the RAGS and related to characterising exposure from selected exposure pathways are included in the Exposure Factors Handbook (EFH). CalTOX is in the process of being updated with revised inputs based on the newest version of the EFH (US-EPA, 1997). CalTOX has the capability of conducting Monte Carlo simulations with a spreadsheet add-in program. Therefore each exposure factor is represented by a probability distribution, with a mean, a coefficient of variation and a distribution type. Used in this way, CalTOX will present

a range of risks or health-based soil target clean-up levels that reflect the uncertainty and the variability of the estimates.

3.3 Ingestion of contaminated soil particles

3.3.1 CLEA

Human exposure

The soil ingestion rate and the exposure duration is dependent on the chosen exposure scenario. For each scenario the different (average) soil ingestion rates are presented in Table 3.2. From the documentation of CLEA (1998) it is not clear which considerations and exact data are the basis for the soil ingestion rates presented in Table 3.2. Nevertheless, in CLEA (1998) there are short summaries presented of known studies and articles on soil ingestion of for instance Binder et al. (1986), van Wijnen et al. (1990), Calabrese et al (1989) and Davis et al. (1990). For the scenarios “residential with gardens” and “recreational allotments” of CLEA, not only the inadvertent soil ingestion is considered, but also the occasionally deliberate soil ingestion. For the age category from 1 to 6 years the deliberate soil ingestion is only accounted for in the second year of one’s life.

The occasionally deliberate (exploratory) soil ingestion rate is based on a reasonable estimate for geophagic or pica children (soil ingestion is a deliberate persistent and purposeful habit) of 10 g/d. Nevertheless it seems very unlikely that the much larger number of children who go through a phase of exploratory soil-eating will ingest soil at this rate. For those children 5 g/d has been chosen as the provisional deliberate soil ingestion rate, over and above that due to inadvertent hand-to-mouth contact. According to CLEA (1998) even a rather short-term exploratory soil-eating of 5 g/d can have a significant impact on childhood contaminant intakes from soil. For the scenario “residential with garden” a deliberate soil ingestion of 5 g/d during 15 days over the period of 1-6 years the yearly average intake increases with more than 40%.

Table 3.2 Soil ingestion rates used in CLEA (CLEA, 1998)

Exposure scenario	Age category (year)	Soil ingestion (avg.) (mg/d)	Exposure duration (day/year)	Deliberate soil ingestion (mg/d)	Yearly average exposure (mg/d)	Distribution
<i>Residential with gardens</i>	1-6	80	365	5000 ¹⁾	114 ²⁾	Lognormal
	7-16	60	365	0	60	Lognormal
	>16	60	365	0	60	Constant
<i>Residential without gardens</i>	1-6	80	365	0	80	Lognormal
	7-16	60	365	0	60	Lognormal
	>16	5	365	0	5	Constant
<i>Recreational allotments</i>	1-6	80	54	5000 ¹⁾	46 ²⁾	Lognormal
	7-16	60	54	0	9	Lognormal
	>16	70	365	0	70	Constant

- 1) The deliberate intake component is assumed to apply only in the second year of life. The rate is taken as 5 g/d for n days, where n is a Monte Carlo variable drawn from a uniform distribution (distribution is characterised by an upper and lower limit and all parameter values have equal probability) between $n=0$ and $n=30$.
- 2) The yearly average exposure is calculated with a deliberate soil ingestion of 5 g/d for 15 days during the period of 1-6 years

In CLEA the expected daily intake (EDI) via the outdoor ingestion of soil is calculated using the following equation:

$$EDI = \frac{1}{\sum (\Delta T)_i} \sum_{i=1}^n \frac{C_i (IR)_i (ED)_i}{W_i}$$

$\Sigma(\Delta T)_i$:	total number of days over which exposure is averaged	[day]
n:	number of age intervals	[-]
C_i :	average concentration of contaminant in soil over time interval $(\Delta T)_i$	[mg/g]
$(IR)_i$:	soil ingestion rate for time interval $(\Delta T)_i$	[g/day]
$(ED)_i$:	number of days of exposure to outdoor soil in time interval $(\Delta T)_i$	[day]
W_i :	body weight for time interval $(\Delta T)_i$	[kg]

3.3.2 UMS

Human exposure

The soil ingestion and exposure duration are dependent on the exposure scenario. For the UMS system not only the direct uptake of soil is taken into account, but also the indirect uptake via inhalation and subsequently swallowing of dust particles. In UMS it is assumed that 60% of the inhaled dust is transported back to the oral cavity, after which it is orally taken up. For the direct and the indirect uptake route a different daily intake rate (DIR) is used. The DIR for the indirect soil ingestion is negligible compared to the direct route. The most recent direct soil ingestion rates are presented in Table 3.4 (UMS, 1997). The DIR values for the indirect route are at least a factor 100 smaller than those of the direct route and are considered to be negligible.

In the UMS documentation a large range of 50 mg/d - 100 g/d is described for the daily soil intake values for children (see Appendix 3). The UMS values for the average soil intake for the different scenarios for little children of 250 mg/d and for children of 150 mg/d, are mainly based on the values presented in Table 3.3 (AGLMB, 1995). In the UMS system the deliberately soil ingestion by children, including geophagic or pica behaviour, is not taken into account. For the residential home scenario only for children the intake of soil particles and home dust is used for the UMS model. Dependent on the outdoor playing time different authors estimate the intake of soil and dust for children at about 100 mg/d (Hawley, 1985; Davis et al. 1990; Paustenbach et al. 1996). The default soil ingestion values presented in Table 3.4 are realistic worst case estimates for town centre homes.

The soil intake values for juveniles and adults (e.g. garden scenario) is based on reported values ranging from 50 mg/d to 500 mg/d (e.g. US-EPA, 1989; Ruck, 1990; Calabrese et al. 1989). For this age category an oral soil intake rate of 100 mg per stay is used for intensive use of the garden. It is not explained how the actual soil intake value of 30 mg/d is calculated for juveniles and adults.

For each scenario the exposure frequency rates for children are mainly based on the study of Stubenrauch et al. (1994). The exposure frequency rates for the other age categories are derived from this value for children.

Table 3.3 Average oral soil intake values (AGLMB, 1995)

Age	<1	1-3	4-6	7-9	10-14	15-19	20-75
Soil intake (mg/d) probable case	20-100	20-100	20-100	5-25	5-25	2-10	2-10
Soil intake (mg/d) worst case	100-500	100-500	100-500	25-125	25-125	10-50	10-50

In the UMS model the potential daily resorbed dose (PDI) via soil ingestion is calculated with the following equation:

$$PDI = DIR \cdot EAF \cdot CCM \cdot AV \cdot R \cdot U \quad [mg / kg \cdot d]$$

with

$$DIR = \frac{IR \cdot EFR \cdot ED}{BW \cdot AT}$$

DIR:	daily intake rate, yearly average	[mg/kg _{bw} .day]
EAF:	exposure adjusted factor, default value=1	[-]
CCM:	concentration in contact medium (soil)	[mg/kg]
AV:	availability from soil matrix, default value=1	[-]
R:	resorption rate, default value=1	[-]
U:	conversion factor = 10 ⁻⁶	[kg/mg]
IR:	soil ingestion rate	[mg/day]
ED:	exposure duration (dependent on scenario)	[year]
EFR:	exposure frequency rate	[day/year]
BW:	body weight	[kg]
AT:	carcinogenic substances: AT=70·365	
	non-carcinogenic substances: AT=ED·365	[day/year]

The calculated daily soil ingestion intake rates are presented in Table 3.4.

Table 3.4 The daily soil ingestion intake rates used in UMS (UMS, 1997)

Exposure Scenario	Age (years)	Bodyweight (BW) (kg)	Soil ingestion (IR) (mg/d)	Exposure duration (EFR) (d/y)	Yearly average exposure (mg/d)	Yearly average daily intake rate (DIR) (mg/kg BW.d)
<i>garden</i>	1-3	10	250	180	123	12.33
	4-8	20	150	180	74	3.70
	9-16	40	30	190	16	0.40
	>16	70	30	190	16	0.22
<i>residential home</i>	1-3	10	250	150	103	10.3
	4-8	20	150	150	62	3.1

3.3.3 CalTOX

Human exposure

In the CalTOX documentation it is reported that the daily soil ingestion is only applicable to residential land uses. The soil ingestion rate is only adjusted for two age categories, because a number of studies have shown that inadvertent ingestion of soil is common among children (Calabrese et al., 1989; Davis et al., 1990; Van Wijnen et al., 1990). CalTOX uses a soil ingestion factor, which is based on the daily soil ingestion, bodyweight and exposure duration for children from 0 to 15 years old and adults from 16 to 70 years old. On the basis of location specific information the soil ingestion rate can be adjusted.

In the current input file for CalTOX 22 mg/d is used as the lifetime equivalent soil ingestion. This value was obtained from the US-EPA Exposure Factors Handbook (EFH) of 1989 and from early work by Calabrese and others. Combining the information in the 1989 EFH with recommendations by Calabrese et al. (1991) and LaGoy (1987) (T. McKone, pers. comm.), the following soil-ingestion estimates are obtained:

- 60 mg/d (2.2·10⁻⁶ kg(soil)/kg·d) for children 0 to 15 y

- 10 mg/d ($1.4 \cdot 10^{-7}$ kg(soil)/kg-d) for adults 16 to 70 y
- 20 mg/d ($3.5 \cdot 10^{-7}$ kg(soil)/kg-d) for a lifetime equivalent during ages 0 to 70.

Together with EPA the most recent soil ingestion data are reviewed to develop age-specific distributions of soil intake for the use in CalTOX. The most recent recommendations for soil ingestion described by the US-EPA in the EFH are presented in Table 3.5 (US-EPA, 1997). So far, these values are not used in the CalTOX model.

Table 3.5 Summary of recommended values for soil ingestion (US-EPA, 1997)

Population	Mean	Upper Percentile
Children	100 mg/day ^{a)}	400 mg/day ^{b)}
Adults	50 mg/day	--
Pica-child	10 g/day ^{c)}	--

a) 200 mg/day may be used as a conservative estimate of the mean (see US-EPA 1997).

b) Study period was short; therefore, these values are not estimates of usual intake.

c) To be used in acute exposure assessments. Based on only one pica child (Calabrese et al., 1989).

In the CalTOX manual (CalTOX, 1993) the equation for incidental ingestion of soil is written as follows:

$$Intake_{soil} = C_g \cdot \frac{IR_{soil}}{BW} \cdot FI \cdot \frac{EF \cdot ED}{AT} \cdot CF$$

Intake _{soil} :	Intake by exposed individual via ingestion of soil	[mg/kg _{bw} .d]
IR _{soil} :	ingestion rate of soil	[mg/d]
C _g :	concentration in surface soil	[mg/kg]
BW:	body weight	[kg]
FI:	fraction of soil ingested from contaminant source	[1]
EF:	exposure frequency	[d/y]
ED:	exposure duration	[y]
AT:	averaging time	[d]
CF:	conversion factor	[10 ⁻⁶ kg/mg]

3.3.4 CSOIL

Human exposure

The present values in CSOIL for soil ingestion of children (1-6 year) and adults (7-70 year) are 150 mg/d and 50 mg/d, respectively (Van den Berg, 1995). These values are mainly based on the studies of Hawley (1985), Linders (1990) and Van Wijnen (1990). In Hawley (1985) the exposure for young children is estimated to be 150 mg/d, based on a soil ingestion outside of 250 mg during 130 days, and a value inside of 100 mg/day (182 days) in the winter and 50 mg/d (182 days) in the summer. The ingestion by adults is also based on Hawley (1985), estimating an ingestion of 480 mg per day during for 2 days a week and 5 months a year (=57 mg/day). Linders (1990) uses a soil ingestion rate 200 mg/d during 3 days per week (about 86 mg/d yearly average).

In the CSOIL the exposure or daily intake rate (DI) via soil ingestion is calculated with the following equation:

$$DI = \frac{AID \cdot Cs \cdot fa}{W}$$

AID:	daily intake amount of soil for adults/children	[50/150 mg/d]
Cs:	content in the soil	[mg/kg]
fa:	relative absorption factor (default=1)	[-]
W:	body weight for adults/children	[70/15 kg]

3.3.5 Model comparison

Soil ingestion rate

The UMS model not only uses the direct uptake of soil but also an indirect uptake via inhalation and subsequently swallowing of dust particles. The daily soil intake via the indirect route appeared to be negligible compared to the direct route. CLEA, CalTOX and CSOIL only use the direct uptake of soil.

In CLEA the occasionally deliberate (exploratory) soil ingestion rate is based on a reasonable estimate for geophagic or pica children of 10 g/d. Even a rather short-term exploratory soil-eating of 5 g/d can have a significant impact on childhood contaminant intakes from soil. For the CLEA scenario “residential with garden” a deliberate soil ingestion of 5 g/d during 15 days over the period of 1-6 years the yearly average intake increases with more than 40%. No information is available on a comparison of the short-term exposure of the deliberate soil-eating against acute toxicity data.

All models use an age adjusted soil ingestion factor, because inadvertent soil ingestion is different for children and adults. The used age categories 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/d is higher than the ingestion rates of the other models (Table 3.6). For the relevant scenarios of the other models the yearly averaged soil ingestion rates for children are 123 mg/d and 74 mg/d for UMS, 114 mg/d for the CLEA and 60 mg/d for CalTOX. For adults the ingestion rate of the UK is comparable with the CSOIL value of 50 mg/d. The ingestion rates of the UMS and CalTOX model are lower with a value of 16 mg/d and 10 mg/d, respectively. Further it must be noted that only the CLEA model accounts for an additional deliberate soil ingestion rate in the second year of life.

Table 3.6 Soil ingestion rates and use of deliberate soil ingestion for the models compared

Model	Yearly average soil ingestion rate for adults (mg/d)	Yearly average soil ingestion rate for children (mg/d)	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 ⁴⁾	123 (1-3 year) 74 (4-8 year) ⁵⁾	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/d for a maximum of 30 days in the second year of life

3) The uptake in the human body

4) Based on a soil ingestion of 30 mg/d and an exposure duration of 190 d/y

5) Based on a soil ingestion of 250 mg/d (1-3) and 150 mg/d (4-8) and an exposure duration of 180 d/y

Human exposure

The concept for calculating the daily intake or exposure is fundamentally the same for all the models. CLEA, UMS and CalTOX can account for a separate exposure frequency combined with a daily intake rate. For those models it is possible to use a scenario with an exposure duration of less than 365 days per year, which results in a lower yearly average intake rate. Only CSOIL uses a fixed yearly average soil intake rate and it is not possible to change the CSOIL scenario for exposure durations of less than 365 days per year. For the residential scenarios of CLEA an exposure duration of 365 d/y is used and is therefore not different from CSOIL. The UMS model uses a considerably lower exposure duration of 150 – 190 d/y, dependent on the used scenario. For the UMS model the yearly average intake rates are

therefore lower than the daily intake rates. A separate exposure frequency combined with a daily intake rate is also implemented in CalTOX. For the comparison it is assumed that CalTOX uses an exposure frequency of 365 days.

3.4 Indoor inhalation of vapours of contaminants

3.4.1 CLEA

Indoor inhalation of vapours

For inhalation the following four routes are defined in CLEA:

1. Outdoor inhalation of fugitive dust;
2. Outdoor inhalation of soil vapour;
3. Indoor inhalation of soil vapour;
4. Indoor inhalation of vapour derived from water mains.

For a comparison with CSOIL only the indoor inhalation of soil vapour is relevant and therefore the other routes are not further explained in this document.

For calculating potential risks it is assumed that the ambient air is uncontaminated and that there are no indoor sources of air contaminations. The key mechanisms of transport and dispersion are:

1. Contaminant partitioning into the soil-vapour phase;
2. Molecular diffusion;
3. Ventilation;
4. Suction flow (pressure driven flow).

For calculating the indoor inhalation of soil vapour a three compartment and a four compartment approach is used in the CLEA model. With the three compartment approach houses are modelled without a crawl space under the dwelling, where in the four compartment approach a crawl space is added. Both approaches are used for deriving guideline values (personal communication N. Earl, 1999).

For a comparison with CSOIL only the four compartment approach is relevant and therefore the three compartment approach is not described. In the CLEA model the air fluxes in the house are described using balance equations, because under equilibrium conditions the total amount of air entering each separate volume of a house should be equal to the amount of air leaving the same volume.

The following compartments are defined in the four compartment approach (Figure 3.1):

0. Soil;
1. Crawl space under the dwelling;
2. Living space;
3. Outdoor space.

In CLEA different fluxes, molecular diffusion, ventilation and suction flow, are used for calculating the resulting equilibrium concentration in indoor air. In Figure 3.1 all fluxes are presented. These fluxes use simple linear relations (Ferguson et al. 1995; Krylov and Ferguson, 1998). All fluxes are briefly described in the following paragraphs. In Appendix 4 a complete description of the fluxes is presented.

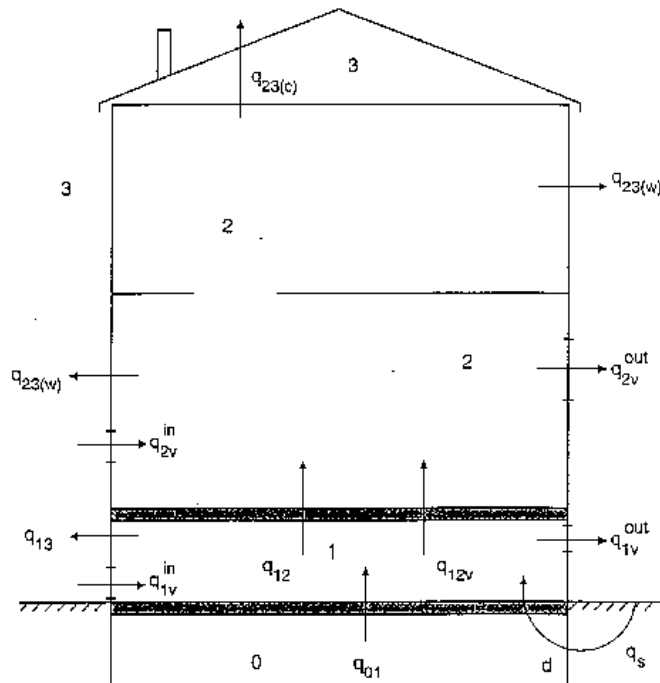


Figure 3.1 Schematic diagram of the detached house considered in CLEA.
Arrows indicate possible fluxes of a chemical.

Molecular diffusion

In CLEA three diffusion fluxes are described:

- Diffusion through the ground to the soil surface;
- Diffusion from crawl space to the living space;
- Diffusion through walls and ceiling.

Ventilation

Natural ventilation is mainly caused by pressure differences between inside and outside air induced by wind. There are two ventilation volumes: the living space and the crawl space. To calculate all the ventilation fluxes it is necessary to estimate the pressure differences between outside and inside air separately for living space and void and, additionally, the pressure difference between void and living space can be determined. Results are in good agreement validated with BREVENT, a numerical model developed by Building Research Establishment. In CLEA the wind induced pressure, the stack effect and the resulting air fluxes in a house are describes.

Suction flow (pressure driven flow)

Suction flow results when the soil-gas pressure exceeds the air pressure inside a void and causes a chemical flux from soil-air to the air in the void. The pressure gradient in soil causes fluxes from soil to void air via connected pore spaces, gaps and cracks. Suction flow may be a response to wind induced pressure differentials, or differentials created by heating and air-conditioning systems. The main difference between suction flow and the above mentioned ventilation is that ventilation describes the flows inside a building and the suction flow only describes the flux from soil-air to the air in the void. In contrast with the stack effect suction flow is not thermally induced. The aerodynamically induced suction flow in a house with a void occurs throughout the year.

Equilibrium concentrations of toxic vapour

A house is assumed to be one living space with a single homogenous volume, because it is assumed that internal doors are opened sufficiently frequent to allow free interchange of air between rooms. At equilibrium the air concentration of a chemical in each separate volume of a house will be constant. Windows and doors are considered as impenetrable by contaminants. It is further assumed that the outdoor air is unpolluted and that indoor sources of contaminants are absent.

Human exposure

The inhalation volumes for children and adults used in the CLEA model are presented in Table 3.7. For calculating the exposure to indoor inhalation of vapours of contaminants only the passive inhalation volumes are used.

Table 3.7 Inhalation volumes used in CLEA

		Inhalation volume (m ³ /h)	Male Weight 50 th % (kg)	Female Weight 50 th % (kg)	Calc. inh. rates ¹⁾	
					(m ³ /h)	(m ³ /d)
Children	Active	0.03*Weight	6.12-56.5	5.70-52.5	0.45	10.8
	Passive	0.011*Weight	(3 months-15.5 yrs.)	(3 months-15.5 yrs.)	0.17	4
Adults	Active	0.018*Weight	65-75.5	55.5-63.5	1.3	30.2
	Passive	0.006*Weight	(16-75 yrs.)	(16-75 yrs.)	0.42	10.1

1) Respiration rates are calculated with the CSOIL default values for weight, which is 15 kg for a child and 70 kg for an adult.

In CLEA the expected daily intake (EDI) via the indoor inhalation of vapour is calculated using the following equation:

$$EDI = \frac{1}{\sum (\Delta T)_i} \sum_{i=1}^n \frac{(AC)_i (RV)_i (ED)_i}{W_i}$$

(AC)_i: average indoor air concentration in time interval (ΔT)_i [mg/m³]
 (RV)_i: daily respiration volume for indoor activities in time interval (ΔT)_i [m³/day]
 (ED)_i: number of days of exposure to indoor air in time interval (ΔT)_i [day]
 W_i: body weight for time interval (ΔT)_i [kg]

3.4.2 UMS

Indoor inhalation of vapours

The starting point for estimating the indoor concentration in air is the concentration of the substance in soil air. The soil-air concentration is calculated from the soil concentration with a partitioning coefficient soil-air (Nazaroff et al., 1992). It is assumed that the concentration of a substance in the living room is only a result of the concentration in soil air directly under the house. The direct transport of substances from outdoor air into the house is not taken into account in the UMS model. For the assessment of substances in indoor air the transfer of substances is divided in a step to overcome the distance from the place of contamination to the house, followed by a step of direct transport through cracks and pores into the house. It is further assumed that substances are not adsorbed to building materials or foundations.

The detailed models of Jury (1990), Mendoza and Frind (1990), Garbesi et al. (1993) and Nazaroff et al (1992) are considered not to be useful in the scope of the UMS model (UMS,

1993). For a real estimation of the transfer of substances across soil air these models are considered to be too complex. A validation of the different models available has shown that the model results are sometimes realistic, but mostly unreal. The simplified assumptions of these models are used in the UMS model for estimating the transfer of substances from soil air to indoor air. Based on the studies of e.g. Nazaroff and Garbesi, describing radon transport in buildings or using pressure driven flow, the transfer factor soil air/indoor air is estimated. For the radon transport a coefficient alpha is used for describing the concentration in indoor air from the concentration in soil air. The pressure driven flow is based on the relative lower pressure of the house against the relative higher pressure in soil. According to UMS the thermal differences, the wind pressure and the structure of the house account for this pressure difference. The UMS model uses an unchangeable factor of 0.01 between the soil-air concentration and the indoor air concentration. This factor is mainly chosen by evaluation of data from contaminated sites. It must be noted that using this factor for most of the substances probably the indoor concentration will be estimated higher than the actual value. This factor must be used for an overview or discussion if there might be a risk in cellars or ground floor apartments. It must not be used as a real total value that causes remediation action (personal communication D. Grünhoff).

In equations the concentration in indoor air is calculated as follows:

$$C_{IA} = C_{SA} \cdot 1,000,000 \cdot TF_{SA-IA}$$

$$C_{SA} = \frac{C_S \cdot K_H}{(K_{d+} SWC)}$$

C_{IA} :	concentration in indoor air	[$\mu\text{g}/\text{m}^3$]
C_{SA} :	soil-air concentration	[mg/l]
C_S :	soil concentration	[mg/kg]
TF_{SA-IA} :	transfer factor soil air/indoor air	[0.01]
K_H :	Henry constant	[-]
K_d :	partition coefficient soil-pore water	[-]
SWC :	soil moisture	[0.2 l/kg]

Human exposure

The inhalation rates of the UMS model used for the residential scenario are presented in Table 3.8.

In the UMS model the potential daily resorbed dose (PDI) via inhalation is calculated with the following equation:

$$PDI = DIR_{IA} \cdot C_{IA} \cdot R_{inhal}$$

$$\text{with: } DIR_{IA} = \frac{IR_{Atem} \cdot EFR_d \cdot EFR \cdot RF_{EFRg}}{365 \text{ days/year} \cdot BW}$$

C_{IA} :	concentration in indoor air	[$\mu\text{g}/\text{m}^3$]
R_{inhal} :	substance specific resorption rate	[-]
DIR_{IA} :	daily inhalation rate, yearly average	[$\text{m}^3/\text{kg} \cdot \text{day}$]
IR_{Atem} :	inhalation rate	[m^3/h]
EFR_d :	exposure duration	[h/day]
EFR :	exposure frequency rate (365 days/year)	[day/year]
RF_{EFRg} :	reduction factor for exposure duration based on building use; a building with no possibility to be outside $RF = 1$, when a building has a balcony or garden then RF is decreasing.	[-]
BW :	body weight	[kg]

The calculated daily intake rates via inhalation are presented in Table 3.8.

Table 3.8 Average daily intake rates via inhalation for the residential home scenario (UMS, 1997)

Population	Age <i>years</i>	Exposure frequency (EFR _d) <i>h/d</i>	Inhalation rate (IR _{Atem}) <i>m³/h</i>	Body weight (BW) <i>kg</i>	Average daily intake (DIR _{IA}) <i>m³/kg.d</i>
Infants	<1	21	0.1	5	0.42
Little children	1-3	21	0.25	10	0.53
Children	3-8	18	0.5	20	0.45
Juveniles	8-16	15	0.7	40	0.26
Adults	16-46	21	0.8	70	0.24

3.4.3 CalTOX

Indoor inhalation of vapours

In CalTOX the concentration in indoor air is not based on fugacity models, but is based on the application of a simple mass balance to a volume element or box of air. In this box model approach the region to be studied is divided into cells or boxes. The concentration in each box is assumed to be uniform and is a function of the box volume, the emission rates within the box and the rate at which material is imported and exported from the box. Dispersion in the air compartment of the CalTOX model is based on this box-model approach. In the CalTOX model six environmental compartments or boxes can give rise to chemicals in air inhaled by people:

1. Particulate phase of ambient air outdoors;
2. Vapour phase of ambient air outdoors;
3. Ground-surface soil;
4. Root-zone soil;
5. Volatile compounds dissolved in groundwater;
6. Volatile compounds dissolved in surface water.

The analytical methods for estimating the diffusion coefficients in air are based on Reid et al. (1987) and Lyman et al. (1982). In CalTOX it is assumed that turbulent diffusion within air is so efficient that the bulk concentration is equal in the entire air compartment. At the boundary between air and ground-surface soil the diffusive mass transfer is more complex and is modelled using a boundary-layer model. The concept of this model is that a well-mixed turbulent air mass exists over a well-mixed stagnant layer of air that is in contact with soil.

The simple mass-balance model for the indoor environment considers four sources:

1. Transfer of air contaminants (gas and dust particles) from outdoor to indoor air.
2. Transfer of volatile chemicals from soil below a house to indoor air
3. Tracking of contaminated soil from outside to the indoor environment
4. Transfer of volatile chemicals from tap water to indoor air

Chemical specific concentration ratios are used for the first three transfer routes. For the transfer of volatile chemicals from soil below a house to indoor air, the indoor air/soil gas ratio is based on radon (the so-called “alpha factor”). A two compartment indoor air model is used for the transfer of volatile chemicals from tap water to indoor air. Pressure driven or suction flow is only used to the extent that it is implicitly included in the alpha factor that was developed for radon. The CalTOX inhalation equations for indoor air of an on-site building are

divided into an indoor air part, excluding the bathroom, and into a bathroom air part. For the bathroom air also the transfer of volatile chemicals from tap water are relevant.

Human exposure

The default inhalation rate in CalTOX is 20 m³/day for adults (CalTOX, 1993). This value exceeds the recommended values (Table 3.9) of the Exposure Factors Handbook (US-EPA, 1997). The EFH values are based on studies that have been classified as key or relevant. The key studies are used as the basis for deriving recommendations and the relevant studies are included to provide additional background and perspective. So far, the values Table 3.9 of are not used in the CalTOX model.

Table 3.9 Summary of recommended values for inhalation for long-term exposures (US-EPA, 1997)

Population	Age (years)	Males/Females	Mean (m ³ /day)
Infants	<1		4.5
Children	1-2		6.8
	3-5		8.3
	6-8		10
	9-11	Males	14
		Females	13
	12-14	Males	15
		Females	12
	15-18	Males	17
		Females	12
Adults	19-65+	Males	15.2
		Females	11.3

The exposure or intake via the inhalation of vapour phase chemicals is calculated according to the following equations:

$$Intake_{air} = C_{air} \cdot \left(\frac{IR_{air}}{BW} \right) \cdot \left(\frac{EF \cdot ED}{AT} \right)$$

Intake _{air} :	daily inhalation rate	[m ³ /kg.day]
C _{air} :	concentration of chemical of concern in air	[mg/m ³]
IR _{air} :	inhalation rate	[m ³ /day]
BW:	body weight	[kg]
EF:	exposure frequency	[350 days/year]
ED:	exposure duration	[years]
AT:	averaging time (non-carc: AT=ED, carc. or chronic effects: AT=70 years = 25,550 days, ref.: US-EPA, 1997)	

The time consideration is independent of the inhalation pathway of inhalation and relates to whether the chemical is a carcinogen: $\left(\frac{EF \cdot ED}{AT} \right)$. The average daily intake rate: $\left(\frac{IR_{air}}{BW} \right)$ and the concentration in air (C_{air}) are both dependent on the location and can be divided in outdoor exposure, indoor exposure and bathroom exposure.

Inhalation of indoor air (excluding bathroom air) is described with:

$$\frac{IR_{air}}{BW} = ((ET_{ind} - ET_{sb}) \cdot f_{ind,l} \cdot BR_l) + ((ET_{ind} - ET_{sb}) \cdot (1 - f_{ind,l}) \cdot BR_s)$$

ET_{ind} :	total hours spend indoors incl. bathroom at contaminated site	[hours/day]
ET_{sb} :	total hours spend in the bathroom at contaminated site	[hours/day]
$f_{ind,l}$:	fraction of total hours spend indoors with breathing rate associated with light activity	[-]
BR_l :	light activity breathing rate per kg body weight	[m ³ /kg.hour]
BR_s :	sleeping activity breathing rate per kg body weight	[m ³ /kg.hour]

3.4.4 CSOIL

See chapter 4. Evaluation volatilisation module of CSOIL with other concepts.

3.4.5 Model comparison

Concepts

The used concepts of the models compared are presented in Table 3.10.

Only in the CLEA and CSOIL model it is possible to calculate indoor air concentrations for houses with crawl spaces.

The CLEA and CalTOX models use molecular diffusion for describing the fluxes through the ground to the soil surface and through the floors, walls and ceiling. CLEA and CalTOX are the only models using flows from outside air to the indoor environment. The UMS and CSOIL model are mainly based on molecular diffusion. In those models it is assumed that the concentration of a substance in indoor air is only a result of the concentration in soil air directly under the building. Different from the other models CSOIL describes the evaporation of soil moisture and CLEA uses additional ventilation fluxes. The concepts of the mentioned diffusive fluxes are all comparable, but the magnitude of the fluxes remains unknown.

From all models only CLEA explicitly uses the pressure driven flow for calculating the indoor concentration in air. The CalTOX and UMS model only implicitly use the pressure driven flow concept.

Table 3.10 Conceptual information used by the models compared

Model	Molecular diffusion	Pressure driven flow	Crawl-space under dwelling	Other concepts	Flow from outside air to indoor air	Transformation or degradation	Absorption/resorption rate ³⁾
CLEA	Yes	Yes	Yes	Ventilation ²⁾	Yes	Yes	No
CalTOX	Yes	Yes ⁴⁾	No	No	Yes	Yes	No
UMS	Yes ¹⁾	Yes ¹⁾	No	No	No	No	Yes (default 1)
CSOIL	Yes	No	Yes	Evaporation from soil moisture	No	No	Yes (default 1)

- 1) A constant factor between soil-air concentration and indoor air concentration is derived from studies describing radon transport inside building which implicitly includes molecular diffusion and the pressure driven flow concept
- 2) Natural ventilation inside the house as a result of wind induced pressure and resulting air flows and the stack effect (an upward air flux resulting from the pressure difference between warm and cold air in the winter)
- 3) Factors for describing the substance specific uptake in the human body via the lungs
- 4) Pressure driven or suction flow is only used to the extent that it is implicitly included in the used "alpha factor" that was developed for radon.

The UMS model uses an unchangeable factor of 0.01 between the soil-air concentration and the indoor air concentration. CSOIL uses a fixed factor of 0.1 between the air concentration in the crawl space and the indoor air concentration.

CLEA and CalTOX both account for transformation/degradation processes as for instance photolysis, hydrolysis or microbial transformation.

Human exposure

On the basis of the presented respiration rates for the international models compared, it can be concluded that the present value in CSOIL of 20 m³/d is rather large for adults. The present value in CalTOX is also 20 m³/d, but this value will be revised according to the EFH. For adults the most recent respiration rates for the models of the UK, Germany and the US (EFH value, for male and female) are 10, 17 and 15/11 m³/d, respectively. For children (1-6 years) the values of the US (EFH value) and German models are comparable with the CSOIL value of 7.6 m³/d. Only the respiration rate of the UK model is lower, with a value of 4 m³/d.

Table 3.11 Inhalation rates used by the models compared

Model	Inhalation rate for children (m ³ /d)	Inhalation rate for adults (m ³ /d)
CLEA	4	10
CalTOX	Present value unknown 6.8 (1-2 y); 8.3 (3-5y) (EFH)	20 (default) 15 male / 11 female (EFH)
UMS	5.3 (1-3 y); 9 (3-8y)	17
CSOIL	7.6	20

For all models the exposure via the inhalation of vapours of contaminants is fundamentally based on the concentration in air multiplied with the daily inhalation rate, both divided by the body weight. The differences between the models compared are the used absorption rates and the exposure duration for certain scenarios.

3.5 Exposure to contaminants via the consumption of crops

3.5.1 CLEA

Concentration in crops

In the CLEA model the exposure from the ingestion of home-grown crops is calculated for the land use “residential with garden” and “allotments”. The uptake of soil contaminants is modelled only via the pathway of root uptake and subsequently translocation by the transpiration stream. CLEA does not account for the uptake from dust particles deposited on plant surfaces or other pathways, mainly because most uptake studies make no attempt to discriminate between these pathways. For inorganic contaminants uptake algorithms (BCF values) are substance specific. A more general approach is used for many organic contaminants.

The intake of contaminants can also be calculated by the ingestion of soil attached to crops that have not been removed by normal food preparation and cooking processes. In CLEA a value of 30 g soil / kg dry leaf (= 3%) is used, which corresponds to about 0.3% fresh weight for a typical plant moisture content of 90%. This value is based on the suggested estimated soil load concluded by Sheppard and Evenden (1992). Wind erosion processes were excluded from this study to account for the portion of soil on leaves only coming from the underlying soil. In the Sheppard and Evenden study plant material was rigorously washed with a stream of distilled

water, dried and ashed, weighted and analysed for radionuclides. They assumed that all of the acid insoluble ash in the washed leaf samples was soil, and that all of the contaminant content was the result of soil adhesion. The results of the Sheppard and Evenden study clearly showed that adhesion to leaves is an important component of plant accumulation of sparingly soluble contaminants, and this contaminant may not be removed by rigorous cleaning. It should be noted that in the CLEA model the adherent soil is calculated using a random variant from a beta distribution and a standard deviation. For crops growing beneath the soil surface (potatoes, carrots, onions, leeks) the Sheppard and Evenden data can not be used. In those cases the attached soil fraction, chosen by expert judgement, is 0.1% of fresh weight for potatoes and carrots and 0.5% of fresh weight for onions and leeks.

Plant uptake of metals from soil

According to CLEA (1998) it is unlikely that any general regression approach is reliable for modelling the plant uptake of metals, given the complexities of plant-soil solution systems and the widely different responses of different plant species. The procedure adopted in CLEA combines general regression equations with available field data for the relevant metal and crop type. CLEA uses the soil to plant concentration factor defined as the ratio of plant tissue contaminant concentration to total contaminant concentration in soil. The general regressions, defining the upper and lower boundary for leafy and root crops of Baes et al. (1984) are used to find a relation between the soil to plant concentration factor and the partitioning coefficient for soil. Other studies (i.e. Anderson and Christensen, 1988) are used for combining the dependence of the partitioning coefficient for soil with the soil pH. The derived relationships, including the soil pH, are used to provide upper and lower bounds. These bounds are compared with the field uptake data for the specific crop, to check if the model is reasonable for that metal-crop combination. Further, the uptake of metals from soil is modelled using Monte Carlo simulation from a uniform distribution between the upper and lower boundaries. In CLEA field data are collected for cabbage, lettuce, potato, carrot and onion, but are not published in the available literature.

Plant uptake of organic compounds

Because of the reasonably good empirical support, in CLEA the plant uptake algorithm is based on the Briggs-Ryan model. The Paterson-Mackay model is coded in the CLEA model, which is found to be an elegant alternative, but should not be used until empirical support is forthcoming. With a log Kow value a transpiration stream concentration factor (TSCF) and a root concentration factor (RCF) is calculated for organic substances. With a TSCF a stem concentration factor (SCF) can be calculated. With the RCF and the SCF the concentration in the different parts of the plant are calculated for organic contaminants, according to Briggs et al (1982). Ryan (1988) has extended the Briggs approach to include the effect of soil sorption on soil solution concentrations. The Briggs-Ryan model is essentially a regression model based on uptake of relatively hydrophilic chemicals (log Kow ranging from -0.57 to 3.7) by barley seedlings. Therefore, it should not be relied on for other plant species or for more hydrophobic chemicals.

Human exposure

Because eating habits differ considerably from one country to another, only sources of information relevant to the UK are used in CLEA. One of the main sources is the National Food Survey, which involves domestic food consumption estimates throughout the year (Table 3.12). The crops that are mentioned in Table 3.12 were chosen because a high proportion of the population ate them and probably contribute to the bulk of home-grown crops in the UK. The average home-grown consumption rate is based on the difference between the average

consumption and the average purchases. The home-grown fraction of the crop consumption rate is modelled separately in CLEA. In the CLEA model a preparation factor of 0.25 is assigned to cabbage and sprouts.

Table 3.12 Yearly food consumption rates (freshweight) in the UK (MAFF, 1990)

Crops	Average consumption rate (g/d)	Average home-grown consumption rate (g/d)	Upper bound home-grown consumption rate (g/d)
<i>Root crops:</i>			
Potatoes	142	6.6 (4.6%)	112 (78.9%)
Carrots	16	1.3 (8.1%)	12 (75%)
Onions, shallots, leeks	13	1.3 (10%)	13 (100%)
<i>Leafy crops:</i>			
Cabbages	12	1.5 (12.5%)	12 (100%)
Brussels sprouts	4.0	0.4 (10%)	3.8 (95%)
Leafy salads	7.2	0.5 (6.9%)	4.8 (66.7%)

In CLEA the expected daily intake (EDI) of home-grown crops is calculated using the following equation:

$$EDI = \frac{1}{\sum (\Delta T)_i} \sum_{i=1}^n \frac{C_i (ED)_i}{W_i} \sum_{k=1}^m (CR)_{ik} (HF)_k U_k$$

m:	number of crop species	[m=6]
C _i :	concentration in home-grown crops	[mg/kg]
(CR) _{ik} :	consumption rate of the k th crop type in time interval (ΔT) _i	[g/day]
(HF) _k :	home-grown fraction of the k th crop type	[-]
U _k :	uptake coefficient for the k th crop type	[-]
(ED) _i :	number of days of exposure to home-grown crops in time interval (ΔT) _i	[365 days]

The current number of exposure days (ED)_i is set at 365 days per year and the length of the growing season (and related factors) is adjusted by the variable (HF)_k. The user has the choice of adjusting both variable values to suit the available data.

3.5.2 UMS

Concentration in crops

The oral plant intake is only an exposure route for the scenario “garden”. This scenario includes all use activities in residential gardens and in allotment gardens. From the possible uptake routes for plants only the uptake from the soil compartment via the roots are calculated in UMS. The route from soil to plant is considered the most important one for the assessment of contamination dating from years back (a main goal of UMS). Not taken into account are the uptake routes for plants via the deposition of contaminants from air on the leaf surface or the gaseous uptake from air via the stomata. Transfer factors (bioconcentration factors) are used to specify the proportion between the contaminant concentration in soil (pore water) and the contaminant concentration in plants. With these factors the contaminant concentration in plants can be calculated for a soil depth of less than one meter. For soil depths of more than one meter an additional factor of 0.2 is used.

Plant uptake of metals from soil

For metal contamination the transfer factor is determined for crops (75%) and fruits (25%). Crops are further distributed between potatoes for 57% (4/7) and other crops for 43% (3/7). The total distribution is then 32% crops, 43% potatoes and 25% fruits. For the use in UMS first a transfer factor (TF) for crops is calculated, because the database for crops is better than for fruits. Compared to transfer in crops the transfer in fruits is more complex and complicated to describe. For some heavy metals it is known from literature that the transfer into fruits is a per cent part from the transfer into crops. The transfer factor metals is calculated according to:

$$TF_V = \frac{\frac{3 \cdot (a + b + c + d)}{n} + 4 \cdot TF_p}{7}$$

$$TF = X\% \text{ of } TF_V$$

$$TF_{SM} = \frac{75 \cdot TF_V + 25 \cdot TF_F}{100}$$

TF _V :	transfer factor for crops	[-]
TF _F :	transfer factor for fruits	[-]
TF _p :	transfer factor for potatoes	[-]
a-d:	empirical weighted TF values for different crops	[-]
n:	number of used crops	[-]
X%:	the % part of the transfer factor for crops to derive the transfer factor for fruits	[-]

As far as possible measured data are used for the determination of the transfer factors a-d and TF_p (e.g. Sauerbeck, 1989; Sauerbeck and Lübben, 1991).

Plant uptake of organic compounds

For organic substances it is assumed that they are transported and stored in plants without structural changes and the possible metabolites are not evaluated. For organic substances with an available partition coefficient (K_d in l/kg) first a concentration is calculated in pore water (C_{sw} in mg/l) from a concentration in soil (C_s in mg/kg):

$$C_{sw} = \frac{C_s}{K_d}$$

The concentration in plants is calculated starting from the concentration in porewater.

With a root concentration factor (RCF) or a sprout (stem, leaf, fruit) concentration factor (SCF) the concentration in the different parts of the plant are calculated for organic contaminants. The concentration in roots and sprouts is calculated according to Briggs et al (1982,1983):

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

$$TSCF = 0.784 \cdot 10^{\left(-0.434 \cdot \frac{(\log Kow - 1.78)^2}{2.44} \right)}$$

$$SCF = RCF \cdot TSCF$$

According to the UMS model the log Kow is limited to the range of -0.7 to 4.3. In the UMS model a correction is used for substances with a high logKow value (method unknown). Additionally, the work of Trapp and Matthies (1994) is used in UMS accounting for the plant uptake of organic chemicals via pore water and the exchange via air.

For organic substances crops are divided in potatoes for 47%, fruit for 24%, and the remaining 29% is equally divided over roots and sprouts, according to the UMS manual (DGE, 1992). From this it is assumed that for at least 85% the transfer factor must be used for sprouts and that the remaining 15% must be used for roots. Therefore in UMS potatoes are not assumed to be root crops. For organic contaminants the transfer factor from porewater to plants is calculated according to:

$$TF_{org} = RCF \cdot 0.15 + SCF \cdot 0.85$$

For estimating the concentration in the digestible parts of plants, the above mentioned calculations are in a modified form summarised in the UMS model. Not only is accounted for the use percentages of sprouts and roots, but also for the preparation of food (scraping, peeling, cooking etc.). For organic substances the developed new equation in the UMS model for calculating the concentration in plants is:

$$C_{P-org} = \frac{0.15}{\log Kow^{0.95}} \cdot (10^{0.77 \cdot (\log Kow)^{0.82} - 1.52} + 5) \cdot C_{SW}$$

C_{P-org} :	concentration in plants for organic substances	[mg/kg frw]
K_{ow} :	octanol-water partition coefficient	[-]
C_{sw} :	concentration in porewater	[mg/l]

Human exposure

The total average daily plant intake rates are based on a home-grown food use percentage of 41% for crops and 45% for fruits (see Table 3.13). Regarding to the German mean value the total intake rates for crops and fruits (Table 3.13) is corrected with a factor of 1.9 and 1.7, respectively. This correction is used because it appeared that people consume more crops and fruits when they have an own allotment or garden. When the home-grown food use percentages were used on the uncorrected German mean intake rates, the home-grown intake rates would be estimated too low. The separate intake rates of crops and fruits are not only corrected for the percentage used, but also for the preparation of food (scraping, peeling, cooking etc.) by multiplying them with a factor of 0.5 (UMS, 1997).

Table 3.13 Freshweight intake rates for crops and fruits for the garden scenario (UMS, 1997)

Population	Age (years)	Body weight (kg)	Total intake rate crops ¹⁾ (g/d)	Total intake rate fruits ²⁾ (g/d)	Intake home- grown crops ³⁾ (g/d)	Intake home- grown fruits ⁴⁾ (g/d)	Total average daily intake (mg/kg.d)
Infants	<1	5	-	-	-	-	-
Little children	1-3	10	115	50	47	23	7000 ⁵⁾
Children	3-8	20	230	95	94	43	6850 ⁵⁾
Juveniles	8-16	40	380	110	156	50	5125 ⁵⁾
Adults	16-46	70	475	120	195	54	3560 ⁵⁾

1) 1.9 times the German mean value determined by the Deutschen Gesellschaft für Ernährung (DGE), (Mekel, 1996)

2) 1.7 times the German mean value determined by the Deutschen Gesellschaft für Ernährung (DGE) (Mekel, 1996)

3) Intake is based on a home-grown food use percentage of 41% for crops (Mekel, 1996)

4) Intake is based on a home-grown food use percentage of 45% for fruits (Mekel, 1996)

5) This total average daily intake rate for the garden scenario must further be multiplied with a factor of 0.5 for the correction of food preparation (scraping, peeling, cooking etc.)

The daily intake values for plants (crops and fruits) are the same for heavy metals and organic substances. Different is the way how the concentration in plants is derived for heavy metals and organic substances. In the UMS model the concentration for crops are expressed on a

freshweight basis. Dry weight concentrations for crops are assumed to be 15% of the freshweight concentration. In the UMS model the potential daily dose (PDI) to home-grown crops is calculated with the following equations (UMS, 1993):

$$PDI_{P-S-ol} = DIR_P \cdot C_{P-SM} \cdot R_{ol} \cdot Av$$

$$PDI_{P-org-oral} = DIR_P \cdot C_{P-org} \cdot R_{oral} \cdot Av$$

with

$$C_{P-SM} = C_s \cdot TF_{SM} \cdot F \cdot 0.5 \cdot 0.15$$

$$C_{P-org} = \frac{0.15}{\log Kow^{0.95}} \cdot (10^{0.77 \cdot (\log Kow)^{0.82} - 1.52} + 5) \cdot C_{SW}$$

$$DIR_P = \frac{(IR_V \cdot EA_V) + (IR_F \cdot EA_F)}{BW}$$

C_{P-SM} :	concentration in crops for heavy metals (freshweight)	[mg/kg]
C_{P-org} :	concentration in crops for organic substances (freshweight)	[mg/kg]
R_{oral} :	substance specific oral resorption	[-]
Av :	matrix specific resorption availability (default 1)	[-]
C_s :	concentration in soil	[mg/kg]
C_{sw} :	concentration in porewater	[mg/l]
F_d :	soil depth (0-1 m : $F_d=1$; >1 m : $F_d=0.2$)	[-]
DIR_P :	daily intake rate crops/fruits, yearly average	[g frw/kg.day]
IR_V :	intake rate crops	[g frw/day]
EA_V :	one's own contribution from home-grown crops	[41%]
IR_F :	intake rate fruit	[g frw/day]
EA_F :	one's own contribution from home-grown fruit	[45%]
BW :	body weight	[kg]
0.5:	correction factor for food preparation	[-]
0.15:	calculation factor from freshweight to dryweight	[-]

3.5.3 CalTOX

Concentration in crops

In the CalTOX model, vegetation is modelled as a single compartment consisting of air, water, plant lipids and other materials (minerals etc.). In this model partitioning is defined among the gas, liquid and solid phase of the plant compartments. The plant compartment interacts with the air and root soil compartment. Pathways are defined for:

1. diffusion with the gas phase of the air compartment;
2. particle deposition with the solid phase of the air compartment;
3. advection with the liquid phase of the root-zone soil compartment.

The fugacity capacity of this plant compartment is based on a simplified version of the model proposed by Paterson and Mackay (1989). Paterson and Mackay have proposed a seven compartment fugacity model for plants that, in addition to the leaves, stem and roots, includes compartments for xylem, phloem and cuticle. Expressions relating to exchanges between vegetation and air and between vegetation and soil are obtained for nonionic organic chemicals by requiring that the fugacity of plants is the average of the fugacities in air and soil. It is also determined that for ionic organic chemicals and inorganic species, the fugacity in the plant tissues will approach the fugacity of soil when equilibrium is attained.

A different approach is used for metals, which is based on a balance among deposition, rainsplash, wash-off and plant decay that was developed for radioactive elements. According to CalTOX, BCF correlation models fail to predict the plant uptake reliably. A manuscript will be

published (end 2000) describing the Paterson and Mackay approach used in the CalTOX model.

The CalTOX exposure pathway model calculates the contamination of the exposed media of fruits, crops and grains. Fruits and crops are divided in a group of exposed produce representing aboveground edible plant parts and in a group of protected produce (root crops) and produce protected from the environmental compartment of air, such as citrus fruits. Grains are exposed produce.

Human exposure

In Table 3.14 the fresh weight intake rates are presented for crops and fruits, including the home produced values. These values are recommended in the Exposure Factors Handbook (US-EPA, 1997). In the CalTOX model the EFH values are not used, but instead the total consumption of each food type is considered as presented in the US Department of Agriculture Continuing Survey of Food Intakes by Individuals (CSFII). These values are adjusted by the fraction that is home-grown based on the EFH. The intake rates actually used in CalTOX were not found in the available literature. In the CalTOX model no correction factor is used for the preparation of food.

Table 3.14 Fresh weight intake rates of crops and fruits for home produced crops (US-EPA, 1997)

	Total crop intake	Total crop intake (home produced) ³⁾	Total root crop intake	Total root crop intake (home produced) ³⁾	Total fruit intake	Total fruit intake (home produced) ³⁾
Mean (g/kg.d)	4.3	2.1 (49%)	1.2	1.2 (100%)	3.4	2.7 (79%)
95 % (g/kg.d)	10	7.54 (75%)	4	3.7 (93%)	12	11.1 (93%)
Mean (g/d)	301 ¹⁾	126 ²⁾ (42%)	84 ¹⁾	72 ²⁾ (86%)	238 ¹⁾	162 ²⁾ (68%)
95 % (g/d)	700 ¹⁾	452 ²⁾ (65%)	280 ¹⁾	222 ²⁾ (79%)	840 ¹⁾	666 ²⁾ (79%)

1) A body weight of 70 kg is used.

2) A body weight of 60 kg is used; based on the number of respondents in each age category and the average body weights for these age groups.

3) The percentage between brackets is the part of the total intake value which is home produced.

The CalTOX model calculates the contamination of the exposure media of fruits, crops and grains via transfer factors (~BCF; not further explained here) for chemicals present in the environmental compartments air, water surface soil and root-zone soil. CalTOX uses the following equation for calculating the ingestion of contaminated fruits and crops and grains ($Intake_{fvg}$):

$$Intake_{fvg} = C_{fvg} \cdot \left[\frac{IR_{fvg}}{BW} \right] \cdot FI \cdot \frac{EF \cdot ED}{AT}$$

C_{fvg} :	concentration chemical in crop, fruit or grain	[mg/kg]
IR_{fvg} :	ingestion rate	[kg/day]
BW:	body weight	[kg]
FI:	home-grown based fraction ingested from contaminant source based on EFH (see Table 3.14)	[-]
EF:	exposure frequency	[day/year]
ED:	exposure duration	[years]
AT:	averaging time	[day]

3.5.4 CSOIL

Concentration in crops

For metals, other inorganic substances and organic substances different equations are available for calculating the crop content for root crops and leafy crops. All the equations are based on BCF values. For metals the dryweight concentration in soil is used for calculating the concentration in plants, using the BCF values of Sauerbeck (1989) completed with values obtained from the Baes (1984) equation. Further, for other inorganic and organic substances the concentration in pore water is used for calculating the concentration in plants. For the plant uptake of organic substances from soil the relations of Briggs (1982,1983) are used. For more information about the plant uptake of organic substances is referred to chapter 5. For metals the daily crop consumption is expressed on a dryweight basis and for other (in)organic compounds on a freshweight basis. The freshweight and dryweight intake rates are presented in Table 3.15.

Human exposure

The CSOIL intake rates of root crops and leafy crops are presented in Table 3.15.

Table 3.15 Freshweight and dryweight intake rates of root crops and leafy crops used in the CSOIL model

Crops	Intake root crops g _{dryweight} /d	Intake root crops g _{freshweight} /d	Intake leafy crops g _{dryweight} /d	Intake leafy crops g _{freshweight} /d
Children (1-6)	15.1	74.8	8.9	76.1
Adults (7-70)	27.6	136.7	18.4	157.8

The CSOIL model is corrected for the relative contribution of the daily consumption of leafy and root crops. A fraction of 0.1 is assumed for the use of home-grown crops (fv). No correction factor is used for the preparation of food (scrapping, peeling, cooking etc.) or the soil depth. CSOIL calculates one dose for the daily consumption of leafy and root crops. The uptake of contaminants via crops (VI), for adults and children separately, is based on:

$$VI = \frac{(Q_{fvk'} \cdot C_{pr'} + Q_{fvb'} \cdot C_{ps'}) \cdot fa \cdot fv}{W}$$

C _{pr'} /C _{ps'} :	concentration in roots or leaves of crops	[mg/kg _{wwt}]
Q _{fvk'} :	daily intake of root crops (adult)	[0.1367 kg _{wwt} /d]
Q _{fvb'} :	daily intake of leaf crops (adult)	[0.1578 kg _{wwt} /d]
fa:	relative absorption factor	[1.0]
fv:	fraction contaminated food (fraction of own garden)	[0.1]

3.5.5 Model comparison

Organic substances

For the models CLEA, UMS and CSOIL the calculations for organic substances in crops (roots and leaves) are based on Briggs (1982, 1983). This approach uses a transpiration stream concentration factor (TSCF), a stem concentration factor (SCF) and a root concentration factor (RCF) to calculate the concentration in the different plant parts. The Briggs approach is based on the uptake of relatively hydrophilic and is only used for barley seedlings. It is not clear how more hydrophobic chemicals and other plants or crops are used in those models. Besides the Briggs approach CLEA uses Ryan (1988) to include the effect of soil sorption on soil solution concentrations. The UMS model uses not only Briggs but also Trapp and Matthies (1994) additionally. For more information about the plant uptake of organic substances according to

Trapp and Matthies see section 5.3 Uptake of organic substances according to Trapp and Matthies. In a simplified form CalTOX uses the advanced seven compartment fugacity model of Paterson and Mackay. This model is suitable for all substances except metals. In the CLEA model the Paterson and Mackay approach is available but is not used because it is lacking empirical support.

Metals

Like CSOIL, CLEA and UMS use BCF correlation models to predict the concentration of metals in roots and leaf. In CLEA Baes et al. (1984) and other studies (i.e. Anderson and Christensen, 1988) are used to derive a relation between the soil to plant concentration factor, the partitioning coefficient for soil and the soil pH. Further, field uptake data for specific crops are used to check if the model is reasonable for that metal-crop combination. The approach of CSOIL is based on Sauerbeck and additionally Baes (1984). According to CalTOX, BCF correlation models fail to predict the plant uptake reliably. Therefore a different approach is used for metals, which is based on a balance among deposition, rainsplash, wash-off and plant decay that was developed for radioactive elements.

In a different way the models compared account for soil attached to crops. CLEA accounts for soil attached to crops which cannot be removed by normal food preparation (30 g dry soil / kg dry leaf or 3%). CalTOX uses a rainsplash partitioning coefficient and uses also the concept describing the deposition on plant parts (no further information available). In CSOIL deposition on plant parts is modelled according to Hetrick and McDonnal-Boyer (1984), but is not used to derive guideline values. Adhesion to leaves is an important component of plant accumulation of sparingly soluble contaminants, and this contaminant may not be removed by rigorous cleaning (Sheppard and Evenden, 1992). Therefore it is recommended to add the deposition on plant parts or rainsplash to the CSOIL model.

In Table 3.16 an overview is presented for the used approaches of all models.

Table 3.16 Approaches for calculating the concentration in crops used by the different models

Model	All substances	Metals	Organic substances	Accounts for soil attached (splash)	Correction food preparation
CLEA	Paterson and Mackay (available, not used)	Baes (1984) and other studies. And check with field data.	RCF: Briggs (1982) SCF: Briggs (1983) and Ryan (1988)	Yes, Sheppard, Evenden (1992)	Yes ¹⁾
CalTOX	Simplified Paterson and Mackay	Different approach based on deposition, rainsplash, wash-off and plant decay.	-	Yes, rainsplash partition coefficient?	No
UMS	-	Experimental BCFs (Sauerbeck and Lubben) or transfer factors (unknown reference)	RCF: Briggs (1982) SCF: Briggs (1983) & Trapp and Matthies	No	Yes, 0.5
CSOIL	-	Experimental BCFs (Sauerbeck)	RCF: Briggs (1982) SCF: Briggs (1983)	Yes, deposition: Hetrick, McDonnal-Boyer (1984)	No

1) A preparation factor of 0.25 is assigned to cabbage and sprouts

Human exposure

Only crop intake for adults are compared with each other, because for children intake values were not available for the CLEA and CalTOX model. It should be noted that potatoes are not considered to be root crops in the UMS model. For all models the results are presented in Table 3.17. The differences are rather large between the different models, especially for the home-grown intake rates. The difference between the lowest and highest intake rate is a factor 13 and 30 for home-grown root crops and leafy crops, respectively.

Table 3.17 Freshweight intake rates of root crops and leafy crops

Model	Intake home-grown root crops (g/d)	Intake home-grown leafy crops (g/d)	Total intake root crops (g/d)	Total intake leafy crops (g/d)
CLEA ¹⁾	9.2	2.4	171	23.2
CalTOX ²⁾	126	72	301	84
UMS ³⁾	Crops: 195		Crops: 475	
CSOIL ⁴⁾	13.7	15.8	136.7	157.8

- 1) The separate intakes of different crops are added to obtain the total values (see Table 3.12). 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 by CalTOX are unknown.
- 3) Only the crop values are presented, because root crops and leafy crops are not defined in UMS. The values are without a factor of 0.5 for correcting for the preparation of food
- 4) The intake of home-grown crops is assumed to be 10% of the total crop intake

From Table 3.17 the factors are calculated between the home-grown intake rates and the total intake rates of root crops and leafy crops. The intake of home-grown crops compared to the total crop intake vary from 5.4% to 42% for root crops and 10% to 86% for leafy crops (see Table 3.18).

Table 3.18 Factor between home-grown intake rates and total intake rates of root crops and leafy crops

Model	Factor for root crops	Factor for leafy crops
CLEA	18.6 (5.4%)	9.7 (10.3%)
CalTOX	2.4 (42%)	1.2 (86%)
UMS	crops: 2.4 (41%)	
CSOIL	10 (10%)	10 (10%)

For all models the exposure to contaminants via crops is based on the estimated concentration in leaves and roots multiplied with the daily consumption and both divided by the body weight. The differences are mainly the used absorption or resorption rates and the used time intervals. The UMS and CSOIL model can use a chemical specific resorption or absorption factor for uptake in the human body. CLEA and UMS both use a correction is used for preparing food.

3.6 Conclusions

In this chapter concepts of international models are selected that might be useful for improvement of CSOIL. The recommendations are subdivided into the ingestion of contaminated soil, the inhalation of vapours of contaminants, the ingestion of contaminants via crop consumption and other model concepts. Recommendations for the input parameters are mentioned in the last part of this section, but are actually subject of the evaluation of input parameters (Otte et al., 2001). For some recommendations additional research, the exact equations and detailed descriptions are necessary to get more insight in the exact use of the model concepts.

Ingestion of contaminated soil particles

All models compared use the same concept for calculating the soil ingestion by multiplying a contaminant concentration in soil with a soil ingestion rate which is normalised on the basis of the body weight.

Indirect soil uptake via inhalation and subsequently swallowing of dust particles

The UMS model uses a direct and indirect oral uptake of soil or dust particles. The indirect oral uptake describes first the inhalation of dust particles, after which they are subsequently swallowed. The daily soil intake via the indirect route appeared to be negligible compared to the direct route and therefore it is not useful to implement the indirect route in CSOIL.

Deliberate or exploratory soil ingestion during childhood

The concept of deliberate soil ingestion, together with inadvertent soil ingestion, should be included in CSOIL. There is little doubt that a relative short-term deliberate soil-eating is widespread among children and can have a significant impact on childhood contaminant exposure. A deliberate soil ingestion of 5 g/d during only 15 days over the period of 1-6 years increases the yearly average intake with more than 40%. The considerations for a possible approach of combining inadvertent and deliberate soil ingestion are presented in CLEA (1998). Research is necessary to determine the persistence (duration) of the deliberate soil-eating of children. According to CLEA (1998) this behaviour can persist from a few days to a few months. CSOIL only accounts for lifetime daily mean exposures and therefore the effect of short-term deliberate soil ingestion is probably negligible. Further research on the comparison of the short-term exposure of deliberate soil-eating to acute toxicity data is particularly recommended. Deliberate soil ingestion is especially important when the exposure for children (1-6 years) is separated from the exposure for adults (7-64 years).

Use of yearly average soil ingestion rates or daily rates combined with a separate exposure duration

For CSOIL it is proposed to introduce a separate exposure duration combined with a daily intake rate. All international models use a separate daily soil ingestion rate combined with an exposure duration. In CSOIL only a yearly average soil ingestion rate can be used. Dependent on the exposure duration of the used scenario the international models are therefore flexible for adjusting the yearly average ingestion rate. The CSOIL scenario can then possibly be adjusted for exposures duration of less than 365 d/y. For the potential exposure assessment for the scenario residential with garden the exposure duration remains 365 d/y.

Inhalation of vapours of contaminants

Calculation of the concentration in crawl space; diffusive flows

Besides CSOIL only in CLEA it is possible to calculate indoor air concentrations for houses with crawl spaces. The CLEA approach for calculating the concentration in the crawl space is more detailed than CSOIL. In CLEA not only a diffusion flux from soil and in- and outgoing horizontal ventilation fluxes are used, but different from CSOIL, also a diffusion flux from crawl space to indoor air and in- and outgoing ventilation fluxes through crawl space and an outgoing diffusion flux through walls is used. The diffusion flux through walls seems of minor importance, compared to the ventilation flux. More extensive information on these diffusive flow concepts can be derived by further research.

Calculation of the concentration in crawl space; the pressure driven flow

A possible improvement of CSOIL can be the use of the pressure driven flux for modelling the flow from soil air to indoor air. All models compared explicitly or implicitly use the pressure driven flow concept, except CSOIL. For more information on the pressure driven flux the reader is referred to chapter 4 Evaluation volatilisation module of CSOIL with other concepts.

Use of ventilation fluxes describing the wind induced pressure and the stack effect

Different from the other models CLEA uses additional ventilation fluxes describing the wind induced pressure and the stack effect. For the multi-media concept the CalTOX model uses an exchange of flows between the outside air and the indoor air. Possibly CSOIL could be refined using ventilation fluxes or the exchange of air between the indoor and outdoor environment. Further research is only essential when the fixed ratio between indoor air and crawl space is going to be revised in CSOIL.

Ingestion of contaminants via consumption of crops

Plant uptake of organic substances:

All models compared use the Briggs approach to predict the plant uptake of organic contaminants, except CalTOX. The only difference is that UMS uses Trapp and Matthies. It is not expected that the Ryan approach is different from the Briggs approach as used in CSOIL, except that Ryan has extended the Briggs approach to include the effect of soil sorption on soil solution concentrations. For none of the international models using the Briggs approach is described what the consequences are for substances with $\log K_{ow}$ values of more than about 5 (see plant uptake of organic compounds section 3.5.1 and 3.5.2). The Trapp and Matthies (1994) approach is used in UMS to account for the plant uptake of organic chemicals via pore water and the exchange via air. A possible improvement of CSOIL is the use of the Trapp and Matthies approach (see also section 5.3 and 5.5). At this moment it is advised not to use the advanced seven-compartment fugacity model of Paterson and Mackay, mainly because of the lack of empirical support. Probably at the end of 2000 a study will be published about the use of a simplified Paterson and Mackay model in CalTOX.

Plant uptake of metals:

For the plant uptake of metals CLEA and UMS use the BCF correlation models. In CLEA the Baes concept is supplemented with information from other studies to incorporate the influence of the soil pH. In CLEA also field uptake data for a specific crop are used to check if the model is reasonable for that metal-crop combination. CSOIL could be refined using BCF values that are corrected for the soil pH as is done for CLEA. Research is necessary to determine the importance of the soil pH on the BCF values, because the documentation of CLEA is too limited to make a good comparison with CSOIL. The evaluation of the BCF values currently used in CSOIL is described in Otte et al. (2001). The UMS model uses substance specific experimental BCF values for different crops according to Sauerbeck, which are recalculated to one averaged BCF value for crops and fruits. This concept is almost identical to CSOIL and therefore it offers no advantages compared to the current approach in CSOIL. According to CalTOX BCF correlation models fail to predict the plant uptake reliably. Therefore a different approach (details are lacking) is used for metals based on a balance among deposition, rainsplash, wash-off and plant decay.

Soil attached to plants:

Soil and dust particles can deposit on the different plant parts by rainsplash. Therefore it can be interesting to investigate the contribution of this route compared to the total concentration in plants. For soil attached to crops, which cannot be removed by normal food preparation, CLEA uses a value of 30 g soil / kg dry leaf (= 3%). This value is based on the suggested estimated soil load concluded by Sheppard and Evenden (1992). The results of the Sheppard and Evenden study clearly showed that adhesion to leaves is an important component of plant accumulation. For crops growing beneath the soil different percentages are used (0.1% - 0.5% on a fresh weight basis). With the CLEA assumptions it is possible to determine the importance of this route for the exposure to contaminants via the consumption of crops. Details for a good comparison with CSOIL are lacking on the CalTOX rainsplash partitioning coefficient. Both the concepts of CLEA and CalTOX are different from the deposition to plants as used in CSOIL. It is recommended to add the soil attached to crops route to CSOIL, because the contribution is not expected to be negligible.

Correction factor for the preparation of food

CLEA and UMS use a correction is used for preparing food, i.e. scraping, peeling or cooking. CLEA uses a preparation factor of 0.25 for cabbage and sprouts. UMS multiplies the total average daily intake with a factor of 0.5. Although relevant it is not clear what the results of these habits are on the intake in general. At this moment it is advised not to implement a factor for the preparation of food in CSOIL.

Other model concepts*Box-model concept:*

CalTOX includes a seven compartment transport and transformation box-model with mass exchange processes between the different compartments. CSOIL must be completely revised when this concept would be used. A human exposure model comparison study can show the possible advantages of the CalTOX concept above the CSOIL concept. At this moment it is advised not to implement the box model concept in CSOIL.

Use of resorption or absorption rates:

Based on this model comparison it is advised to make a distinction between oral and inhalative absorption and therefore a different parameter for each route should be included in CSOIL. In UMS and CSOIL a factor is used for the uptake of a contaminant in the human body via the ingestion of soil particles, the inhalation of vapours and the ingestion of crops. This factor is called a resorption factor in UMS and an absorption factor CSOIL. For all the mentioned routes of both models the default value of this factor is 1. The default value of 1 can be discussed for the inhalation route, because due to exhalation the total inhaled quantity of a substance can not be absorbed.

Natural degradation

CLEA and CalTOX use the single first order approach of Jury (1983) for the determination of the natural degradation of organic chemicals. Removal processes can include photolysis, chemical reaction, volatilisation, biodegradation, run-off, erosion, leaching and harvesting of crops. For calculating the potential exposure with CSOIL it is not useful to investigate the importance of degradation, because the exposure must then be calculated as a function of time and because of the differences in observed half live times of a substance. For site specific assessments of readily degrading compounds it can be useful to include natural degradation. In that case it is proposed to measure the on-site degradation.

Background concentration in air or soil

The CLEA model can account for other sources than only the contaminants in soil, like natural or ambient soil or air concentration (background concentrations) and other indoor sources of contaminants (cigarette smoke paints etc.). UMS can also use background soil concentrations. Therefore it can be interesting to investigate the use of natural background concentrations on the Intervention Values. Ambient background concentrations can be significant for site specific assessments, but are not considered for calculating potential risks with CSOIL.

Input parameters

The values for the input parameters of the international models are different from those of CSOIL. The following conclusions should be taken into account in the evaluation of the input-parameters.

Ingestion of contaminated soil particles

All models use an age adjusted soil ingestion factor, because inadvertent soil ingestion is different for children and adults. On the basis of the yearly average soil ingestion rates of the international models compared, it can be concluded that the present value in CSOIL of 150 mg/d is rather high for children. For adults the international model ingestion rates are comparable with the CSOIL value.

Inhalation of vapours of contaminants

On the basis of the presented respiration rates for the international models compared, it can be concluded that the present value in CSOIL of 20 m³/d is rather high for adults. For children (1-6 years) the values of the US and German model are comparable with the CSOIL. Only the respiration rate of the UK model (EFH value) is somewhat lower.

Ingestion of contaminants via consumption of crops

As presented in Table 3.17 the intake values of home-grown root crops and leafy crops and the total intake values of root crops used in CSOIL are lower than the international models. This can be caused by the different eating habits in international countries. The difference between the lowest and highest home-grown intake rate for adults is a factor 13 and 30 for root crops and leafy crops respectively.

Further it can be useful to investigate the use of the standard fraction of 0.1 of CSOIL for correcting the total crop intake to obtain the home-grown fraction. All the international models use the direct result of intake studies and not a standard factor to determine the home-grown crop intake. As can be calculated from Table 3.17, the factor between the total crop and home-grown crop intake always lower than the factor 0.1 used in CSOIL. Only the factor for leafy crops of the CLEA model is almost equal to the CSOIL value (Table 3.18). At this moment it is advised not to change the CSOIL concept, because the use of home-grown crops and eating habits are simply different in foreign countries.

4. Evaluation volatilisation module of CSOIL with other concepts

4.1 Introduction

The volatilisation module in CSOIL estimates the human exposure to volatile compounds in soil and groundwater. This chapter focuses on the human exposure to volatile compounds in indoor air. For indoor air the concentration in the living room of a single-family dwelling is used. In the Netherlands about 2/3 of the housing stock consist of single-family dwellings. The concentration in other rooms is supposed to be the same, although ventilation will be different in all parts of a house. The exposure in outdoor air is negligible (van den Berg, 1995). The estimation of the human exposure can be divided in two parts:

1. calculation of the distribution over soil phases and the contaminant flux to the air;
2. calculation of the indoor air concentration and the human exposure.

The main concept of part 1 in CSOIL is that volatile compounds reach the soil surface by convective transport with the water evaporation flux and by a diffusion flux from soil to crawl-space air. This is an empirically lumped flux in which transport of the compound by capillary rise of the groundwater is combined with the evaporation with the water at the soil surface.

The CSOIL module is based on equilibrium partitioning and stationary transport equations. The following limitations can be mentioned for this module:

- no biological degradation is included;
- the contaminant source in a soil is inexhaustible;
- a soil is homogeneous;
- in the soil exists equilibrium at the depth of the contamination, but above this no equilibrium is assumed;
- no lateral transport or leaching.

Because of these limitations and the fact that CSOIL is not fit for site-specific calculation of the human exposure, the model VOLASOIL was developed (Waitz e.a., 1996). This model is used to determine the actual risk of a soil contamination. The concept of this model might be useful to improve the CSOIL module on volatilisation.

In the following section the CSOIL-model with its limitations is presented (section 4.2). Second the concept of the VOLASOIL model is described (section 4.3). In section 4.4 model concepts of both models are compared. In section 4.5 the concepts (also from international models) are discussed and conclusions are drawn. Section 4.6 concentrates on evaluation of the relevant input-parameters and in section 4.7 the conclusions are summarised.

4.2 The CSOIL module and its limitations

This paragraph describes the main concept of the CSOIL module together with the limitations. More details of the module can be found in the CSOIL-formulas in Appendix 6.

4.2.1 Distribution over soil phases

Non-equilibrium sorption

The distribution between the soil phases in CSOIL is based on the fugacity theory of Mackay (1985). The formulas used for the calculation can be found in Appendix 6. Important for the equilibrium are the organic carbon-water partitioning coefficient (K_{oc}), the solubility (in water);

S) and the vapour pressure (Vp). In the real soil environment the principle of equilibrium sorption does not have to be the case. This becomes clear for example within several sanitation projects, where the concentration in the withdrawn contaminated groundwater (or soil moisture) drops in time, although the concentrations in the soil stay relatively high (van Geer et al, 1997). For aged contamination the assumption of equilibrium between the soil phases probably results in an overestimation of the concentration in soil moisture and the volatilisation flux.

A solution to this problem would be to use non-equilibrium sorption, but this would make the calculation much more complex and more input-parameters would be needed.

Distribution coefficient, solubility and vapour pressure

The partitioning coefficient K_{oc} (distribution between groundwater and organic carbon in the soil) is an important parameter for calculating the concentration in the groundwater (or soil moisture). Different methods are used to determine the value of this parameter (measured or calculated from K_{ow} or solubility). The uncertainty in these values and the methods for estimation are subject of the study on the input-parameters (Otte et al., 2001). Together with the organic carbon content (foc) the K_{oc} -distribution determines the distribution between soil and pore water.

Solubility (S) and vapour pressure (Vp) of a compound is temperature dependent. The standard condition for measurements is 20 °C, but the soil the mean soil temperature is about 10°C (Feddes and Huinink, 1990). The parameters used in the CSOIL model for the first and second series of Intervention Values were *not* corrected for this temperature difference (Van den Berg, 1997). Methods and data for temperature correction of S and Vp are subject of the study on input-parameters (Otte et al., 2001).

4.2.2 Fluxes

In CSOIL different fluxes of volatile compounds can be distinguished. Figure 4.1 gives an overview of these fluxes, indoors as well as outdoors.

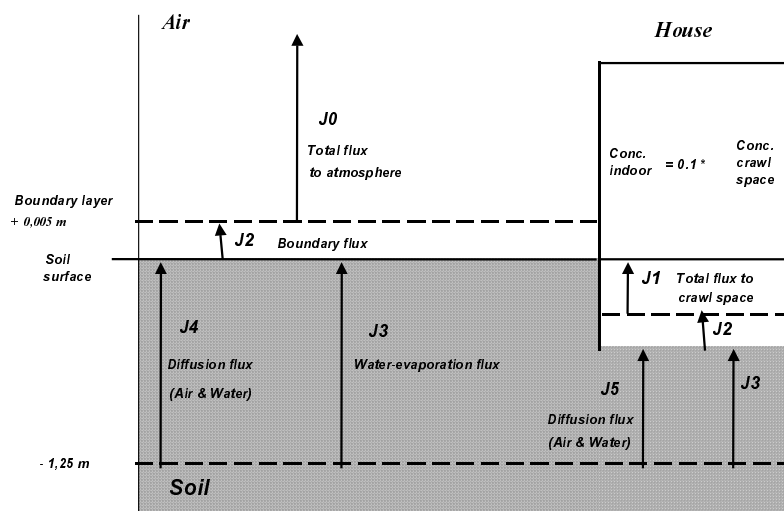


Figure 4.1 Transport fluxes of volatile compounds from soil/ groundwater to indoor and to outdoor air in CSOIL

Because the indoor air concentration is the most important exposure route, we concentrate on the estimation of the indoor air concentration. For the indoor air the following contaminant fluxes are calculated (Figure 4.1):

J1= total flux to the crawl space;

J2= flux through the boundary layer (limits the fluxes from soil to air);

J3= water evaporation flux from soil to the crawl space;

J5= diffusion flux from soil (soil air and pore water) to crawl space.

Diffusion fluxes (J5)

The diffusion fluxes through soil air and pore water are calculated in CSOIL according to the theory of Jury (1984c). The assumption is a linear concentration gradient in the soil with the maximum concentration at a depth of 1,25 m below land surface.

Of these two fluxes the diffusion of volatile compounds by soil air is by far the most important in the open capillary zone of the soil. For this reason the diffusion through pore water will not be paid attention to. The diffusion flux through soil air (J5) can be described as:

$$J5 = \frac{Du \cdot Cs \cdot SD}{dp - Bh}$$

with $Du = (Pa \cdot Dsa / Va) + (Pw \cdot Dsw / Vw)$

with $Dsa = Va^{10/3} \cdot Da / (1-Vs)^2$ with $Da = 0.036 \cdot (76/M)^{1/2}$

and $Dsw = Vw^{10/3} \cdot Dw / (1-Vs)^2$ with $Dw = 3.6 \cdot 10^{-6} \cdot (76/M)^{1/2}$

Du :	diffusion coefficient in the soil	[m ² /h]
Cs :	initial soil content (total soil content in gas, water, solid phase)	[mol/kg dry soil or mg/kg]
SD :	mass volume of the dry soil	[kg dry soil/dm ³ humid soil]
dp :	mean depth of the contamination	[1.25 m]
Bh :	height of the crawl space (under groundlevel)	[0.5 m]
Pa :	mass fraction in soil air	[-]
Pw :	mass fraction in pore water	[-]
Dsa :	diffusion coefficient in the soil-gas phase	[m ² /h]
Dsw :	diffusion coefficient in the soil-water phase	[m ² /h]
Va :	volume fraction air	[-; 0.2]
Vw :	volume fraction water	[-; 0.2]
Vs :	volume fraction solid phase	[-; 0.6]
Da :	diffusion coefficient in free air	[m ² /h]
M :	molecular mass	[g/mol]

Water evaporation flux (J3)

The second process that determines the total flux to the crawl space is the water evaporation flux. The water evaporation flux is calculated based on data from Fast et al (1987). For the Dutch situation it is estimated on 0.1 dm³/m².d. The process includes the transport of water, a phase change from liquid to vapour water and the transfer from the soil surface to the air. There are two reasons why this concept is not entirely scientific correct:

1. Because the crawl-space air is near saturation, there is no concentration gradient in the air that drives the transport of water from the soil to the air.
2. The constant evaporation flux implies that there is a constant capillary rise from the groundwater table. In the real soil this is only possible up to the capillary transition zone, which in many cases would not reach to the soil surface. Above this zone diffusion is the dominant process.

In equations this flux can be described as:

$$J3 = C_{pw} \cdot \frac{Ev}{24}$$

Ev: flux of evaporating water (0.0001 m³/m².d; Fast *et al.*, 1987) [m³/m².d]
 Cpw: soil-moisture concentration (= Cs · SD · Pw/Vw) [mol/dm³ or g/m³]

Boundary flux (J2)

The transport to the crawl-space air can be limited by the boundary layer, a stagnant layer of air above the soil surface in which only diffusion occurs. The boundary flux (J2) can be calculated with:

$$J2 = Da \cdot \frac{Csa}{d}$$

Da : diffusion coefficient in free air [m²/h]
 Csa : soil-air concentration (=Cs · SD · Pa / Va) [mol/dm³ or g/m³]
 d : thickness boundary layer (Jury *et al.*, 1984c: 0.005 m) [m]

Total flux to crawl space (J1)

The sum of the water evaporation flux (J3) and the diffusion flux (J5) may not exceed the calculated boundary flux (J2). The total contaminant flux to the crawl space (J1, in g/m².h) equals J3 + J5, but in case J2 < (J3+J5), J1 is equal to J2. The total flux to the crawl space is used to calculate the indoor air concentration.

Depth of groundwater table (depth of contaminant)

The depth of the groundwater table is not incorporated in CSOIL. Assumed is that the maximum concentration of the contaminant is at 1.25 m. When the groundwater is closer to the soil surface the diffusion will be smaller, because the diffusion flux through water is much smaller than through air.

4.2.3 Crawl-space air and indoor air concentration

The concentration in crawl-space air depends on the total flux from the soil (J1), the surface and the volume of the crawl space and the air-exchange rate of the crawl space (Vv), which empirically is estimated between 0.04 and 7.4 h⁻¹, with a mean of 1.25 h⁻¹ (Fast *et al.*, 1987, 1988).

In equations:

$$Cba = \frac{J1 \cdot Bo}{Bv \cdot Vv}$$

Cba : concentration in the crawl-space air [g/m³]
 Bo : surface area of the crawl space [50 m²]
 Bv : volume of the crawl space [25 m³]
 Vv : air-exchange rate [1.25 h⁻¹]

Secondly the indoor air concentration can be calculated as a mean fraction of the concentration in the crawl space. The contribution of the crawl-space air (fbi) to the indoor air varies between 0 and 0.68, with a mean of 0.11, showing a large difference between houses with wooden (mean 0.19) and concrete floors (mean 0.096) (Fast *et al.*, 1987, 1988). The parameter is at 0.1 in the model.

In equations:

$$C_{ia} = f_{bi} \cdot C_{ba}$$

C_{ia} :	concentration in the indoor air	[g/m ³]
f_{bi} :	contribution of the crawl-space air to the indoor air as fraction	[0.1; -]

Although the empirical estimation of the air-exchange rate of the crawl-space air (V_v) and the contribution of crawl-space air to indoor air (f_{bi}) show large ranges, the concept of calculating the indoor air is accepted.

4.2.4 Human exposure by inhalation

Inhalation of indoor air

The intake of volatile compounds depends on:

- the concentration of indoor air (C_{ia}) (and outdoor air: C_{oa});
- time spend indoor (and outdoor) for adults and children: t_{ia} and t_{ic} (t_{oa} and t_{oc});
- annual average time fractions for stay indoor (and outdoor): tf_{ia} and tf_{ic} (tf_{oa} , tf_{oc});
- breathing volume adults and children (AV_a and AV_c);
- absorption of contaminants in lungs (f_a);
- body weight (adults and children; W_a and W_c).

These parameters are estimated by Linders et al. (1990). The fraction of absorption of contaminants (f_a) is currently set on 1.

For adults and children the exposure is calculated by:

$$IV = [AV \cdot C_{ia} \cdot tf_i \cdot t_i + AV \cdot C_{oa} \cdot tfo \cdot to] \cdot f_a \cdot 10^3 / W$$

The lifelong daily exposure of volatile compounds ($DOSE_{IV}$) is the weighted average of the dose for children and the dose for adults:

$$DOSE_{IV} = \frac{6IV_{child} + 64IV_{adult}}{70}$$

Inhalation of outdoor air

The inhalation of outdoor air is not evaluated in this chapter because this is not an important exposure route. The VOLASOIL models only indoor air.

4.3 Relevant concepts of the VOLASOIL model

4.3.1 Main concept and distribution over the soil phases

The VOLASOIL model is developed to estimate the actual human risk of volatile compounds. It is used to determine if a location has high priority for clean up based on human risks. Calculation with this model is often combined with measurements in the indoor and crawl-space air. The complete description of the model and the formulas can be found in Waitz et al. (1996).

The VOLASOIL model is based on stationary transport and has, to some extent, the same assumptions and limitations as the CSOIL module:

- no biological degradation is included;
- the contaminant source in a soil is inexhaustible;

- a soil is homogeneous;
- equilibrium sorption at the depth of the contamination, but above this no (non-equilibrium) sorption is assumed;
- no lateral transport or leaching.

In VOLASOIL difference has been made between the groundwater, the full capillary zone and the open capillary zone (separated by the groundwater table and the capillary transition boundary, CTB, respectively). Two important transport processes are quantified in the open capillary zone:

- diffusion in soil air;
- pressure driven vapour flow.

Below the CTB diffusion and dispersion in pore water and the convective transport by water flow are the most important transport mechanisms. In Figure 4.2 the different zones and fluxes are shown. Only the bold fluxes are incorporated in VOLASOIL.

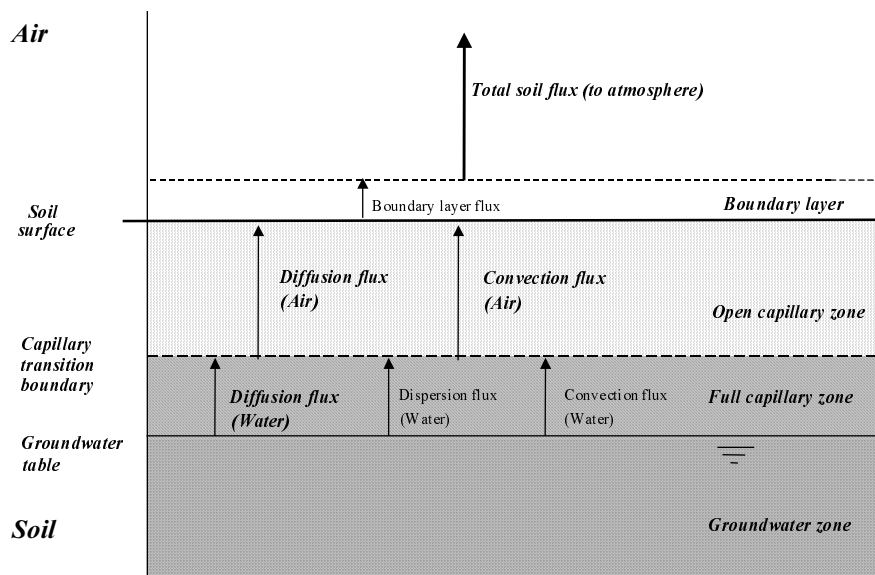


Figure 4.2 Zones and fluxes (bold) within VOLASOIL

In VOLASOIL eight cases have been distinguished. Case A (groundwater contamination, well-mixed container) is the basic scenario and is closest to the assumptions within the CSOIL module. Within VOLASOIL the depth of the groundwater table can be changed, just like other site-specific parameters.

For the calculations of fluxes to the soil surface it is important to determine the height of the capillary transition boundary (CTB) above the groundwater table. For the 18 soils of the Staring series (Wösten et al, 1994) the height lies between 12 and 84 cm. The value for clayey loam, the closest to standard soil is 84 cm. The arithmetic mean of all soils is, just like for sand 50 cm.

The concentration in the soil air at the capillary transition boundary is calculated by:

$$C_{sa} = K_{lw} \cdot C_{sw}$$

Csa :	soil-air concentration	[g/m ³]
Klw :	air-water distribution coefficient or dimensionless Henry constant [(mol/m ³ air)/(mol/m ³ water)]	[-]
Csw :	soil-moisture concentration	[g/m ³]

The dimensionless Henry constant ($K_{lw}=H/R \cdot T$) is corrected for the average standard soil temperature of 10°C. A few correction methods for the Henry constant (H , in Pa.m³/mol) are described in an appendix of Waitz et al. (1996).

4.3.2 Fluxes from soil to crawl space and crawl-space air concentration

Fluxes to crawl space

Two fluxes are calculated in the open capillary zone:

- diffusion in soil air (diffusive transport);
- pressure-driven vapour flow (convective transport).

When only the *diffusion flux* is considered, this can be described as:

$$Jd_{ss} = D_{sa} \frac{C_{sa}}{L_s}$$

Jdss :	diffusion flux from soil to soil surface	[g/m ² h]
Dsa :	diffusion coefficient in the soil air	[m ² /h]
Csa :	concentration in soil air at dp	[mol/dm ³ or g/m ³]
Ls :	magnitude of soil column (= dp-dc; average depth of contaminant - depth of crawl space below land surface)	[m]

The average depth of the contaminant is assumed to be at the capillary transition boundary (CTB). The diffusion coefficient in soil air (D_{sa}) is derived from the diffusion coefficient in free air (D_a , based on the molecular weight), the volume fraction soil air (V_a) and volume fraction pore water (V_w). These are identical to the calculation of these parameters in CSOIL.

Second the *pressure-driven air flow* in VOLASOIL is described as:

$$Fsc = K_s \frac{\Delta p_{cs}}{L_s}$$

Fsc :	air flux from soil to crawl space	[m ³ /m ² .h]
Ks :	air conductivity of soil	[m ² /Pa.h]
Δpcs :	air pressure difference between crawl space and soil	[Pa]
Ls :	magnitude of soil column (= dp-dc; average depth of contaminant - depth of crawl space below land surface)	[m]

The factor K_s , the air conductivity, depends on the air permeability (κ) and the dynamic viscosity of air (η).

$$K_s = \frac{\kappa}{\eta}$$

The air permeability of different soils is found in several references with a range of 10^{-10} - 10^{-16} m², from coarse sand to clay (Waitz et al, 1996).

The *total contaminant flux* to the crawl space is a combination of the convective flux and the diffusive flux, which are closely related. Therefore one equation is derived from the equations for diffusion and convection. With a negligibly low concentration (zero) at the surface (C_0) as an upper boundary condition, the flux from soil to crawl space (J_1) is:

$$J_1 = \frac{-F_{sc} \cdot C_{sa}}{\exp\left(\frac{-F_{sc}}{D_{sa}} L_s\right) - 1}$$

J_1 :	total contaminant flux from soil to crawl space	[g/m ² .h]
F_{sc} :	air flux from soil to crawl space	[m ³ /m ² .h]
C_{sa} :	concentration in soil air at d_p	[mol/dm ³ or g/m ³]
L_s :	magnitude of soil column (= $d_p - d_c$; average depth of contaminant - depth of crawl space below land surface)	[m]
D_{sa} :	diffusion coefficient in the soil air	[m ² /h]

Crawl-space air concentration

The concentration in the crawl space can be calculated on the basis of the total contaminant flux from soil to crawl space, the air-exchange rate and the dimensions of the crawl space, (assuming that the surface area of the crawl space is equal to that of the floor):

$$C_{ca} = J_1 \frac{A_f}{V_c \cdot vv_c}$$

C_{ca} :	concentration in crawl-space air	[g/m ³]
J_1 :	total contaminant flux from soil to crawl space	[g/m ² .h]
A_f :	surface area of floor	[m ²]
V_c :	volume of crawl space	[m ³]
vv_c :	air-exchange rate of crawl space	[h ⁻¹]

The air-exchange rate (vv_c) used in VOLASOIL was measured by Fast et al (1987) with a geometric mean of 1.05 h⁻¹.

4.3.3 Flux from crawl space to indoor air and indoor air concentration

Flux to indoor air

Within VOLASOIL an air flux is derived for the flux from the crawl space through the gaps, cracks and holes in the floor. This air flux (F_{ci}) can be calculated with:

$$F_{ci} = \frac{f_{of}^2}{n\pi \cdot 8\eta} \frac{\Delta p_{ic}}{L_f}$$

F_{ci} :	air flux from crawl space through floor to indoor space	[m ³ /m ² .h]
f_{of} :	fraction openings in the floor	[m ² /m ²]
η :	dynamic viscosity of air	[Pa.h]
n :	number of openings per floor area	[m ⁻²]
Δp_{ic} :	air pressure difference between indoor space and crawl space	[Pa]
L_f :	floor thickness	[m]

With the air flux the contaminant flux to the indoor air can be calculated as well:

$$J_{c_i} = F_{ci} \cdot C_{ca}$$

J_{c_i} :	convective flux from crawl space to indoor air space	[g/m ² .h]
F_{ci} :	air flux from crawl space to indoor space	[m ³ /m ² .h]
C_{ca} :	concentration in crawl-space air	[g/m ³]

Indoor air concentration

The indoor air concentration can be calculated on the basis of the total contaminant flux from soil to crawl space, the air-exchange rate and the dimensions of the crawl space, (assuming that the surface area of the crawl space is equal to that of the floor):

$$C_{ia} = Jc_{ci} \frac{A_f}{V_i \cdot vv_i}$$

C_{ia} :	indoor air concentration	[g/m ³]
Jc_{ci} :	total contaminant flux crawl space to indoor space	[g/m ² .h]
A_f :	surface area of floor	[m ²]
V_i :	volume of indoor space	[m ³]
vv_i :	air-exchange rate of indoor space	[h ⁻¹]

The human exposure is no part of VOLASOIL; the calculated air concentration is directly compared with the TCA (Tolerable Concentration in Air) (Waitz et al.,1996).

4.4 Comparison exposure with CSOIL and with VOLASOIL

4.4.1 Parameter values

In Table 4.1 the CSOIL parameters used for the calculation of the indoor air concentration are summarised, including the default values used in the CSOIL-model. The corresponding VOLASOIL parameters are given as well.

Table 4.1 CSOIL parameters and corresponding VOLASOIL parameters

Symbol CSOIL	Symbol VOLASOIL	Default CSOIL	Unit
distribution over soil phases			
M	M	input	g/mol
Cs	C _t	input	mg/kg dry soil
fnd	-	output	-
foc	-	0.058	kg _{org.} C/kg dry soil
Va	V _a	0.2	- ; volume fraction
Vw	V _w	0.2	- ; volume fraction
Vs	V _s	0.6	- ; volume fraction
SD	-	1.5	kg _{dry soil} C/dm _{humid soil}
Pa	-	output	- ; mass fraction
Pw	-	output	- ; mass fraction
flux to crawl space			
Csa	C _{sa}	output	mol/dm ³ or g/m ³
Cpw	C _{sw}	output	mol/dm ³ or g/m ³
Dsa	D _{sa}	output	m ² /h
Da	D _a	output	m ² /h
Dsw	-	output	m ² /h
Dw	D _w	output	m ² /h
Du	-	output	m ² /h
J1/Ji	J1	output	g/m ² .h
J2	-	output	g/m ² .h
J3	-	output	g/m ² .h
J5	Jd _{sc}	output	g/m ² .h
d	-	0.005	m
Ev	-	0.0001	m ³ /m ² .d
dp	dp	1.25	m

Symbol CSOIL	Symbol VOLASOIL	Default CSOIL	Unit
concentration crawl space and indoor air			
Bh	dc	0.5	m
Cba	C _{ca}	output	g/m ³
Bo	A _f	50	m ²
Bv	V _c	25	m ³
Vv	vv _c	1.25	h ⁻¹
Cia	C _{ia}	output	g/m ³
fbi	-	0.1	-
human exposure			
Ava / Avc	-	20 / 7.6	m ³ /d
ti adult/child	-	8 / 16	h
tfi adult/child	-	2.856/ 1.322	-
fa	-	1	-
Iva / Ivc	-	output	mg/kg.d
Wa / Wc	-	70 / 15	kg

4.4.2 Comparison of CSOIL and VOLASOIL with default parameters

For four organic compounds the indoor air concentration with the current CSOIL model and with VOLASOIL is calculated. The current Intervention Value soil is used to calculate the pore water (porewater) concentration. This (equilibrium) porewater concentration is also used as input parameter for VOLASOIL. In CSOIL the standard parameters are used. In VOLASOIL the default parameters for a normal situation are used and the parameters in Table 4.2. For the substance-related parameters the values of CSOIL are used.

Table 4.2 Values of parameters used in exposure calculations with CSOIL and VOLASOIL

Parameters crawl-space air concentration	Symbol VOLASOIL	Unit	Current CSOIL	Location-specific range and default value VOLASOIL
depth of contamination (below land surface)	dp	m	1.25	input (dg-z) used: 1.25
depth of groundwater level (below land surface)	dg	m	n.a.	input used: 1.75
height of capillary transition boundary above groundw. table	z	m	n.a.	0.12-0.84 used: 0.5 (=sand & average)
air permeability of soil (depending on soil type)	κ	m ²	n.a.	10 ⁻¹⁰ -10 ⁻¹⁶ used: 10 ^{-11.5} (=fine sand)
pressure difference soil air and crawl-space air	Δp _{cs}	Pa	n.a.	2
dynamic viscosity of air	η	Pa.h	n.a.	6E-9
depth of crawl space below land surface	dc	m	0.5	0.4 used: 0.5
volume of crawl space	V _c	m ³	25	25
floor area	A _f	m ²	50	50
basic ventilation rate crawl space	vr _{c,b}	m ³ /h	n.a.	20
air-exchange rate crawl space	vv _c	h ⁻¹	1.25 used: 0.93	0.93
Parameters indoor air concentration				
total area of openings in floor	A _{of}	m ²	n.a.	0.005-0.00005 used: 0.0005 (= normal)
fraction of openings in floor	f _{of}	m ² /m ²	n.a.	0.0001-0.000001 used: 0.00001 (=normal)
floor thickness	L _f	m	n.a.	0.1
pressure difference crawl-space air and indoor air	Δp _{ic}	Pa	n.a.	2
ventilation rate of indoor space	vr _i	m ³ /h	n.a.	25-150; used: 75

Remarks to the calculations:

- For the comparison the solubility (S) and vapour pressure (Vp) of VOLASOIL are used, because these values are already corrected for the temperature difference between soil (10 °C) and given in the literature (20 °C);
- For the comparison the air-exchange rate of the crawl space (vv_c) of VOLASOIL (default 0.93 h^{-1}) is also used in CSOIL (default 1.25 h^{-1});
- Starting from the soil concentration (used in CSOIL) the porewater concentration is calculated. In VOLASOIL and CSOIL the same porewater concentrations are used. Because the Intervention Value groundwater is deducted from the porewater concentration by dividing by 10, the presented groundwater concentration differs in both models.
- In VOLASOIL case A 'groundwater contamination: well-mixed container' is used.

The results of the calculations (see Table 4.3) show:

- the concentration in soil air is the same in both models;
- the diffusion flux (J5 and Jd) is also identical in both models (same calculation);
- the pressure driven flow (= convection flux = Jc) in VOLASOIL is higher than the evaporation flux (J3) in CSOIL (factor 3400);
- the total flux in CSOIL is calculated by addition of the diffusion flux (J5) and the evaporation flux (J3) and the total flux in VOLASOIL is calculated by combination of the diffusion flux (Jd) and the convection flux (Jc);
- the total flux in CSOIL is determined for 96 to 99.5 % by the diffusion flux. For VOLASOIL this is not known, because the diffusion and convection flux influence each other.
- the total flux (J1) in VOLASOIL is a factor 10 to 15 higher than of CSOIL;
- the calculated concentration in the crawling space is identical in both models ($2.15 \cdot J1$);
- the indoor air concentration is lower than in the crawling space, for CSOIL this factor is 10, for VOLASOIL the (default) factor is 24;
- the indoor air concentration of VOLASOIL is a factor 4 (benzene) to 6 (tetrachloroethene) higher than of CSOIL.

Table 4.3 Calculated fluxes and concentrations in air with CSOIL and VOLASOIL ($\mu\text{g}/\text{m}^3$)

substance	groundwater level depth of contamination	TCL	CSOIL n.a. -1.25 m	n.a. - 3 m	VOLASOIL -1.75 m -1.25 m	-3.5 m -3.0 m
benzene	conc. soil (mg/kg)	30	1	1	-	-
92% contribution to IV soil	conc groundwater ($\mu\text{g}/\text{l}$)		29.7	29.7	297	297
	conc pore water ($\mu\text{g}/\text{l}$)		297	297	297	297
	conc soil air		43900	43900	43960	43960
	J5 / Jd (diffusion)		60.9	18.3	60.9	18.3
	J3 / Jc (convection)		1.24	1.24	4217	1267
	J1 (total)		62.1	19.5	623	188
	crawl space air		134	42	1341	9472
	indoor air		13.4	4.2	56.8	17
toluene	conc. soil (mg/kg)	3000	130	-	-	-
87% contribution to IV soil	conc groundwater ($\mu\text{g}/\text{l}$)		1100		11000	
	conc pore water ($\mu\text{g}/\text{l}$)		11000		11000	
	conc soil air		1890000		1890000	
	J5 / Jd (diffusion)		2430		2440	
	J3 / Jc (convection)		45.8		156200	
	J1 (total)		2480		26900	
	crawl space air		5330		57600	
	indoor air		533		2440	
tetrachloroethene	conc. soil (mg/kg)	2500	4	-	-	-
96% contribution to IV soil	conc groundwater ($\mu\text{g}/\text{l}$)		41.2		412	
	conc pore water ($\mu\text{g}/\text{l}$)		412		412	
	conc soil air		286000		286000	
	J5 / Jd (diffusion)		272		266	
	J3 / Jc (convection)		1,72		5850	
	J1 (total)		273		4050	
	crawl space air		588		8686	
	indoor air		58.8		367	
monochloro- benzene	conc. soil (mg/kg)	1000	30	-	-	-
69% contribution to IV soil	conc groundwater ($\mu\text{g}/\text{l}$)		193		1930	
	conc pore water ($\mu\text{g}/\text{l}$)		1930		1930	
	conc soil air		170000		170000	
	J5 / Jd (diffusion)		196		196	
	J3 / Jc (convection)		8.05		27406	
	J1 (total)		204		2417	
	crawl space air		439		5182	
	indoor air		43.9		219	

$$J_c (\mu\text{g}/\text{m}^2 \cdot \text{h}) = F_{sc} (\text{m}^3/\text{m}^2 \cdot \text{h}) \cdot \text{conc. porewater} (\text{g}/\text{m}^3) \cdot 10^6$$

When the starting point for the calculations would be the groundwater concentration in CSOIL (being a factor 10 lower than the porewater), the indoor air concentrations calculated with VOLASOIL calculation would be a factor 2.5 (benzene) to 1.6 (tetrachloroethene) lower than in CSOIL.

4.4.3 Influence of input-parameters on the calculated flux

For the important input parameters an impression is given of the influence of these parameters on the calculated flux with benzene as an example.

Depth of the contaminant (dp) and depth of the groundwater table (dg)

In CSOIL the depth of the contaminant is 1.25 m; in VOLASOIL the depth is calculated from the groundwater table (dg) and the capillary transition boundary (z): $dp = dg - z$. The magnitude of the soil column (L; below the crawl space) is in both models used to calculate the diffusive

flux. The lower the groundwater table (d_g)(and d_p), the longer is the column (L_s) and the smaller is the diffusion flux. A longer soil column results in VOLASOIL also in a smaller convection flux (J_c). In Table 4.3 the influence of the depth of the contaminant (and the groundwater table) is shown for benzene

Height of capillary transition boundary (z)

The height of the capillary transition boundary (CTB) depends on the soil type. Together with the depth of the groundwater table it determines the depth of the contaminant. The higher the CTB is, the smaller are the depth of the contaminant, the soil column and the calculated fluxes.

Soil permeability (κ) for a sandy soil

The air permeability of the soil (κ) depends also on the soil type. This parameter influences the calculated convection flux strongly. In Table 4.4 the influence of the air permeability (κ)(and the CTB, z) on the indoor air concentration is shown. The higher the permeability, the higher are the convection flux and the total flux.

Table 4.4 Influence of the permeability (κ) and the CTB (z) on the calculated fluxes ($\mu\text{g}/\text{m}^2\cdot\text{h}$) and the concentrations ($\mu\text{g}/\text{m}^3$)(of benzene)

soil type	parameter	CSOIL	VOLASOIL
clay, $\kappa = 1.10^{-16}$ $z = 0.2$ $d_p = 1.55$ $L_s = 1.05$	J5 cq Jd (diffusion)	43.5	43.5
	J3 cq Jc	1.24	0.009
	J1	44.7	43.5
	conc. crawl space	96.2	93.3
	conc. indoor air	9.62	3.95
sand, fine $\kappa = 3.2.10^{-12}$ $z = 0.5$ $d_p = 1.25$ $L_s = 0.75$	J5 cq Jd (diffusion)	60.9	60.9
	J3 cq Jc	1.24	421
	J1	62.1	97.4
	conc. crawl space	134	209
	conc. indoor air	13.4	8.8
sand, middle $\kappa = 3.2.10^{-11}$ $z = 0.5$ $d_p = 1.25$ $L_s = 0.75$	J5 cq Jd (diffusion)	idem	60.9
	J3 cq Jc		4217
	J1		625
	conc. crawl space		1341
	conc. indoor air		56.8
sand, coarse $\kappa = 1.10^{-10}$ $z = 0.5$ $d_p = 1.25$ $L_s = 0.75$	J5 cq Jd (diffusion)	idem	60.9
	J3 cq Jc		13187
	J1		1954
	conc. crawl space		4190
	conc. indoor air		177

Pressure differences (Δp)

The higher the pressure difference between soil and crawl space (Δp_{sc}), the higher the calculated indoor air concentration with VOLASOIL. In Table 4.5 the influence is shown for benzene.

Table 4.5 Influence of Δp_{sc} on the calculated indoor air concentration ($\mu\text{g}/\text{m}^3$)

Δp_{sc} (Pa)	CSOIL	VOLASOIL
1.10^{-9}	14	5.5
10	14	280

In Table 4.6 the influence of the pressure difference between crawling space and indoor air (Δp_{sc}) on the concentration in the crawl space (C_{ca}) and the indoor air (C_{ia}) is given. The pressure difference in VOLASOIL also influences the air-exchange rate of the crawl space

(vv_c). The factor concentration in crawl space air/ indoor air is given for VOLASOIL (in CSOIL this factor is a constant, 10). A higher pressure difference results in a higher concentration in indoor air.

Table 4.6 Influence of Δp_{ic} on calculated indoor air concentrations of benzene ($\mu\text{g}/\text{m}^3$)

Δp_{ic} (Pa)	Vv_c (h^{-1})	CSOIL		VOLASOIL		
		C_{ca}	C_{ia}	C_{ca}	C_{ia}	C_{ca}/C_{ia}
0.1	0.8	155	15.5	1550	3.4	456
14	1.73	72	7.2	724	171	4.2

Quality of the floor

In VOLASOIL the quality of the floor is quantified by the total area of openings in the floor (A_{of}): good, $5 \cdot 10^{-5} \text{ m}^2$; normal, $5 \cdot 10^{-4} \text{ m}^2$; bad $5 \cdot 10^{-3} \text{ m}^2$. With this parameter the air flux from crawling space to indoor air (F_{ci}) is calculated, followed by calculating the contaminant flux from the crawl space to the indoor air ($J_{c,i}$) and the indoor air concentration (C_{ia}). Also the air-exchange rate of the crawling space (vv_c) depends on the area of openings in the floor. In CSOIL vv_c has a fixed value. In Table 4.7 is shown that a larger A_{of} leads to lower concentrations in the crawl space and in the indoor air. The factor concentration crawl space air/indoor air (f_{bi}) decreases strongly (default 10 in CSOIL).

Table 4.7 Influence of the quality of the floor on the concentration (of benzene) ($\mu\text{g}/\text{m}^3$) in the crawl space (C_{ca}) and in the indoor air (C_{ia})

A_{of} (m^2)	Vv_c (h^{-1})	CSOIL		VOLASOIL		
		C_{ca}	C_{ia}	C_{ca}	C_{ia}	factor
$5 \cdot 10^{-3}$	14	8.8	0.88	89	73	1.2
$5 \cdot 10^{-4}$	0.93	134	13.4	1341	57	24
$5 \cdot 10^{-5}$	0.80	155	15.5	1560	0.69	2261

Influence ventilation rate indoor (vr_i)

The basic indoor ventilation rate (vr_i) in VOLASOIL is used to calculate the indoor ventilation rate of the indoor space (vv_i), followed by the calculation of the indoor air concentration. CSOIL uses a fixed ratio between crawl space air and indoor air (10). In VOLASOIL a basic ventilation rate between bad ($25 \text{ m}^3/\text{h}$) and very good ($150 \text{ m}^3/\text{h}$) can be chosen (default $75 \text{ m}^3/\text{h}$, being the minimum according to NEN 1087). Table 4.8 shows that a higher ventilation rate leads to lower indoor air concentrations a higher ratio (f_{bi}).

Table 4.8 Influence of ventilation rate on the indoor air concentration ($\mu\text{g}/\text{m}^3$) in VOLASOIL

vr_i	indoor air concentration	conc. crawl space/indoor air.
25 = bad	157	8.5
50	83	16
75	57	24
100	43	31
150 = very good	29	46

4.5 Comparison and discussion of model concepts

In this paragraph the model concept is evaluated based on the current CSOIL, VOLASOIL and international models and proposals are made for changes of the model concept. The following parts of the concept are distinguished:

- exposure scenario;
- soil-air concentration;

- flux to crawl space and crawl space air concentration;
- flux to indoor air and indoor air concentration;
- parameter values;
- human exposure.

4.5.1 Exposure scenario

Contaminants can be present in soil and in groundwater. The current Intervention Values are calculated based on contamination in soil. In the site specific risk assessment with VOLASOIL the source of the contamination is in the groundwater. It is proposed to apply the model concept to derivation of the Intervention Value of both compartments. The exposure models UMS, CLEA only concern derivation of a value for soil, CalTOX also concerns groundwater.

Intervention Value soil

For the Intervention Value it is assumed that the contamination is present in the porewater, starting at a specific depth below land surface. Important parameter is the average depth of the contaminant. The depth of the groundwater table is in this case of no importance, but could best be set at the same depth as the depth of the contaminant for reasons of consistency.

Intervention Value groundwater

For the derivation of Intervention Value for groundwater it is assumed that the contamination is present in a well-mixed container of groundwater. The concentration at the top of the capillary transition boundary (CTB) depends on the concentration in the groundwater. In field experiments it was found that the concentration in the top layer of the groundwater often is lower than the concentration in the groundwater one meter below the groundwater table (Waitz et al, 1999). For risk assessment there are two possibilities:

- the concentration in the CTB is assumed to be equal to the concentration in the upper groundwater; in this case the concentration should be measured in the top of the groundwater;
- the concentration in the CTB is assumed to be lower than the concentration in the groundwater 1 m below the groundwater table (where the concentration is measured); results from field experiments should be used to estimate the difference.

For the purpose of potential risk assessment the first option is the most appropriate.

4.5.2 Soil-air concentration

The calculations in CSOIL start with the total soil content of a contaminant, in VOLASOIL the calculations start with the concentration in the groundwater. The calculation of the soil-air concentration from the pore water concentration in CSOIL, VOLASOIL and the other international models are identical and are based on the fugacity theory of Mackay and equilibrium partitioning. In CLEA and CalTOX also transformation and degradation is included, although it is not clear if this is used for deriving guidelines (see sections 3.2.1 and 3.2.3).

Problem is that in the field equilibrium between the soil phases often does not occur. Several reasons can be mentioned for this difference:

- there can be a hysteresis effect (difference between adsorption and desorption). Although it is decided to use measured Koc's it is not known how these Koc's are measured (probably adsorption experiments).

- there can be ageing effects, because contaminants are in the soil/sediment for a longer time. Slower desorption can result in lower concentrations in the porewater than expected based on the partitioning coefficient (Cornelissen, 1999). If this is the case the partitioning could be corrected for this.

A solution could be the measurement of the K_{oc} for each location (as is done for the organic matter content), but this can financially be impossible. As long as there is no general accepted approach for this problem, it is proposed to use the equilibrium partitioning method.

Consequence can be that the risks are over estimated. Therefore further research on this subject is necessary.

The relation between porewater and soil air in the field does not have to correspond with the expected equilibrium based on the Henry coefficient either. Nevertheless the relation between porewater and soil air is calculated with a temperature corrected Henry coefficient (with a soil temperature of $T = 10^{\circ}\text{C}$).

4.5.3 Flux from soil air to crawl-space air and crawl-space air concentration

Fluxes

In CSOIL a diffusion flux (J_5) and an evaporation flux (J_3) are estimated. The calculation of the *diffusion flux* in CSOIL and VOLASOIL is identical, with the exception that in VOLASOIL diffusion through the water phase is neglected. The boundary flux (J_2) is not calculated in VOLASOIL, because this flux is not a limitation on the total flux. For the upper boundary condition for diffusion it is assumed that the concentration in the crawl space and at the soil surface is negligibly low compared to the concentration in soil air. The international model comparison (section 3.4) shows that a diffusion flux is included in CLEA (UK) and that in UMS (Germany) and CalTOX (USA) it is implicitly included in the parameter values, based on studies for radon in dwellings.

Not included in CSOIL is the (pressure driven) convective flux (air flux). This flux is a result of pressure differences by wind and temperature differences between indoor, outdoor and crawl space air (Godish, 1990). Other processes that can lead to convective flow from soil air into a crawl space (or house), are barometric pressure differences and precipitation (Nazaroff et al., 1988). In a study on radon pressure driven flow was even more important than diffusion (Nazaroff et al., 1985). The evaporation flux in the present CSOIL model is not included in VOLASOIL and the other models.

A reason to include a pressure driven vapour flow in CSOIL is that in many references is stated that diffusion as well as convective flow contribute to indoor air concentrations. The relative contribution of both processes strongly depends on the type of soil and pressure differences (e.g. Nazaroff et al., 1988; Ferguson et al. 1995; Johnson and Ettinger, 1991). The international model comparison (section 3.4) shows that in CLEA (UK) a convective flux is included and that in UMS (Germany) and CalTOX (USA) it is implicitly included in the parameter values, based on studies for radon in dwellings.

The evaporation flux to crawl space air in CSOIL is of minor importance, because:

- in a crawling space the water content in the air is often near saturation;
- the capillary rise from the groundwater does not (always) reach the soil surface.

Therefore it is proposed to exclude the current evaporation flux to the crawl space. As part of the total convective flux (F_{sc}) the evaporation could be included, although of minor

importance. It is also proposed to exclude the evaporation flux to outdoor air, because evaporation is more than compensated by precipitation in the Netherlands.

It is proposed to include the convective flow (of air and water) besides the molecular diffusion in the model concept. To implement this change in the exposure model, choices on the exposure scenario and important parameter-values have to be made (see section 4.6).

Crawl space air concentration

The calculation of crawl space air concentration in CSOIL and VOLASOIL are almost identical, except from the fact that VOLASOIL corrects for the air flux from crawl space to indoor space and the air flux from soil to crawl space. *Besides parameter-values (section 4.6), the flux should be corrected for the air flux from soil to crawl space.*

4.5.4 Flux from crawl space to indoor air and indoor air concentration

Fluxes and indoor air concentration

In CSOIL no flux is calculated, but a 10% contribution of the crawl-space air to the indoor air (fbi) is assumed, based on measurements (Fast et al., 1987, 1988; Kliet et al., 1989). In VOLASOIL the flux is calculated depending on the quality of the floor and the ventilation characteristics, and therefore describes the influence on the actual airflow in a better way. Internationally UMS (0.01) and CalTOX (α -factor) use a fixed ratio between soil air and indoor air (see sections 3.4.2 and 3.4.3). The CLEA-model uses a sophisticated ventilation model (section 3.4.1), which is comparable with VOLASOIL.

A more acceptable module, as in CLEA or VOLASOIL could be used in CSOIL, but using a standard scenario and fixed assumptions (for an average house in the Netherlands) results in a ratio between the two compartments. For a potential risk assessment a (well-founded) ratio of the contribution of crawl space air to indoor air is found to be sufficient.

In VOLASOIL the *concentration in indoor air* is calculated with the flux and the air-exchange rate in the house. This approach describes the process better and gives the option to adjust parameters when new data become available.

It is proposed to maintain a fixed ratio between the concentration in crawl space air and indoor air for calculation of the indoor air concentration. This ratio should be based on measurements in Dutch houses (see section 4.6).

4.5.5 Human exposure

In all models the inhalation of vapours (from indoor air) is fundamentally calculated in the same way. The main differences are the use of adsorption rates and exposure times (section 3.4.5). The default values for CSOIL are stated in Appendix 6.8 (Linders, 1990, Waitz et al., 1996).

In VOLASOIL (for location-specific risk assessment) the estimated indoor air concentration is directly compared with the TCA. Then exposure time parameters are not needed for calculation of the risk limit. Disadvantage is that time fractions are not included and the total exposure is not calculated.

For CSOIL it is proposed to integrate the parameters t_i (duration of exposure inside) and the factor t_{fi} (annual average time fractions for staying indoors) to one exposure time parameter (T_i).

4.5.6 Preliminary conclusions on model concepts for vapour exposure

Based on the concepts in EUSES (section 2) the international model concepts (section 3) and the concepts in VOLASOIL (sections 4.3 and 4.4), the following is concluded.

The calculation of the soil-air concentration (from the total soil concentration) in CSOIL and the other models are identical (all equilibrium partitioning), and no modification is proposed. Nevertheless it is clear that this is only an estimation and field measurements can lead to other concentrations.

The diffusion fluxes in the *flux from soil air to crawl-space air* in CSOIL, VOLASOIL and probably CLEA are identical. A pressure driven convective air flux is a good supplement to the diffusive flux. Therefore it is proposed to include a convective flux (pressure driven air flux) into the volatilisation module of CSOIL. Before this can be implemented, new input-parameters have to be selected (see section 4.6). The *evaporation flux* in CSOIL is not used in other models, has only a small contribution and is found not to be appropriate for this objective. To avoid differences between *fluxes to indoor and to outdoor air* and because precipitation exceeds evaporation in general, it is decided to exclude the evaporation flux also from the estimated flux to outdoor air. The *boundary flux* in CSOIL does not lead to limitations in the total flux ($J_2 \gg J_3 + J_5$) and can be left out.

The calculation of the *crawl space air concentration* in VOLASOIL (and CLEA) is slightly different from CSOIL. In UMS and CalTOX these concentrations are not calculated. It is proposed to also correct for the air flux from soil, besides values of parameter to be evaluated (see section 4.6 and Otte et al., 2001).

For the calculation of the *flux from crawl space to indoor air* and the *indoor air concentration* it is proposed to maintain a fixed ratio between indoor air and crawl space air. The value of this ratio has to be evaluated based on the assumptions in the standard scenario's of VOLASOIL (ratio = 24) and the current ratio in CSOIL (ratio = 10).

The two parameters for the exposure time for the calculation of the *human exposure* can be integrated to one exposure time parameter (T_i).

4.6 Evaluation of important parameters

4.6.1 Introduction

To implement new model concepts into the volatilisation module of CSOIL, input-parameters have to be evaluated and selected to be able to create a standard ("average") scenario for a contamination in a "standard" soil. The following parameters have to be known to calculate the crawl-space air concentration based on the total concentration in soil and the concentration in groundwater:

- pressure difference soil air and crawl space air (Δp_{cs});
- air permeability (κ);
- dynamic viscosity of air (η);
- depth of contamination (d_p);
- depth of groundwater level (d_g);
- capillary transition boundary (z);
- depth of crawl space below land surface (d_c);
- ventilation rate crawl space (V_v).

To calculate the indoor air concentration, based on the crawl space air concentration, the contribution of crawl space air to indoor air (f_{bi}) is necessary.

The parameters Δp_{cs} , κ and η are new compared to the current model concept. The uncertainty analysis showed that Δp_{cs} and κ contribute largely to the uncertainty of the calculated indoor air concentration (Waitz et al., 1996). Especially for these parameters it is important to determine the best values for the Dutch situation (see section 4.6.2 and 4.6.3). The parameter η is a physical parameter of air, which is $18E-6 \text{ N.m}^{-2}.\text{s}$ (Pa.s) or $5E-9 \text{ Pa.h}$ (Chang, 1981; CRC, 1998). The evaluations of the other six parameters, as described in Otte et al. (2001) are summarised in section 4.6.4.

4.6.2 Pressure difference soil air/crawl space air and crawl space air/indoor air (Δp_{cs} ; Δp_{ic})

Difference can be made between soil (or outside air) to crawl space (Δp_{cs}) and crawl space to indoor air (Δp_{ic}), but in some studies these are not separated (when e.g. no crawl space is present) (see Figure 4.3). The main focus is on Δp_{cs} . In fact the ∇P (pressure gradient; Pa/m) should be estimated and changed to Δp_{cs} with the magnitude of the soil column ($\nabla P = \Delta p/d$). House depressurisation increases the pressure driven flow. Several sources of house depressurisation can be identified (Fugler, 1997a+b; Garbesi et al., 1989, Nazaroff, 1988).

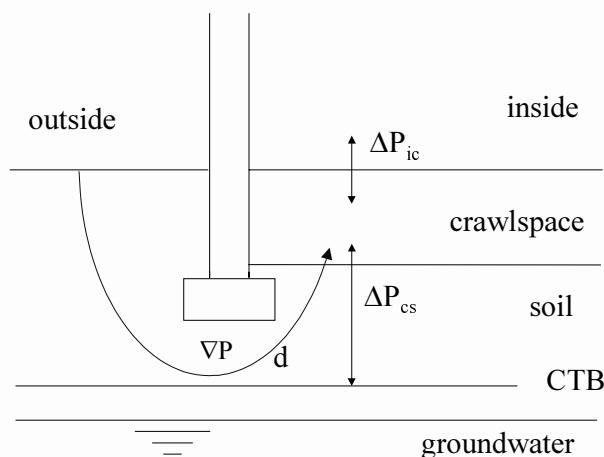


Figure 4.3 Pressure differences and airflow from soil to crawl space

The stack effect (temperature difference).

This occurs because buildings behave like chimneys. Warmer air rises and escapes at upper level, the resulting low pressure in the basement causes the flow of soil gas into the building. The pressure difference (Pa) due to temperature difference (stack effect) can be calculated by (Nazaroff et al., 1987, 1988):

$$\Delta P_s = \alpha(z - z_0)\Delta T$$

α :	stack effect	[0.040 Pa/m.K]
$z - z_0$:	height above the level at which indoor and outdoor pressure are equal	[m]
ΔT :	temperature difference between indoor and outdoor	[K]

This pressure difference is approximately 2 Pa in winter (Nazaroff et al., 1987; Krylov and Furguson, 1998) or 2 - 6 Pa (Garbesi et al., 1989).

Wind.

The pressure difference (Pa) due to wind can be calculated by (Nazaroff et al., 1987, 1988):

$$\Delta P_w = C_j \frac{1}{2} \rho v^2$$

C_j :	surface pressure coefficient ($-1 < C_j < 1$)	[Pa.m.s ² /kg]
ρ :	air density	[kg/m ³]
v :	wind speed	[m/s]

This pressure difference is approximately 2 Pa in winter (Nazaroff et al., 1987). The pressure gradient in the soil due to wind can be estimated with:

$$\nabla P = (P_1 - P_2)/d$$

P_0 :	the dynamic soil-gas pressure (considered zero)
P_1 :	the dynamic gas pressure in the crawl space
d :	the characteristic path length between soil and crawl space.

With $d = 1$ m and a wind of 3 m/s the pressure gradient is estimated -0.5 Pa (Krylov and Furguson, 1998).

Mechanical systems (heating, ventilation, air conditioning and fireplaces).

This systems replace indoor air, which must be replaced with outside or crawl space air. No special attention is given to these sources.

Other sources of convective flow from the soil to the indoor air are barometric pressure differences and rainfall (Nazaroff, 1988).

Data from literature

Nazaroff et al (1985) measured the **outdoor/ indoor (basement) pressure difference** during the period February till June in a house in Chicago. The pressure difference was between 0.6 and 4.3 Pa with a mean of 2.3 Pa (winter 3.3, spring 1.3 Pa). They also stated that the entry rate is generally higher for higher temperature differences. When the temperature difference is small, higher entry rates are associated with high wind speeds, when the temperature difference is large higher entry rates are associated with low wind speeds.

Put and Meijer (1989) measured the **outdoor/crawl space pressure difference** on 5 May in a house in The Netherlands. The mean pressure difference was 4 Pa. Sometimes a peak up to 20 Pa occurs and overpressure in the crawl space of 4 Pa. Measurements of the indoor/crawl space pressure difference show an average of 2.5 Pa.

Aldenkamp et al (1994) measured an **outdoor/crawl space pressure difference** during 11-17 June in a house in The Netherlands. The pressure difference varies with a semi-diurnal periodicity (12 hour cycle) between 0 Pa and 1 Pa with a mean of 0.5 Pa.

Table 4.9 Maximum pressure difference across below grade building envelopes

house type	typical Δp mild winter	typical Δp moderate winter	Typical Δp severe winter
slab-on-grade (no chimney)	1	2	3
slab-on-grade (chimney)	3	4	5
1 or 2 storey (no chimney)	4	5	6
1 or 2 storey (chimney)	8	9	10

Adjustments:

- If the house has a fresh air intake duct or combustion air supply, reduce the difference pressure by 2 Pa.
- If the house has a fireplace, central exhaust system or other large of frequently used exhaust equipment, increase the difference pressure by 2 Pa.

Fugler et al (1997a) included a table with maximum **pressure difference across below grade building envelopes** for different types of Canadian houses (Table 4.9). **The average pressure difference** across the below grade building envelope during the heating season can be estimated as 50% of the maximum value given in Table 4.9 (after appropriate adjustments). For the Dutch situation mild winters apply.

In Janssen et al (1998) the ventilation characteristics of new and old dwellings were modelled with a Dutch model dwelling (including ventilation holes to the crawl space) and a distribution of Dutch weather conditions. The **outdoor to crawl space pressure difference** based on all these conditions varies between 1.92 and -0.54 Pa (mean 0.33 Pa) with 90% of between 1.0 and -0.1 Pa. For old dwelling the pressures over the soil are 2.5 to -0.25 Pa.

Hintenlang et al (1992) and Robinson et al (1995a) demonstrated that even under neutral pressure conditions (outdoor/indoor pressure difference is less than 0.5 Pa), atmospheric pressure changes can provide a driving force for soil gas to enter the house. When no depressurisation occurs, indoor pressure responds nearly instantaneously to variations of the outdoor pressure ($-0.5 \text{ Pa} < \Delta p \text{ indoor/outdoor} < 0.5 \text{ Pa}$). The **indoor/sub slab pressure differences** ($-3 \text{ Pa} < \Delta p < 5 \text{ Pa}$ (Hintenlang et al., 1992)) and the **indoor/soil pressure differences** ($-1.5 \text{ Pa} < \Delta p < 2.5 \text{ Pa}$ (at 1.7 m below floor slab) (Robinson et al., 1995b)) are larger than the indoor/outdoor pressure differences.

The indoor/outdoor pressure differences are not well coupled to the indoor/subslab pressure differences (Hintenlang et al., 1992; Gids et al., 1986). The indoor/sub-slab pressure difference is quite constant, about 4 Pa in a Dutch dwelling at 8-10 March (Gids et al., 1986). The atmospheric pressure and the indoor/sub slab pressure difference vary with a semi diurnal periodicity although the indoor/sub-slab pressure difference lag in phase behind the atmospheric pressure.

The **response time** of pressure differences is in the order of tens of minutes (Hintenlang et al., 1992) or minutes (Robinson et al., 1995a). Falling atmospheric pressure draws soil gas into the house; rising atmospheric pressure drives air out of the house into the soil. Although the time averaged gas flow between soil and the house (driven by fluctuations in atmospheric pressure) is approximately zero under neutral pressure conditions, these fluctuations can build up an indoor gas concentration. Reasons are that the concentration in soil air generally is orders of magnitude larger than that of the indoor air and that little outdoor air is infiltrated since the indoor/outdoor pressure equalise so quickly.

Overall it can be stated that the pressure difference between soil (often soil surface) and crawl space fluctuates between about -0.5 to +4 Pa, with an average value around 1 or 2 Pa, caused by wind, temperature differences and barometric changes (Nazaroff et al, 1985; Put and Meijer, 1989; Aldenkamp et al, 1994; Fugler et al, 1997a; Janssen et al, 1998). The pressure difference between the soil (at the depth of the contaminant) and crawl space will be smaller than from outdoor air to crawl space air, because the magnitude of the pressure difference is smaller. Therefore, for potential risk assessment (in the case of no depressurisation) it seems appropriate to use a value of 1 Pa to account for the convection flux in soil. For a reasonable worst case 2 Pa could be used and for a worst case approach and in winter (with depressurisation due to the stack effect), the pressure difference can be set higher.

4.6.3 Air permeability of the soil (κ)

The air permeability depends largely on the soil type. The difference between coarse sand and clay is six orders of magnitude $1 \cdot 10^{-16}$ - $1 \cdot 10^{-10}$. Therefore the data from several references are summarised in Table 4.10. References a, d and f being the original. In general it is proposed to use a mean value of the soil characteristics and exposure parameters. Because often the ground is raised by using sand and for avoiding best case circumstances (in the case of clay) it is appropriate not to use values for clay, but to use the permeability of sand. At a few sites the permeability was measured (Garbesi, 1989, 1993). Values found for κ were 0.02 - $1.7 \cdot 10^{-11}$ (av. 0.65) and 0.03 - $2 \cdot 10^{-11}$ (average 0.3) for natural soil and 0.07 - $0.89 \cdot 10^{-11}$ (av 0.3) for 'backfill' soil. Another important factor for the permeability is the moisture content of the soil. For sandy soils though it is found that at field capacity the air permeability not strongly affected compared to dry soils (0.6 to 0.8 of the permeability of the dry soil)(Nazaroff et al, 1988).

Based on these data and the fact that sand close to the saturated zone is relatively wet, it is proposed to use an air permeability of $1 \cdot 10^{-11} \text{ m}^2$, being the lower boundary of medium sand. For a reasonable worst case or worst case approach the value of respectively $1 \cdot 10^{-10.5}$ (medium sand) and $1 \cdot 10^{-10}$ (coarse sand) can be chosen.

Table 4.10 Air permeability of soils (m^2)

Soil type	Permeability (m^2)	Reference
coarse sand	10^{-10} - $5 \cdot 10^{-9}$	a;e;f
medium sand	10^{-11} - 10^{-10}	a;b;d
fine sand (uniform)	10^{-12} - 10^{-11}	a;b;d;f
sandy loam-loamy sand	10^{-13} - 10^{-11}	c
silty sand	10^{-13} - 10^{-12}	b;d
silt	10^{-14} - 10^{-13}	a;b;c;d
clay	10^{-16}	a;e;f
clay	10^{-16} - 10^{-15}	b

a: Nazaroff *et al.*, 1988

b: Ferguson *et al.*, 1995

c: Garbresi and Sextro, 1989

d: Johnson and Ettinger, 1991

e: Sextro *et al.*, 1986

f: Put and Meijer, 1989

4.6.4 Other location parameters (dp , dg , z , V_v , dc , fbi)

Capillary transition boundary (z)

The height of the capillary transition boundary (CTB) above the groundwater table (z) determines the height above the groundwater table below which the blocking of the air-filled pores leads to no relevant gas diffusion (and the convective flow). This height depends on the water retention curve (pF-curve) of the soil and the capillary upward flow. For the 18 soils of the Staring series (Wösten et al, 1994) the height (z) is calculated between 12 and 84 cm at pF 2.2 and the average Dutch upward flow of $0.1 \text{ cm} \cdot \text{d}^{-1}$ (Waitz et al, 1996). The arithmetic mean of all soils (47 cm) is almost the same as that of sand, 50 cm.

Mean depth of the contamination (dp) and depth of groundwater (dg)

The depth of a volatile contaminant can be related to the depth of the groundwater table, but can also be present in the unsaturated zone of the soil. For both situations it is proposed to use the depth of the groundwater table (dg) and the capillary transition boundary (z) to estimate de

depth of the contaminant ($dp = dg + z$). The current *mean depth of the contamination* in CSOIL is 1.25 m below land surface.

To get an impression of the distribution of the groundwater depth in the Netherlands data from three databases were compared in Otte et al. (2001): the National Groundwater Monitoring Network (LMG) from 1990 till 1998, a database for monitoring the effects of the policy on nutrients and the OLGA-database used in the National Groundwater Model (LGM). The results are summarised in Table 4.11. In general the groundwater level in built-up areas is lower than for all locations. Based on the LMG-database (mean of all data and data only on built-up areas) it is proposed to set the generic depth of the groundwater table (dg) at 1.75 m mls (minus 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 mls.

Table 4.11 Depth of groundwater tables in the Netherlands (in m below land surface)

Database/selection	average (STD)	50-perc.	75-perc.	90-perc
LMG total	2.09 (2.15)	1.60	1.09	0.73
LMG built-up area	2.45 (1.82)	1.82	1.32	1.0
Monitoring database (agriculture)	1.39 (0.59)	1.28	0.99	0.8
LGM	2.82	1.52	1.02	0.5

In Table 4.12 the data from paragraph 4.6 are summarised:

- current value used in CSOIL (if available);
- range of values in VOLASOIL;
- proposed value for CSOIL (based on an average Dutch situation).

The *height of the crawl space (Bh)* is maintained at 0.5 m. The *air-exchange rate of the crawl space (Vv)* in CSOIL was 1.25 h^{-1} , based on Fast et al (1987). It is proposed to use an average ventilation rate (Vv) of 1.1 h^{-1} in the model as the air-exchange rate of the crawl space (Vv), based on Fast et al. (1987) and Stoop et al. (1998). The *contribution of the crawl-space air to indoor air* was 0.1, based on Fast et al. (1987). It is proposed to maintain this value of 0.1 based on Fast et al.(1987) and Stoop et al. (1998) (Otte et al., 2001).

Table 4.12 Existing and new CSOIL-parameters with proposed values

Parameters crawl-space air concentration	Symbol	Unit	current CSOIL	default/ range VOLASOIL	PROPOSAL CSOIL
pressure difference soil air and crawl-space air	Δp_{cs}	Pa	n.a.	2	1
air permeability of soil (depending on soil type)	κ	m^2	n.a.	10^{-10} - 10^{-16}	$1 \cdot 10^{-11}$
depth of groundwater level	dg	m mls	n.a.	input	1.75
height of capillary transition boundary above groundwater table	z	m	n.a.	0.12-0.84	0.5
depth of contamination	dp	m mls	1.25	input ($dg - z$)	1.25 (= $dg - z$)
Height of crawl space (depth of crawl space below land surface)	Bh	m	0.5	0.4	0.5
air-exchange rate crawl space	Vv	h^{-1}	1.25	1.05 (geom. mean)	1.1
Parameter indoor air concentration					
contribution of crawl space air to indoor air	fbi	-	0.1	output	0.1

4.7 Conclusions

These conclusions are based on the model concepts in EUSES (section 2), the international model comparison (section 3) and the concepts in VOLASOIL (sections 4.3 and 4.4).

The calculation of the *soil-air concentration* (from the total soil concentration) in CSOIL and the other models are identical (all equilibrium partitioning). Therefore no modification is proposed. From measurements of field concentrations it has become clear that the (calculated) equilibrium is often not present and that e.g. process of ageing influences the equilibrium. Measurement of soil air and indoor air concentrations stay important in the (site-specific) risk assessment.

The starting point of the calculation of the risk assessment is the depth of the contaminant (d_p). It is set at 1.25 m below land surface, being equal to the current value in CSOIL. This depth is the result of the depth of the groundwater table (d_g ; being set at 1.75 m mls, based on the median of all areas and of built-up areas) and the height of the capillary transition boundary, CTB (z , average value 0.5 m).

The diffusion fluxes in the *flux from soil air to crawl-space air* in CSOIL, VOLASOIL and probably CLEA are identical. A pressure driven *convective air flux* is a good supplement to the diffusive flux. Therefore it is proposed to include a convective flux (pressure driven air flux) into the volatilisation module of CSOIL. To implement this, new input-parameters have been proposed. The *evaporation flux* in CSOIL is not used in other models, has only a small contribution and is found not to be appropriate for this objective. To avoid differences between fluxes to indoor and to outdoor air and because precipitation exceeds evaporation in general, it is proposed to exclude the evaporation flux from the flux to outdoor air as well. The *boundary flux* in CSOIL does not lead to limitations in the total flux and can be left out.

The pressure difference between soil air and crawl-space air (Δp_{cs}) can be estimated based on limited literature data. The value proposed to use for an average situation in CSOIL is 1 Pa. The air permeability of soil (κ) depends largely on the soil type and highly influences the calculated convection flux. It is proposed to use an average value for a sandy soil, being 1.10^{-11} m^2 .

The calculation of the *crawl space air concentration* in VOLASOIL (and CLEA) is slightly different from CSOIL. In UMS and CalTOX these concentrations are not calculated. It is proposed to maintain the current concept with only horizontal ventilation of the crawl space. It is recommended to change the air-exchange rate of the crawl space (vv_c) slightly to 1.1 h^{-1} (was 1.25), based on a much larger database on crawl space ventilation rates in Dutch dwellings.

For the calculation of the *flux from crawl space to indoor air* and the *indoor air concentration* it is proposed to maintain a fixed ratio between indoor air and crawl space air. For the contribution of crawl space air to indoor air (f_{bi}) it is proposed to maintain the average value of 0.1, based on 2 data sets from tracer studies in Dutch dwellings.

The two parameters for the exposure time for the calculation of the *human exposure* can be integrated to one exposure time parameter (T_i). The absorption factor (f_a) for ingestion of soil, food, and inhalation of vapour has to be split in a factor for ingestion (for soil and food separately) and for inhalation (F_{inh}).

5. Concept of uptake of organic substances by plants

5.1 Introduction

This chapter describes and evaluates the current module in CSOIL for uptake of organic substances in plants. This module is part of the exposure route ‘consumption of contaminated crops’, consisting of:

- uptake of organic substances from soil in plants (this chapter);
- uptake of metals from soil in plants (Otte et al, 2001);
- deposition (or rainsplash) on and uptake by plants (this chapter);
- human exposure by consumption of contaminated crops.

For the uptake of organic compounds a description and comparison is made of the current and alternative methods:

- method in current CSOIL, according to Briggs (1982, 1983);
- method according to Trapp and Matthies (1995, 1996);
- method used in the model EUSES;
- methods used in other countries (USA, UK and Germany).

The comparison is followed by preliminary conclusions about the concept.

Next a further investigation of the model of Trapp and Matthies (and EUSES) is carried out by implementing the concept in CSOIL and selection of default-parameters for potential risk assessment.

Finally the uptake by plants in the current module (Briggs) is compared with the approach according to Trapp and Matthies. These estimations are compared with limited literature data to get an impression of the general performance of the models.

5.2 Uptake of organic substances by plants in CSOIL

In the CSOIL-model a difference has been made between uptake in subterranean plant parts (roots) and uptake in aboveground plant parts (stem or leaf).

Briggs (1982,1983) deduced a relationship from experiments with fine roots of barley seedlings. The empirical relations according to Briggs (1982, 1983) used in CSOIL for the **uptake of organic substances in roots** is (van den Berg, 1995):

$$BCF_{root} = 10^{0.77 \cdot \log Kow - 1.52} + 0.82 \quad [\text{mg/kg fresh weight} : \text{mg/dm}^3 \text{ porewater}]$$

For roots this relationship is deduced for substances with a log Kow between -0.6 and 4.6, with a difference between calculated and measured of a factor of 2 (Briggs, 1982).

For the **aboveground plant parts** a relationship of Briggs (1982,1983) for stems is used, being an extension of the relationship deduced for roots:

$$BCF_{stem} = \left(10^{0.95 \cdot \log Kow - 2.05} + 0.82 \right) \cdot \left(0.784 \cdot 10^{(-0.434 \cdot (\log Kow - 1.78)^2 / 2.44)} \right)$$

[mg/kg fresh weight : mg/dm³ porewater]

For aboveground plant parts the relationship is deduced for substances with a logKow between -0.6 and 3.7. Differences between measured and calculated of factor 3 are found (Briggs, 1983).

The contribution of the aboveground plant parts to the total exposure by contaminated crops (calculated with CSOIL) is respectively about 30%, 13% 3% and less than 1% for compounds with a logKow of 3,4,5 and 6. In the current concept, this makes the root uptake quantitatively more important for most compounds.

Deposition

Currently the deposition model by Hetrick and McDonnell-Boyer (1984) and Dutch data on deposition velocities is used (van den Berg, 1995) for estimating the deposition of metals and organic substances on plants. Many parameters are important in that model. In this approach it is assumed that all particles originate from soil. After using all the data it results in the following relationship:

$$C_{dp} = 1.089 \cdot 10^{-3} \cdot C_s \quad [\text{mg/kg dry plant}]$$

with C_{dp} as the concentration in the plant and C_s as total soil content. The contribution to the total concentration in plants is small (<1%) for all substances. Although the evaluation of the deposition (deposition from air or as 'rainsplash') is not included in this evaluation, it is recommended to give attention to this subject in the future.

Crop consumption

In CSOIL the exposure by consumption of contaminated crops is calculated with:

$$VI = (Q_{fvk} \cdot C_{pr} + Q_{fvb} \cdot C_{ps}) \cdot f_v \cdot f_a / W$$

With: Q_{fvk} and Q_{fvb} as the crop consumption of root and leafy crops (in g fresh weight per day), C_{pr} and C_{ps} the concentration in root and leaf (and stem)(in mg/kg fresh weight). f_v the fraction contaminated crops, f_a the absorption factor and W the human bodyweight.

In the current CSOIL roots are represented by potatoes. Although potatoes are not really roots, all edible underground plant parts will be treated as root crops.

5.3 Uptake of organic substances according to Trapp and Matthies

5.3.1 Equations

Roots

The partitioning between water and plant tissue is based on sorption to plant fats. Trapp and Matthies (1995) give the following relation for plant tissue:

$$K_{\text{plant-water}} = F_{\text{water}} + F_{\text{fat}} \cdot K_{\text{ow}}^b$$

$K_{\text{plant-water}}$:	partition coefficient between plant and water	[kg/m ³ plant: kg /m ³ water]
F_{water} :	volume fraction of water	[m ³ water/m ³ plant]
F_{fat} :	volume fraction of plant fat	[m ³ fat/m ³ plant]
K_{ow} :	octanol water partition coefficient	[ml water/ml octanol]
b :	correction exponent for differences between plant fat and octanol [-]	

For the concentration in fine roots (C_{root}) a relation can be given with the concentration in porewater:

$$C_{\text{root}} = \frac{K_{\text{plant-water}} \cdot C_w}{\rho_{\text{plant}}} \quad [\text{kg/kg}_{\text{wwt}}]$$

$K_{\text{plant-water}}$:	partition coefficient between root and water	[kg/m ³ plant to kg/m ³ water]
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	see also calculation of $K_{plant-water}$ via previous equation	
ρ_{plant} :	plant density	[kg/m ³]
C_w :	concentration in the porewater	[kg/m ³]

Because this equation is comparable to that of Briggs, the feasibility study of Versluijs et al., 1998a) concludes that the calculation of the concentration in the roots is satisfactory.

Mass transport to aboveground plant tissue

The mass transport in the xylem (N_{xy}) from the porewater is defined as:

$$N_{xy} = C_w \cdot TSCF \cdot Q \quad [\text{kg/d}]$$

C_w :	concentration in the porewater (calculated with C_s/K_d)	[in kg/m ³]
TSCF:	Transpiration Stream Concentration Factor	[-]
Q:	transpiration stream	[m ³ /d]

The TSCF can be calculated in two ways:

$$TSCF = 0.784 \cdot \exp \left[\frac{-(\log K_{ow} - 1.78)^2}{2.44} \right] \quad (\text{Briggs et al, 1982})$$

$$TSCF = 0.7 \cdot \exp \left[\frac{-(\log K_{ow} - 3.07)^2}{2.78} \right] \quad (\text{Hsu et al, 1991})$$

The highest result of both equations is used for further calculations [Trapp and Matthies, 1995]. In EUSES only the relation of Briggs is used.

Exchange with air

The partition coefficient between leaf and air determines the exchange with air:

$$K_{leaf-air} = \frac{K_{plant-water}}{K_{air-water}} + F_{air} \quad [\text{m}^3/\text{m}^3]$$

$K_{plant-water}$:	partition coefficient plant vs. water	[-]
$K_{air-water}$:	partition coefficient between air and water (dimensionless Henry: $V_p/(S.R.T)$);	
F_{air} :	volume fraction air in the plant	[m ³ /m ³]

F_{air} can be left out, because it never makes a difference in calculations (pers. comm. Trapp, 2000). The net flux between leaf and air is:

$$N_A = A \cdot g [C_A - C_L / K_{leaf-air}] \quad [\text{kg/s}]$$

A:	leaf surface	[m ²]
g:	conductance	[m/s]
C_A :	concentration in air	[kg/m ³]
C_L :	concentration in the plant	[kg/m ³]
$K_{leaf-air}$:	partition coefficient between leaf and air.	[m ³ /m ³].

Mass balance

The total mass consists off:

Change in the quantity of substance in aboveground plant parts, $d(C_L V_{leaf})/dt =$

- + flux from soil via the xylem to the stems, N_{xy}
- +/- flux from/to air, N_A
- photo-degradation, λ_p
- metabolism, λ_m

This can be written as a first order linear differential equation:

$$dC_L / dt = -aC_L + b$$

$$a = \frac{A \cdot g}{K_{leaf-air} V_{leaf}} + \lambda_E + \lambda_G \quad (\text{loss})$$

$$b = C_w \cdot \text{TSCF} (Q_{transp} / V_{leaf}) + C_A g (A / V_{leaf}) \quad (\text{source})$$

g:	conductance	[m/d]
A:	leaf surface	[m ²]
V _L :	leaf volume	[m ³]
λ _E :	elimination (metabolism and photo-degradation)	[d ⁻¹]
λ _G :	growth rate constant	[d ⁻¹]
C _A :	concentration in air	[mg/m ³]

The analytical solution (at a given C_L(0)) is:

$$C_L(t) = C_L(0)e^{-at} + b / a(1 - e^{-at})$$

De steady-state concentration in the plant (aboveground) can be calculated from:

$$C_L(\infty) = b / a$$

5.3.2 Background

This paragraph describes the background and restrictions of the model of Trapp and Matthies. In the model of Trapp and Matthies the uptake of organic substances via porewater and the uptake/elimination via air is included. Deposition from air can also be important, but is not taken into account in this model. The exposure routes of the plant are summarised in Figure 5.1.

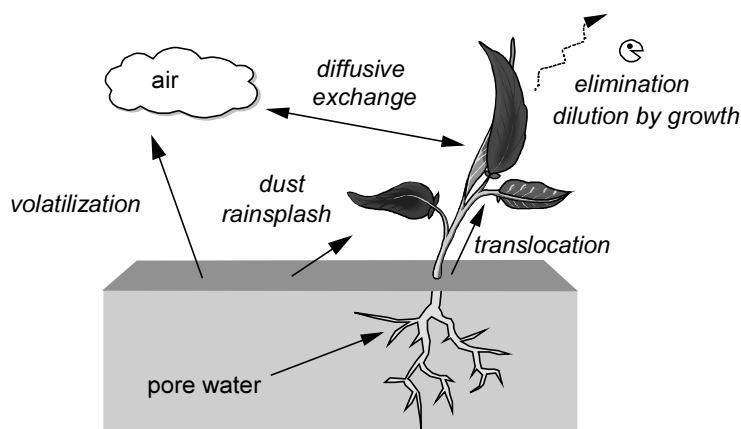


Figure 5.1 Routes of uptake of plants.

Porewater ⇒ *root* ⇒ *leaf*. Uptake from soil is for most substances a passive process, directed by the transpiration stream in the xylem of the plant. Water-soluble substances that can pass the membranes in the root are transported to the leaf with the transpiration stream. In the leaf water will evaporate and substances can accumulate. For most (neutral) substances the phloem flow back to the root is negligible (Bromilow and Chamberlain, 1995).

Soil ⇒ *air (gas phase)* ⇒ *plant*. This route is often neglected but can play an important role in heavily contaminated soils. For example PCDD/F's are poorly transported with the

transpiration stream but can be taken up with this route in substantial amounts (Trapp and Matthies, 1994). Because dilution by wind is an important factor, air concentrations stay low. Nevertheless, for closed vegetation close to the ground this can be an important factor (e.g. grasses, lettuce).

Soil⇒air (particle-bound)⇒plant. Soil and dust parts can be deposited on the plant by wind or rain (also called rainsplash or soil resuspension). The contribution is difficult to estimate and depends on many factors (e.g. the geometry of the plant). Nevertheless this route can be important in case of contaminated soils. Soil can be directly deposited or a concentration can be built up in air, after which the plant can be exposed. It is difficult to estimate to what extent the internal concentration is influenced.

Elimination processes. Elimination of substances from the leaf can be important for volatile compounds. Photo-degradation and metabolism of organic substances can occur in the plant, although prediction of these processes is poor using physical-chemical properties of the compound. Also dilution by growth will influence the concentration in the plant.

Boundary conditions and restrictions

This model can only be used for **non-dissociating** (neutral) **organic compounds**. For these compounds the highest concentrations are expected for roots and leaf, whereas fruits, seeds and stems show lower concentrations (because of the fact they are fed from the phloem). Using the concentration in the leaf tissue for fruits etc. can be seen as a worst-case approach for fruits. The concentrations in the root will probably not be much higher than in the soil (because the affinity of organic substances for soil and root material is comparable, assuming $F_{oc}=F_{fat}$; often $F_{oc}>F_{fat}$) (Trapp and Matthies, 1994).

Of the ionogenic (**dissociating**) **organic compounds** especially compound with a high mobility in the phloem of plants (e.g. systemic herbicides) are of importance for soil pollution. Most of the phloem mobile compounds are weak acids with low logKow (<2) (Bromilow and Chamberlain, 1995). The behaviour of these kinds of substances is difficult, but sinks are roots, new leaves and fruits or seeds. Uptake of dissociating compounds in general is difficult to predict, despite the fact that porewater concentrations can be calculated. Dissociating compounds (phenols) need a different treatment in a model. They behave different, than would be expected from their logKow. The real uptake and distribution in a plant depends on the acidity of the porewater and on the different parts of the plant. Because of this complexity and the fact that this could lead to substantial higher concentrations, these compounds will need more attention in the future.

The concentration in air is an input-parameter in the model of Trapp and Matthies. It is not calculated in relation to the concentration in the soil. So either a relation has to be set or the concentration has to be fixed at a certain level (e.g. zero or background). The concentrations in air can be very important for some substances.

The model of Trapp and Matthies does not include deposition by rain and particles from air. Still there are some options for estimating dry and wet deposition fluxes to the plant (Trapp and Matthies, 1994; Smith and Jones, 1999; McLachlan, 1999). These fluxes do account for weathering (removal of particles from the leaves by weather influences), but not for the fact that chemicals attached to particles are not necessarily taken up, but may only stick to the outside of leaves. In relation to soil pollution these sources of pollution are not of direct interest.

Not taken into account, and probably of more importance, is the resuspension of soil particles to the crops by wind and rain ('rainsplash'). It is suggested by Trapp et al. (1998) to use a fixed percentage of the soil concentration (e.g. 1% of soil per dry weight plant). By washing crops this partly can be removed.

The model assumes continuous exponential growth (otherwise there is no analytical solution of the equation). This means the model only applies to plants that are eaten before they stop growing. For crops with a longer growing period (e.g. cabbage with 120 days) and plants of which the fruits/seed are consumed, the growth can be substantially lower at the end of the season. In practice this doesn't seem to give a problem because dilution by growth only is important in the mass balance for compounds with a very high $K_{\text{leaf-air}}$ [Jager and Hamers, 1997](compounds with a low K_{oa} ; a low $K_{\text{air-water}}$ and a high $\log K_{\text{ow}}$).

The next restrictions are mentioned for the application of the model:

- there is no spatial distribution in the plant;
- the soil-air-plant path, being important for volatile lipophilic compound needs an other solution;
- the empirical parameters TSCF and b (for estimating $K_{\text{leaf-air}}$) are derived from a small amount of experiments;
- for substances with a high $\log K_{\text{ow}}$ no experimental data are available.

Model validation

The model is validated to a limited extent by the original authors (Trapp and Matthies, 1995) by comparing with a more extended model and data for Bromacil and TCDD. The reliability of the RCF (root concentration factor), TSCF and $K_{\text{leaf-air}}$ is investigated by Polder et al. (1995, 1996). This showed that the estimated RCF based on Briggs e.a. (1982) was in general within a factor 10 (Jager and Hamers, 1997). The estimate of the TSCF is more difficult. Clear is that the TSCF is between 0 and 1 and there seems to be an optimum between $\log K_{\text{ow}}$ 1-4. The uncertainty of this parameter is substantial, by which application of a Gauss-curve as proposed by Briggs et al. (1982) and used by Trapp and Matthies (1995) can be discussed. The estimation of $K_{\text{leaf-air}}$ based on physical-chemical properties is quite reliable (within a factor 10).

5.4 Comparison of concepts for uptake of organic chemicals

5.4.1 Uptake of organic substances according EUSES

In section 2.3.3 the plant uptake in the EUSES is described. The module in EUSES is based on the model of Trapp and Matthies. This model is used in the evaluation of new and existing substances (EC, 1996). The model concept for calculating the concentration in the aboveground plant parts and calculation of the concentration in the roots is identical in both approaches. Deposition (of dry or wet particles) is not included in the model.

5.4.2 Uptake of organic substances in other exposure models

In the section 3.5 the model concepts for uptake of organic chemicals used in the UK, the US and Germany are described. In CLEA (UK) the method Briggs-Ryan is used (section 3.5.1), in UMS (Germany) the approach of Trapp and Matthies is used (section 3.5.2) and in the CalTOX model the approach of Paterson and Mackay (see section 3.5.3) is used. These model concepts are compared with CSOIL in 3.5.5.

5.4.3 Comparison and preliminary conclusions

To assess the described model concepts for their potential improvement in the CSOIL exposure model, some qualitative criteria are used:

- extent in which a concept is well founded;
- possibility for an uniform utilisation of the concept (all substances, all plants);
- extent in which the method technically describes the processes in the plant;
- extent in which the model calculation corresponds with literature data.

In all methods the plant content is calculated based on the logKow of the compound and the concentration in the porewater. The concentration in the porewater is calculated with the organic carbon content and the logKoc.

Uptake in root crops

Accumulation in root crops is very relevant, because the estimated concentrations (especially for compounds with higher logKow) are much higher than in the aboveground plant parts. The estimation of the accumulation of organic substances in the current CSOIL (according to Briggs, 1982,1983) was found to be accurate enough to use in the calculation of potential and location specific risks (Versluijs et al., 1998a; Polder et al 1995). Briggs is also used in the model CLEA (UK). Nevertheless the relation of Briggs is based on experiments with only young barley roots. The Briggs-relation is in fact comparable with the relation of Trapp and Matthies (Jager and Hamers, 1997). The Trapp and Matthies approach is used in EUSES and in UMS (Germany). Because Briggs (1982, 1983) is an empirical relation and in the relation of Trapp and Matthies (1995) the parameterisation is uncertain, Briggs could be maintained for potential risk assessment. Paterson and Mackay, used in CalTOX (USA), use a fugacity approach, which probably includes the same elements as used in Trapp and Matthies. It is useful to compare Briggs and Trapp and Matthies in more detail, also in relation to empirical data (paragraph 5.5 and 5.6)

Uptake in aboveground plant parts

The estimation of the uptake by aboveground plant parts is currently based on Briggs (1982,1983). This empirical relation is also used in CLEA (UK) (Ryan, 1988). This relation does only relate to the Kow, is based on experiments with barley seedlings and estimates the concentration in the stem (Versluijs et al., 1998a; Polder et al 1996). The model concept of Trapp and Matthies (1995) gives a better description of the transport processes (soil and air path are separated) and parameters involved, including plant parameters. This model concept is also used in EUSES (EC, 1996) and in UMS (Germany). It includes uptake from porewater and uptake/elimination via air, but is also restricted to the total content of the aboveground plant parts. More complex models also can differentiate between different aboveground plant parts (stem, leaf and fruit). The approach of Paterson and Mackay (1989), used in CalTOX (USA), is probably comparable with respect to the uptake and elimination routes.

There is a relation between Kleaf-air and the logKoa ($=\log Kow / \log Kaw$; McLachlan, 1999) and therefore the concentration in the plant strongly relates to the Koa. In the model of Trapp and Matthies the Kleaf-air is estimated from Kow and Kaw (dimensionless Henry coefficient, H).

It is concluded that the model concept of Trapp and Matthies for aboveground plant parts is an improvement compared with the empirical approach of Briggs and could be incorporated in CSOIL. To what extent both approaches estimate measured concentrations in field experiments and in laboratory studies needs more investigation.

Soil particle resuspension

Root uptake and dry gaseous deposition (concentration in air) are taken into account in the concept of Trapp and Matthies, EUSES and probably UMS. Other exposure routes of plants are dry particle deposition, wet particle deposition and soil particle re-suspension (rainsplash) (Smith and Jones, 1999; McLachlan, 1999). Dry and wet particle deposition, originating from air pollution, can be excluded from the risk assessment for soil. Estimation of the soil particle resuspension (rainsplash), as used in CLEA, can be an important source of contaminants in plants for some compounds (section 3.5.1). Especially for compounds with a high log K_{oa} particle bound deposition can be important for the concentration in the plant (McLachlan, 1999). Smith and Jones (1999) mention a mass loading of 0.2 to > 20% of soil per dry weight plant (geometric mean 1.2%), although not giving the part which might be washed off. Sheppard and Evenden (1992) proposed a fraction of 3% of soil per dry weight plant to account for soil not to be washed off. Trapp and Matthies (1998) suggest 1% of soil per dry weight plant to account for this route as a rough estimate. It is proposed to use the value of 1% to account for this route, because 3% is a more conservative value.

5.5 Further investigation of the model of Trapp and Matthies

5.5.1 Selection of parameters and uncertainty analysis

This paragraph investigates the parameters necessary to incorporate the module of Trapp and Matthies (1995) in CSOIL (as reported in (Versluijs et al., 1998b)). Therefore the new parameters necessary for the equations used in the model are summarised and default values are selected. Based on the selected input-parameters also an uncertainty analysis of the calculated concentration in the aboveground plant parts is carried out.

The following parameters can be distinguished in the model of Trapp and Matthies:

- general parameters (e.g. soil parameters);
- substance-specific parameters;
- plant parameters (plant properties).

For most plant parameters data had to be collected to be able to choose default values.

The general parameter **C_A, concentration in air**, partly determines the flux from leaf to air. Besides the calculated concentration in CSOIL in the outdoor air at 1 and 1.5 m, based on a flux from the soil, the concentration at 0.3 meters was calculated. It is recommended to reconsider this calculation in a later stage. An uncertainty analysis showed that for some volatile compounds the route soil → air → plant contributes to a large extent to the calculated plant concentration (and contaminants in soil are of minor importance; Versluijs et al., 1998b). Especially for these compounds the concentration in air is critical. Another possibility is to use a (local) background concentration or to set C_A=0. Because for many substances there are no (or hardly any) data on background concentrations, this is not an option.

For the **plant parameters (aboveground)**, not used in CSOIL (see Table 5.1), data from other sources are used. The parameters are collected for selected crops (consumption of home-grown crops). Table 5.1 shows the values used in an uncertainty analysis (Versluijs et al., 1998b). These values originate from earlier RIVM-publications (Jager and Hamers, 1997; Polder et al, 1994, 1996) and a limited literature research (reported in Versluijs et al., 1998b). Based on data of separate crops it was not possible to differentiate between the crops. Therefore the median (likeliest) values and spread for all crops are used in the uncertainty analysis (see Table 5.1). In the last column the default values are proposed. These values are based on the default values in

EUSES (EC, 1996) and Trapp and Matthies and partly on the additional literature data. Most default values correspond to the likeliest value, only the volume fraction fat (F_{lipid}) of roots is more related to the upper boundary of the range.

Table 5.1 Plant parameters of aboveground plant parts in the model of Trapp and Matthies, with values from the uncertainty analysis, the EUSES-model and the proposed default values

PARAMETER	Symbol	Unit	uncertainty analysis			EUSES default	Proposed default
			likeliest value	min value	max value		
water content of the plant	F_{water}	m^3/m^3	0.70	0.55	0.9	0.65	0.65
lipid content of the plant	F_{lipid}	m^3/m^3	0.002	0.001	0.01	0.01	0.01
air content of the plant	F_{air}	m^3/m^3	0.25	0.10	0.40	0.3	0.3
correction exponent plant lipid/octanol	b	-	0.95	0.75	1.0	0.95	0.95
density plant tissue	$\text{RHO}_{\text{plant}}$	kg/m^3	800	600	950	700	800
water density	d_w	kg/m^3	1				1
transpiration stream	Q	m^3/d	0.001	0.0005	0.005	0.001	0.001
conductivity (leaf)	g	m/d	80	30	400	86.4	80
leaf volume (or plant volume)	V_{leaf}	m^3	0.005	0.002	0.010	0.002	0.002
leaf area (or of total plant)	AREA	m^2	5	2.5	10	5	5
elimination constant	k_{elim}	d^{-1}	0			0	0
growth constant (for dilution by growth)	k_{growth}	d^{-1}	0.035	0.005	0.2	0.035	0.035
TSCF ¹	TSCF	-	x	x-0.2	x+0.2		

¹Transpiration-Stream Concentration Factor (depending on logKow, value between 0 and 1)

Volume fractions **water** (F_{water}), **fat** (F_{lipid}) and **air** (F_{air}) in the plant and the density of the harvested crop ($\text{RHO}_{\text{plant}}$) are quite well known (Sprenger instituut, w.y.). Trapp and Matthies themselves set the correction factor 'b', for the difference between octanol and plant fat, at 0.95 (for aboveground plant parts).

The **transpiration stream** (Q) strongly depends on the growth circumstances of the plant and the weather. Therefore a substantial spread of the values is possible

The **conductance** of the leaf (g) also strongly depends on the time of day and the circumstances. When the air is humid and the soil is humid, the conductance is higher than in a dry period in which the stomata are closed to keep the water inside. The spread in values probably is larger due to conditions than due to the kind of crop.

The leaf volume (V_{leaf}) and leaf surface (AREA) is strongly related to the kind of crop and the growth stage of the crop. The values represent the values just before harvesting.

The uncertainty analysis showed that some parameters are much more critical than others, also depending on the compound. Important parameters, with a contribution to the variance of more than 25% for 1 or more of the 12 investigated substances², are:

- lipid content of the plant, F_{lipid} ;
- correction exponent plant fat/octanol, b ;
- transpiration stream, Q ;
- conductance (leaf), g ;
- growth rate constant, k_{growth} .

For strongly lipophilic and low volatile compounds dilution by growth (k_{growth}) is an important factor, for other substances it is not important. For compounds not being very lipophilic, but

² benzene, phenol, phenantrene, benzo(a)pyrene, 1,2-dichloroethane, trichloroethene, monochlorobenzene, pentachlorophenol, atrazine, 1,3,6,8-TCDD, and DEHP.

moderately to strongly volatile the conductance (g) is important. Transpiration is (Q) is for most compounds important (Versluijs e.a., 1998b).

The analysis showed that for most investigated substances the difference between the 20- and 80-percentile of the calculated plant concentration was a factor 2 to 5. It should be noticed that the uncertainty due to substance-specific parameters ($\log K_{ow}$ and $\log K_{air-water}$) and general parameters is not included. In further research attention should be paid to the most sensitive parameters.

5.5.2 Model calculations with Briggs and Trapp and Matthies

To compare the estimations of Briggs (current CSOIL) with Trapp and Matthies (with default parameter values given in Table 5.1), the bioconcentration factors for leaf (BCF_{leaf}) and for root (BCF_{root}) were calculated. This is done for compounds with a $\log K_{ow}$ of 0.5 to 8 and with a dimensionless Henry coefficient of $1 \cdot 10^{-7}$ to 0.1. This corresponds with a $\log K_{oa}$ of 3 to 14.

BCF_{root}

In Trapp and Matthies the BCF_{root} depends, besides the $\log K_{ow}$, on the water and the lipid content of the plant, the density of the root and the exponent b. The values can differ from the values for aboveground plant parts. The water content of roots is higher than aboveground plant parts and is set at 0.93 (Jager & Hamers, 1997). The lipid content of roots generally seems to be lower than for shoots (see Table 5.2), currently a good estimate of the lipid content is 0.5% (Flindt, 1988; Tam et al, 1996). A good estimate for the density of the root is 1000 kg/m³ (Jager and Hamers, 1997). The exponent b is the most uncertain factor giving difference between plant lipids and octanol. Trapp and Matthies (1995) mention values of 0.75 and 0.77 (for roots) to 0.95 and 0.97 (for barley shoots and citrus cuticles). Because of these large differences, a value of 0.8 as well as 0.95 (current default EUSES) is worked out. The value of 0.8 is arbitrarily derived from the value of 0.77, because the value of 0.77 suggests too much accuracy. The results from this comparison in relation with the $\log K_{ow}$ are given in Figure 5.2 and Figure 5.3.

Table 5.2 Composition of root crops (average % of edible parts; Flindt, 1988; Tam et al, 1996)

	lipid kg/kg fwt	Flipid m ³ /m ³ ^a	% water
Sweet potato	0.0060	0.0073	69
Tapioca	0.0035	0.0042	65
Yam	0.0024	0.0029	72
Potato	0.0015	0.0018	78
Soybean	0.0038	0.0046	92
Average	0.0034	0.0042	

^a (density root 1000 kg/m³, density octanol 827 kg/m³)

In both model concepts (Briggs and Trapp and Matthies) the BCF_{root} depends on the $\log K_{ow}$, which clearly can be seen in Figure 5.2. Comparing the BCF_{root} of Briggs and of Trapp and Matthies (with $b=0.95$) shows that at a $\log K_{ow}$ of 0.5 to 4 the BCF_{root} of Briggs is (less than a factor 2) lower than calculated with Trapp and Matthies. At higher values of $\log K_{ow}$ the BCF_{root} value calculated with Trapp and Matthies is higher than of Briggs, maximally a factor 5 higher at a $\log K_{ow}$ of 8. A value of 0.8 for the exponent b leads for compounds with $\log K_{ow}=2$ to a factor 2 lower BCF_{root} with Trapp and Matthies than Briggs and a factor 4 lower BCF_{root} for compounds with $\log K_{ow}$ 4 to 7. It can be concluded that using other values for the mentioned parameters, especially the exponent b (but also the lipid content of roots) largely influences the results

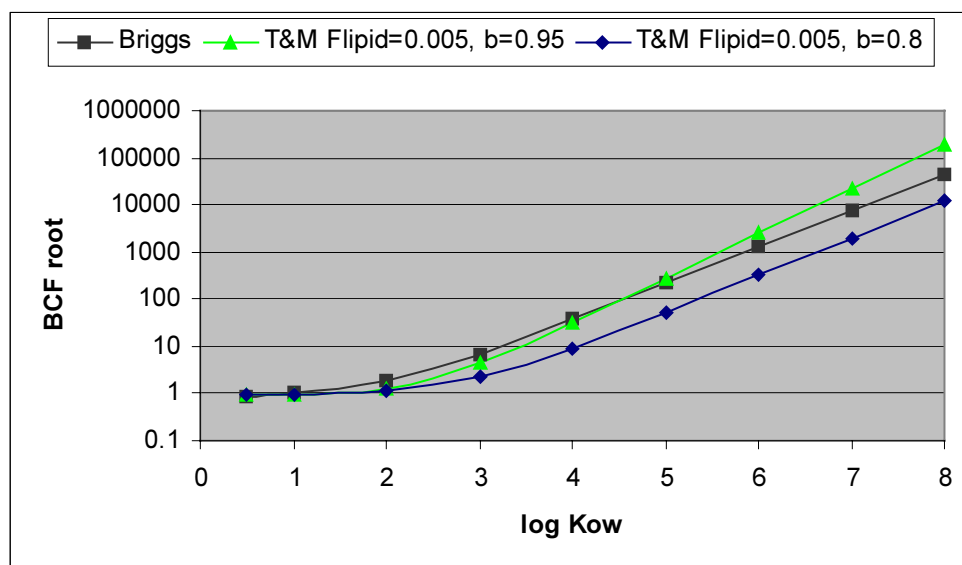


Figure 5.2 BCF_{root} (l/kg_{wwt}) from porewater against $\log Kow$ calculated with the current CSOIL-model (Briggs) and with the model of Trapp and Matthies

BCFleaf

The BCF_{leaf} in CSOIL (calculated with Briggs) is independent of the Henry-coefficient, and only depends on the $\log Kow$. With the module of Trapp and Matthies the dependency of the the Henry-coefficient (H) and $\log Kow$ (and therefore the $\log Koa$) is visualised for 7 values of H in Figure 5.3. For low values of H (10^{-7} , 10^{-6} , 10^{-5}) an optimum of BCF_{leaf} can be seen, both for Briggs as for Trapp and Matthies. For $H < 10^{-5}$ and $\log Kow < 5$ or ≥ 7 Trapp and Matthies calculates a higher BCF than Briggs. In all other cases the BCF by Briggs is higher.

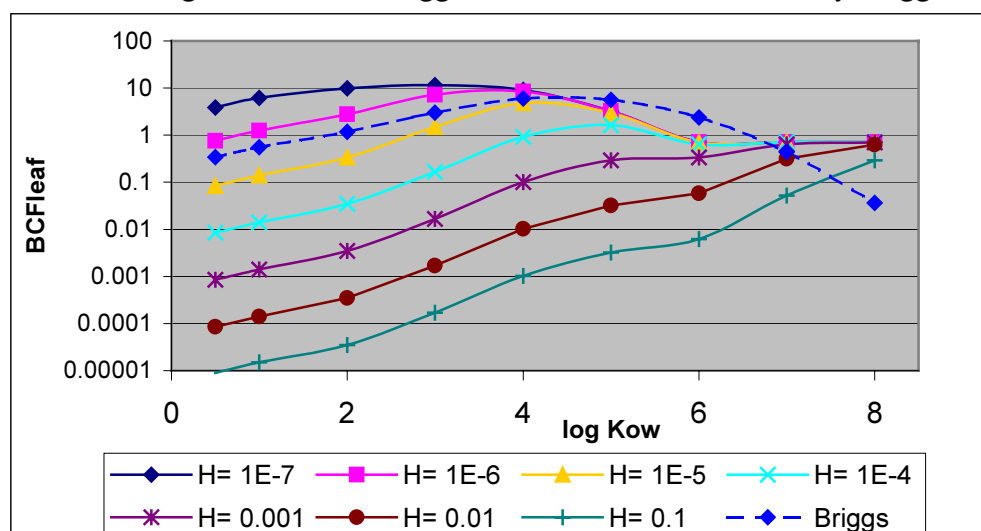


Figure 5.3 BCF_{leaf} (l/kg_{wwt}) against $\log Kow$ calculated with the current CSOIL-model and with the model of Trapp and Matthies (with default values) and different values of the dimensionless Henry coefficient (H)

Results BCF_{leaf} for different groups of compounds

Besides a general comparison, calculations have been made for compounds with a substantial (>25 %) contribution of crop consumption to the total human exposure. The calculated BCF_{root} according to Briggs (current CSOIL) and Trapp and Matthies (with default values) is given in Figure 5.4. Figure 5.5 shows the estimated BCF_{leaf} according to both methods and

Figure 5.6 shows the BCF-leaf plotted against the log K_{oa} (log K_{ow}/log K_{aw}). For each group the results of the BCFleaf are discussed below.

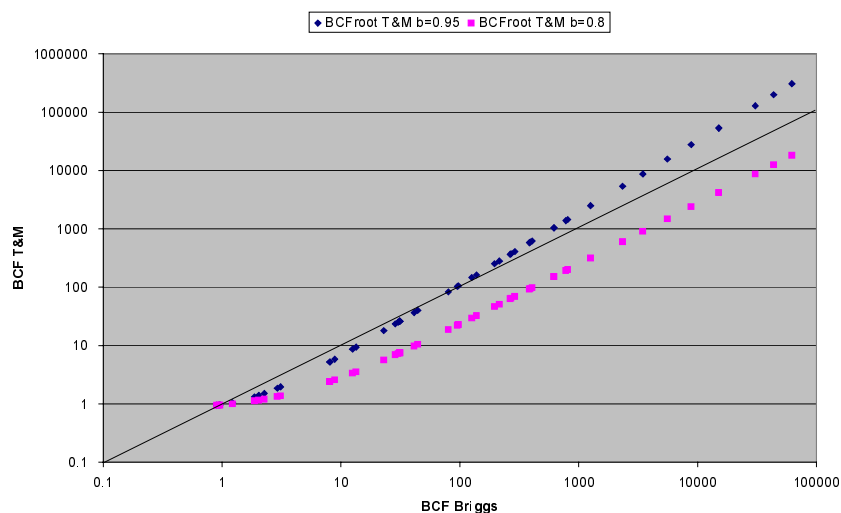


Figure 5.4 *BCFroot (l/kg_{wwt}) from porewater calculated according to Briggs (CSOIL) and Trapp and Matthies (with 2 values for factor *b*; the line represents the 1:1 relation)*

Aromatic compounds. The log K_{ow} values of these compounds are between 0.55 and 2. The BCF-leaf calculated with Trapp and Matthies is for all compounds a factor 3 to 5 lower than of Briggs, Only for hydrochinon the BCF is even a factor 40 lower, the main reason being the Henry coefficient, which is a factor 10 higher than the other compounds.

PAH. The log K_{ow} values of PAH are between 3.4 and 6.8. The BCF-leaf calculated with Trapp and Matthies is for all PAH between 0.7 and 1.6, except for naphthalene (0.01). With Briggs a BCF-leaf is calculated between 0.6 and 6.4. Only for benzo(k)fluoranthene (logK_{ow} 6.8 and H= 5E-7) the BCF is for both methods almost the same (0.6 and 0.7). In general the difference between both methods is only a factor 4, only for naphthalene (H=4E-3) this difference is a factor 460.

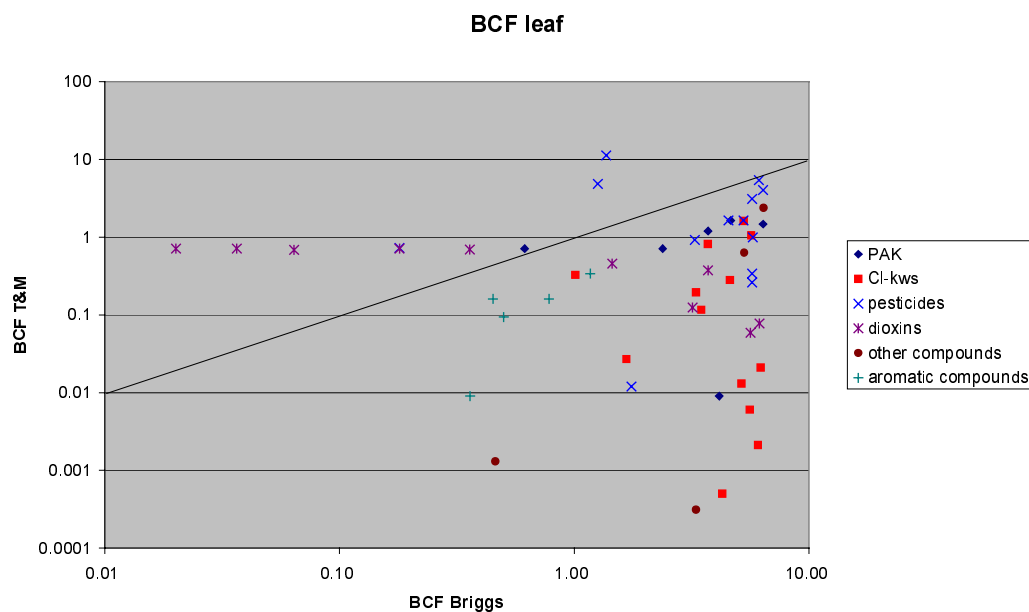


Figure 5.5 *BCF-leaf (l/kg_{wwt}) calculated according to Briggs and Trapp and Matthies (with default values; the line gives the 1:1 relation)*

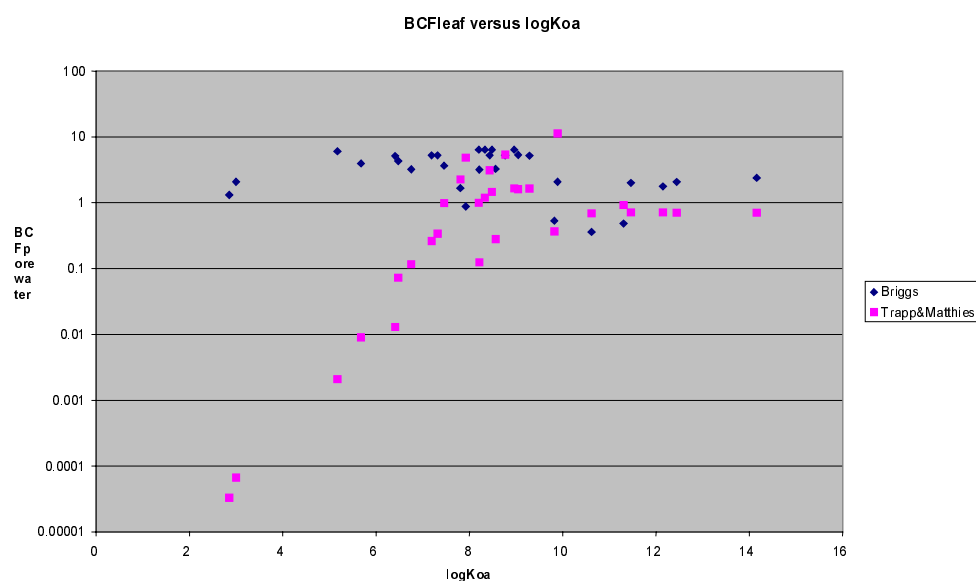


Figure 5.6 *BCF-leaf* (l/kg_{wwt}) calculated according to Briggs (CSOIL) and Trapp and Matthies (with default values of Table 5.1) against $\log K_{oa}$

Chlorinated hydrocarbons. The $\log K_{ow}$ of chlorinated hydrocarbons PAH is between 2.4 and 6.6. The *BCFleaf* with Trapp and Matthies is always lower than with Briggs (CSOIL). The least volatile is trichlorophenol ($H=8.10^{-5}$), for which the difference between both method is a factor 5 (1.1 and 5.7). The most volatile compound is p-dichlorobenzene ($H=0.1$); the difference between the two methods is a factor 8500 (0.0005 and 4.3). This makes clear that volatility influences the differences to a large extent.

Pesticides. The $\log K_{ow}$ differs largely between the pesticides. The *BCFleaf* with Trapp and Matthies is lower than Briggs for DDE, dieldrin, endrin, α -HCH, γ -HCH, and carbaryl. For propoxur and δ -HCH the result of both methods is the same. It must be noted that for aldrin, atrazine and carbofuran the result with Trapp and Matthies is *higher* than with Briggs (CSOIL). Reason for atrazine and carbofuran is the low volatility in combination with a low $\log K_{ow}$. For aldrin the reason is the combination of a relatively high volatility in combination with a high $\log K_{ow}$.

Dioxins. For dioxins the $\log K_{ow}$ is between 4.8 and 8.2. The *BCFleaf* calculated with Trapp and Matthies is much lower (factor 80) for the mono and di-chlorinated dioxins. For the higher chlorinated dioxins (TeCDD) the *BCFleaf* is equal or even higher for the high-chlorinated dioxins. This is notable, and can probably be explained with the fact that these dioxins accumulate in the plant by the route soil \rightarrow air \rightarrow plant, because of the high $\log K_{ow}$ and moderate volatility ($H=3.10^{-4}$).

Other compounds. For cyclohexanon ($\log K_{ow} = 0.8$) and styrene ($\log K_{ow} = 3.1$) the *BCFleaf* with Trapp and Matthies is much lower (> a factor 100). For phthalates ($\log K_{ow} = 4.4$ and 5.1) the *BCFleaf* with Trapp and Matthies is a factor 3 to 8 lower than with Briggs.

Calculations according to Trapp and Matthies give lower values for the *BCFleaf* than calculations according to Briggs for compounds with a $\log K_{oa} < 8$. Values in the same order of magnitude are calculated in for compounds with a $\log K_{oa} > 8$. Up to $\log K_{oa} = 8$ a higher K_{oa}

leads to higher BCF values. In general BCF-values are higher for compounds with a higher logKow and with a lower volatility (H).

5.6 Comparison of estimations with literature data

By comparing the results of both methods with literature data, it is possible to get an impression of the extent in which the calculations fit measurements. In 1999 a limited literature search was performed of the accumulation of organic compounds in plants (Cornelese, 2000). The data of measured BCF (wet weight plant/ porewater) or the estimated BCF based on measured concentrations are summarised in this document. The references used for this comparison are given in Table 5.3. These data are used for comparison with the presented calculations.

Table 5.3 References used for comparison of measured BCF with estimated BCF

Compound	number of references	References
PAHs	2	<i>Wild et al, 1992; Delschen, 1996</i>
PCBs	6	<i>Ye et al, 1991; Trapp et al, 1990; O'Connor et al, 1990; Bellin et al, 1990; Webber et al, 1994; Delschen, 1996</i>
Pesticides	12	<i>Harris et al, 1969; Heinrich et al, 1996; Voerman et al, 1975; Beall et al, 1971; Pylypiw et al, 1993; Shone et al, 1974; Burken et al, 1996; Rouchaud et al, 1991; Trapp et al, 1990; Aplada-Sarlis et al, 1994; Nair et al, 1992</i>
Dioxins	1	<i>Isensee et al, 1971</i>
Chlorofenols	2	<i>Bellin et al, 1990; Casterline et al, 1985</i>
Chlorobenzenes	1	<i>Topp et al, 1989, Tam et al, 1996.</i>
Trichloroethene	1	<i>Schnabel et al, 1997</i>
Benzene	1	<i>Topp et al, 1989</i>
Phthalates	1	<i>O'Connor, 1996</i>

5.6.1 Roots

In Figure 5.7 the relation between logKow and BCF-root is given for both concepts and the data from the literature search. The values found in literature are mostly lower than the estimated values with Briggs and Trapp and Matthies with $b=0.95$. The estimated values with Briggs can be seen as the upper boundary of the data found in literature and is therefore more a worst case estimate. Probably an important reason for the differences between the calculated and the literature data are that the model calculates concentrations in the fine roots, where most literature data concern root crops. The literature data that match with these lines concern (fine) roots of grasses and beans (4 pesticides) and uptake from aqueous solutions (all chlorobenzenes). For these roots the models seems to perform quite well.

Consumption crops, like potato and carrot, appear to have lower bioconcentration factors. In Polder et al (1994) and Jager&Hamers (1997) most literature data are lower than the calculations too, except from experiments in nutrient media. The main reason will be that there is no equilibrium of the larger roots (and root crops) with the porewater (only with the peel). The calculations with Trapp and Matthies with a value of 0.8 for factor b seem to give a better fit for the BCF-values found for consumption crops. Although the fact that there is probably no equilibrium has no direct relation with the exponent b in the concept of Trapp and Matthies. Using this concept leads to a more realistic estimate of the bioconcentration factors for root crops. Therefore it is proposed to –provisionally- use the concept of Trapp and Matthies with $Flipid = 0.005$ and $b=0.8$.

For a worst case approach Briggs still can be used.

It is strongly recommended to investigate the uptake by root crops by a combination of experiments, model modifications and parameterisation.

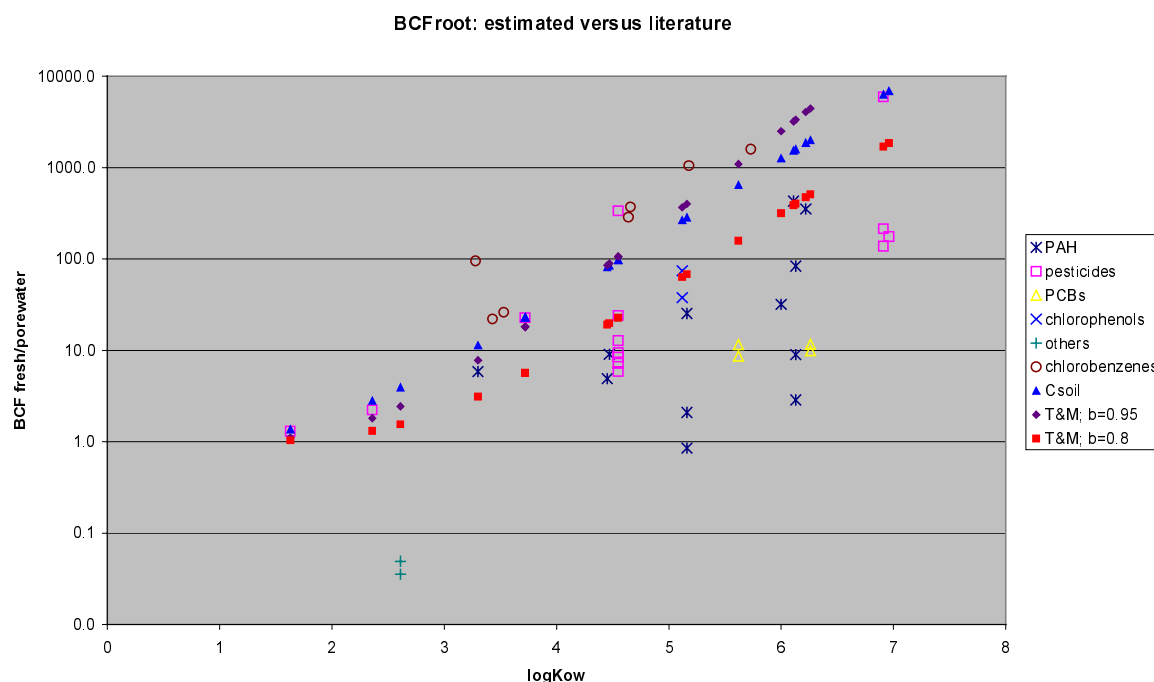


Figure 5.7 Estimated BCF-root (l/kg_{ww}) with Briggs and Trapp and Matthies ($Flipid=0.005$, $b=0.95$; $Flipid=0.005$, $b=0.8$) compared with values based on literature data

5.6.2 Aboveground plant parts

The estimated BCF (Briggs and Trapp&Matthies) for the aboveground plant parts are also compared with BCF-data from literature. In Figure 5.8 the BCF values are plotted against the logKoa.

Figure 5.8 shows that in general BCF-values from the literature are higher than calculated with Briggs and with Trapp&Matthies. To some extent the BCF-values from literature increase with higher Koa. The high concentrations found in literature could originate from deposition (dry and wet), from soil resuspension (rain splash) or from air born contaminants (see paragraph 5.4.3). In the model calculations shown in Figure 5.5 and Figure 5.6 deposition or resuspension is not included. Besides, air concentrations during the experiments could have been higher than used in the model calculations.

Because it was recommended to include soil resuspension into the model calculation (see paragraph 5.4.3), the contribution of soil resuspension (1% on dry weight bases) is added to the estimated BCF with Trapp&Matthies. In Figure 5.9 this model calculation is plotted against the literature data. The figure shows that the differences between the estimated BCF and the measured BCF are smaller than in Figure 5.8. This supports the fact that soil resuspension can be an explanation for these differences (besides the other mentioned reasons). Also an increase of the BCF with higher Koa can be seen for both the estimation with Trapp & Matthies and the BCF based on literature data.

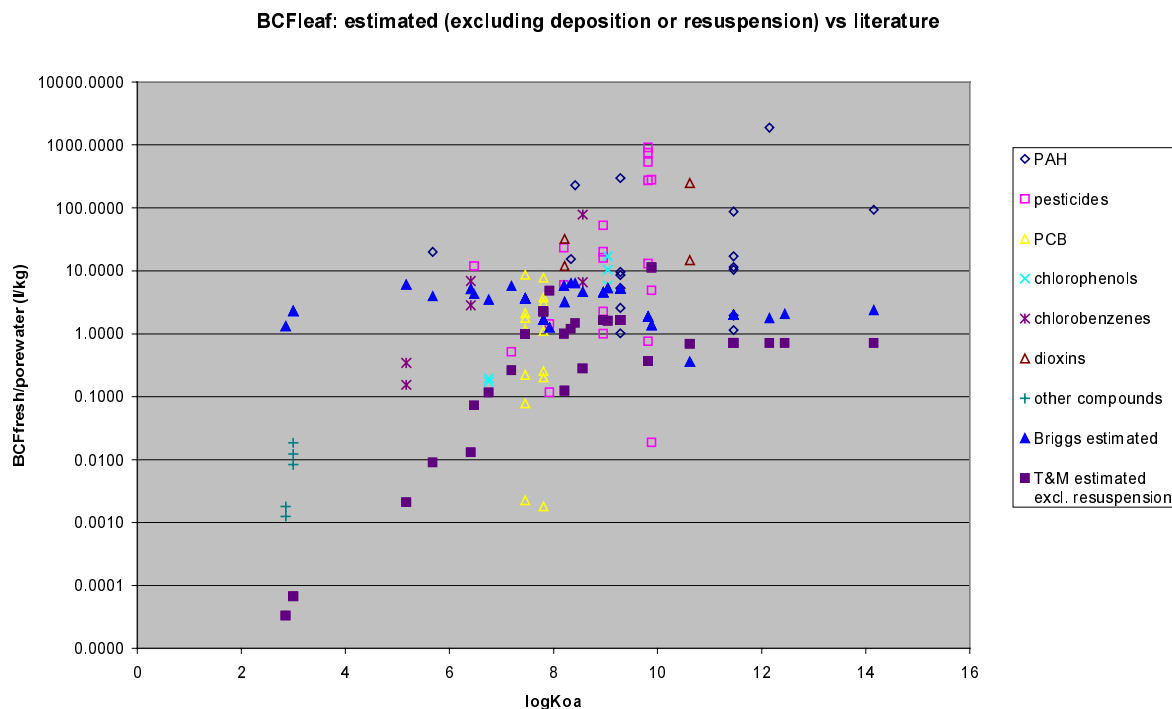


Figure 5.8 Estimated BCF-leaf (l/kg_{ww}) with Briggs and Trapp&Matthies (with default values excluding soil resuspension) compared with BCF-values based on literature data

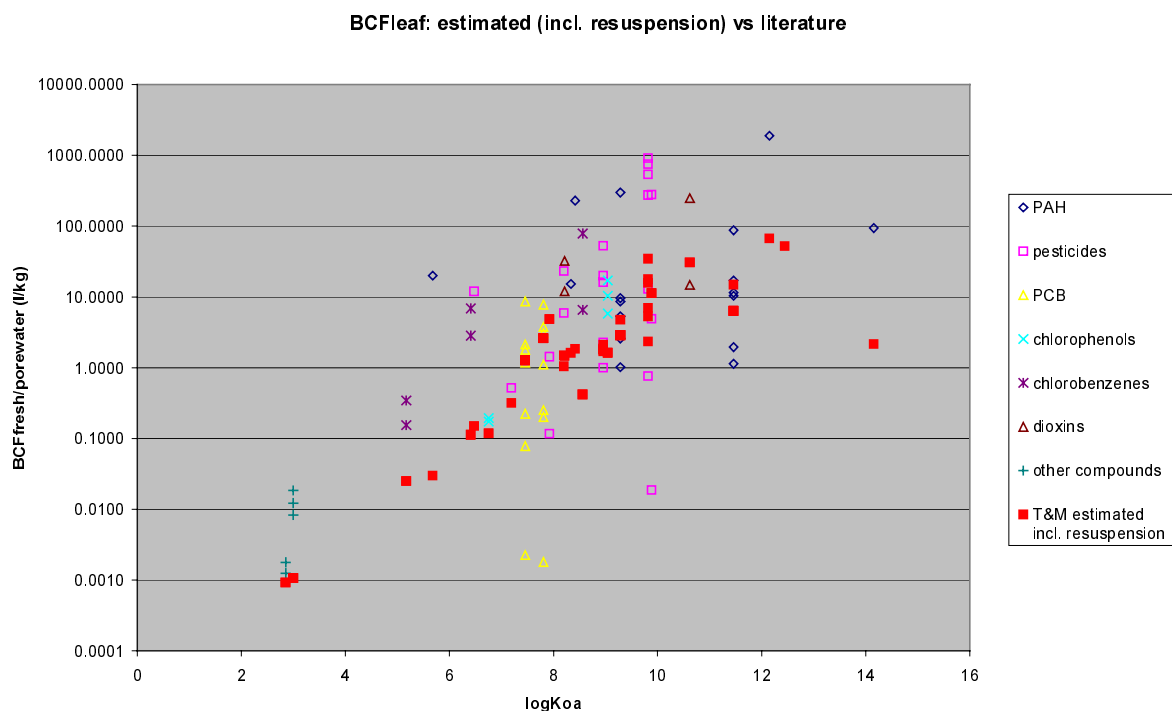


Figure 5.9 Estimated BCF-leaf (l/kg_{ww}) with Trapp&Matthies (with default values including soil resuspension) compared with values based on literature data

When the literature data with a (little) positive relationship between the soil content and the concentration in the plant are selected, this results in a small data set, because many experiments were done at only 1 concentration. The remaining data set shows in general only the lower BCF-values. The BCFleaf based on literature data for compounds with log K_{oa} 7 to

10 are in the same order of magnitude as calculated with Briggs and with Trapp and Matthies. For trichloroethene (log K_{oa} 3) the measured data is between the estimations with both methods. Based on this limited data set there is no evidence of which model concept approaches the best the BCF_{leaf} based on measured data in literature.

5.7 Conclusions

For the uptake of organic compounds in roots the concepts used in both model concepts are to a large extent comparable and are related to the logK_{ow} of compounds. The estimated uptake in roots is higher than the uptake in aboveground plant parts (especially for compounds with a high logK_{ow}). With the parameters used, the estimation of the BCF with Trapp and Matthies (1995) (with Fl_{lipid} = 0.005; b = 0.95) is maximally a factor 3 larger than with Briggs (1983). The estimation of the BCF with Trapp and Matthies (1995) (with b = 0.8) is maximally a factor 4 lower than with Briggs for compounds with higher logK_{ow}s. Comparing these results with BCF derived from literature data, it seems there is an overestimation with Briggs and Trapp and Matthies (with b = 0.95) of the exposure at higher logK_{ow}. The main reason is probably that there is no equilibrium between the root crops and porewater, where for fine roots this equilibrium seems to exist. To account for the lower BCF-values based on literature data it is proposed to use the concept of Trapp and Matthies, but with an exponent of b = 0.8 and a lipid content of 0.005. For a worst case approach Briggs (1983) still can be used. It is strongly recommended to further investigate the uptake by root crops by a combination of experiments, model modifications and parameterisation.

For the uptake of organic compounds aboveground plant parts (from porewater) the model concept of Trapp and Matthies (1995) is found to be more acceptable than the relation of Briggs (1983). In other risk assessment models both approaches are found. Comparing the estimations with BCF based on literature data, there seems an underestimation of the BCF for both approaches. Reason could be that the air concentrations contribute largely to the plant concentrations found in literature. Nevertheless the BCF with Trapp and Matthies shows a larger differentiation between compound (depending on K_{ow} and K_{aw}).

It is proposed to use the concept of Trapp and Matthies, because it describes the relevant processes (uptake from soil and uptake/elimination from air) and parameters, among which the lipophilicity (based on the logK_{ow}) and the volatility (based on the logK_{aw}). Besides these characteristics seem to be important for the BCF found in literature data. Because of these reasons Trapp and Matthies offers the opportunity to estimate the uptake in the aboveground plant parts depending on the circumstances, plant species and compounds characteristics.

It is recommended to investigate the important parameters in the model, also in relation to different plant species. Secondly it is recommended to investigate validity of this approach compared to more experimental data. In that effort the circumstances within the studies already used from literature need verification as well.

Besides this model for aboveground plant parts, it is proposed to add a factor to account for soil particle resuspension, according to Sheppard and Evenden (1992) and as proposed by Trapp et al (1997). The contribution of this exposure route can provisionally be set at 1% dry soil per dry plant, as discussed in § 5.4.3, but should be considered in more detail in the future.

6. General conclusions and recommendations

Exposure routes

This project has focused on the evaluation of the most relevant model concepts used for determining potential human exposure. Model concepts on the actual site-specific human exposure are not considered in this report, while concepts of other models that might be useful for improvement of CSOIL have been selected. Therefore CSOIL first had to be compared to other exposure models. Table 6.1 shows which routes are described in the other models and makes clear the minor differences between the routes taken into account. All the important routes in CSOIL are also considered in all the other models, except EUSES. The exposure to bathing water and via the consumption of fish are not included in CSOIL, since this model is limited to terrestrial soils. The consumption of meat and milk are not described in CSOIL because these routes are considered irrelevant for a local site-specific assessment in the Dutch situation.

This chapter describes the conclusions and recommendation of the evaluation of the three most relevant exposure routes. Human exposure is described separately for each of the following routes:

1. the ingestion of contaminated soil particles;
2. the inhalation of volatile compounds in indoor air;
3. the consumption of contaminated crops.

The *dermal uptake via soil contact* and the *ingestion of contaminants via drinking water* both make a small contribution to total exposure. No attention has been given to these exposure routes. Although the dermal uptake via soil and ingestion of contaminants via drinking water are not examined in this report, it is recommended to take these into account in a possible follow-up to this project. Neither is the *consumption of contaminants via mothers' milk* discussed here. Perhaps this route needs more attention in a discussion on the derivation of the human toxicologically derived Maximum Permissible Risk (MPR).

Table 6.1 The available routes of the different exposure models

Exposure route	CSOIL	CLEA	UMS	CalTOX	EUSES
Ingestion of contaminated soil particles (outdoor)	Yes	Yes	Yes	Yes	-
<i>Ingestion of contaminated soil particles / dust (indoor)</i>	Yes	Yes	Yes	-	-
<i>Dermal contact with soil contaminants (outdoor)</i>	Yes	Yes	Yes	Yes	-
<i>Dermal contact with soil contaminants / dust (indoor)</i>	Yes	Yes	-	-	-
<i>Inhalation of contaminated soil particles / dust (outdoor)</i>	Yes	Yes	Yes	Yes	-
<i>Inhalation of contaminated soil particles / dust (indoor)</i>	Yes	Yes	Yes	Yes	-
<i>Inhalation of vapours from contaminants (outdoor)</i>	Yes	Yes	-	Yes	Yes
Inhalation of vapours from contaminants (indoor)	Yes	Yes	Yes	Yes	-
Consumption of (home-grown) crops	Yes	Yes	Yes	Yes	Yes
<i>Consumption of soil attached to crops</i>	-	Yes	-	-	-
<i>Consumption of contaminants via drinking water</i>	Yes	Yes	Yes	Yes	Yes
<i>Ingestion of contaminants via bathing water</i>	-	-	Yes	Yes	-
<i>Inhalation of vapours from drinking water from shower</i>	Yes	Yes	-	Yes	-
<i>Dermal contact with drinking water from shower/bath</i>	Yes	Yes	-	Yes	-
<i>Dermal contact with contaminants via bathing water</i>	-	-	-	Yes	-
<i>Consumption of contaminants via consumption of fish</i>	-	-	Yes	Yes	Yes
<i>Consumption of contaminants via consumption of milk</i>	-	-	-	Yes	Yes
<i>Consumption of contaminants via consumption of meat</i>	-	-	-	Yes	Yes
<i>Consumption of contaminants via mothers' milk</i>	-	-	-	Yes	-

-: Exposure route not available

Soil ingestion

For this route, CSOIL has been compared with the three international exposure models. There is little doubt that relatively short-term *deliberate soil-eating* is widespread among children. Occasional soil-eating can have a significant impact on childhood contaminant exposure. For children the concept of deliberate soil ingestion, together with inadvertent soil ingestion, should therefore be included in CSOIL. Considerations for a possible approach to combining inadvertent and deliberate soil ingestion are presented in CLEA (1998). Research is necessary to determine the persistence or duration of deliberate soil-eating by children, which can vary from a few days to a few months. CSOIL only accounts for lifetime daily mean exposures and therefore the effect of short-term deliberate soil ingestion is probably negligible. Further research on the comparison of the short-term exposure of deliberate soil-eating to acute toxicity data is particularly recommended (Calabrese et al., 1997). Deliberate soil ingestion is especially important when the exposure of children (1-6 years) is separated from the exposure of adults (7-64 years); this might be the case for site-specific assessments. Implementing the concept of deliberate soil ingestion for children is proposed if, in further research, the persistence or duration of this habit is quantified in more detail.

The UMS model uses a direct and *indirect oral uptake* of soil or dust particles. The indirect oral uptake describes first the inhalation of dust particles, after which they are subsequently swallowed. The daily soil intake via the indirect route appeared to be negligible compared to the direct route and therefore it is not useful to implement the indirect route in CSOIL. For calculating the soil ingestion, all models compared use the same concept, only the values for the input parameters are different. The contaminant concentration in soil is multiplied by a soil ingestion rate that is normalised on the basis of the body weight for adults or children. The only difference with CSOIL is that all international models use a *separate daily soil ingestion rate with an exposure frequency*. For CSOIL only a (yearly) average daily soil ingestion rate is proposed (Otte et al., 2001). Depending on the exposure duration of the scenario used, the international models are therefore flexible for adjusting the yearly average ingestion rate. For CSOIL it has been proposed to introduce separate exposure duration combined with a daily intake rate. The CSOIL scenario can then possibly be adjusted for exposure frequencies of less than 365 days per year. For the potential exposure assessment the exposure duration can remain 365 days per year.

Further, it has been proposed to make a distinction between the oral and inhalative absorption, because the actual oral and inhalative uptake is different. The default fraction of uptake will be 1 for calculating the potential exposure for both routes; however, for some contaminants, the absorption for the ingestion of soil may be adjusted.

Inhalation of vapours

The calculation of the soil-air concentration (from the total soil concentration) in CSOIL and the other models are identical (all equilibrium partitioning), and no modification is proposed. Nevertheless, it is clear that this is only an estimation and field measurements can lead to other concentrations.

The diffusion fluxes in the *flux from soil air to crawl space air* in CSOIL, VOLASOIL and probably CLEA are identical. In CalTOX and UMS it is not possible to calculate the indoor air concentrations for houses with sub-floor voids (crawl space). CLEA and VOLASOIL explicitly use a convective flux (pressure-driven air flux), besides the diffusive fluxes mentioned. CalTOX and UMS implicitly account for a convective flux. Including a convective flux (pressure driven air flux) into the volatilisation module of CSOIL is proposed, since, in many

references (mainly on radon), diffusion as well as convective flow is stated to influence the indoor air concentrations.

Excluding the *evaporation flux* from the volatilisation module of CSOIL has also been proposed. None of the other models compared use this flux. The contribution of this evaporation flux has appeared low and not correctly implemented in CSOIL. To avoid differences between *fluxes to indoor and outdoor air*, and because precipitation exceeds evaporation in general, it was decided to exclude the evaporation flux also from the flux to outdoor air. The *boundary flux* in CSOIL does not lead to limitations in the total flux and will be left out.

The calculation of the *crawl-space air concentration* (based on the flux to the crawl space and the ventilation rate) in VOLASOIL (and CLEA) is slightly different from CSOIL. In UMS and CalTOX crawl-space air concentrations cannot be calculated. The ventilation rate does not have to be corrected for the contribution of the air flux from soil (negligible). For the calculation of the *flux from crawl space to indoor air* and the *indoor air concentration*, it is proposed to maintain a fixed ratio between indoor air and crawl space air. In CalTOX and UMS the indoor air concentrations are based on a diffusion flux from soil air to indoor air. More information about the fluxes mentioned is presented in sections 4.2 and 4.3. For convenience of organisation the two-exposure-time parameters used for the calculation of the *human exposure* should be integrated into one-exposure-time parameter.

For the implementation of the convective flux, proposals for newly introduced input parameters have been made (see section 4.6). The relevant new parameters are the depth of groundwater (dg), the pressure difference soil air and crawl-space air (Δp_{cs}) and the air permeability of the soil (κ). The evaluation of the relevant new parameters has led to the following conclusions. The depth of the contaminant (dp) is set at 1.2 m below land surface, which is practically the same as the current value in CSOIL. It results from the depth of the groundwater table (dg; set at 1.75 m minus land surface) and the height of the zone with no air diffusion / convection (z; 0.5 m). The magnitude of the soil column through which diffusion and convection take place (0.7 m) is a result of dp and the depth of the crawl space (dc; set at 0.5 m). This leads to the same magnitude as currently used in CSOIL. The pressure difference between soil air and crawl-space air (Δp_{cs}) can be estimated based on limited literature data. The value proposed for an average situation in CSOIL is 1 Pa. The air permeability of soil (κ) largely depends on the soil type and strongly influences the calculated convection flux. The use of an average value for a sandy soil, $1 \cdot 10^{-11} \text{ m}^2$, is proposed. The evaluation of the current CSOIL parameters air-exchange rate of the crawl space (vv_c) and the contribution of crawl-space air to indoor air (fbi) form the subject of the report of Otte et al. (2001).

For all models, the exposure via the inhalation of vapours of contaminants is fundamentally based on the same concept, where the concentration in air is multiplied by the daily inhalation rate and divided by the body weight. The main differences between the models compared are the use of respirable fractions and absorption rates.

Only the EUSES model uses a separate correction factor for the respirable fraction and the absorption rate. CSOIL and UMS only account for a correction factor for the *absorption rate* (default = 1). In EUSES the default fraction for the absorption in the human body for the inhalative route is 0.75 (not 1), because it is assumed that actually no substance is totally absorbed via exhalation. Discussion of the default value of 1, which is used for the absorption via the inhalative route, is recommended. For the time being, maintaining the default value of 1 in CSOIL is proposed.

Use of the respirable fraction in CSOIL separate from the absorption rate should also be discussed. The *respirable fraction* is the part of the total inhaled quantity of a substance, which actually reaches the lungs or alveoli. It should be noted that this recommendation accounts mainly for site-specific assessments, since the advised default values for calculating potential exposure for both fractions would be 1.

Consumption of contaminated crops

In CSOIL the uptake of *metals in roots and aboveground plant parts* is based on an average BCF derived per individual metal based on literature data. Just like CSOIL, CLEA and UMS use BCF correlation models to predict the concentration of metals in roots and leaf. An important difference is that CLEA incorporates the influence of the soil pH. Only CalTOX uses a different approach for the uptake of *metals in crops*, which is based on a balance among deposition, rainsplash, wash-off and plant decay that was developed for radioactive elements. Details are lacking on this CalTOX approach and its advantages are unknown. The evaluation of the BCF currently used in CSOIL and the revised method for deriving this BCF from field measurements is described in Otte et al. (2001). The main approach is: after selection of data per plant species, a weighted average BCF value is derived which is related to pH, organic matter and clay, followed by a calculation of a weighted average for each compound.

For the uptake of *organic compounds in roots* the concepts used in the different models (Briggs, 1982, 1983; Trapp and Matthies, 1995) are to a large extent comparable. In all concepts the BCF is related to the logKow of compounds. When these results are compared with BCF values based on literature data, there seems to be an overestimation of the exposure at higher logKow. Because there is probably no equilibrium of the root crops with the porewater (like there is between fine roots and porewater), it is proposed to use the model of Trapp and Matthies with a lower exponent b of 0.8 (as was suggested for roots). This can account for the current overestimation found with the relation of Briggs compared to the data from literature. It is strongly recommended to further investigate the uptake by root crops through a combination of experiments, model modifications and parameterisation.

For the uptake of *organic compounds in aboveground plant parts*, use of the model concept of Trapp and Matthies (1995) is proposed instead of the relation of Briggs, mainly because it is more acceptable than the relation of Briggs (1982, 1983). This is because Trapp and Matthies describe the relevant processes and parameters, including the lipophilicity (based on the logKow) and the volatility (based on the log Kaw). In other risk assessment models both approaches are found. Comparing the estimations with BCF based on literature data, there is apparently an underestimation of the BCF for both approaches. There is no substantial evidence that one of both estimations is closer to the measured data; the BCF of Trapp and Matthies only shows a larger differentiation between compounds. Investigating the validity of this approach compared to more experimental data is recommended, along with investigation of the value of the important parameters in the model, also in relation to different plant species.

For the uptake of *organic compounds in roots and aboveground plant parts* only CalTOX uses a different approach, which is a simplified form of the seven-compartment fugacity model of Paterson and Mackay. At the moment it is not advisable to use the seven-compartment fugacity model of Paterson and Mackay, mainly because of the lack of empirical support.

The *rainsplash concept* should be added to CSOIL. Soil and dust particles can deposit on the different plant parts by rainsplash. CLEA and CalTOX only use rainsplash. Details for a good comparison with CSOIL are lacking on CalTOX rainsplash. CLEA uses 30 g dry soil per kg dry plant (= 3%) for soil attached to crops; this is based on a mean estimated soil load on plants

as in Sheppard and Evenden (1992). This value is based on the attached soil that cannot be removed by normal food preparation. Trapp & Matthies suggest a less conservative value of 1% dry soil per dry plant. Setting the contribution of this route at a provisional value of 1% dry soil per dry plant is proposed, but this value should be considered in more detail in the future.

For all models the exposure to contaminants via crops is based on the concentration in leaves and roots multiplied by the daily consumption and both divided by the body weight. The main difference is the use of absorption rates. The UMS and CSOIL model use a compound specific absorption factor for uptake in the human body. CLEA and UMS use a correction for preparing food, i.e. scraping, peeling or cooking. Details are lacking on this approach and the advantages are unknown. For potential assessments it is proposed not to use this correction factor in CSOIL, because it suggests too much accuracy.

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Appendix 1 Mailing list

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- 73 NARIP, via Dr. H. Leenaers (NITG-TNO, Delft)
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Appendix 2 Overview of the available international human exposure models

Country	Model developed	Model used for soil and groundwater quality standards	Model used for other purposes
Austria	None	None	none
Belgium	None	Vlier-humaan (a clone of HESP)	Yes
Denmark	CETOX-human	None	none
Finland	None	None	CalTOX RISC-Human
France	No name given	No name given	
Germany	UMS	None	
Greece	None	None	none
Ireland	None	None	EUSES POEM
Italy	ROME (in analogy met CONCAWE)	ROME	ASTM RBCA
The Netherlands	CSOIL, SEDISOIL, VOLASOIL	CSOIL (terrestrial soils), SEDISOIL (sediments)	USES, RISC Human, HESP
Norway	GRUF-model (based on Naturvardverket, CSOIL)	GRUF-model	
Portugal	None	None	
Spain	No name given	No name given	
Sweden	No name given	No name given	yes
Switzerland	None	None*	none
United Kingdom	CLEA	CLEA	
USA	CalTOX	CalTOX	
Canada	No name given	No name given	
Australia	None	None	none

*No model is used, but guidelines for metals has been based on *worst case* exposure

Appendix 3 Selected oral soil intake values for children according to UMS (1993)

Source	Oral soil intake (g/d)	Remarks
CSOIL (1991)	0.15	
Eikmann & Kloke (1991)	1	Value adopted from SRU, 1991; Absorption rate 5-100%
EPA (1989)	0.2-0.8	No value for adults available, because of lacking data
EPA (1993)	0.2	For children from 1-6 years old
ECETOC (1990)	0.248	
Hawley (1988)	0.09 (2-5 years) 21 (>6 years)	Daily exposure of 0.25 (2-5 y) and 0.05 (>6 y) is reduced by exposure duration of 130 and 152 d/y, respectively
Kaiser & Roßkamp (1991)	0.2	Exposure of 150 d/y
Lappenbusch (1988)	0.1	
RIVM (1990)	0.2	
SRU (1991)	1	Children from 9-18 months and 3-5 years
Ruck (1990)	1 (2-7 years) 0.1 (lifetime)	Different exposure times and age categories
Kramer et al. (1990)	0.2 1 (at playgrounds)	Relevant soil depth is 35 cm, and 25 cm is reachable with children tools
Clausing (1990)	0-0.9 (at a crèche or day-care centre)	
Some BRD (federal) states	0.2 (1 state) 0.5 (3 states)	Age categories from 1-6 years, body weight 10-15 kg
Clausing (1987)	0.05-0.1	Age differentiation: 9-18 months and 3.5-5 years = 0.05 and 1.5-3.5 years = 1
Sedman (1989)	0.59	
Range	0.05-1	

Appendix 4 Calculating air concentration in CLEA

Description of the fluxes for calculating the equilibrium air concentration in the living space.

Molecular diffusion

- Diffusion through the ground surface: two basic constructions
 1. Ground surface covered by hard core, blinding sand, and oversite concrete beneath a suspended timber floor
 2. Ground surface covered by hard core and blinding sand, beneath a propriety beam and block floor system

For each layer or cover a diffusion coefficient is identified controlling the diffusion flux from soil to crawl space. When a layer or cover is not appropriate, the diffusion coefficient for that part is equal to zero.

$$\frac{1}{D_{01}} = \frac{1}{D_{layer1}} + \frac{1}{D_{layer2}} + \frac{1}{D_{layer3}} + etc.$$

- Diffusion from crawl space to the living space: two basic constructions:
 1. Fibre insulation layer / Suspended timber floor
 2. Beam and block floor system / Screed / Insulation layer / PVC damp proof membrane / Wooden decking

A diffusion coefficient is identified for the above subscripts controlling the diffusion flux from crawl space to living space.

$$\frac{1}{D_{12}} = \frac{1}{D_{layer1}} + \frac{1}{D_{layer2}} + etc.$$

- Diffusion through walls and ceiling. The wall construction consists of a 5 layer sandwich of brick / air gap / insulation layer / lightweight block / and surface coating. The bricklayer largely determines the diffusion coefficient. It is assumed that there is no effective diffusion barrier between roof space and outside air.

$$\frac{1}{D_{23}} = \frac{1}{D_{layer1}} + \frac{1}{D_{layer2}} + \frac{1}{D_{layer3}} + etc.$$

Ventilation

- Wind induced pressure and resulting air flows: the wind speed (v) at a certain height above the ground surface (H) is calculated according to the power-law model (BSI, 1991):

$$v = v_0 \cdot \left(\frac{H}{H_0} \right)^\alpha$$

The typical wind velocity (v_0) is 3 m/s at a reference height (H_0) of 10 m. The default height for living space is 5.4 m and for a crawl space is 0.2 m. The value of α is 0.17 (open flat spaces), 0.20 (countryside with occasional obstacles), 0.25 (build up areas; default value) or 0.33 (city areas).

Further the dynamic air pressure associated with wind acting on the house, air velocity through openings in the house (cracks gaps) and the effective air permeability of the floor material (floor air resistance) is determined:

$$P = \frac{1}{2} \rho v^2 k$$

ρ :	mass density outdoor air	(1.29 kg/m ³)
v :	velocity of air flow	(m/h)
k :	position dependent coefficient (range -1 to 1)	
	Default values front: $k_f=0.915$ and rear: $k_r=-0.8$	(-)

For the different spaces, void (1) or living (2), and the different sites, front (f) or rear (r), the subscript of P is a combination of the symbols between brackets, e.g. P_{1f} is the dynamic air pressure for the front side of a crawl space.

- The stack effect describes an upward air flux resulting from the pressure difference (ΔP_s) between the columns of warm and cold air and is only important in the winter. The pressure difference of about 2 Pa would be applied to the floor separating the living space from the void.

$$\Delta P_s = g \cdot H_{av} \cdot \rho \cdot \left(\frac{T_2 - T_1}{T_2} \right)$$

T_1 T_2 : temperatures inside (1) and outside (2) the house
default value winter: $T_1=283$ $T_2=292$ (K)

H_{av} : average height of all openings in the house
Default: whole height of living space (5.4 m) (m)

g : acceleration due to gravity (9.8 m/s)

- The air flux in a house The horizontal flow rates [m^3/h] through the void (I_1) and living space (I_2) are described by:

$$I_1 = 3600 \cdot \sqrt{\frac{P_{1f} - P_{1r}}{0.5 \cdot \rho \cdot \left(\frac{1}{(A_1^{in})^2} + \frac{1}{(A_1^{out})^2} \right)}} \quad \text{and} \quad I_2 = 3600 \cdot \sqrt{\frac{P_{2f} - P_{2r}}{0.5 \cdot \rho \cdot \left(\frac{1}{(A_2^{in})^2} + \frac{1}{(A_2^{out})^2} \right)}}$$

3600: converts units from [m^3/s] to [m^3/h] (-)

P_{1f} P_{1r} : dynamic air pressure front/rear side void (Pa)

P_{2f} P_{2r} : dynamic air pressure front/rear side living space (Pa)

A_1^{in} A_1^{out} : living: total area of openings in walls for in- and outgoing fluxes (m^2)

A_2^{in} A_2^{out} : void: total area of openings in walls for in- and outgoing fluxes (m^2)

The resulting air flow rates correspond to the following air-exchange rates [h^{-1}] for void (E_{x1}) and living space (E_{x2}):

$$E_{x1} = \frac{I_1}{V_1} \quad \text{and} \quad E_{x2} = \frac{I_2}{V_2}$$

The default volume of the living space (V_2) is 400 m^3 .

The dynamic pressures inside the void (P_1) and living space (P_2) are determined as:

$$P_1 = P_{1r} + \frac{P_{1f} - P_{1r}}{1 + \frac{(A_1^{out})^2}{(A_1^{in})^2}} \quad \text{and} \quad P_2 = P_{2r} + \frac{P_{2f} - P_{2r}}{1 + \frac{(A_2^{out})^2}{(A_2^{in})^2}}$$

Finally, with these pressures the air flow rate through the floor, or floor leakage, I_{12} [m^3/h] can be determined:

$$I_{12} = \frac{\Delta P_s + (P_1 - P_2)}{R_{12}} \quad \text{with:} \quad R_{12} = \frac{G}{A_{12}}$$

R_{12} : linear resistance through a floor (Nh/m)

G : floor air resistance; default: timber floor 27.8 complex screed floor 139 (Nh/ m^3)

A_{12} : floor area (m^2)

ΔP_s : pressure difference resulting from stack effect; default value summer $\Delta P_s=0$ (Pa)

Because the stack effect is only relevant for the winter two I_{12} values can be calculated: I_{12s} for summer and I_{12w} for winter.

Suction flow (pressure driven flow)

Suction flow results when the soil-gas pressure exceeds the air pressure inside a void and causes a chemical flux from soil-air to the air in the void. The pressure gradient in soil (∇P), causes fluxes from soil to void air via connected pore spaces, gaps and cracks.

$$V_s = -\frac{k_{eff}}{\mu} \nabla P$$

$$\nabla P = -\frac{(P_1 - P_{0d})}{d}$$

k_{eff} :	effective air permeability of floor material	
	reasonable worst case: $1 \cdot 10^{-11}$ (medium sand)	(m ²)
μ :	air viscosity. default $5 \cdot 10^{-9}$	(Nh/m ²)
P_1 :	dynamic air pressure inside void	(Pa)
P_{0d} :	dynamic soil-gas pressure (considered as equal to 0)	(Pa)
d :	characteristic path length of the flux of the vapour molecules beneath outside walls from soil to void. default = 1 m	(m)

Equilibrium concentrations of toxic vapour

Substituting the above mentioned equations the following expression is obtained for concentration of toxic vapour in the living space:

$$C_2 = \frac{\left(\frac{\left(\frac{D_{12} + I_{12}}{A} \right) \cdot \left(\frac{D_{01} + V_s \cdot p \cdot L}{S_a \cdot A} \right) \cdot K_b \cdot C_b}{E_{x1} \cdot H_1 + D_{13} \cdot \left(\frac{A_{wa1} - A_h}{A} \right) + D_{01} + D_{12} + \frac{I_{12}}{A}} \right)}{\left(E_{x2} \cdot H_2 + D_{23(c)} + D_{23(w)} \cdot \left(\frac{A_{wa2} - A_{wd}}{A} \right) + D_{12} - \frac{D_{12} \cdot \left(\frac{D_{12} + I_{12}}{A} \right)}{E_{x1} \cdot H_1 + D_{13} \cdot \left(\frac{A_{wa1} - A_h}{A} \right) + D_{01} + D_{12} + \frac{I_{12}}{A}} \right)}$$

C_2 :	concentration air in living space	(ppb)
D_{01} :	diffusion coefficient through ground surface	(m/h)
D_{12} :	diffusion coefficient through all floor layers (timber floor $\sim 6 \cdot 10^{-2}$; beam/block floor $\sim 2 \cdot 10^{-2}$)	(m/h)
D_{13} :	diffusion coefficient from void to outside air	(m/h)
$D_{23(w)}$:	diffusion coefficient through walls	(m/h)
$D_{23(c)}$:	diffusion coefficient through ceiling	(m/h)
I_{12} :	resulting air flow rate through floor	(m ³ /h)
V_s :	suction flow velocity	(m/h)
p :	perimeter length of the house (default value: 34.4 m)	(m)
L :	characteristic length of ground outside house over which suction flow is effective (default value: 0.5 m)	(m)
	$p \cdot L$: area through which suction flow takes place	
S_a :	air filled porosity of soil	(0.2)
A :	surface area subfloor ground, floor and ceiling; $A=A_g=A_f=A_c$	(m ²)
A_{wa1} :	surface area walls crawl space	(m ²)
A_{wa2} :	surface area walls living space	(m ²)
A_{wd} :	surface area windows/doors	(m ²)
A_h :	surface area holes (air bricks) in crawl space	(m ²)
E_{x1} :	air-exchange rate of crawl space	(h ⁻¹)
E_{x2} :	air-exchange rate of living space	(h ⁻¹)
H_1 :	height of crawl space; default 0.2 m	(m)
H_2 :	height of living space; default 5 m	(m)
K_b :	partitioning coefficient bulk soil- vapour phase	(-)
C_b :	concentration bulk soil	(mg/kg)

Appendix 5.1 EUSES equations for calculating the concentration in leaves of plants

EUSES: equations for calculating the concentration in leaves of plants

The transpiration stream concentration factor (TSCF) is the ratio between the concentration in the transpiration stream and the concentration in pore water. The domain of physical chemical properties is log Kow -0.5 to 4.5 (outside this range the minimum or maximum Kow is used).

$$TSCF = 0.784 \cdot \exp \left[\frac{-(\log Kow - 1.78)^2}{2.44} \right]$$

Gaseous exchange between leaves and air can be described by a leaf-air partition coefficient:

$$K_{leaf-air} = Fair_{plant} + \frac{K_{plant-water}}{K_{air-water}}$$

Elimination of the substance may take place by metabolism or photolysis. If the rate constants are known they may be added:

$$kelim_{plant} = kmetab_{plant} + kphoto_{plant}$$

The sink term is formed by diffusive transfer from leaf to air, elimination in the plant tissue and dilution by growth:

$$ALPHA = \frac{AREA_{plant} \cdot g_{plant}}{K_{leaf-air} \cdot V_{leaf}} + kelim_{plant} + Kgrowth_{plant}$$

The source term is formed by the uptake and translocation from soil and the gaseous uptake from air:

$$BETA_{agric} = C_{agric,porew} \cdot TSCF \cdot \frac{Qtransp}{V_{leaf}} + (1 - F_{ass_{aer}}) \cdot C_{air} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}$$

The steady-state concentration is calculated as the source term divided by the sink term:

$$C_{leaf} = \frac{BETA_{agric}}{ALPHA} \cdot \frac{1}{RHO_{plant}}$$

TSCF:	transpiration stream concentration factor	[-]
$K_{leaf-air}$:	partition coefficient between plant tissue and water	[m ³ /m ³]
$F_{air_{plant}}$:	volume fraction of air in plant tissue	[0.30 m ³ /m ³]
$K_{plant-water}$:	partition coefficient between plant tissue and water	[m ³ /m ³]
$K_{air-water}$:	air-water partition coefficient	[m ³ /m ³]
$kelim_{plant}$:	rate constant for total elimination in plants	[d ⁻¹]
$kmetab_{plant}$:	rate constant for metabolism in plants	[0 d ⁻¹]
$kphoto_{plant}$:	rate constant for photolysis in plants	[0 d ⁻¹]
ALPHA:	sink term of differential equation	[d ⁻¹]
$AREA_{plant}$:	leaf surface area	[5 m ²]
g_{plant} :	conductance	[86.4 m/d]
V_{leaf} :	shoot volume	[0.002 m ³]
$kgrowth_{plant}$:	rate constant for dilution by growth	[0.035 d ⁻¹]
Qtransp:	transpiration stream	[1.10 ⁻³ m ³ /d]
$F_{ass_{aer}}$:	fraction of substance adsorbed to aerosol	[-]
C_{leaf} :	concentration in leaves of plants	[kg/kg _{wwt}]
RHO_{plant} :	bulk density of plant tissue (wet weight)	[700 kg _{wwt} /m ³]

Appendix 5.2 A CSOIL equations for calculating the pore water concentration

$$Z_w = \frac{S}{V_p}$$

$$Z_a = \frac{1}{R \cdot T}$$

$$Z_s = \frac{K_d \cdot SD \cdot Z_w}{V_s}$$

$$K_{lw} = \frac{Z_a}{Z_w}$$

$$K_{oc} = 0.411 \cdot K_{ow}$$

$$K_d = f_{oc} \cdot K_{oc}$$

$$P_w = \frac{Z_w \cdot V_w}{Z_a \cdot V_a + Z_w \cdot V_w + Z_s \cdot V_s}$$

$$C_{pw} = \frac{C_s \cdot SD \cdot P_w}{V_w}$$

Symbol (CSOIL)	Symbol (EUSES)	Value	Unit (CSOIL)
Cs	C _{soil}	input	mg/kg _{dw}
S	SOL	input	mol/m ³
Vp	VP	input	Pa
SD	RHO _{soil}	1.5	kg _{dw} /dm ³
R	R	8.314	Pa.m ³ /mol.K
T	TEMP	283	K
Va	Fair _{soil}	0.2	-
Vw	Fwater _{soil}	0.2	-
Vs	Fsolid _{soil}	0.6	-
foc	Foc _{soil}	0.058	kg/kg
Zw ¹⁾	-	calculated	mol/Pa.m ³
Za ²⁾	-	calculated	mol/Pa.m ³
Zs ³⁾	-	calculated	mol/Pa.m ³
Klw	K _{air-water}	calculated	m ³ _{air} /m ³ _{water}
Koc	Koc	calculated	dm ³ /kg
Kd	Kp _{soil}	calculated	dm ³ /kg
Pw ⁴⁾	-	calculated	-
Cpw	C _{soil,porew}	calculated	mol/dm ³ = g/m ³

1) Fugacity capacity constant water

2) Fugacity capacity constant air

3) Fugacity capacity constant soil

4) Weight fraction in soil pore water

Appendix 5.2 B EUSES equations for calculating the pore water concentration

$$HENRY = \frac{VP \cdot MOLW}{SOL}$$

$$K_{air-water} = \frac{HENRY}{R \cdot TEMP}$$

$$Koc = \frac{1.26 \cdot Kow^{0.81}}{1000}$$

$$Kp_{soil} = Foc_{soil} \cdot Koc$$

$$K_{soil-water} = Fair_{soil} \cdot K_{air-water} + Fwater_{soil} + Fsolid_{soil} \cdot Kp_{soil} \cdot RHO_{solid}$$

$$C_{si, rewater} = \frac{C_{si} \cdot RHO_{si}}{K_{si-water}}$$

Symbol (EUSES)	Symbol (CSOIL)	Value	Unit (EUSES)
C _{soil}	Cs	input	kg/kg _{wwt}
SOL	S	input	kg/m ³
VP	Vp	input	Pa
RHO _{soil}	SD	1700	kg _{wwt} /m ³
RHO _{solid}	-	2500	kg _{solid} /m ³ _{solid}
R	R	8.314	Pa.m ³ /mol.K
TEMP	T	285	K
Fair _{soil}	Va	0.2	-
Fwater _{soil}	Vw	0.2	-
Fsolid _{soil}	Vs	0.6	-
Foc _{soil}	foc	0.02	kg/kg
HENRY	-	calculated	Pa.m ³ /mol
K _{air-water}	Klw	calculated	m ³ /m ³
Koc	Koc	calculated	m ³ /kg
Kp _{soil}	Kd	calculated	m ³ /kg
K _{soil-water}	-	calculated	m ³ /m ³
C _{soil.porew}	Cpw	calculated	kg/m ³

Appendix 6 Current CSOIL Formulas

The CSOIL exposure model is developed for the derivation of Intervention Values for soil and groundwater clean-up. These Intervention Values are, for example, based on potential risk assessment for humans exposed to soil contaminants [Van den Berg, 1995]. Physicochemical properties of the contaminant, together with soil properties, plant uptake characteristics, human physical characteristics, human behaviour, climatological/meteorological standards and other assumptions lead to quantification of the potential exposure. The exposure is compared with the human toxicologically based Maximum Permissible Risk (MPR).

Matching the MPR with the soil concentration gives the human toxicologically based Intervention Value (former C-value) for soil and groundwater for a standardised situation [DGM, 1994a,b]. Exceedance of the Intervention Values means "serious soil contamination", an unacceptably increased risk to humans or the environment, taking into account all possible exposure pathways [Van den Berg *et al.*, 1993].

The following formulas have been adjusted on the basis of the TCB [1992] recommendations; the information on the uptake of heavy metals by plants has been adjusted to Bockting and Van den Berg [1992] as well as other information. Mistakes have been corrected.

Appendix 6.1	Formulas fugacity calculations.
Appendix 6.2	Formulas air flux calculations.
Appendix 6.3	Formulas dilution air flux outdoor.
Appendix 6.4	Formulas air concentration calculation.
Appendix 6.5	Formulas crop content.
Appendix 6.6	Formulas calculation concentration in drinking water after permeation.
Appendix 6.7	Formulas for the calculation of the air concentration in the bathroom during showering.
Appendix 6.8	Formulas for the quantification of the exposure.
Appendix 6.9	Primary set of data.
Appendix 6.10	Conversion formulas.

Appendix 6.1 Formulas fugacity calculations

Organic substances

$$Z_a = 1 / (R \cdot T)$$

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

$$Z_w = S/V_p$$

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

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

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

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

$$= 1 - V_a - V_w$$

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

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

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

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

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

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

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

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

Dissociating organic substances

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

f_{nd} : fraction non-dissociated substance

$$f_{nd} = 1 / (1 + 10^{[pH - pK_a]})$$

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

pK_a : acid dissociation constant of the substance

Calculation mass fractions

$$P_a = (Z_a * V_a) / (Z_a * V_a + Z_w * V_w + Z_s * V_s)$$

$$P_w = (Z_w * V_w) / (Z_a * V_a + Z_w * V_w + Z_s * V_s)$$

$$P_s = (Z_s * V_s) / (Z_a * V_a + Z_w * V_w + Z_s * V_s)$$

P_a : mass fraction in soil air [-]

P_w : mass fraction in soil moisture [-]

P_s : mass fraction in solid phase soil [-]

Inorganic substances

$$Z_a = 0; C_{sa} = 0; P_a = 0$$

$$P_w = 1; P_s = 0$$

Metals and arsenic

$$Z_a = 0; C_{sa} = 0; P_a = 0$$

$$P_w = V_w / (V_w + K_d * SD)$$

$$P_s = 1 - P_w$$

Calculation concentrations

$$C_{sa} = C_s * SD * P_a / V_a$$

C_{sa} : soil-air concentration [mol.dm⁻³ or g.m⁻³]

C_s : initial soil content (total soil content in gas, water, and solid phase) [mol.kg⁻¹ dry soil or mg.kg⁻¹]

$$C_{pw} = C_s * SD * P_w / V_w$$

if : $C_{pw} > S$ then: $C_{pw} = S$

$$C_{sa} = S * V_w * P_a / (P_w * V_a)$$

C_{pw} : soil-moisture concentration [mol.dm⁻³ or g.m⁻³]

Appendix 6.2 Formulas air flux calculations

$$D_{sa} = V_a^{10/3} * D_a / (1 - V_s)^2 \text{ with } D_a = 0.036 * (76/M)^{1/2}$$

D_{sa} : diffusion coefficient in the soil-gas phase [m².h⁻¹]

D_a : diffusion coefficient in free air [m².h⁻¹]

M : molecular mass [g.mol⁻¹]

$$D_{sw} = V_w^{10/3} * D_w / (1 - V_s)^2 \text{ with } D_w = 3.6 * 10^{-6} * (76/M)^{1/2}$$

D_{sw} : diffusion coefficient in the soil-water phase [m².h⁻¹]

D_w : diffusion coefficient in free water [m².h⁻¹]

$$D_u = (P_a * D_{sa} / V_a) + (P_w * D_{sw} / V_w)$$

D_u : diffusion coefficient in the soil [m².h⁻¹]

$$J_2 = D_a * C_{sa} / d$$

$$J_3 = C_{pw} * E_v / 24$$

$$J_4 = D_u * C_s * SD / dp$$

$$J_5 = D_u * C_s * SD / (dp - Bh)$$

if : $C_{pw} > S$ then : $J_4 = D_u * S * V_w / (dp * P_w)$

if : $C_{pw} > S$ then : $J_5 = D_u * S * V_w / [(dp - Bh) * P_w]$

J2	: boundary-layer flux	[g.m ⁻² .h ⁻¹]
J3	: water-evaporation flux	[g.m ⁻² .h ⁻¹]
J4	: diffusion flux water-soil to surface level	[g.m ⁻² .h ⁻¹]
J5	: diffusion flux water-soil to crawl space	[g.m ⁻² .h ⁻¹]
Ev	: flux of evaporating water	[Fast <i>et al.</i> , 1987: 0.0001 m ³ .m ⁻² .d ⁻¹]
d	: thickness boundary layer	[Jury <i>et al.</i> , 1984: 0.005 m]
dp	: mean depth of the contamination	[1.25 m]
Bh	: height of the crawl space	[0.5 m]

if : J3+J4 < J2 then: Jo = J4 + J3

if : J3+J4 >= J2 then: Jo = J2

if : J3+J5 < J2 then: Ji = J5 + J3

if : J3+J5 >= J2 then: Ji = J2

Jo	: total soil flux to outdoor air	[g.m ⁻² .h ⁻¹]
Ji	: total soil flux to crawl space	[g.m ⁻² .h ⁻¹]

Appendix 6.3 Formulas dilution air flux outdoor

$$V_f = V_g * S_z / L_p$$

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

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

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

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

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

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

Z10	: altitude	[10 m]
V10	: wind velocity at 10 m altitude	[18 000 m.h ⁻¹]

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

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

Co : correction factor for the roughness length [-]

model calculation for $L_p = 100$ m:

	children	adults	
Z	= 1.0	1.5	[m]
V'	= 3127	3127	[m.h ⁻¹]
V1	= 0	3170	[m.h ⁻¹]
Vg	= 1563	3148	[m.h ⁻¹]
Co	= 1.56	1.56	[-]
Sz	= 10.31	10.31	[m]
Vfc	= 161.3		[m.h ⁻¹]
Vfa	=	324.6	[m.h ⁻¹]

Appendix 6.4 Formulas air concentration calculation

$$Co_{aa} = J_o / V_{fa}$$

Co_{aa} : concentration in the outdoor air for an adult at 1.5 m altitude [g.m⁻³]
V_{fa} : dilution velocity adult [m.h⁻¹]

$$Co_{ac} = J_o / V_{fc}$$

Co_{ac} : concentration in the outdoor air for a child at 1 m altitude [g.m⁻³]
V_{fc} : dilution velocity child [m.h⁻¹]

$$C_{ba} = J_i * B_o / (B_v * V_v)$$

C_{ba} : concentration in the crawl-space air [g.m⁻³]
B_o : surface area of the crawl space [50 m²]
B_v : volume of the crawl space [25 m³]
V_v : air-exchange rate [1.25 h⁻¹]
(experimental data (Fast *et al.*, 1987): min. 0.03 - max. 7.4 - av. 1.25)

$$C_{ia} = f_{bi} * C_{ba}$$

C_{ia} : concentration in the indoor air [g.m⁻³]
f_{bi} : contribution of the crawl-space air to the indoor air as fraction [0.1 -]
(experimental data (Fast *et al.*, 1987): min. 0 - max. 0.68 - av. 0.11 - 95 perc. 0.39)

if : C_{ia} < Co_{ac} then: C_{ia} = Co_{ac}

Appendix 6.5 Formulas crop content

Deposition

$$C_{dp} = \frac{TSP_o * DR_o * f_{rs} * C_s * [f_{in} / (Y_v * f_{Ei})] * \{1 - (1 - \exp[-f_{Ei} * t_e]) / (f_{Ei} * t_e)\}}{1}$$

C_{dp} : crop content originating from deposition [mg subst.kg⁻¹ dw crop]
f_{in} : fraction interception by crop [0.4 -]
Y_v : crop yield [0.28 kg dw.m⁻²]
f_{Ei} : weathering constant [0.033 d⁻¹]
TSP_o : concentration particles in outdoor air [0.07 mg.m⁻³]

frs : fraction soil in particles [0.5 -]
 DRo : deposition velocity [1 cm.s⁻¹ = 864 m.d⁻¹]
 te : growing period crop [180 d]

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

Crop content

Metals

root crops:

$$Cpr = BCFr * Cs$$

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

leafy crops:

$$Cps = BCFs * Cs + Cdp$$

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

if no BCFr or BCFs are given:

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

Other inorganic substances

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

root crops:

$$Cpr' = Cpw * (1 - fdwr)$$

Cpr' : content of the root crop [mg subst.kg⁻¹ fresh weight crop]
 fdwr : ratio dry weight—fresh weight root crops [0.202 kg dw.kg⁻¹ fresh]

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

BCFr' : bioconcentration factor root [(mg subst.kg⁻¹ fresh crop)/(mg subst.dm⁻³ soil moisture)]

leafy crops:

$$Cps' = Cpw * (1 - fdws) + Cdp * fdws$$

Cps' : content of the leafy crop [mg subst.kg⁻¹ fresh weight crop]
 fdws : ratio dry weight—fresh weight leafy crops [0.117 kg dw.kg⁻¹ fresh]

$$BCFs' = (1 - fdws)$$

BCFs' : bioconcentration factor stem [(mg subst.kg⁻¹ fresh crop)/(mg subst.dm⁻³ soil moisture)]

Organic substances*root crops:*

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

BCFr' : bioconcentration factor root [(mg subst.kg⁻¹ fresh crop)/(mg subst.dm⁻³ soil moisture)]

$$\text{Cpr}' = \text{BCFr}' * \text{Cpw}$$

Cpr' : content of the root crop [mg subst.kg⁻¹ fresh weight crop]

stems:

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

BCFs' : bioconcentration factor stem [(mg subst.kg⁻¹ fresh crop)/(mg subst.dm⁻³ soil moisture)]

$$\text{Cps}' = \text{BCFs}' * \text{Cpw} + \text{Cdp} * \text{fdws}$$

Cps' : content of the leafy crop [mg subst.kg⁻¹ fresh weight crop]

Appendix 6.6 Formulas calculation concentration in drinking water after permeation

$$\text{Cmax} = \text{Cpw} * 2 * \text{Dpe} * t / (r * d)$$

Cmax : maximum concentration in the drinking water after t days stagnation [mg.dm⁻³]

Dpe : permeation coefficient [m².d⁻¹]

t : time period of water stagnation [Vonk, 1985a,b: 8 h = 1/3 d]

r : radius of the pipe [0.0098 m]

d : thickness of pipe wall [0.0027 m]

24 hrs permeation:

$$\text{Cdw} = \text{Cmax} * 3 * \pi * r^2 * L / \text{Qwd}$$

Cdw : 24 h mean drinking-water concentration [mg.dm⁻³]

t : in this case 24 h = 1 d, hence correction factor 3

L : length of the pipe along which permeation can occur = size location [100 m]

Qwd : mean daily water consumption [500 dm³]

$$\text{Cdw} = 4.56 * 10^3 * \text{Dpe} * \text{Cpw} \quad [\text{mg.dm}^{-3}]$$

Appendix 6.7 Formulas for the calculation of air concentration in the bathroom during showering

$$\text{kwa} = [(H_{sh}/RT_{sh}) * kL * kG] / [(H_{sh}/RT_{sh}) * kG + kL] * [Ad/Vd] * tf$$

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

Temperature correction for the Henry constant:

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

H _{sh}	: Henry constant at a temperature of 313 K (T _{sh})	[Pa.m ³ .mol ⁻¹]
H ₀	: Henry constant for the reference situation (T ₀ = 283-293 K)	[Pa.m ³ .mol ⁻¹]

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

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

$$Ad/Vd = 3 / r$$

r	: radius of the drop	[0.5 mm = 0.0005 m]
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$$kL = Kl * (44/M)^{1/2} / 3600 [m.s^{-1}]$$

$$kG = Kg * (18/M)^{1/2} / 3600 [m.s^{-1}]$$

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

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

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

$$C_{bk} = kwa * C_{dw} * 5 * 10^{-3} [g.m^{-3}]$$

Appendix 6.8 Formulas quantification exposure

Soil ingestion

$$DI = AID * C_s * f_a / W$$

DI	: uptake via soil ingestion	[mg subst.kg ⁻¹ .d ⁻¹]
AID	: daily intake amount soil	[kg dry subst.d ⁻¹]
	adults	: 50 * 10 ⁻⁶
	children	: 150 * 10 ⁻⁶
W	: body weight	adults : 70 kg
		children : 15 kg

fa : relative absorption factor, set at 1 [-]
 Cs : initial soil content (total soil content in gas, water, and solid phase) [mol.kg⁻¹ dry soil or mg.kg⁻¹]

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

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

Dermal contact soil

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

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

DA : uptake via dermal contact with soil [mg.kg-1.d-1]
 A exp : exposed surface area [m2]
 indoor outdoor
 adult 0.09 0.17
 children 0.05 0.28
 fm : matrix factor [0.15 -]
 DAE : degree of coverage [mg soil.cm-2 = * 0.01 kg.m-2]
 indoor outdoor
 adults 0.056 3.75
 children 0.056 0.51
 DAR : absorption velocity [h-1]
 adults 0.005
 children 0.01
 t : duration of exposure [h d-1]
 indoor outdoor
 adults 8 8
 children 8 8
 tf : time fraction exposure [-]
 correction of daily to annual average exposure
 indoor outdoor
 adults 1.857 0.143
 children 1.143 0.357
 frs : fraction soil in dust [-]
 frsi: indoor: 0.8

$$DAa = 5.92 * 10^{-6} * Cs / Wa$$

$$DAc = 6.43 * 10^{-6} * Cs / Wc$$

Inhalation of soil (particles)

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

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

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

TSP : amount of air-suspended particles [mg.m-3]
 TSPo: outdoor : 70 ug.m-3

TSPi: indoor : $0.75 * 70 = 52.5 \text{ ug.m}^{-3}$
 frs : soil fraction in particles in the air [-]
 frso: outdoor : 0.5
 frsi: indoor : 0.8
 AV : breathing volume [m³.d⁻¹]
 AVa: adults : $20 = 0.83 \text{ m}^3.\text{h}^{-1}$
 AVc: children : $7.6 = 0.32 \text{ m}^3.\text{h}^{-1}$
 t : duration of exposure [h]
 indoor outdoor
 adults 8 8
 children 16 8
 tf : time fraction exposure [-]
 correction from daily to annual average exposure
 indoor outdoor
 adults 2.856 0.143
 children 1.322 0.357

$$\text{IPa} = 0.625 * 10^{-6} * \text{Cs} / \text{Wa}$$

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

Inhalation of air

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

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

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

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

Background of daily indoor/outdoor exposure times

Exposed	Exposure location	Weekday			Weekend			Week, total hours [h.w ⁻¹]	Day, mean hours [h.d ⁻¹]	name of parameter
		days	hours	total hours	days	hours	total hours			
		[-]	[h.d ⁻¹]	[h]	[-]	[h.d ⁻¹]	[h]			
adult	indoor	5	24	120	2	20	40	160	22.86	Tia
	outdoor	5	0	0	2	4	8	8	1.14	Toa
child	indoor	5	22	110	2	19	38	148	21.14	Tic
	outdoor	5	2	10	2	5	10	20	2.86	Toc

Ingestion of crops: leafy and root crops

metals

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

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

$$VIa = (0.002761 * Cpr + 0.001843 * Cps) / Wa$$

$$VIc = (0.001511 * Cpr + 0.000890 * Cps) / Wc$$

other (in)organic substances

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

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

$$VIa = (0.01367 * Cpr' + 0.01578 * Cps') / Wa$$

$$VIc = (0.00748 * Cpr' + 0.00761 * Cps') / Wc$$

Ingestion of drinking water

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

DIw : intake of contaminated drinking water by drinking [mg.kg-1.d-1]
 Qdw : daily drinking-water intake [m3.d-1]
 adults : 0.002 = 2 dm3.d-1
 children : 0.001 = 1 dm3.d-1
 Cdw : drinking-water concentration [mg.dm-3 = g.m-3]

$$DIwa = 2 * Cdw / Wa$$

$$DIwc = 1 * Cdw / Wc$$

Inhalation of vapours during showering

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

IVw : intake contamination by inhaling vapour during showering [mg.kg-1.d-1]
 Cbk : concentration in the bathroom air [g.m-3]
 td : duration of stay in the bathroom [h]
 15 min. showering + 15 min. drying/dressing = [0.5 h]

$$IV_{wa} = 2.08 * C_{dw} * k_{wa} / W_a$$

$$IV_{wc} = 0.792 * C_{dw} * k_{wa} / W_c$$

Dermal contact during showering

$$DA_w = A_{tot} * f_{exp} * DAR * t_{dc} * (1 - k_{wa}) * C_{dw} * f_a / W$$

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

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

adults : 1.8

children : 0.95

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

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

t_{dc} : contact time = showering time [0.25 h.d-1]

(1 - k_{wa}) : substance remaining in water after evaporation [-]

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

$$P_1 = (0.038 + 0.153 * K_{ow})$$

$$P_1 = 5000 * P_1 / (5000 + P_1), \text{ maximization according to Brown \& Rossi (1989)}$$

$$P_2 = \exp(-0.016 * M) / 1.5$$

$$DA_{wa} = 0.18 * DAR * (1 - k_{wa}) * C_{dw} / W_a$$

$$DA_{wc} = 0.095 * DAR * (1 - k_{wa}) * C_{dw} / W_c$$

Total exposure

$$TAD = DI_a + DA_a + IP_a + IV_a + VI_a + DIW_a + IV_{wa} + DA_{wa}$$

$$TCH = DI_c + DA_c + IP_c + IV_c + VI_c + DIW_c + IV_{wc} + DA_{wc}$$

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

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

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

DOSIS: lifetime mean daily exposure [mg.kg-1.d-1]

Appendix 6.9 Primary set of data

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

S : water solubility [mol.m⁻³] or [mg.l⁻¹]

V_p : vapour pressure pure substance [Pa] or [atm] or [mm Hg]

or

K_{lw} : air—water distribution coefficient [-]

(this may also be calculated from the other data, see Appendix 6.10)

M	: molecular mass	[g.mol ⁻¹]
K _{ow}	: octanol—water distribution coefficient (for organic substances)	[(mol.dm ⁻³)/mol.dm ⁻³]
K _d	: soil—water distribution coefficient (for metals)	[dm ³ .kg ⁻¹]
D _{pe}	: permeation coefficient	[m ² .d ⁻¹]

Appendix 6.10 Conversion formulas

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

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

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

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

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

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

$$K_{lw} = H * 1.013 * 10^5 / (R_1 * T)$$

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

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

M : molecular mass [g.mol⁻¹]

$$f_{oc} = 0.58 * f_{om} \text{ or } f_{om} = 1.724 * f_{oc} \text{ or } OS = 172.4 * f_{oc}$$

f_{om} : fraction of mass organic matter

OS : percentage organic matter

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