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CSOIL 2000: an exposure model for human risk assessment of soil contamination

A model description

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Abstract

CSOIL 2000: an exposure model for assessing human risks due to soil contamination.
A model description

This RIVM description of the CSOIL 2000 model deals, for the first time, with all aspects of the model. CSOIL 2000 can be used to derive intervention values.
Intervention values are calculated for contaminated soil and represent a measure for determining when contaminated soil needs to be remediated.

CSOIL 2000 calculates the risks that humans are exposed to if they come into contact with soil contamination. Humans can be exposed to contaminated soil via different exposure routes (soil, air, water and crops). The soil use, such as a vegetable garden, determines the measure of exposure. Physical-chemical properties of the contaminant in soil air, soil particles and groundwater also have an influence on the exposure.

CSOIL 2000 also calculates the maximum concentration of a contaminant in the soil at which it is still safe for humans. This maximum concentration influences the level of the intervention value. In soil contamination the intervention value differentiates between lightly and seriously contaminated soils. The urgency of remediation is therefore determined by the level at which soil contamination exceeds the intervention value.

Key words: CSOIL 2000, intervention values, human risk assessment, Serious Risk Concentration (SRChuman), user scenarios

Rapport in het kort

CSOIL 2000 een blootstellingsmodel voor humane risicobeoordeling van bodemverontreiniging. Een modelbeschrijving

Het RIVM heeft een beschrijving opgesteld van het model CSOIL 2000, waarmee de interventiewaarden voor bodemverontreiniging worden berekend. Interventiewaarden geven aan wanneer verontreinigde grond moet worden gesaneerd. In het rapport zijn voor het eerst alle onderdelen van dit model samen beschreven.

Met CSOIL 2000 worden de risico's voor de mens die aan verontreiniging in de bodem wordt blootgesteld berekend. De mens kan via verschillende blootstellingsroutes (bodem, lucht, water en gewas) aan bodemverontreiniging worden blootgesteld. Het gebruik van de bodem, bijvoorbeeld moestuinen, bepaalt vervolgens de mate van blootstelling. Van invloed zijn ook de fysisch-chemische eigenschappen van de verontreinigingen in de bodemlucht, de bodemdeeltjes en het grondwater.

Het model berekent daarnaast de maximale concentratie van een verontreiniging in de bodem die veilig is voor de mens. Deze bodemconcentratie is van invloed op de hoogte van de interventiewaarde.

De interventiewaarde voor bodemverontreiniging maakt onderscheid tussen lichte en ernstig verontreinigde bodems. Bij overschrijding van de interventiewaarden wordt bepaald of spoedig saneren noodzakelijk is.

Trefwoorden: CSOIL 2000, interventiewaarden, humane risicobeoordeling, risicogrenzen, gebruikersscenario's

Preface

In 1994 the exposure model CSOIL was developed and used to determine the Dutch intervention values. Since 1994 new developments have taken place and it was therefore time to make an evaluation and revision of the model parameter set. This was done in 2001 as part of the project 'Risks in relation to soil quality'. This project was commissioned by the Directorate General of Environment to the National Institute for Public Health and the Environment (RIVM). A part of this project consists of writing a manual about the new version, the model CSOIL 2000. The present report represents this manual of the model CSOIL 2000.

The writer owes gratitude to F.A. Swartjes for his information, advice and remarks, during the writing of this report. The writer would also like to thank E.M. Dirven-van Breemen and M.G.J. Rikken for their welcome comments on the earlier versions of the report.

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Samenvatting

Sinds 1994 maakt men in Nederland gebruik van interventiewaarden bodemsanering ter bescherming van mensen en ecosystemen. Interventiewaarden zijn generieke risicogrenzen voor bodem- en grondwaterkwaliteit, en zijn gebaseerd op potentiële risico's voor mens en ecosysteem. Interventiewaarden worden gebruikt, om een bodemverontreiniging te classificeren als ernstig verontreinigd. Vanaf 1994 werden de eerste interventiewaarden afgeleid en in 2001 werd een deel van deze waarden geëvalueerd.
De afleiding van deze interventiewaarden gebeurde met behulp van het humane risicomodel CSOIL. In 2001 werd naast de evaluatie van de interventiewaarden ook de dataset van het model CSOIL geëvalueerd en aangepast aan recente (toxiciteits)data en nieuwe inzichten in de risicobeoordeling. Het geëvalueerde model werd CSOIL 2000 genoemd. Dit nieuwe model werd uiteindelijk gebruikt ter evaluatie van de interventiewaarden en voor risicoanalyse.

Voor de afleiding van de humaan-toxicologische risicogrenzen in CSOIL 2000, wordt uitgegaan van het standaard blootstellingscenario 'wonen met tuin'. Naast dit blootstellingscenario is CSOIL 2000 ook in staat om de risicogrenzen voor zes andere blootstellingsscenario's te bepalen. De blootstellingsscenario's van het huidige CSOIL 2000 zijn aangepast aan het nieuwe bodembeleid, zoals besproken in de projectgroep Normstelling en Bodemkwaliteitsbeoordeling (NOBO). Enkele scenario's zijn uitgebreid of opgesplitst. Tevens zijn er twee nieuwe scenario's bijgekomen. De nieuwe blootstellingsscenario's, naast het standaard scenario, zijn:

- plaatsen waar kinderen spelen;
- volks, - moestuinen;
- landbouw zonder boerderij/erf;
- natuur;
- groen met natuurwaarden;
- ander groen, bebouwing, infrastructuur en industrie.

De blootstelling van mensen aan verontreinigingen is niet alleen afhankelijk van het blootstellingscenario, maar ook van de blootstellingroute. In het huidige model zijn de blootstellingroutes niet sterk gewijzigd ten opzichte van de modelversie van voor 2000. De achterliggende berekeningen en formules zijn echter wel aangepast.
CSOIL 2000 kent de volgende zes blootstellingsroutes:

- ingestie van verontreinigde bodemdeeltjes;
- dermaal contact met verontreinigde bodemdeeltjes binnen en buiten;
- inhalatie van verontreinigde bodemdeeltjes;
- inhalatie van verontreinigde dampen;
- consumptie van verontreinigde groenten;
- contact via verontreinigd drinkwater.

Deze blootstellingroutes worden in het model nog verder opgesplitst.

Voor de bepaling van de risico's wordt door het model ook gebruik gemaakt van vaste parameters welke eveneens in dit rapport worden beschreven. Deze parameters zijn, indien dit noodzakelijk was, aangepast aan nieuwe toxicologische data.
Ook de formules die in CSOIL 2000 worden gebruikt zijn weergegeven in deze rapportage.

Summary

Since 1994 intervention values are used in the Netherlands for the protection of humans and ecosystems. Intervention Values are generic soil quality standards that are based on the potential risk for both humans and ecosystems. The intervention values are used to classify historical soil contamination as ‘seriously contaminated’. In 1994 the first series of intervention values were derived and in 2001 a part of these values were evaluated in line with the most recent views on risk assessment and (toxicological) data. The derivation of these values was done with the human risk model CSOIL. Next to the evaluation of the intervention values the dataset of the CSOIL model was also adapted to the new scientific knowledge. The evaluated model was called CSOIL 2000. This newer model was eventually used to evaluate the intervention values in 2001.

For the derivation of the human toxicological risk limits, CSOIL 2000 uses the standard user scenario ‘Residential with garden’. Next to this standard user scenario, CSOIL 2000 can also determine the risk limits for six other user scenarios. The scenarios that CSOIL 2000 uses are recently adapted to the revised Dutch Soil Legislation, in agreement with the policy workgroup NOBO (Policy workgroup on Soil quality standards and Soil quality assessment). Previous user scenarios have been extended or split up and two new scenarios have been introduced.
The new user scenarios, besides the standard scenario, are:

- places where children play;
- kitchen, -vegetable garden;
- agriculture without farm (yard);
- nature;
- green with nature, sports, recreation and city parks;
- other greens, buildings, infrastructure and industry.

The exposure of humans to contaminations does not only depend on the user scenario, but also on the exposure route. CSOIL 2000 distinguishes six main exposure routes. These routes have not considerably been changed in relation to the earlier version of the model. The equations used in the exposure routes have however been changed and will be described in this report. CSOIL 2000 recognises the following exposure routes:

- ingestion of contaminated soil particles;
- dermal contact with contaminated soil particles;
- inhalation of contaminated soil particles;
- inhalation of contaminated vapours;
- consumption of contaminated crops;
- contact via contaminated drinking water.

These exposure routes are further divided in the model.

CSOIL 2000 makes use of default parameters to determine the risk to humans. These parameters have been changed to the recent toxicological data. These parameters and the equations that use them are also described in this report.

1 Introduction

1.1 Scope and objectives

The project 'Risks in relation to soil quality' has the objective to create a basis and support for soil policy development and implementation, with special interest in adverse effects of contaminated soil.

The 'Directorate General for Environmental Protection' commissioned the RIVM (National Institute for Public Health and the Environment) to carry out the project 'Implementation of human risk assessment'. The purpose of this project is to develop a knowledge base for human risk evaluation. This is essential for a good explanation of risk evaluation and extending the risk evaluation in different frameworks e.g. risk in relation to soil quality. It leads to transparency and foundations of the soil standards. Writing the current report about the human exposure model CSOIL 2000 is one of the desired products!

The first CSOIL model was developed in 1994 for the purpose of deriving intervention values. Recently some changes were implemented in the CSOIL model, because since 1994 new data, exposure models and calculation methods have become available (Rikken et al. 2001, Otte et al. 2001).
The current report will give an explanation and a description about, how the new exposure model CSOIL 2000 is constructed and will also explain some changes that have been made. This on behalf of the derivation of intervention values in which CSOIL 2000 still plays a part (Rikken et al. 2001, Otte et al. 2001, Lijzen et al. 2001).
The model used was never reported as such. With this report this omission is solved.

The results and conclusions of this report will be used as a foundation and support for (future) soil policy. The report is in the first place written, for people working with CSOIL 2000. However everybody who has an interest in the model and has a basic knowledge on soil topics can use the report to learn about CSOIL 2000.

1.2 Exposure modelling

Due to the production and extensive use of various chemicals and products, contaminated soils are now present in large parts of the Netherlands. These so called contaminated sites can pose serious risk to humans and nature. The contaminants can accumulate in the ecosystem and end up in the human food chain (Bontje et al. 2005). Through the food chain people are exposed to the contaminants. However there are also other ways of contact, like soil ingestion, dermal contact or inhalation.
Models can be used to calculate the risks related to human behaviour and soil contamination. In the Netherlands CSOIL was developed in 1994, to estimate the exposure of humans who live on contaminated sites. The CSOIL model was developed with the help of previous models like HESP, SOILRISK, RIVM model (Linders 1990) and extensive studies of the literature behind these models. The background, similarity and differences of these models were analysed.

Both models HESP and SOILRISK were meant for the determination of actual exposure risks via contact with contaminated soils. This can be concluded from the exposure routes, parameters and constants that were chosen within these models. These variables were location related. In the models the testing of the results was done afterwards, in which the normative aspect was not the central aspect. Unlike the present model, CSOIL 2000 (Van den Berg 1995).
The RIVM model was more a description of the procedure that had to be followed, to determine the potential risk for humans, when exposed to contaminants in the environment. This procedure could be used for the calculation of C-testing values (intervention values) and for the calculation of actual risks (Van den Berg 1995).

Intervention values are generic soil quality standards used to classify historically contaminated soils, sediments and groundwater (i.e. before 1987) as seriously contaminated in the framework of the Dutch Soil Protection Act. In 1994 intervention values were published for the first series of compounds. Intervention Values are based on potential risks for both human health and ecosystems (Van den Berg et al. 1994). The ecological risks are not calculated in CSOIL 2000 and will therefore not be discussed in this report.

1.3 Readers guide to the report

Chapter 2 will discuss CSOIL 2000 in general. Chapter 3 will give a description of all the exposure routes of CSOIL 2000. Chapter 4 will describe the model parameters for the different exposure routes. Chapter 5 will describe the user scenario and the related user parameters that CSOIL 2000 uses to calculate the human exposure. Chapter 6 will show a list of reports that are related to CSOIL 2000 and chapter 7 will end with abbreviations and a glossary.

2 Model CSOIL 2000

2.1 Lay-out of the model

CSOIL 2000 consists of an Excel file with several worksheets. There are two general sheets. One input sheet and a general compound/contaminant sheet. The general compound sheet contains all compounds and the specific data that CSOIL 2000 uses during calculation.
The input sheet contains the default settings for the different contaminants. All the default settings can be changed if necessary. If no changes are made the default settings will be used to do the calculations.
There is also a calculation worksheet, here the secondary calculations are shown. There are two sheets that present the final calculated data. One sheet shows the data in a graph and the second one gives an overview of all parameters that have been calculated.
The last worksheet contains a selected compound list on which the data such as octanol-water partition coefficient (K_{ow}), solubility, molecular weight et cetera, are mentioned. Note that this sheet is not the same as the general compound sheet mentioned earlier. The last compound sheet only shows the compounds which are selected for the calculation.

2.2 Exposure routes of the model

A standard exposure scenario has been defined to describe the standardized conditions. In this scenario, all possible exposure pathways in CSOIL 2000 are assumed to be operational on the basis of exposure to contaminants in a residential situation.
The direct and indirect exposure routes that are taken into account by CSOIL 2000 are:

Soil
- ingestion of contaminated soil particles;
- dermal contact with soil contaminants (indoor);
- dermal contact with soil contaminants (outdoor);
- inhalation of contaminated soil particles;

Air
- inhalation of vapours of contaminants via crawl space (indoor);
- inhalation of vapours of contaminants (outdoor);

Crops
- ingestion of contaminants via consumption of locally grown crops;

Drinking water
- ingestions of soil contaminants via drinking water;
- inhalation of vapours of contaminants in the drinking water during showering;
- dermal contact with contaminants in the drinking water during showering and bathing (Rikken et al. 2001).

The exposure routes are also represented in Figure 2.1.

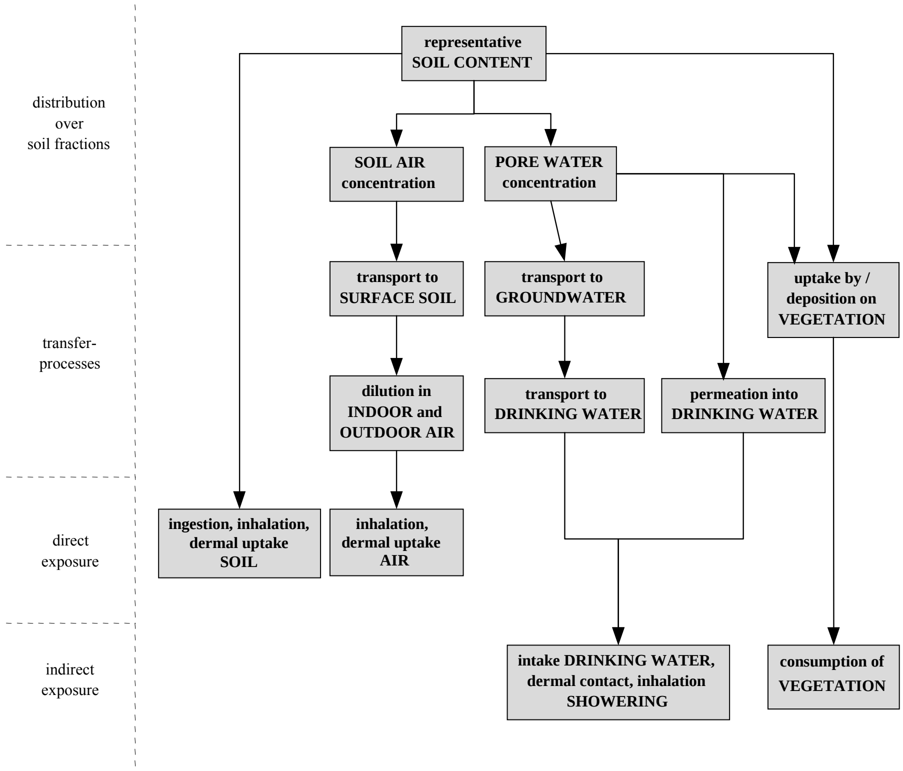

Figure 2.1: Diagram showing the exposure routes of the model, CSOIL 2000.

The following three exposure routes are responsible for at least 90% of the total exposure for almost all compounds. This can be concluded from calculations done with the model (Otte et al. 2001).
The three exposure routes are:

- the human exposure via the ingestion of contaminated soil particles;
- the human exposure to volatile compounds in the indoor air;
- the human exposure via the consumption of contaminated crops.

The following exposure routes however contribute very little to the total exposure.

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

Although not every exposure route has a significant contribution to the total human exposure, the basic principle is that all possible exposure routes are taken into account.

The model concept consists of roughly three parts:

1. the description of the behaviour of the compound in the soil and the partitioning over the soil phases;
2. the transfer processes and parameterisation of the different exposure routes (direct and indirect);
3. the quantification of the lifetime average exposure (Otte et al. 2001).

The model concepts can be cluster related to the exposure/contact with: soil, air, crops and drinking water.

The input parameters can, on basis of this concept, roughly be divided into:

- compound-specific input parameters; mainly physicochemical properties e.g. K_{ow};
- site and soil properties, related to potential exposure e.g. pH;
- exposure parameters which describe the receptor characteristics and behaviour e.g. breathing volume or ingestion frequency (Otte et al. 2001).

2.3 Human toxicological risk limits (MPR)

CSOIL 2000 is used to calculate the human toxicological risk limit (MPR). The human toxicological definition for serious soil contamination is taken as: the soil quality resulting in exceeding of the Maximum Permissible Risk for intake (MPR_{human}). MPR_{human} is defined as the amount of substance that any human individual can be exposed to daily, during a full lifetime without significant health risk. The MPR_{human} can be expressed as a tolerable daily intake (TDI) or an excess carcinogenic risk via intake (CR_{oral}), both are covering exposure by oral ingestion and dermal contact. But it can also be expressed as a tolerable concentration in air (TCA) or an excess carcinogenic risk via air (CR_{inhal}), both covering exposure by inhalation (Lijzen et al. 2001). The TDI represents the estimated amount of the chemical that humans can ingest daily during their lifetime without resultant adverse effects. The TCA represents the air concentration of the chemical that humans can inhale during their entire life without resultant adverse effects.

To derive human toxicological risk limits, the oral/dermal and inhalative exposure is calculated separately, under standardized conditions (*potential* exposure). The oral MPR_{human} (TDI or CR_{oral} in $\mu g.kg^{-1}$ bw day^{-1}) are used for the risk assessment of the oral and dermal exposures. The TCA or CR_{inhal} (in $\mu g.m^{-3}$) are used for the risk assessment of exposure via air. However TCA and TDI are not equal, and can therefore not be used directly. To be able to use the TCA or CR_{inhal} in CSOIL they are transformed to the unit $\mu g.kg^{-1}$ bw day^{-1}, just as the oral and dermal exposures and toxicological risk limit (Lijzen et al. 2001).
Finally the human toxicological risk limit is defined as the concentration of a contaminant in the soil for which the sum of the oral (inclusive dermal) and inhalative risk indexes equal 1 (Lijzen et al. 2001). See the equation below.

$$(\Sigma \text{ oral exposure}/ MPR_{humanoral}) + (\Sigma \text{ inhalative exposure}/ MPR_{humaninhalative}) \leq 1$$

Figure 2.2 shows the equation in a graph. The orange and yellow lines represent the organic contaminants (oral/dermal and inhalative). The blue lines show the metal contaminants (oral/dermal and inhalative). The four lines represent the increase in human risk at an increase in soil concentration. If the contaminants exceed the cross point of the critical concentration and the reference dose, a risk is imminent.
For metals this process is linear. For organic contaminants a kink is present. This kink represents the point, where the solubility of the organic contaminant is exceeded. This results in a limiting contribution of the oral plant uptake to the total dermal/oral uptake from this point on. Hence if the solubility of a contaminant is exceeded, an increase in concentration, does not lead to an increase in exposure via uptake by plants. Therefore the oral/dermal exposure keeps rising (due to the increase in exposure by direct ingestion), but it rises more slowly.

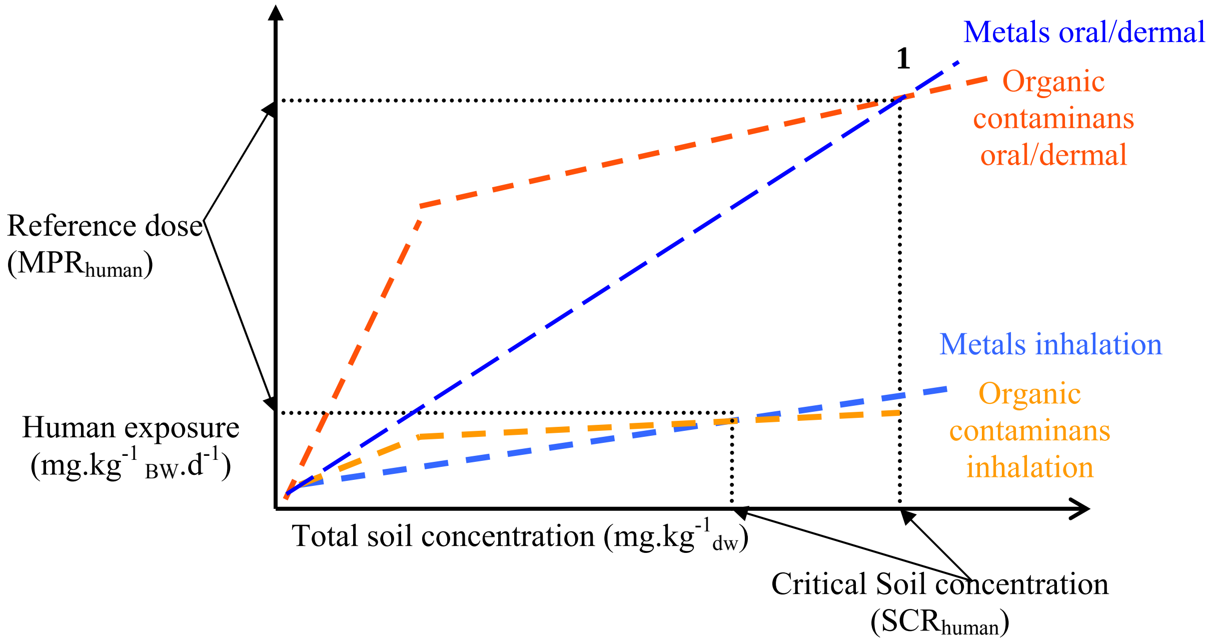

Figure 2.2: The derivation of the risk limit depends on inhalative and oral uptake.

3 Model concepts

When a contaminant enters the soil, it can be partitioned over different soil phases. From these phases the contaminant can enter different transfer routes, from which it can expose humans.
In the first paragraph of this chapter the partitioning of contaminants over the different soil phases is described. The other paragraphs describe the different transfer routes that the contaminants can have.
In chapter 2 four transfer routes to humane exposure are distinguished. These transfer routes are soil, air, crops and drinking water.
The equations that are needed to calculate the exposure that humans encounter via these transfer routes are mentioned in Appendixes 1-7.

3.1 Partition soil, water and air

Contaminants do not remain in the solid phase of a soil. In CSOIL 2000 the concentration of the contaminant in water phase (Cpw mg.dm^{-3}), air phase (Csa in mg.dm^{-3} soil air) and the soil phase (Cs mg.kg^{-1} dry matter) is calculated (Figure 3.1).
The partition amounts in the different phases can be calculated if assumed that there is equilibrium in the three soil phases (Van den Berg 1995).

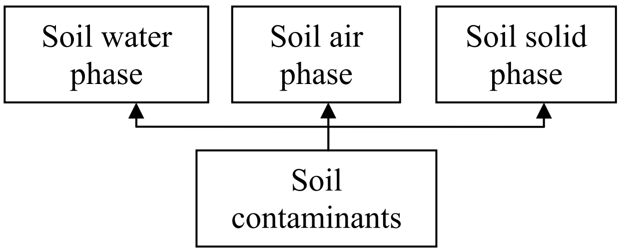

Figure 3.1: Partition of soil contaminants.

With knowledge about the soil-water partition coefficient (Kd in mg.kg^{-1} dry matter/mg.dm^{-3} or dm^3.kg^{-1}), air-water Henry-coefficient (H in mg.dm^{-3}/mg.dm^{-3} or dm^3.dm^{-3}) and the soil parameters, the concentrations of the contaminant can be calculated in the different soil phases (Van den Berg 1995).
A precondition for the calculation is that the concentration of the contaminant in the water phase is not higher than its solubility. If this is true, the concentration in the water phase should be taken equal to the solubility of a contaminant. Additional adaptations also have to be made to the concentration of a contaminant in the gas phase.

The partitioning of a contaminant is not only dependent on different soil phases, but distinction also has to be made between three types of contaminants, namely metals, organic and inorganic contaminants.
Metals are non-volatile and are therefore not present in the gas phase (with the exception of mercury). Their concentrations are divided over the water phase and solid phase of the soil.
Organic contaminants can be located in the water, air and soil phase.
Non-volatile, soluble substances like inorganic contaminants will remain in the water phase. Due to the fact that there is no information about the speciation of inorganic contaminants it is assumed, that 100% of the inorganic contaminant is dissolved in the water phase.
The equations used to calculate the partition and concentrations over the different soil phases are mentioned in Appendix 1.

Within CSOIL 2000 the fugacity calculations are done according to the Mackay and Paterson theory (Van den Berg 1995, Mackay et al. 1985). In the fugacity calculations organic carbon plays a significant role with the sorption/partition of the organic contaminants. Therefore the Kd is usually a soil organic carbon related parameter K_{oc}
(see also Appendix 1) (Van den Berg 1995).

3.2 Soil module

3.2.1 Soil ingestion

Soil ingestion has a major contribution to the total exposure of humans to contaminants. Adults and especially children ingest soil on purpose or by accident (Figure 3.2). This soil is then digested and the contaminant is released into the digestive tract, after which the chemical can be adsorbed into the body. This exposure route contributes significantly to the exposure of humans especially for immobile contaminants.
The ingestion can happen during the licking of contact media, for example fingers (Van den Berg 1995).
Several studies have been performed to determine the amounts of soil that adults and children might ingest during a day (e.g. Hawley 1985, Wijnen et al. 1990, Calabrese et al. 1989, 1990, 1997 and Stanek et al. 1997). Otte et al. performed in 2001 a review to determine the yearly averaged daily soil ingestion of children and adults. Although the amount of data from direct measurements should be extended, the insight in the (distribution) of the parameters is sufficient for exposure modelling.
Equations to calculate the exposure of humans via soil ingestion are given in part 2.1 of Appendix 2.

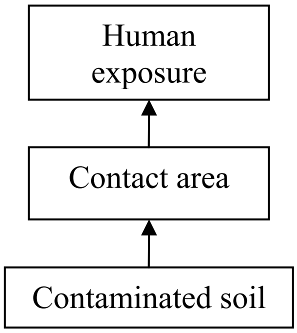

Figure 3.2: Route of exposure via soil ingestion.

3.2.2 Soil inhalation

Soil particles are part of all particles in the air. Via inhalation by humans, absorption of these particles in the body is possible (Figure 3.3).
The relative importance of soil inhalation depends on the type of contaminant. Volatile contaminants are more likely to evaporate and be inhaled as gases, than when they are attached to soil particles. Metal and non-volatile contaminants however will remain bound to the soil particles and can enter the human system via this route of exposure.
With the inhalation of soil particles, all particles <10 μm are included
(Van den Berg 1995).

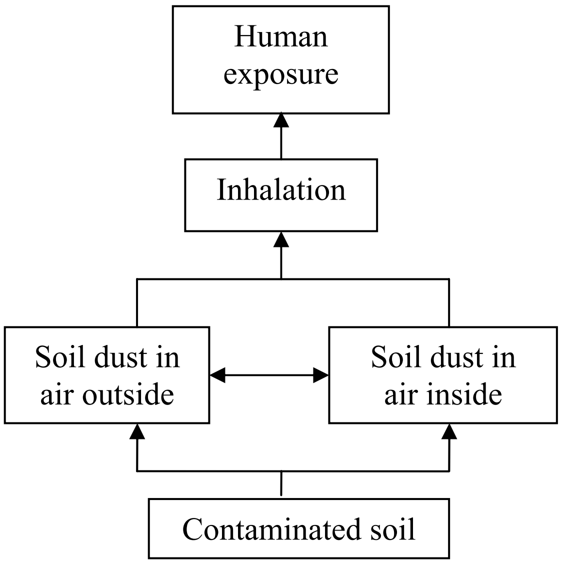

Figure 3.3: Routes of exposure via soil inhalation.

A distinction is made between indoor and outdoor soil particle inhalation. Outdoors the concentration of dust particles is higher, but the fraction of soil in these particles is lower. Indoors the concentration of particles is lower, but the soil content is higher (Otte et al. 2001). Within this module only soil dust is considered to be important. Dust particles that have another origin than soil from the assessed location are not considered in CSOIL 2000. Neither is the contaminant contribution of these dust particles to the local soil particles included. Equations used to calculate the amount of inhaled soil can be found in part 2.2 of Appendix 2.

3.2.3 Soil dermal uptake

Dermal uptake of contaminants through contact with the contaminated soil is a relative small exposure pathway. However absorption is possible and therefore CSOIL 2000 takes this exposure route into account (Figure 3.4). The amount of exposed surface area (skin) is higher outdoors and lower indoors. Indoors the amount of particles per square meter of skin is also lower than outdoors (Otte et al. 2001).

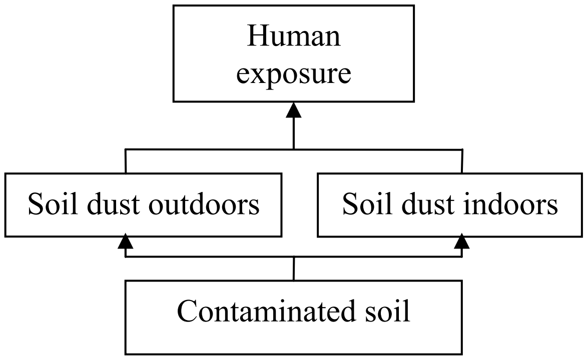

Figure 3.4: Routes of exposure via dermal contact with soil inhalation.

The skin consists of an outer layer that protects humans against different external factors. It is however possible for some contaminants to absorb into the skin. From here the contaminants are taken up by the blood vessels that are located in the interstitial tissue. Once the contaminants are in the blood stream they can cause different health problems. Damaging of the skin can increase the absorption speed of contaminants.
Organic substances can be absorbed via dermal uptake.
For inorganic substances it is assumed that the absorption is equal to zero, meaning that there is no exposure for inorganic contaminants via this route. This also applies for metal contaminants (Van den Berg 1995).
In part 2.3 of Appendix 2 the equations, that can be used to calculate the dermal uptake, are given.

3.3 Air module

In the air module the evaporation of the contaminant to the air is described (Figure 3.5). Soil particles do not play a part in this type of transfer. CSOIL 2000 describes the migration process of substances from the soil phase to the air phase as a result of a number of stationary equilibrium processes (Van den Berg 1995, Waitz et al. 1996).

In the model it is assumed, that at a depth of 1.25 m a contaminant is present which is, due to equilibrium processes, distributed over a liquid, gas and solid phase. Due to vertical transport of the contaminant through the soil, emissions can take place from the soil system (Waitz et al. 1996). These emissions are diluted in the outdoor air and to a lesser extend also in the indoor air. Indoor air concentrations of the contaminant can occur due to the transport of volatile compounds from the soil into the crawlspace air and from there into the indoor airspace (Waitz et al. 1996). Due to ventilation with outdoor air via the registers of the house, the indoor air concentrations are diluted.

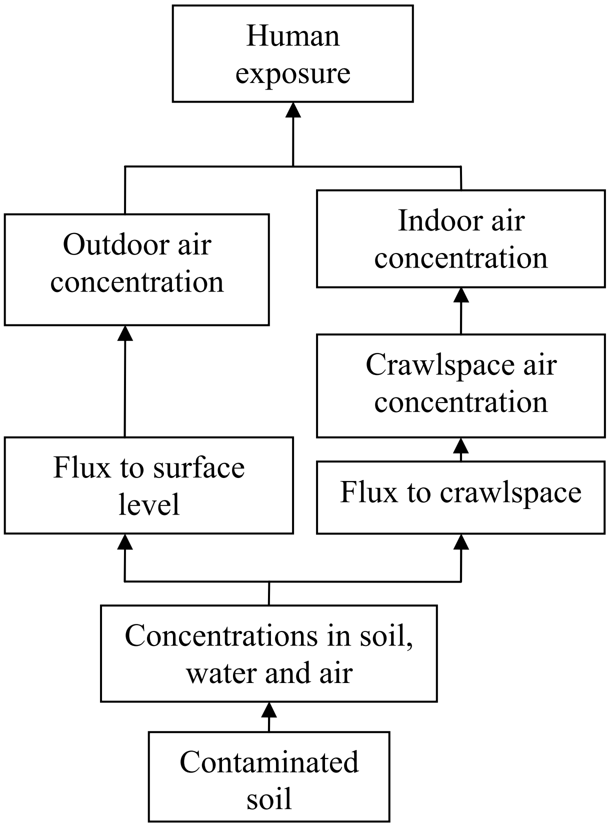

Figure 3.5: Routes of exposure via inhalation of volatile compounds.

The exposure of humans via inhalation of a volatile compound depends on the indoor/outdoor concentration in air, daily duration of indoor/outdoor exposure, annual average time fractions for residential time indoors/outdoors, relative absorption factor and human physiological characteristics, like breathing volume and bodyweight (Waitz et al. 1996).

This route of exposure only plays a significant role for organic contaminants. Metals, with the exception for mercury, and inorganic contaminants are not or not considered volatile and will therefore not evaporate to the air phase.
Equations that are used to calculate the exposures are given in Appendix 3.

3.4 Water module

A compound can also be transferred from the solid phase to the liquid phase. From here it can take several routes, however CSOIL 2000 uses only three: transport to groundwater, permeation through water pipelines and uptake by vegetation (Figure 3.6). The uptake by vegetation is discussed in section 3.5.

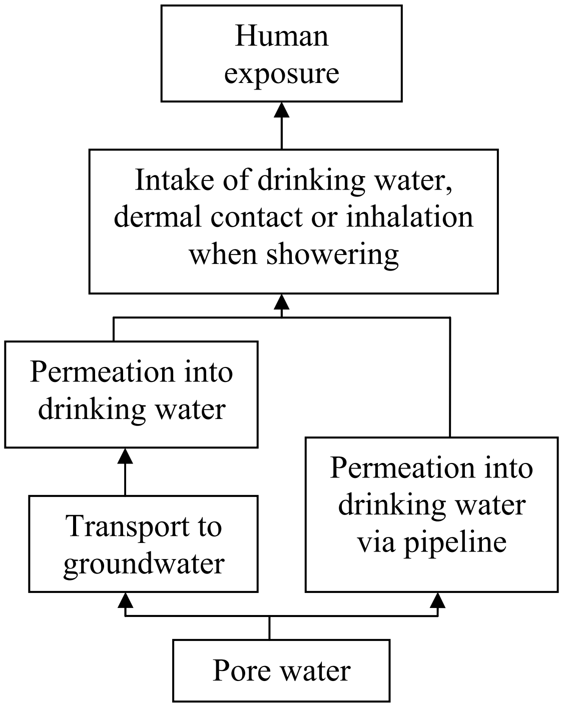

Figure 3.6: Routes of exposure via drinking, inhalation, dermal contact with drinking water.

3.4.1 Drinking water

From the pore water the compounds can be transported to the groundwater. If the contaminated groundwater is used for drinking water, the compound is automatically transported to humans.

Once the drinking water is contaminated humans can be exposed by drinking the contaminated water, inhaling the water vapours when showering/bathing and/or by dermal contact when showering/bathing.

If the contaminated site is near a drinking water pipeline, some compounds can permeate through the tubing of the pipeline, contaminating the clean drinking water inside (Van den Berg 1995).
Contaminants from the pore water or air phase will usually only permeate through a pipeline into the drinking water if the pipeline is made out of LDPE. These pipelines are found in the neighbourhood of houses or other buildings (Van den Berg 1995). For inorganic compounds and metals permeation of pipelines is not possible, and therefore only organic substances are considered (Van den Berg 1995). The speed with which a compound permeates through a pipeline is, in CSOIL 2000, described with the permeation coefficient ($m^2.d^{-1}$).
See also Vonk (1985) for some of the permeation coefficients.

The drinking water that originates from surface water (e.g. rivers and lakes) is not part of CSOIL 2000 and will therefore not be discussed in this report. The equations that can be used to calculate the exposure via drinking water is described in parts 4.1 and 4.2 of Appendix 4.

3.4.2 Showering

Showering is done with tap water. If this water is contaminated, originating from the process in section 3.4.1, humans can be exposed via two possible routes, dermal contact and inhalation of water vapours (Figure 3.7). The main parameters that are used during inhalation and dermal exposure calculations are: Henry's law constant, molecular mass and K_{ow}.

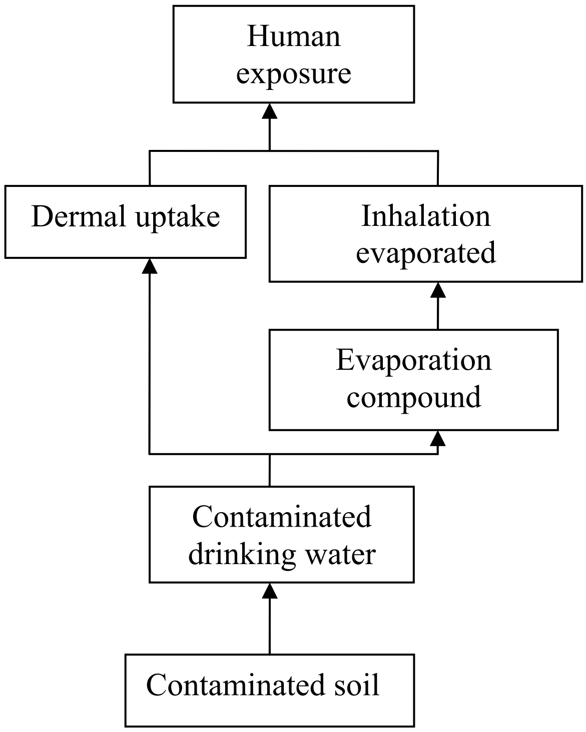

Figure 3.7: Routes of exposure via showering.

Inhalation of water vapours

During showering the volatile organic compounds can evaporate from the tap water and be inhaled with the water vapours. Droplet forming of the water will increase the surface-volume ratio. This droplet forming will increase the evaporation rate of the compound from the water. The temperature of the water also influences the evaporation rate of the compound, the warmer the water, the higher the evaporation (Bontje et al. 2005).
To calculate the human exposure, the concentration in the water vapour, breathing volume and the residence time must be known (Van den Berg 1995). The equations to make the calculation are given in parts 4.3 and 4.4 of Appendix 4.

Dermal contact

'During showering/bathing, contaminants from the water can be absorbed through the skin' (Van den Berg 1995). Although this route has a relatively small influence on the total human exposure, it is still considered in CSOIL 2000. The rate of the absorption is mainly determent by the concentration of the compound in the water, the surface of the skin that comes into contact with the water (fraction exposed skin), the time that a person takes a shower/bath and the dermal absorption speed. The equations that use these parameters to calculate the dermal uptake are given in part 4.5 of Appendix 4.

3.5 Crop module

There are two main exposure routes for vegetation described in CSOIL 2000. These are via the air (deposition of soil dust/soil re-suspension/ rain splash and deposition of local volatized contaminant) and via uptake by plant roots (Figure 3.8). From every plant different parts are eaten and therefore a difference is made between roots and leaves of the plant. The term leaves includes all parts of the plant that are above ground, this means leafs and stem.

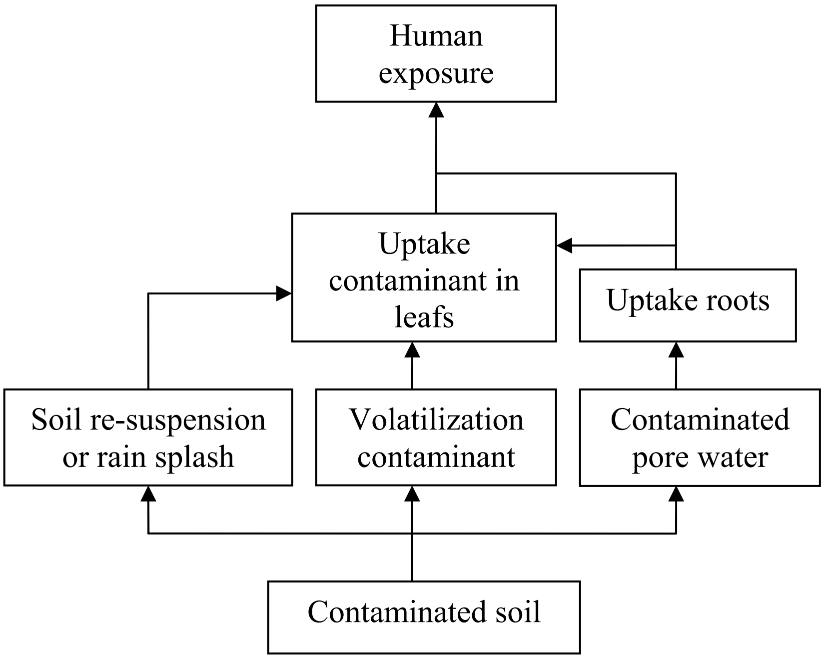

Figure 3.8: Routes of exposure via vegetation.

CSOIL 2000 also calculates the transport of the compound from the roots to the leaves of the plant. The concentration of the contaminant in plants depends on the deposition on the leaves and the accumulation of the contaminant in the roots of the plants. The concentration in the plant is calculated by adding up the concentrations in both roots and leaves (Bontje et al. 2005, Trapp and Matthies 1995).
The exposure to humans depends on the concentration in the crops, the amount of consumption and the fraction of the total vegetation that comes from a contaminated soil (Rikken et al. 2001).

3.5.1 Uptake by roots

The uptake of a contaminant by the roots of a plant is the most important exposure route in the vegetation exposure. The uptake from the soil is largely a passive process. It is driven by the transpiration stream in the xylem of the plant (Versluijs and Otte 2001). The water soluble compounds pass the root membranes and can be transported upwards to the leaves of the plant by the transpiration stream. In some cases the compounds will remain in the roots. In the leaves the water will evaporate and the compounds can accumulate (Rikken et al. 2001, Bromilow and Chamberlain 1995).

Within this exposure route a difference is made between organic compounds, inorganic compounds and metal compounds, this is done due to the different behaviour of the compounds.

For the organic compounds the relation between the concentration in the soil and the concentrations in the roots of a plant and the relation between the concentrations in the roots and in the leaves of a plant is according to the Trapp and Matthies (1995) model. This model was assessed by Rikken et al. in 2001.
The concentrations of the contaminant in the plant can be calculated with the octanol-water partition coefficient and the concentration of the compound in the soil water phase.
The roots of a plant consist of a water fraction and a lipid fraction. The pore water in the soil is considered to be in equilibrium with the water fraction in the crops. The concentrations of the compound in both liquids are therefore considered equal. The lipid fraction is assumed to behave like octanol. The root lipids will finally come in equilibrium with the pore water that surrounds the root. The time before this equilibrium is reached depends on the K_{ow} (lipophilicity) (Rikken et al. 2001).

For metals an empirical approach is used in which the uptake by the plant is within the use of a BioConcentration Factor (BCF). This is due to the poor understanding of the mechanisms of accumulation for metals. To get the bioconcentration factor, experimental data are used. If these data are not present the BCF can be calculated with the equation of Baes et al. (1984). Part 5.1 of Appendix 5 gives the equations to calculate the BCF in the leaves and roots of the plant.

Most inorganic substances are very soluble and therefore the assumption is made, that the concentration of the contaminant in the roots is the same as the concentration in the pore water. The concentration of the inorganic substances is assumed to be a worst-case scenario, in which the total dissolved concentrations of the compounds are equal to the overall total concentration. For cyanides it was concluded that this is a worst-case approach and that these compounds are broken down in the plant (Köster 2001).
Part 5.3 of Appendix 5 gives the equations for exposure via vegetation.

3.5.2 Soil re-suspension and rain splash (organic compounds)

Due to wind and rain contaminated soil- and dust particles can be deposited in the leaves of a plant. This is also called re-suspension or rain splash (Rikken et al. 2001). The compound can than be transferred from the soil particles into the leaf of the plant. However it is very difficult to estimate to what extent the concentration inside the leaf is influenced by this deposition (Rikken et al. 2001).
If the vegetable is not properly washed, the contaminated soil particles, which are now located on the plant, are eaten. Washing of the crops can reduce the exposure via this route greatly (Rikken et al. 2001, Versluijs and Otte 2001).
The contribution of this exposure pathway is difficult to estimate. As soon as the dust particles are airborne they are diluted due to the wind. Within CSOIL 2000 only the dust particles from the locally contaminated soil are used to make a calculation. Contaminated dust from elsewhere is therefore not considered (Rikken et al. 2001). The amount of dust deposit also depends on the geometry of the vegetable type.
In part 5.2 of Appendix 5 the equations that are used by CSOIL 2000 to calculate the influence of soil re-suspension and rain splash on the BCF value, are given.

3.5.3 Deposition of local volatile contaminants (organic compounds)

Deposition of local volatile contaminants only includes the volatile contaminants that originate from the (locally) contaminated location and does not include deposition of aerosols originating from elsewhere.
This type of contamination is not well known and is often neglected because of its limited contribution to the concentration in a plant. However it can play a role on heavily contaminated soil. For example the transport of PCDD/F's (dioxins) via this route can be substantial. These substances are not or poorly transported via the xylem of the plant (Rikken et al. 2001). Due to wind, the concentrations of these volatile contaminants are rapidly diluted, however for plants close to the ground this type of contamination could be an important factor. The concentration of the compound in the leaf is calculated with help of a mechanistic model. See part 5.3 of Appendix 5 for the equation that can be used to calculate the exposure.

The total exposure can now be calculated by adding up all the different exposure routes. How this is done is shown in Appendix 6.

3.6 Direct consumption of contaminated groundwater

Direct consumption of contaminated drinking water is included in CSOIL 2000. This principle is used for setting groundwater quality standards and for deriving intervention values. Groundwater can be directly consumed as drinking water (Figure 3.9). It can however also be used as a strategic drinking water source. This means that in theory, groundwater should be drinkable without treatment.
The exposure of humans via drinking contaminated groundwater can be calculated with CSOIL 2000, however the model is mostly used to calculate the Intervention Value for groundwater. The direct consumption of groundwater is only very scarcely done. Therefore the exposure of humans via drinking contaminated groundwater is not included in the total human exposure of CSOIL 2000.

Appendix 7 gives the equation that can be used to determine the maximal permissible concentration in groundwater.

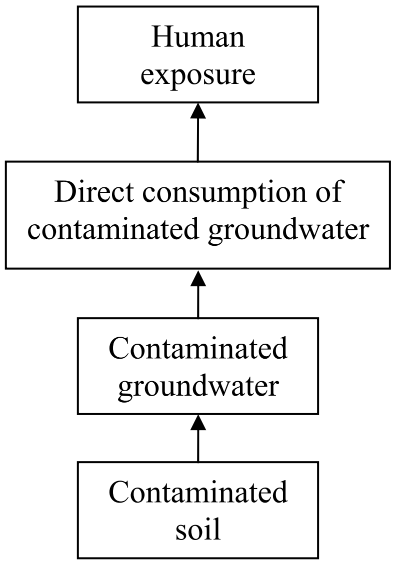

Figure 3.9: Route of exposure via direct consumption contaminated groundwater.

4 Model parameters

4.1 Constants and site parameters

CSOIL 2000 uses general parameters (e.g. gas constants et cetera.) to calculate the human risk. This paragraph gives an overview of the general constants and parameters. The following paragraphs will show the specific human related parameters that belong to the different exposure routes mentioned in chapter 3.

Table 4.1 shows the constants and site specific parameters for the user scenario 'Residential with garden'. It was chosen to only describe the parameters for 'Residential with garden', because this is the standard user scenario for deriving the intervention values soil.

Table 4.1: The constants and site specific parameters for 'Residential with garden' (Otte et al. 2001).

Parameters	Module	Abbreviation/ code	Value	Unit
Gas constant	Air	R	8.3144	[$Pa.m^3. mol^{-1}.K^{-1}$]
Viscosity of air	Air	ETA	$5 \cdot 10^{-09}$	[Pa.h]
Mean depth of contamination	Air	dp	1.25	[m]
Air permeability of soil	Air	KAPPA	$1 \cdot 10^{-11}$	[m^2]
Depth of groundwater table	Air	Dg	1.75	[m]
Height of the capillary transition boundary	Air	z	0.5	[m]
Air pressure difference crawl space	Air	DELTAPCS	1	[Pa]
Fraction dry matter root crops	Crop	fdwr	0.167	[-]
Fraction dry matter leafy crops	Crop	fdws	0.098	[-]
Deposition constant	Crop	dpconst	0.01	[-]
Temperature bathing water	Water	Tsh	313	[K]
Liquid exchange speed	Water	Kl	0.2	[$m.h^{-1}$]
Gas phase mass transport coefficient	Water	Kg	29.88	[$m.h^{-1}$]

4.2 Soil (partitioning) parameters

Soil characteristics are known to have a high influence on the calculated risk limits. It was therefore necessary to evaluate these parameters. The model is equipped with a default soil that contains, a pH of 6, organic matter content of 10% and a clay content 25% (Lijzen et al. 2001). Still it is possible to change these default settings to the specific soil in question.

The general influence of the different parameters decrease in the following order: density of the solid phase > organic matter content > depth of contamination > depth of groundwater table > contribution of crop consumption from own vegetable garden to total vegetable consumption > pore air fraction.

Table 4.2 shows the soil specific parameters for the user scenario 'Residential with garden'.

Table 4.2: Soil parameters for partition soil, water and air in 'Residential with garden' (Otte et al. 2001).

Soil parameters	Abbreviation/code	Value	Unit
Soil temperature	T	283	[K]
Volume fraction air	Va	0.2	[-]
Volume fraction water	Vw	0.3	[-]
Volume fractions soil	Vs	0.5	[-]
Fraction organic carbon	F_{oc}	0.058*	[-]
Percentage clay	L	25*	[%]
Dry bulk density	SP	1.2	[kg.dm^{-3}]
pH	pH	6*	[-]

** These values differ from the recommended value see also Lijzen et al.(2001).*

4.3 Soil ingestion, inhalation and dermal uptake module

4.3.1 Soil ingestion

Exposure to contaminants via soil ingestion depends mainly on the amount of soil that is ingested daily by children/adults (AIDc,a). The amount of ingested contaminant via this route also depends on the concentration in the soil (Cs), the relative absorption factor (Fa) and the bodyweight of the child (BWc,a). See Appendix 2.1. In Otte et al. (2001) the background of the soil ingestion is discussed.
The relative absorption factor Fa is default set at 1. This means that the absorption is assumed to be evenly high as the absorption that was present in the toxicological study on which the MPR was based. Only for lead this value can be adjusted.
Table 4.3 shows the default parameters used to calculate the exposure via soil ingestion.

Table 4.3: Exposure parameters for soil ingestion for a child/ adult for 'Residential with garden' (Otte et al. 2001).

Exposure parameters soil ingestion	Abbreviation/code		Value		Unit
	Child	Adult	Child	Adult	
Soil ingestion	AIDc	AIDa	$1.00 \cdot 10^{-4}$	$5.00 \cdot 10^{-5}$	[kg dry weight.day^{-1}]
Relative absorption factor	Fa	Fa	1	1	[-]
Bodyweight	BWc	BWa	15	70	[kg]

4.3.2 Soil inhalation

The inhalation of soil particles (indoors/outdoors) depends on the concentration of the contaminant in the soil (Cs), the amount of inhaled dust particles for a child/adult (ITSPc/ITSPa), the relative absorption factor (Fa), the retention factor of the soil particles in the lungs (Fr) and the bodyweight of the child/adult(BWc/ BWa). See Appendix 2.2.

The amount of inhaled dust particles (indoors/outdoors) for a child/adult is set as a default parameter value. This parameter was calculated with the following default values: amount of suspended particles in air (TSp) indoors/outdoors, the fraction of soil particles in the air (frs) indoors/outdoors, the air volume of a child/adult (AVc/AVa), the length of time a child/adult is exposed indoors/outdoors (t) and a correction factor of the time exposure from daily to yearly (tf) for an child/adult when indoors/outdoors.

Table 4.4 shows the default exposure parameters for the exposure during soil inhalation.

Table 4.4: Exposure parameters for soil inhalation for a child/adult when indoors/outdoors for 'Residential with garden' (Otte et al. 2001).

Exposure parameters soil inhalation	Abbreviation/ code		Value				Unit
	Child	Adult	Child		Adult		
Amount of inhaled dust	ITSPc	ITSPa	$3.13 \cdot 10^{-7}$		$8.33 \cdot 10^{-7}$		[kg.day^{-1}]
Relative sorption factor	Fa	Fa	1		1		[-]
Retention factor soil in lungs	Fr	Fr	0.75		0.75		[-]
Air volume	AVc	AVa	0.317		0.833		[m^3.h^{-1}]
			Indoor	Outdoor	Indoor	Outdoor	
Amount of suspended particles in air	TSP	TSP	52.5	70	52.5	70	[µg.m^{-3}]
Fraction soil particles in air	frs	frs	0.8	0.5	0.8	0.5	[-]
Length of time of exposure	t	t	16	8	8	8	[h]
Correction factor daily → yearly	tf	tf	1.322	0.357	2.856	0.143	[-]

4.3.3 Dermal uptake

Within the exposure route dermal uptake, a difference is made between contact indoors and contact outdoors. The difference between these routes is the fraction of soil indoors (Frsi). The dermal exposure further depends on the concentration in soil (Cs), exposed surface area of skin for a child/adult when indoors/outdoors (AEXPci,o/AEXPai,o), the matrix factor dermal uptake (fm), degree of covered skin indoors/outdoors for child/adult (DAEci,o/DAEai,o), the dermal absorption velocity of a child/adult(DARc,a) and the period of exposure through contact with soil indoors/outdoors for child/adult (TBci,o/TBai,o). See Appendix 2.3.

The period of exposure through contact with soil is calculated with the help of the parameters, time of exposure indoors/outdoors for a child/adult (t_ci,o/t_ai,o) and a correction factor of the time exposure from daily to yearly (tf_ci,o/tf_ai,o) for a child/adult when indoors/outdoors.
Table 4.5 shows the exposure parameters for dermal uptake.

Table 4.5: Exposure parameters for dermal uptake for a child/adult when indoors/outdoors for 'Residential with garden' (Otte et al. 2001).

Exposure parameters dermal uptake	Abbreviation/ code		Value				Unit
	Child	Adult	Child		Adult		
Fraction of soil indoors	Frsi	FRSi	0.8		0.8		[-]
Dermal absorption velocity	DARc	DARa	0.01		0.005		[h^{-1}]
The matrix factor dermal uptake	Fm	Fm	0.15		0.15		[-]
			Indoor	Outdoor	Indoor	Outdoor	
Exposed surface area of skin	AEXPci,o	AEXPai,o	0.05	0.28	0.09	0.17	[m^2]
Degree of coverage skin	DAEci,o	DAEai,o	$5.6 \cdot 10^{-4}$	$5.1 \cdot 10^{-3}$	$5.6 \cdot 10^{-4}$	$3.8 \cdot 10^{-2}$	[$kg.m^{-2}$]
Average period of exposure with soil	TBci,o	TBai,o	9.14	2.86	14.86	1.14	[$h.day^{-1}$]
Duration of exposure	t_ci,o	t_ai,o	8	8	8	8	[$h.day^{-1}$]
Correction factor daily → yearly	tf_ci,o	tf_ai,o	1.143	0.357	1.857	0.143	[$h.day^{-1}$]

4.4 Air module

In the exposure route inhalation of air, a difference is made for inhalation of indoor air and outdoor air, due to differences in concentrations (Waitz et al. 1996). The inhalation of air depends on the concentration of the compound in the air indoors/outdoors (CIA2/COAc,a), inhalation period of a child/adult indoors/outdoors (TIIc,a/TIOc,a), the air volume of a child/adult when indoors/outdoors (AVc,a), the relative sorption factor (Fa) and the bodyweight of a child/adult (BWc,a). See Appendix 3.3 and 3.4.
Table 4.6 shows the exposure parameters for inhalation of air indoors/outdoors.

Table 4.6: Exposure parameters for inhalation of air for a child/adult when indoors/outdoors for 'Residential with garden' (Otte et al. 2001).

Exposure parameters Inhalation of air	Abbreviation/code		Value				Unit
	Child	Adult	Child		Adult		
			Indoor	Outdoor	Indoor	Outdoor	
Inhalation period	TIi,oc	TIi,oa	21.14	2.86	22.86	1.14	[$h.d^{-1}$]
Air volume	AVc	AVa	0.317		0.883		[$m^3.h^{-1}$]
Relative sorption factor	Fa	Fa	1		1		[-]

The concentration of compound in the indoor/outdoor air is calculated by CSOIL 2000. The concentration in the outdoor air is determined by, dilution velocity of a child/adult (VFc,a) and the diffusion flux from the soil-water to surface level (Dfs). The concentration of compound in the indoor air is influenced by the concentration in the air of the crawlspace of a

building (CBA), the total contaminant flux from the soil to the crawl space (Jcs), the height of the crawlspace (Bh) and the ventilation void of crawlspace air (Vv).
The indoor air concentration can than be determined if the fraction of indoor air from crawlspace air (fbi) is known.
Table 4.7 shows the parameters of the concentration in air. See Appendix 3.1 and 3.2.

Table 4.7: Exposure parameters for compound concentration in air for a child/adult when indoors/outdoors for 'Residential with garden' (Otte et al. 2001).

Exposure parameters concentration of air	Abbreviation/code		Value		Unit
	Child	Adult	Child	Adult	
Dilution velocity	VFc	VFa	161.3	324.6	[m.h^{-1}]
Height crawl space	Bh	Bh	0.5	0.5	[m]
Air exchange rate crawlspace	Vv	Vv	1.1	1.1	[h^{-1}]
Contribution of the crawl space air to indoor air	fbi	fbi	0.1	0.1	[-]

4.5 Water module

4.5.1 Permeation in drinking water

Within the water module two exposure routes are calculated, the uptake by drinking contaminated water and the dermal uptake and inhalation of water vapours during showering. First the concentration in drinking water is determined; this depends on the type of water pipeline (waterl), the drinking water constant (dwconst), permeation coefficient (DPe), content of pore water (Cpw) and the diameter of the contaminated area (LP).
Van den Berg gave a justification of the derived permeation coefficients based on the report of Vonk (1985), together with a detailed description of the interpretation of data. The selected values were accordingly reported by Van den Berg (1997).

The drinking water constant is determined by the duration of water stagnation in the pipeline (d1), the radius of the pipeline (r), the thickness of the pipe wall (d2) and the average daily water use (Qwd). If the average consumption of drinking water for a child/adult (QDWc,a) is known the exposure of humans can be calculated. See Appendix 4.1.
Table 4.8 shows the parameters of the exposure route permeation in drinking water.

Table 4.8: Exposure parameters of permeation in drinking water for 'Residential with garden' (Otte et al. 2001).

Exposure parameters permeation in drinking water	Abbreviation/code	Value		Unit
Drinking water constant	dwconst	45.6		[-]
Diameter contaminated area	LP	100		[m]
Duration of water stagnation	d1	0.33		[d]
Radius of pipeline	r	0.0098		[m]
Thickness of pipe wall	d2	0.0027		[m]
Average daily water use	Qwd	0.5		[m^3]
		Child	Adult	
Drinking water consumption	QDWc,a	1	2	[dm^3.d^{-1}]

4.5.2 Inhalation and dermal uptake during showering and bathing

If the concentration of the compound in the drinking water is known, CSOIL 2000 can calculate the exposure via inhalation of water vapours and dermal uptake during showering/bathing. More information about these parameters can be found in Otte et al. (2001). The concentration in the bathroom air depends on, the concentration in drinking water (Cdw) and the evaporation of the compound (Kwa). The exposure via the bathroom air (Cbk) can than be calculated with the air volume of a child/adult (Avc,a) and the residence time in the bathroom (Td).
Table 4.9 shows the exposure parameters of the inhalation of water vapours during showering. See Appendix 4.4.

Table 4.9: Exposure parameters for a child/adult for inhalation of water vapours during showering for 'Residential with garden' (Otte et al. 2001).

Exposure parameters inhalation of water vapours during showering	Abbreviation/code		Value		Unit
	Child	Adult	Child	Adult	
Air volume	AVc	AVa	0.317	0.833	$m^3.h^{-1}$
Residence time bathroom	Td	Td	0.5	0.5	$h.d^{-1}$

The exposure of dermal contact depends on the concentration in the drinking water (Cdw), the body surface of a child/adult (ATOTc,a) the fraction exposed skin during showering/bathing (Fexp), the showering/bathing time per event (tdc), dermal absorption speed while showering/bathing (DARw), the evaporation of the compound (Kwa), the relative sorption factor (Fa) and the bodyweight of a child/adult (BWc,a).
Table 4.10 shows the parameters of the exposure dermal contact during showering.
See Appendix 4.5.

Table 4.10: Exposure parameters of dermal contact during showering for a child/adult For 'Residential with garden'(Otte et al. 2001).

Exposure parameters dermal contact during showering	Abbreviation/code		Value		Unit
	Child	Adult	Child	Adult	
Body surface	ATOTc	ATOTa	0.95	1.80	m^2
Fraction exposed skin	Fexp	Fexp	0.40	0.40	[-]
Showering time	tdc	tdc	0.25	0.25	$h.d^{-1}$
Bathing time	td	td	0.5	0.5	$h.d^{-1}$
Relative sorption factor	Fa	Fa	1	1	[-]

4.6 Crop module

The exposure due to consumption of crops is divided in the exposure via the root of the plants and exposure via the leafs of the plants. First the concentration in the vegetation has to be calculated. This concentration is for organic compounds dependent on the concentration of the compound in the soil pore water (Cpw), the bioconcentration factor of the root/leaf (BCFroot/BCFleaf) and the relation between dry weight and fresh weight of the root/leaf (Fdwr/Fdws). For the leafs two extra parameters must be included, the deposition constant (Dpconst) and the concentration of the compound in the soil (Cs).

Metals

For metals the average consumption amount in the vegetation (Cpr1) only depends on the empirically found average bioconcentration factor (BCFrme) and the concentration in the soil (Cs).

Once the concentration in the vegetation in known, the exposure can be calculated. The exposure for metal compounds depends on the daily consumption of root/leafy crops by a child/adult (DCCc/DCCa), the average metal consumption in the vegetation (Cpr1), the relative absorption factor (Fa) and the bodyweight of a child/adult (BWc,a). The average daily consumption of root crops and leafy crops (DCCc/DCCa) is determined by, the amount of consumed root crops/leafy crops (QKc,a/QBc,a), the dry weight of root/leafy crops (Fdwr/Fdws) and the fraction contaminated root/leafy crops (fvk/fvb). See Appendix 5.3.

Organic compounds

For the organic compounds the exposure depends on the concentration of organic compounds in the root/leafy crops (Cpro/Cpso), the amount of consumed root crops/leafy crops (QKc,a/QBc,a), the fraction contaminated root/leafy crop (fvk/fvb), the relative sorption factor (Fa) and the bodyweight of a child/adult (BWc,a). See Appendix 5.3.

Table 4.11 shows the parameters for the exposure via vegetation.

Table 4.11: Exposure parameters for exposure via vegetation for child/adult for 'Residential with garden' (Otte et al. 2001).

Exposure parameters vegetation	Abbreviation/ code				Value				Unit
	Root		Leaf		Root		Leaf		
Deposition constant (organic compounds)	Dpconst		Dpconst		0.01		0.01		Kg dw soil.kg^{-1} dw plant
Fraction con. crops	fvk		fvb		0.1		0.1		[-]
Organic compounds	Child	Adult	Child	Adult	Child	Adult	Child	Adult	
Consumption of crops	QKc	QKa	QBc	QBa	59.5	122.0	58.3	139.0	[g dw.d^{-1}]
Relative sorption factor	Fa				1				[-]
Dilution velocity plant	VFp				84				[m.h^{-1}]
Metals									
Daily consumption root/leafy crops	DCCc	DCCa	DCCc	DCCa	1.565		3.40		[g dry weight.d^{-1}]
Dry weight crops	Fdwr		Fdws		0.167		0.098		[-]

4.7 Compound specific parameters

CSOIL 2000 uses compound specific parameters to make fugacity calculations. These parameters are set as default in the model. However it is possible for the user to adjust some of these parameters to fit the conditions at the contaminated location.

Table 4.12 shows the compound specific parameters and abbreviations. The values are not given in this report. For the most recent values the report of Otte et al. (2001) can be used as a reference. Values for other compounds can be found in earlier reports (Van den Berg et al. 1994, Kreule et al. 1995, Kreule and Swartjes 1998).

Table 4.12: The compound specific parameters (Otte et al. 2001).

Parameter	Abbreviation/code	Unit
Molecular weight	M	[$g.mol^{-1}$]
Solubility	S	[$mg.dm^{-3}$]
Vapour pressure	Vp	[Pa]
Octanol-water coefficient	Log K_{ow}	[-]
Organic carbon normalised soil-water partition coefficient	Log K_{oc}	[$dm^3.kg^{-1}$]
Acid dissociation constant	PKa	[-]
Permeation coefficient	Dpe	[m^2 per day]
Soil water partition coefficient for metals	Kp	[$dm^3.kg^{-1}$]
Bioconcentration factor for metals in crops	BCF	[$kg.kg^{-1}$]

In Otte et al. (2001) the values and the principle of the kind of data (search) that is used, can be found. For some empirical data are preferred, when for other QSARS or relations are used.

5 Human exposure

5.1 Human toxicological risk limits

The MPR_{human} is defined as the amount of a substance (usually a chemical substance) that any human individual can be exposed to daily during a full lifetime without significant health risk. It covers both oral and inhalation exposure (and if necessary also dermal exposure), and classical toxic risks as well as carcinogenic risks. The MPR_{human} can be expressed as a tolerable daily intake (TDI) or an excess carcinogenic risk via intake (CR_{oral}), both covering exposure by oral ingestion. The MPR_{human} can also be expressed as a tolerable concentration in air (TCA) or an excess carcinogenic risk via air (CR_{inhal}), both covering exposure by inhalation (Baars et al. 2001). The procedure to derive MPR_{human} is outlined in detail by Janssen and Speijers (1997). See also section 2.3 for an explanation how to calculate with these risk limits.

5.2 Total human exposure

The total human exposure is determined by the combined exposure of each different exposure route. CSOIL 2000 calculates the actual exposure and the relative exposure of the different exposure routes for children, adults and average lifetime. The total human exposure is calculated in several steps.

Step 1: Individual exposure per route
CSOIL 2000 first calculates the individual exposure of each route separately. This includes for example the exposure due to soil ingestion.

Step 2: Summation of exposure route
After the individual calculations the exposures are divided over two semi total exposures, these are total exposure by inhalation and total exposure by oral and dermal contact.
In the exposure via inhalation, the individual exposures inhalation of soil particles, inhalation of indoor air, inhalation of outdoor air and via inhalation of vapours during showering are included and added up.
In the exposure via oral and dermal contact, the individual exposure via ingestion of soil, dermal contact soil indoors, dermal contact outdoors, ingestion of crops, permeation of drinking water and dermal contact with drinking water during showering are included and added up. See also Appendix 6.

Step 3: Combination of exposure via inhalation and via oral and dermal contact
In the Netherlands the exposure via inhalation is compared with the TCA (Total Concentration in Air). The exposure via oral and dermal contact is compared with the MPR_{oral} (Acceptable Daily Intake). However, the TCA and MPR are not the same and can therefore not be added without a correction. The TCA can be, with help of the inhaled air volume and bodyweight converted, in a MPR_Ac,a for a child or adult
(MPR = Maximal Permissible Risk). This is only done to prevent that both the TCA and MPR are filled up and the exposure gets to high. See section 2.3 and Appendix 6.3.

Step 4: Corrected risk
Based on the summed risk it is now possible to calculate the for MPR_Ac,a corrected total exposure for a child or adult. See Appendix 6.3.

5.3 Standard scenario

The different routes of exposure are not the only variables that determine the average exposure to a contaminant. The user scenarios or soil functions also influence this exposure. CSOIL 2000 is equipped with a standard scenario and, when no changes are made in the input sheet, this scenario is used to calculate the soil quality criteria.

The standard scenario is called ‘Residential with garden’ and it describes a residential area where it is assumed, that a house has a garden. This garden may be used to grow crops however the garden has a bigger recreational function, than a cultivation function. The garden is therefore not a kitchen, -vegetable garden. For the differences between a normal garden and a kitchen, -vegetable garden scenario see section 5.4.
The exposure within the standard user scenario is possible via every exposure route described in chapter 3.
The standard scenario was used to calculate the proposals for Dutch soil quality criteria in 2001.

The standard scenario has also some default parameters concerning exposure routes.
Table 5.1 shows these parameters.

Table 5.1: Default parameters for the standard soil user scenario ‘Residential with garden’.

Default parameters	Child	Adult	Unit
Contact frequency	125	50	[days.year^{-1}]
Soil ingestion yearly average	100	50	[mg.day^{-1}]
Contact time per event	8	8	[h]
Time indoors	21.14	22.86	[h.day^{-1}]
Time outdoors	2.86	1.14	[h.day^{-1}]
Percentage root crops from own garden	10	10	[%]
Percentage leafy crops from own garden	10	10	[%]

5.4 Other soil user scenarios

Next to the standard scenario, CSOIL 2000 also includes different soil user scenarios for the calculation of critical soil concentrations. These scenarios vary from close contact to minimal contact for children and adults. It is important to make this difference in user scenarios, because not every scenario poses the same risk to humans. The soil function determines if and to what extend people come into contact with soil contamination. For example a garden may have a higher influence on the exposure, than an industrial area. This is due to the contact of people with soil. In a garden the contact with soil is much higher than in an industrial area.

Within CSOIL 2000 there are currently six different soil user scenarios next to the standard scenario. In 2005 and earlier 8 scenario's were distinguished. These scenarios and their relation with the revised scenarios are given in Appendix 8.
The soil user scenarios that CSOIL 2000 recognizes are:

1) residential with garden (standard scenario);
2) places where children play;
3) kitchen, -vegetable garden;
4) agriculture without farm (yard);
5) nature;
6) green with nature, sports, recreation and city parks;
7) other greens, buildings, infrastructure and industry.

The seven soil user scenarios are newly subscribed by the policy workgroup NOBO (Policy workgroup on Soil quality standards and Soil quality assessment) and will be implemented in CSOIL 2000.
Some of the scenarios are combined with older scenarios (dating from the previous model). Below the new scenarios will be shortly explained.

1) Residential with garden (standard scenario)
See section 5.3 for a description of the standard scenario

2) Places where children play
This scenario includes places that children often use to play; examples are playgrounds, grass plots, playing fields, gardens near schools and other green places that children use. For both adults and children the ingestion frequency is equal to the scenario 'Residential with garden'. Exposure within this scenario can take place along every described route with the exception of uptake by plants. The exposure is calculated for children and adults.

3) Kitchen, -vegetable garden
Residential with kitchen, -vegetable garden is similar to the user scenario 'Residential with garden', except that it includes a vegetable garden in which more vegetables and potatoes are grown than in a normal garden. The diet of people who own a vegetable garden contains most likely a large part of the crops cultivated in this garden. The vegetables are grown for own consumption (and not for commercial purposes). The exposure can take place via each of the exposure routes.
The contact frequency and soil ingestion of children and adults is equal to the standard user scenario 'Residential with garden'.

4) Agriculture without farm (yard)
The user scenario agriculture without farm (yard) includes the production area of a farmer without a farm or premises. It is possible to make a difference between various types of agriculture namely: grassland, arable farming and crop farming.
The soil contact frequency is equal to the scenario 'Residential with garden'. It must be mentioned that the soil contact frequency for the farmer can be much higher. However this is seen as an occupational hazard.

5) Nature
Within the user scenario nature the exposure only takes place outdoors. It is also assumed that humans are not exposed via drinking water and growth of crops. In average people remain in a nature reserve for one hour a day. The contact frequency is five times lower, than in the scenario 'Residential with garden'.

6) Green with nature values, sports, recreation and city parks
Within this user scenario many recreational utilities are included. Examples are sports fields, city parks and beaches. No vegetables are grown in these areas and therefore this is the only route of exposure, which does not contribute to the total human exposure.
There is a lower chance of soil ingestion and therefore the exposure frequency is 5 times lower than the scenario 'Residential with garden'.
If there are special places for children to play, these locations should be treated as the scenario 'Places where children play'.

7) Other greens, buildings, infrastructure and industry
Within the scenario other greens, buildings, infrastructure and industry no vegetables are grown and therefore exposure can take place via every route, except for uptake by plants. The time that people spend on each of the sublocations (industrial, infrastructure et cetera) is highly diverse. Buildings and industry usually includes a working day for people (40 hours per week inside and 7 hours per week outside). However for infrastructure this time reduces to one hour a day. If really only adults are present at the location, the exposure for children is not taken into account.

5.5 Parameters soil user scenarios

The parameters that have been described in section 5.2 for the standard scenario also apply for the other user scenarios. However for some of the scenarios these parameters have been adapted. Table 5.2 shows the parameters for all soil user scenarios.

Table 5.2: Default parameters for the different user scenarios other than the standard scenario of CSOIL 2000.

Soil user scenario	Child or adult	Contact frequency (days. year^{-1})	Soil ingestion yearly average (mg.day^{-1})	Contact time per event (h)	Time indoors (h.d^{-1})	Time outdoors (h.d^{-1})	Percentage root crops from own garden (%)	Percentage leafy crops from own garden (%)
1*	Child	125	100	8	21.14	2.86	10	10
	Adult	100	50	8	14.86	1.14		
2*	Child	125	100	8	9.14	2.86	0	0
	Adult	50	50	8	14.86	1.14		
3*	Child	125	100	8	21.14	2.86	50	100
	Adult	50	50	8	22.86	1.14		
4*	Child	125	100	8	0	2.86	10	10
	Adult	50	50	8	0	1.14		
5*	Child	25	20	8	0	1	0	0
	Adult	10	10	8	0	1		
6*	Child	25	20	8	0	1	0	0
	Adult	10	10	8	0	1		
7*	Child	25	20	8	6	1	0	0
	Adult	10	10	8	6	1		

* 1) residential with garden;
2) places where children play;
3) kitchen, -vegetable garden;
4) agriculture;
5) nature;
6) green with nature values, sports, recreation and city parks;
7) other greens, buildings, infrastructure and industry.

6 Related reports

On one hand this report is based on various reports. For the different subjects it is already referred to throughout this report. On the other hand, the model CSOIL is used in several projects during the last 10 years. In this chapter both aspects are summarised by referring to related reports of these projects. Other useful reports are mentioned in the references.

The most important reports that support CSOIL can be divided in reports before and after 2001. The relevant report related to CSOIL **before 2001** are:

- Berg van den R., and Roels, J.M. (1991). Risk assessment to man and the environment in case of exposure to soil contamination. Integration of different aspects. RIVM, Bilthoven, The Netherlands. RIVM report No. 725201013.
  This is the first report in which CSOIL is used for deriving human-toxicological risk limits, that are integrated with eco(toxico)logical risk assessment
- Berg van den R. (1995). Exposure of man to soil contamination. A qualitative and quantitative analysis, resulting in proposals for human-toxicological C values. RIVM, Bilthoven, The Netherlands. Partly revised version, RIVM report No. 725201011 (in Dutch RIVM-report 725201006)
  This is the report that describes the old CSOIL version. Nevertheless it is an important resource to understand the background and initial version of CSOIL and the parts that have not been revised.
- Berg van den R., Bockting G.J.M., Crommentuijn G.H., Jansen P.J.C.M. (1994). Proposals for intervention values for soil clean-up: Second series of chemicals. RIVM, Bilthoven, The Netherlands. RIVM Report No. 715810004.
  In this report the same methodology is applied for the second series of compounds as was done for the first series in 1991.
- Kreule P., Berg van den R., Waitz M.F.W., Swartjes F.A. (1995). Calculation of human-toxicological serious soil contamination concentrations and proposals for the intervention values for clean-up of soil and groundwater: Third series of compounds. RIVM, Bilthoven, The Netherlands. RIVM Report No. 715810010.
  In this report the same methodology is applied for the third series of compounds.
- Kreule P. and Swartjes F.A. (1998). Proposals for intervention values for soil and groundwater, including the calculation of the human toxicological serious soil contamination concentrations: Fourth series of compounds. RIVM, Bilthoven, The Netherlands. RIVM Report No. 711701005.
  In this report the same methodology is applied for the fourth series of compounds.
- Waitz M.F.W., Freijer J.I., Kreule P., Swartjes F.A. (1996). The VOLASOIL risk assessment model based on CSOIL for soils contaminated with volatile compounds. RIVM Bilthoven, The Netherlands. RIVM, report No.715810014.
  VOLASOIL is a different model that is an improvement of the volatilisation model of CSOIL. Further development of the model will be incorporated in a revised site-specific version of CSOIL in 2007.

- Vissenberg, H.A. and Swartjes F.A. (1996). Evaluatie van de met CSOIL berekende blootstelling, middels een op Monte Carlo-technieken gebaseerde gevoeligheids- en onzekerheidsanalyse. RIVM, Bilthoven, The Netherlands. RIVM report No.715810018.
  In this report an uncertainty and sensitivity analysis is carried out to make clear what the most important parameters in CSOIL are. With the new CSOIL version it is not expected to change substantially.
- Lijzen J.P.A., Baars A.J., Crommentuijn G.H., Otte P.F., Plassche van de E., Rikken M.G.J., Rompelberg C.J.M., Sips A.J.A.M., Swartjes F.A. (1999). Revision of the Intervention value for lead; evaluation of the intervention values derived for soil/sediment and groundwater. RIVM, Bilthoven, The Netherlands. RIVM report No.711701013 (in Dutch).
  Prior to the evaluation of many compounds in 2001 the risk limits for lead were evaluated and reported with a partially revised CSOIL version.

The relevant report related to CSOIL in and **after 2001** are:

- Versluijs C.W. and Otte P.F. (2001). Accumulatie van metalen in planten. Een bijdrage aan de technische evaluatie van de interventiewaarden en de locatiespecifieke risicobeoordeling van verontreinigde bodem. RIVM, Bilthoven, The Netherlands RIVM report No.711701024.
  In the report data for uptake of metals in plants are analyzed and relationships between plant concentrations and soil characteristics are derived where possible. Also the proposals for generic bioconcentration factors (BCF) are given in this report. The proposed values are implemented in CSOIL 2000.
- Otte P.F., Lijzen J.P.A., Otte J.G., Swartjes F.A., Versluijs C.W. (2001). Evaluation and revision of the CSOIL parameters set. RIVM, Bilthoven, The Netherlands. RIVM report No.711701021.
  In this report the most relevant parameters of the CSOIL model are evaluated in the project of evaluation of intervention values of 1999-2001. Compound specific data for compounds of the first series can also be found in this report.
- Rikken M.G.J, Lijzen J.P.A., Cornelese A.A. (2001). Evaluation of model concepts on human exposure. Proposals for updating the most relevant exposure routes for CSOIL. RIVM, Bilthoven, The Netherlands RIVM report No.711701022.
  In this report the most relevant model concepts of the CSOIL model are evaluated in the project of evaluation of intervention values of 1999-2001.
- Baars A.J., Theelen R.M.C., Janssen P.J.C.M., Hesse J.M., Apeldoorn van M.E., Meijerink M.C.M., Verdam L., Zeilmaker M.J. (2001). Re-evaluation of human-toxicological maximum permissible risk levels. RIVM, Bilthoven, The Netherlands. RIVM report No. 711701025.
  In this report the procedure for deriving MPR-values is described; also the revised MPR- values for the first series of compounds are presented.
- Lijzen J.P.A., Baars A.J., Otte P.F., Rikken M., Swartjes F.A., Verbruggen E.M.J, Wezel van A.P. (2001). Technical evaluation of the intervention values for soil/sediments and groundwater. Human and ecotoxicological risk assessment and derivation of risk limits for soil, aquatic sediment and groundwater. RIVM, Bilthoven, The Netherlands. RIVM report No.711701023.
  This is the integration report of all reports that are made for the evaluation of the Interventions values soil and groundwater for the first series of compounds. It also described the general procedure for deriving proposals for intervention values soil and groundwater.

- Lijzen J.P.A., Mesman M., Aldenberg T., Mulder C.D., Otte P.F., Posthumus R., Roex E., Swartjes F.A., Versluijs C.W., Vlaardingen van P.L.A., Wezel van A.P., Wijnen van H.J. (2002). Evaluation of the underpinning of the Soil-use specific remediation objectives (SROs). RIVM, Bilthoven, The Netherlands. RIVM report No. 711701029 (in Dutch).
  In 1999 Land-use specific remediation objectives (BGW in Dutch) were derived. The human risk assessment of these risk limits have been revised using the CSOIL 2000 values. These values were not implemented.
- Wezel van A.P., Vries de W., Beek M., Otte P.F., Lijzen J.P.A., Mesman M., Vlaardingen van P.L.A., Tuinstra J., Elswijk van M., Römkens P., Bonten L. (2003). Bodemgebruikswaarden voor Landbouw, Natuur en Waterbodem. Technisch wetenschappelijke afleiding van getalswaarden. RIVM, Bilthoven, The Netherlands. RIVM report No.711701031.
  In this report also exposure scenarios for agricultural soil use were added and human-toxicological risk limits for soil were derived with CSOIL for these scenarios. The land-use specific quality standards derived in this way are not implemented.
- Swartjes, F.A. et al. in prep. Towards a protocol for the site-specific human health risk assessment for the consumption of vegetables of contaminated sites. RIVM, Bilthoven, The Netherlands. RIVM report No. 711701040.
  CSOIL 2000 will be extended for site specific risk assessment. With the recommendations of this report the module on plant uptake will be adjusted and improved.
- Bakker J. et al. in prep. Site specific human-toxicological risk assessment of soil contamination with volatile compounds. RIVM, Bilthoven, The Netherlands. RIVM report No. 711701049.
  CSOIL 2000 will be extended for site specific risk assessment. With the recommendations of this report the module on volatilisation to indoor air will be expanded with more scenarios.
- Dirven-Van Breemen, E.M. et al. in prep. Landelijke Referentiewaarden ter onderbouwing van Maximale waarden. RIVM, Bilthoven, The Netherlands. RIVM report No. 711701053 (in Dutch).
  In this report the soil use specific quality criteria are derived in analogy with Lijzen et al. (2002) and Van Wezel et al. (2003). These values will be implemented in the Dutch soil policy in 2007 for the reallocation of soil and as soil use specific remediation objectives. CSOIL was used to derive the human-toxicological risk limits for soil based on adjusted human exposure scenarios.

7 Abbreviations and glossary

7.1 Abbreviations

ADI	Acceptable Daily Intake: the measurement of the amount of any chemical substance that can be safely consumed by a human being in a day.
BCF	Bioconcentration Factor: the ratio of the substance concentration in (part of) an organism (e.g. plant, fish) to the concentration in a medium (e.g soil, water) at steady state.
$CR_{oral/inhal}$	Excess carcinogenic risk via oral, dermal or inhalative risk.
CSOIL	Exposure model used to derive human-toxicological risk limits for soil and groundwater. CSOIL 2000 refers to the most recent version of the model.
LDPE	Low Density Polyethylene: a plastic that is used to make water pipelines, plastic bottles et cetera.
MPR_{human}	Maximal Permissible Risk: for substances without a threshold below which there are no effects (e.g. carcinogens), the MPR is defined as the concentration at which there is annually 1 death per million. For substances with a threshold level, the MPR for humans is set to the exposure level without effect NOAEL.
NOAEL	No Observed Adverse Effect Level: greatest concentration or amount of a substance, found by observation or experiment, which causes no detectable adverse effect. Effects may be detected at this level, which are not judged to be adverse.
NOBO	Policy workgroup on Soil quality standards and Soil quality assessment.
PCDD/F	Polychlorinated dibenzodioxin and dibenzofuran: two members of the dioxin family which are unwanted by products of combustion of organic material.
QSAR	Quantitative Structure-Activity Relationship: toxicity tests with many chemicals have generated enough data to make equations that can be used to calculate toxicity and biodegradation based on chemical structure. The equations used are referred to as Quantitative Structure Activity Relationships or QSARs.
RIVM	Rijksinstituut voor Volksgezondheid en Milieu (Dutch), National Institute for Public Health and the Environment
$SCR_{human/eco}$	Serious Risk Concentrations: concentrations related to serious human or ecological risks.

TCA	Tolerable Concentration in Air: estimate of the amount of a substance that can be inhaled over a specified period of time without appreciable health risk.
TDI	Tolerable Daily Intake: estimate of the amount of a substance that can be ingested or absorbed over a specified period of time without appreciable health risk.

7.2 Glossary

Absorption	The uptake of water, other fluids, or dissolved chemicals by a cell or an organism (as tree roots absorb dissolved nutrients in soil).
Contamination	Introduction into or onto water, air, soil or other media of micro-organisms, chemicals, toxic substances, wastes, wastewater or other pollutants in a concentration that makes the medium unfit for its next intended use.
Critical exposure	General term referring to the concentration limit beyond which a substance can cause dangerous effects to living organisms. See also MPR.
Ecosystem	A dynamic complex of plant, animal and micro-organism communities and their non-living environment interacting as a functional unit.
Equilibrium	Equilibrium is any of a number of related phenomena in the natural and social sciences. In general, a system is said to be in a state of equilibrium if all influences on the system are cancelled by the effects of others. A related concept is stability; an equilibrium may or may not be stable.
Human health	The avoidance of disease and injury and the promotion of normalcy through efficient use of the environment, a properly functioning society, and an inner sense of wellbeing.
Indoor environment	Environment situated in the inside of a house or other building.
Leaves	The main organ of photosynthesis and transpiration in higher plants, usually consisting of a flat green blade attached to the stem directly or by a stalk. Within the model CSOIL 2000 the stem of a plant is also included in theconcept of leaves.
Lipophilicity	Measure of fat loving characteristics of a compound.

Outdoor environment	Environment situated in the outside of a house or other building.
Partition	Division of a compound over different soil phases.
Permeation	The ability of a membrane or other material to permit a substance to pass through it.
Rain splash	The relocation of soil particles on leaves of plants due to rain fall.
Risk assessment	The procedure in which the risks posed by inherent hazards involved in processes or situations are estimated either quantitatively or qualitatively.
Roots	The absorbing and anchoring organ of a plant. Roots used as food vegetables or fodder include carrots, parsnips and turnips; starchy root crops include potatoes, cassavas and yams.
Soil re-suspension	See rain splash
Solubility	The ability of a substance to form a solution with another substance.
Sorption	The action of soaking up or attracting substances; process used in many pollution control systems.
User scenario	The functions that a soil can have. Examples are industrial and residential functions.

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Appendix 1: Equations partition soil, water and air

1.1 Fugacity calculations

1.1.1 Organic compounds

♦ Za =1/R*T

Za	: fugacity constant air	[mol.m^{-3}.Pa^{-1}]
R	: gas constant	[8.3144 Pa.m^{3}.mol^{-1}.K^{-1}]
T	: temperature	[283 K]

♦ Zw =S/Vp

Zw	: fugacity constant water	[mol.m^{-3}.Pa^{-1}]
S	: solubility at soil temperature	[mol.m^{-3}]
Vp	: vapour pressure pure product	[Pa]

♦ Zs =Kd*SD*Zw/Vs

Zs	: fugacity constant soil	[mol.m^{-3}.Pa^{-1}]
Kd	: partition constant soil-water	[(mol.kg^{-1}dw)/(mol.dm^{-3})]
SD	: dry bulk density	[kg dw.dm^{-3} soil]
Zw	: fugacity constant water	[mol.m^{-3}.Pa^{-1}]
Vs	: volume fraction soil	[-]

Vs =1-porosity
=1-Va-Vw

Va	= volume fraction air	[-]
Vw	= volume fraction water	[-]

♦ Kd = K_{oc}*F_{oc}

Kd	: partition coefficient soil-water	[(mol.kg^{-1}dw)/(mol.dm^{-3})]
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} dw]

K_{oc} =0,411*K_{ow}*Fnd

K_{ow}	: octanol-water partition coefficient	[-]
Fnd	: fraction not dissociated compound	[-]

♦	Klw	= Vp/(S*R*T) or = Za/Zw	[-]

Klw	: air-water partition coefficient	[mol.m^{-3} air /mol.dm^{-3}water]
S	: solubility at soil temperature	[mol.m^{-3}]
R	: gas constant	[8.3144 Pa.m^{3}.mol^{-1}.K^{-1}]
T	: temperature	[283 K]
Za	: fugacity constant air	[mol.m^{-3}.Pa^{-1}]
Zw	: fugacity constant water	[mol.m^{-3}.Pa^{-1}]

1.2 Mass fraction calculations

1.2.1 Organic compounds and some inorganic compounds

- ♦ Pa = (Za*Va)/(Za*Va+Zw*Vw+Zs*Vs)
- ♦ Pw = (Zw*Vw)/(Za*Va+Zw*Vw+Zs*Vs)
- ♦ Ps = (Zs*Vs)/(Za*Va+Zw*Vw+Zs*Vs)

Pa	: mass fraction soil air	[-]
Pw	: mass fraction soil moisture	[-]
Ps	: mass fraction solid phase	[-]
Za	: fugacity constant air	[mol.m^{-3}.Pa^{-1}]
Zw	: fugacity constant water	[mol.m^{-3}.Pa^{-1}]
Zs	: fugacity constant soil	[mol.m^{-3}.Pa^{-1}]
Va	: volume fraction air	[-]
Vw	: volume fraction water	[-]
Vs	: 1-Va-Vw	[-]

1.2.2 Metals and some inorganic compounds

♦	Pa	= 0	[-]
♦	Pw	= Vw/(Vw+Kd*SD)	[-]
♦	Ps	= (1-PW)	[-]

Pa	: mass fraction in soil air	[-]
Pw	: mass fraction in soil moisture	[-]
Ps	: mass fraction in soil solid	[-]
Vw	: volume fraction water	[-]
Kd	: partition coefficient soil-water	[(mol.kg^{-1}dw soil)/ (mol.dm^{-3} water)]
SD	: dry bulk density	[kg dw.dm^{-3} dw soil]

1.3 Concentrations in air, water and soil

1.3.1 Organic compounds in air

♦ Csa = (Cs*SD*Pa)/Va

Csa	: concentration in soil air	[$g.m^{-3}$] or [$mg.dm^{-3}$]
Cs	: initial concentration in soil (total concentration in soil gas-, water and solid)	[$mg.kg^{-1}$]
SD	: dry bulk density	[$kg.dm^{-3}$]
Pa	: mass fraction in soil air	[-]
Va	: volume fraction air	[-]

If the solubility is exceeded:
If Cpw >S*M then:

♦ Csa = (S*M*Vw*Pa)/(Pw*Va)

Csa	: concentration in soil air	[$g.m^{-3}$] or [$mg.dm^{-3}$]
S	: solubility	[$mol.m^{-3}$]
M	: molecular weight	[$g.mol^{-1}$]
Vw	: volume fraction water	[-]
Pa	: mass fraction in soil air	[-]
Pw	: mass fraction on soil moisture	[-]
Va	: volume fraction air	[-]

1.3.2 Organic compounds and metals in water

♦ Cpw = Cs*SD*Pw/Vw

Cpw	: concentration in soil moisture	[$g.m^{-3}$] or [$mg.dm^{-3}$]
Cs	: initial concentration in soil (total concentration in gas-, water and solid)	[$mg.kg^{-1}$]
SD	: dry bulk density	[$kg.dm^{-3}$]
Pw	: mass fraction in soil moisture	[-]
Vw	: volume fraction in water	[-]

If the solubility is exceeded (verification only for organic compounds)
If Cpw >S*M then:

♦ Cpw = S*M

Cpw	: concentration in soil moisture	[$g.m^{-3}$] or [$mg.dm^{-3}$]
S	: solubility	[$mol.m^{-3}$]
M	: molecular weight	[$g.mol^{-1}$]

1.3.3 Inorganic compounds

Csa = 0

Csa : concentration in soil air [g.m^{-3}] or [mg.dm^{-3}]

1.3.4 Metals

Csa = 0

Csa : concentration in soil air [g.m^{-3}] or [mg.dm^{-3}]

Appendix 2: Equations soil ingestion, inhalation and dermal uptake

2.1 Exposure via soil ingestion

Conventions:

c	: child	
a	: adult	
L	: lifelong	
Fa	: relative sorption factor	[-]
BWc,a	: bodyweight (child 15, adult 70)	[kg]
Cs	: initial soil concentration (total concentration in gas-, water- and solid phase)	$[mg.kg^{-1}]$
Exposure, the lifelong average exposure		$[mg.kg^{-1}\ bw.d^{-1}]$
Lifelong		[70 year]

CHILD

♦ DIc = AIDc*Cs*Fa/BWc
= AIDc*Cs*Fag/BWc

DIc	: exposure via ingestion of soil - child	$[mg.kg^{-1}\ bw.d^{-1}]$
AIDc	: daily intake soil – child	$[1.0 \cdot 10^{-4} kg\ dw.d^{-1}]$
Cs	: initial soil concentration (total concentration in gas-, water- and solid phase)	$[mg.kg^{-1}]$
Fa	: relative absorption factor (general)	[-]
Fag	: relative absorption factor soil	[-]
BWc	: bodyweight child	[15 kg]

ADULT

♦ DIa = AIDa*Cs*Fa/BWa
= AIDa*Cs*Fag/BWa

DIa	: exposure via ingestion of soil – adult	$[mg.kg^{-1}\ bw.d^{-1}]$
AIDa	: daily intake soil - adult	$[5.0 \cdot 10^{-5} kg\ dw.d^{-1}]$
Cs	: initial soil concentration (total concentration in gas-, water- and solid phase)	$[mg.kg^{-1}]$
Fa	: relative absorption factor (general)	[-]
Fag	: relative absorption factor soil	[-]
BWa	: bodyweight adult	[70 kg]

LIFELONG AVERAGE

♦ DIL =(6*DIc+64*DIa)/70

DIL	: exposure via ingestion of soil lifelong average	$[mg.kg^{-1}\ bw.d^{-1}]$
DIc	: exposure via ingestion of soil lifelong average - child	$[mg.kg^{-1}\ bw.d^{-1}]$
DIa	: exposure via ingestion of soil – adult	$[mg.kg^{-1}\ bw.d^{-1}]$

2.2 Exposure via inhalation of soil particles

CHILD

♦ IPc = Cs*ITSPc*Fr*Fa/BWc

IPc	: exposure via inhalation of soil particles - child	[$mg.kg^{-1}$ $bw.d^{-1}$]
Cs	: initial soil concentration (total concentration in gas-, water- and solid phase)	[$mg.kg^{-1}$]
ITSPc	: inhaled amount of soil particles – child	[$3.13 \cdot 10^{-7}$ $kg.d^{-1}$]
Fr	: retention factor soil particles in lungs	[0.75 -]
Fa	: relative absorption factor	[-]
BWc	: bodyweight child	[15 kg]

ITSPc = TSP * frs * AVc * t * tf

TSP	: amount of suspended particles in air Indoors 0.75 * 70 = 52.5 $\mu g.m^{-3}$ Outdoors 70 $\mu g.m^{-3}$	[$mg.m^{-3}$]
frs	: fraction soil particles in air Indoors 0.8 Outdoors 0.5	[-]
AVc	: air volume child	[$0.317 m^3.h^{-1}$]
t	: length of time of exposure Indoors 16 h Outdoors 8 h	[h]
tf	: correction factor exposure daily → yearly - child Indoors 1.322 Outdoors 0.357	[-]

ADULT

♦ IPa = Cs*ITSPa*Fr*Fa/BWa

IPa	: exposure via inhalation of soil particles – adult	[$mg.kg^{-1}$ $bw.d^{-1}$]
Cs	: initial soil concentration (total concentration in gas-, water- and solid phase)	[$mg.kg^{-1}$]
ITSPa	: inhaled amount of soil particles – adult	[$8.33 \cdot 10^{-7}$ $kg.d^{-1}$]
Fr	: retention factor soil particles in lungs	[0.75 -]
Fa	: relative absorption factor	[-]
BWa	: bodyweight adult	[70 kg]

ITSPa = TSP * frs * AVa * t * tf

TSP	: amount of suspended particles in air Indoors 0.75 * 70 = 52.5 $\mu g.m^{-3}$ Outdoors 70 $\mu g.m^{-3}$	[$mg.m^{-3}$]
frs	: fraction soil particles in air Indoors 0.8 Outdoors 0.5	[-]
AVa	: air volume adult	[$0.833\ m^3.h^{-1}$]

t	: length of time of exposure Indoors 8 h Outdoors 8 h	[h]
tf	: correction factor exposure daily → yearly – adult Indoors 2.856 Outdoors 0.143	[-]

LIFELONG AVERAGE

♦ IPL = (6*IPc+64*IPa)/70

IPL	: exposure via inhalation of soil particles lifelong average	[$mg.kg^{-1}$ $bw.d^{-1}$]
IPc	: exposure via inhalation of soil particles – child	[$mg.kg^{-1}$ $bw.d^{-1}$]
IPa	: exposure via inhalation of soil particles – adult	[$mg.kg^{-1}$ $bw.d^{-1}$]

2.3 Exposure via dermal uptake

2.3.1 Dermal contact soil indoors (DA i)

CHILD

♦ DAci =AEXPci*Fm*DAEci*DARc*Cs*TBci*FRSi*Fa/BWc

DAci	: exposure via dermal contact soil child – indoors	[$mg.kg^{-1}$ $bw.d^{-1}$]
AEXPci	: exposed surface skin – child – indoors	[0.05 m^2]
Fm	: matrix factor dermal uptake	[0.15 -]
DAEci	: degree of skin covered – child – indoors	[$5.6 \cdot 10^{-4}$ kg $soil.m^{-2}$]
DARc	: dermal absorption velocity – child	[0.01 h^{-1}]
Cs	: initial soil concentration (total concentration in gas-, water- and solid phase)	[$mg.kg^{-1}$]
TBci	: period of exposure through contact soil – child – indoors	[9.14 $h.d^{-1}$]
FRSi	: fraction soil in dust - indoors	[0.8 -]
Fa	: relative absorption factor	[-]
BWc	: bodyweight child	[15 kg]

TBci	= t_ci * tf_ci	
t_ci	: duration of the exposure – child - indoors	[8 h/d]
tf_ci	: correction factor exposure daily → yearly – child	[1.143]

ADULT

♦ DAai =AEXPai*Fm*DAEai*DARa*Cs*TBai*FRSi*Fa/BWa

DAai	: exposure via dermal contact soil – adult - indoors	[$mg.kg^{-1}$ $bw.d^{-1}$]
AEXPai	: exposed surface skin – adult - indoors	[0.09 m^2]
Fm	: matrix factor dermal uptake	[0.15 -]
DAEai	: degree of skin covered – adult - indoors	[$5.6 \cdot 10^{-4}$ kg soil. m^{-2}]
DARa	: dermal absorption velocity - adult	[0.005 h^{-1}]
Cs	: initial soil concentration (total concentration in gas-, water- and solid phase)	[$mg.kg^{-1}$]
TBai	: period of exposure through contact soil – adult - indoors	[14.9 $h.d^{-1}$]
FRSi	: fraction soil in dust - indoors	[0.8 -]
Fa	: relative absorption factor	[-]

BWa : bodyweight adult [70 kg]

TBai = t_ai * tf_ai
t_ai : duration of the exposure – adult - indoors [8 $h.d^{-1}$]
tf_ai : correction factor exposure daily → yearly – adult [1.857]

LIFELONG AVERAGE

♦ DALi =(6*DAci+64*DAai)/70

DALi : exposure via dermal contact soil lifelong average- indoors [$mg.kg^{-1}$ $bw.d^{-1}$]
DAci : exposure via dermal contact soil – child – indoors [$mg.kg^{-1}$ $bw.d^{-1}$]
DAci : exposure via dermal contact soil – adult – indoors [$mg.kg^{-1}$ $bw.d^{-1}$]

2.3.2 Dermal contact soil outdoors

CHILD

♦ DAco = Cs*AEXPco*Fm*DAEco*DARc*TBco*Fa/BWc

DAco : exposure via dermal contact soil – child – outdoors [$mg.kg^{-1}$ $bw.d^{-1}$]
Cs : initial soil concentration (total concentration in gas-, water- and solid phase) [$mg.kg^{-1}$]
AEXPco: exposed surface skin – child – outdoors [0.28 m^2]
Fm : matrix factor dermal uptake [0.15 -]
DAEco: degree of skin covered – child – outdoors [$5.1 \cdot 10^{-3}$ kg $soil.m^{-2}$]
DARc : dermal absorption velocity – child kind [0.01 h^{-1}]
TBco : period of exposure through soil –child -outdoors [2.86 $h.d^{-1}$]
Fa : relative absorption factor [-]
BWc : bodyweight child [15 kg]

TBco = t_co * tf_co
t_co : duration of the exposure – child – outdoors [8 $h.d^{-1}$]
tf_co : correction factor exposure daily → yearly – child [0.357]

ADULT

♦ DAao = Cs*AEXPao*Fm*DAEao*DARa*TBao*Fa/BWa

DAao : exposure via dermal contact soil – adult – outdoors [$mg.kg^{-1}$ $bw.d^{-1}$]
Cs : initial soil concentration (total concentration in gas-, water- and solid phase) [$mg.kg^{-1}$]
AEXPao: exposed surface skin – adult - outdoors [0.17 m^2]
Fm : matrix factor dermal uptake [0.15 -]
DAEao: degree of skin covered – adult –outdoors [$3.75 \cdot 10^{-2}$ kg $soil.m^{-2}$]
DARa : dermal absorption velocity – adult [0.005 h^{-1}]
TBao : period of exposure through soil – adult – outdoors [1.14 $h.d^{-1}$]
Fa : relative absorption factor [-]
BWa : bodyweight adult [70 kg]

TBao = t_ao * tf_ao
t_ao : duration of the exposure – adult – outdoors [8 $h.d^{-1}$]
tf_ao : correction factor exposure daily → yearly – adult [0.143]

LIFELONG AVERAGE

♦ DALo = (6*DAco+64*DAao)/70

DALo : exposure via dermal contact soil lifelong average – outdoors [$mg.kg^{-1}$ $bw.d^{-1}$]
DAco : exposure via dermal contact soil – child – outdoors [$mg.kg^{-1}$ $bw.d^{-1}$]
DAao : exposure via dermal contact soil – adult – outdoors [$mg.kg^{-1}$ $bw.d^{-1}$]

Appendix 3: Equations air module

3.1 Indoor

3.1.1 Air flux from soil to crawlspace

Organic compounds

♦ Jsc =(-Fsc*Csa)/(EXP(-Fsc*Ls/Dsa)-1)

Jsc	: total contaminant flux from soil to crawl space	[$g.m^{-2}.h^{-1}$]
Fsc	: air flux from soil to crawl space	[$m^3.m^{-2}.h^{-1}$]
Csa	: concentration in the soil air	[$g.m^{-3}$]
Ls	: length of soil column	[m]
Dsa	: diffusion coefficient in the soil gas phase	[$m^2.h^{-1}$]

♦ FSC = Ks*DELTAPCS/Ls

Fsc	: air flux from soil to crawl space	[$m^3.m^{-2}.h^{-1}$]
Ks	: conductivity soil air	[$m^2.Pa^{-1}.h^{-1}$]
Ks	= KAPPA/ETA	
KAPPA	: air permeability of the soil	[$1 \cdot 10^{-11}$ m^2]
ETA	: viscosity of air	[$5 \cdot 10^{-9}$ $Pa.h^{-1}$]
DELTAPCS	: air pressure difference between crawl space and soil	[1 Pa]
Ls	: length of soil column	[m]

If Dp-Dc < 0.01 then:

♦ Ls = 0.01

If Dp-Dc > 0.01 then:

♦ Ls = Dp-Dc

Ls	: length of soil column	[m]
Dp	: depth of contamination 1.25 (=Dg-Z)	[m]
Dc	: depth of crawl space below ground surface	[m]
Dg	: depth of ground water table	[m]
Z	: Ht of cap. trans. boundary above groundwater table	[m]

3.1.2 Concentration in crawlspace and indoor air

Organic compounds

♦ Cba = (Jsc/(Bh*Vv)

Cba	: concentration in the crawl space air	[$g.m^{-3}$]
Jsc	: total contaminant flux from soil to crawl space	[$g.m^{-2}.h^{-1}$]
Bh	: height of crawl space	[0.5 m]
Vv	: air exchange rate crawlspace	[1.1 $1.h^{-1}$]

If Cba*fbi < COAc then:

- ♦ CIA2 = COAc

If Cba*fbi > COAc then:

- ♦ CIA2 = fbi*Cba

CIA2	: concentration in indoor air according to revised concept	[g.m^{-3}]
COAc	: concentration in air outdoors - child	[g.m^{-3}]
fbi	: fraction indoor air/crawl space air	[0.1 -]
Cba	: concentration in the crawl space air	[g.m^{-3}]

3.2 Outdoor

3.2.1 Air flux from soil to soil surface

Organic compounds

- ♦ Dfs = Du*(Cpw*Vw)/(Dp*Pw) or (Du*Cs*SD)/Dp

Dfs	: diffusion flux from water-soil to the surface	[g.m^{-2}.h^{-1}]
Du	: diffusion coefficient in the soil	[m^{2}.h^{-1}]
Cpw	: concentration in soil moisture/groundwater	[g.m^{-3}] or [mg.dm^{-3}]
Vw	: volume fraction water	[-]
Dp	: depth of contamination 1.25 (=Dg-Z)	[m]
Dg	: depth of ground water table	[m]
Z	: Ht of cap. trans. boundary above groundwater table	[m]
Pw	: mass fraction in the soil moisture	[-]
Cs	: initial soil concentration (total concentration in gas-, water- and solid phase)	[mg.kg^{-1}]
SD	: dry bulk density	[kg.dm^{-3}]

3.2.2 Concentration in outdoor air

- ♦ VF = Vg*Sz/Lp

VF	: dilution velocity (plant, child or adult)	[m.h^{-1}]
Vg	: average windspeed	[m.h^{-1}]
Sz	: Pasquill dispersion coefficient vertical, related to Pasquill weather stability class D	[m]
Lp	: diameter contaminated area	[m]

- ♦ Vg =(Vx+V’)/2

Vx	: wind speed at x meter high	[m.h^{-1}]
V’	: friction speed	[m.h^{-1}]

♦ Vx = ln(Z/Zo)*V'/k

Z	: height when breathing	[m]
Zo	: roughness surface living area	[1.0-]
k	: Karman constant	[0.4-]

♦ V' k*V10/ln(Z10/Zo)

k	: Karman constant	[0.4-]
Z10	: height	[10m]
V10	: wind speed at 10 m height	[18000 $m.h.^{1}$]
Zo	: roughness surface living area	[1.0-]

♦ Sz $= Co*0.2*Lp^{0.76}$

Sz	: Pasquill dispersion coefficient vertical, related to Pasquill weather stability class D	[m]

Co $= (10*Zo)\hat{}(0.53*Lp^{-0.22})$

Co	: correction factor for roughness length	[-]
Zo	: roughness surface living area	[1.0-]
Lp	: diameter contaminated area	[m]

Example calculation if Lp = 100 (Van den Berg 1995)

		Child	Adult	
Z	=	1.0	1.5	[m]
V'	=	3127	3127	[$m.h^{-1}$]
Vg	=	1563	3148	[$m.h^{-1}$]
Co	=	1.56	1.56	[-]
Sz	=	10.31	10.31	[m]

Organic compounds

PLANT

Cair = Dfs/VFp

Cair	: the concentration in air outdoors - plant	[$g.m^{-3}$]
Dfs	: diffusion flux water-soil to surface level	[$g.m^{-2}.h^{-1}$]
VFp	: dilution velocity plant	[84 $m.h^{-1}$]

CHILD

♦ COAc = Dfs/VFc

COAc	: the concentration in air outdoors - child	[$g.m^{-3}$]
Dfs	: diffusion flux water – soil to surface level	[$g.m^{-2}.h^{-1}$]
VFc	: dilution velocity - child	[161.3 $m.h^{-1}$]

ADULT

♦ COAa =Dfs/VFa

COAa	: concentration in air outdoors adult	[g.m^{-3}]
Dfs	: diffusion flux water-soil to surface level	[g.m^{-2}.h^{-1}]
VFa	: dilution velocity - adult	[324.6 m.h^{-1}]

3.3 Exposure via inhalation of indoor air

CHILD

♦ IVci = TIic*CIA2*AVc*Fa*1000/BWc

IVci	: exposure via inhalation of vapours – child – indoors	[mg.kg^{-1} bw.d^{-1}]
TIic	: inhalation period – child – indoors	[21.1 h.d^{-1}]
CIA2	: concentration in indoor air	[g.m^{3}]
AVc	: air volume – child	[0.317 m3.h^{-1}]
Fa	: relative sorption factor	[-]
BWc	: bodyweight child	[15 kg]

ADULT

♦ IVai = TIia*CIA2*AVa*Fa*1000/BWa

IVai	: exposure via inhalation of vapours – adult – indoors	[mg.kg^{-1} bw.d^{-1}]
TIia	: inhalation period – adult – indoors	[22.9 h.d^{-1}]
CIA2	: concentration in indoor air	[g.m^{-3}]
AVa	: air volume – adult	[0.833 m^{3}.h^{-1}]
Fa	: relative sorption factor	[-]
BWa	: bodyweight adult	[70 kg]

LIFELONG AVERAGE

♦ IVLi = (6*IVci+64*IVai)/70

IVLi	: exposure via inhalation of vapours lifelong average	[mg.kg^{-1} bw.d^{-1}]
IVci	: exposure via inhalation of vapours – child - indoors	[mg.kg^{-1} bw.d^{-1}]
IVai	: exposure via inhalation of vapours – adult – indoors	[mg.kg^{-1} bw.d^{-1}]

3.4 Exposure via inhalation of outdoor air

Child

♦ IVco = TIoc*COac*Fa*AVc*1000/BWc

IVco	: exposure via inhalation of vapours – child - outdoors	[mg.kg^{-1} bw.d^{-1}]
TIoc	: inhalation period – child – outdoor	[2.86 h.d^{-1}]
COac	: concentration in outdoor air - child	[g.m^{-3}]
Fa	: relative sorption factor	[-]
AVc	: air volume child	[0.317 m^{3}.h^{-1}]
BWc	: bodyweight child	[15 kg]

Adult

- IVao = TIoa*COaa*Fa*AVa*1000/BWa

IVao	: exposure via inhalation of vapours – adult - outdoors	[$mg.kg^{-1}$ $bw.d^{-1}$]
TIoa	: inhalation period – adult - outdoors	[1.14 $h.d^{-1}$]
COaa	: concentration in outdoor air - adult	[$g.m^{-3}$]
Fa	: relative sorption factor	[-]
AVa	: air volume adult	[0.833 $m^3.h^{-1}$]
BWa	: bodyweight adult	[70 kg]

LIFELONG AVERAGE

- IVLO = (6*IVco+64*IVao)/70

IVLO	: exposure via inhalation of vapours lifelong average	[$mg.kg^{-1}$ $bw.d^{-1}$]
IVco	: exposure via inhalation – child – outdoors	[$mg.kg^{-1}$ $bw.d^{-1}$]
IVao	: exposure via inhalation of vapours – adult - outdoors	[$mg.kg^{-1}$ $bw.d^{-1}$]

Appendix 4: Equations permeation of drinking water

4.1 Concentration in drinking water

If a polyethylene (or other plastic) water pipeline is present, then:

- ♦ Cdw =Dwconst*Dpe*Cpw*LP

Cdw	: concentration in the drinking water	[$mg.dm^{-3}$]
Dwconst	: drinking water constant	[45.6 $d.m^{-3}$]
Dpe	: permeation coefficient PE pipeline	[$m^2.d^{-1}$]
Cpw	: concentration in the soil moisture	[$mg.dm^{-3}$]
LP	: diameter contaminated area	[100 m]

- ♦ Dwconst = (2 * d1* 3 * pi * r) / (d2 * Qwd)

d1	: time of water stagnation	[0.33 d]
r	: radius of pipeline	[0.0098 m]
d2	: thickness of the pipeline wall	[0.0027 m]
Qwd	: average daily water use	[0.5 m^3]

4.2 Exposure via permeation in drinking water

CHILD

- ♦ DIWc = QDW_c*Cdw*Fa/BWc

DIWc	: exposure via permeation of drinking water – child	[$mg.kg^{-1}$ $bw.d^{-1}$]
QDW_c	: consumption of drinking water – child	[1 $dm^3.d^{-1}$]
Cdw	: concentration in drinking water	[$mg.dm^{-3}$]
Fa	: relative sorption factor	[-]
BWc	: bodyweight child	[15 kg]

ADULT

- ♦ DIWa = QDW_a*Cdw*Fa/BWa

DIWa	: exposure via permeation of drinking water – adult	[$mg.kg^{-1}$ $bw.d^{-1}$]
QDW_a	: consumption of drinking water – adult	[2 $dm^3.d^{-1}$]
Cdw	: concentration in drinking water	[$mg.dm^{-3}$]
Fa	: relative sorption factor	[-]
BWa	: bodyweight adult	[70 kg]

LIFELONG AVERAGE

♦ DIWL = (6*DIWc+64*DIWa)/70

DIWL : exposure via permeation of drinking water lifelong average [mg.kg^{-1} bw.d^{-1}]
DIWc : exposure via permeation of drinking water – child [mg.kg^{-1} bw.d^{-1}]
DIWa : exposure via permeation of drinking water – adult [mg.kg^{-1} bw.d^{-1}]

4.3 Concentration in bathroom air

4.3.1 Organic compounds

♦ Cbk = Cdw*Kwa*0.005

Cbk : concentration in bathroom air [mg.dm^{-3}]
Cdw : concentration in the drinking water [mg.dm^{-3}]
Kwa : measure of evaporation of contaminant [-]

♦ Kwa = (KLW_SH*KL*KG)/(KLW_SH*KG+KL)*6000

KLW_SH: air - water partition coefficient at bathroom temperature [-]
KL : water mass transport coefficient [m.s^{-1}]
KG : vapour mass transport coefficient [m.s^{-1}]

♦ KLW_SH= EXP(LN(KLW*R*T) + 0.024*(Tsh-T)/(R*Tsh)

KLW : air – water partition coefficient at soil temperature [-]
R : gas constant [Pa.m^{3}.mol^{-1}.K^{-1}]
T : soil temperature [283 K]
Tsh : temperature bathing water [313 K]

♦ KL = Kl*(44/M)^0.5/3600
♦ KG = Kg*(18/M)^0.5/3600

Kl : exchange speed liquid phase [0.2 m.h^{-1}]
M : molecular weight [g.mol^{-1}]
Kg : mass transport coefficient gas phase [29.88 m.h^{-1}]

4.4 Exposure via inhalation of vapours during showering

CHILD

♦ IVWc = Cbk*AVc*Td*Fa*1000/BWc

IVWc : exposure via inhalation of vapours during showering – child [mg.kg^{-1} bw.d^{-1}]
Cbk : concentration in bathroom air [g.m^{-3}]
AVc : air volume – child [0.317 m^{3}.h^{-1}]
Td : bathing period [0.5 h.d^{-1}]
Fa : relative sorption factor [-]
BWc : bodyweight child [15 kg]

ADULT

- IVWa = Cbk*AVa*Td*Fa*1000/BWa

IVWa	: exposure via inhalation of vapours during showering – adult	[$mg.kg^{-1}$ $bw.d^{-1}$]
Cbk	: concentration in bathroom air	[$g.m^{-3}$]
AVa	: air volume – adult	[0.833 $m^3.h^{-1}$]
Td	: bating period	[0.5 $h.d^{-1}$]
Fa	: relative sorption factor	[-]
BWa	: bodyweight adult	[70 kg]

LIFELONG AVERAGE.

- IVWL = (6*IVWc+64*IVWa)/70

IVWL	: exposure via inhalation of vapours during showering lifelong average	[$mg.kg^{-1}$ $bw.d^{-1}$]
IVWc	: exposure via inhalation of vapours during showering – child	[$mg.kg^{-1}$ $bw.d^{-1}$]
IVWa	: exposure via inhalation of vapours during showering – adult	[$mg.kg^{-1}$ $bw.d^{-1}$]

4.5 Exposure via dermal contact with drinking water during showering

CHILD

- DAWc = ATOTc*Fexp*Tdc*DARw*(1-Kwa)*Cdw*Fa/BWc

DAWc	: exposure via dermal contact with drinking water during showering – child	[$mg.kg^{-1}bw.d^{1}$]
ATOTc	: body surface – child	[0.95 m^2]
Fexp	: fraction exposed skin during showering	[0.40 -]
Tdc	: showering period	[0.25 $h.d^{-1}$]
Kwa	: evaporation of a compound	[-]
Cdw	: concentration in drinking water	[$mg.dm^{-3}$]
Fa	: relative sorption factor	[-]
BWc	: bodyweight child	[15 kg]
DARw	: dermal absorption velocity during showering	[($mg.m^{-2}$)/ ($mg.dm^{3}$).h^{1}]

DARw = (5000*(0.038 + 0.153*10^log_K_{ow}))/(5000 + (0.038 + .153*10^log_K_{ow}))
*(EXP(-0.016*M)/1.5)

ADULT

- DAWa = ATOTa*Fexp*Tdc*DARw*(1-Kwa)*Cdw*Fa/BWa

DAWa	: exposure via dermal contact with drinking water during showering – adult	[$mg.kg^{-1}bw.d^{-1}$]
ATOTa	: body surface – adult	[1.80 m^2]
Fexp	: fraction exposed skin during showering	[0.40 -]
Tdc	: showering period	[0.25 $h.d^{-1}$]
Kwa	: evaporation of a compound	[-]
Cdw	: concentration in drinking water	[$mg.dm^{-3}$]
Fa	: relative sorption factor	[-]
BWa	: bodyweight adult	[70 kg]

DARw : dermal absorption velocity during showering $[(mg.m^{-2})/(mg.dm^{3}).h^{-1}]$

$$DARw = (5000*(0.038+0.153*10^{\log\_K_{ow}}))/(5000+(0.038+0.153*10^{\log\_K_{ow}}))*(EXP(-0.016*M)/1.5)$$

LIFELONG AVERAGE

- DAWL= (6*DAWc+64*DAWa)/70

DAWL: exposure via dermal contact with drinking water during showering lifelong average $[mg.kg^{-1}\ bw.d^{-1}]$

DAWc : exposure via dermal contact with drinking water during showering – child $[mg.kg^{-1}\ bw.d^{-1}]$

DAWa : exposure via dermal contact with drinking water during showering – adult $[mg.kg^{-1}\ bw.d^{-1}]$

Appendix 5: Equations vegetation module

5.1 Calculation of BCF in crops for organic compounds

5.1.1 Calculation Vapour pressure of a Sub-cooled liquid

If TEMPmelt > T then;

♦ VP_L =Vp/(EXP(6.79*(1-TEMPmelt/T)))

VP_L	: vapour pressure of sub-cooled liquid	[Pa]
Vp	: vapour pressure pure product	[Pa]
TEMPmelt:	melting point	[283 K]
T	: soil temperature	[283 K]

If TEMPmelt < T then;

VP_L = Vp

VP_L	: vapour pressure of sub-cooled liquid	[Pa]
TEMPmelt	: melting point	[283 K]
T	: soil temperature	[283 K]

5.1.2 Calculation dry-bulk density

♦ RHO_soil = Vs*RHOsolid+Vw*RHOwater+Va*RHOair

RHO_soil	: calculated dry bulk density (default 1550)	[$kg.m^{-3}$]
Vs	: volume fraction soil	[-]
RHOsolid:	density solid soil	[2500 $kg.m^{-3}$]
Vw	: volume fraction water	[-]
RHOwater:	density water	[1000 $kg.m^{-3}$]
Va	: volume fraction air	[-]
RHOair:	density air	[1.3 $kg.m^{-3}$]

♦ CONV_soil =RHO_soil/(Vs*RHOsolid)

CONV_soil: conversion factor for soil from wet weight –dry weight [-]

RHO_soil:	calculated dry bulk density (default 1550)	[$kg.m^{-3}$]
Vs	: volume fraction soil	[-]
RHOsolid:	density solid soil	[2500 $kg.m^{-3}$]

5.1.3 Calculation bioconcentration factors

- K_plantwater =Fwater_plant+Flipid_plant*K_{ow}^{b}

K_plantwater:	partition coefficient plant-water	[-]
Fwater_plant:	volume fraction water in plant tissue	[0.65 -]
Flipid_plant:	volume fraction lipid in plant tissue	[0.01 -]
K_{ow}	: octanol-water partition coefficient	[-]
b	: correction exponent for differences between plant lipid/octanol	[0.95]

- K_rootwater = Fwater_root+Flipid_root*$K_{ow}^{b\_root}$

K_rootwater:	partition coefficient root-water	[-]
Fwater_root:	volume fraction water in root (=1-Fdwr)	[0.833 -]
Fdwr	: fraction dry matter leafy crops	[0.167 kg dw.kg^{-1} fw]
Flipid_root:	volume fraction lipid in root	[0.005 -]
K_{ow}	: octanol-water partition coefficient	[-]
b_root	: correction exponent for differences between root lipid/octanol	[0.8 -]

- K_leafair = K_plantwater/Klw

K_leafair:	partition coefficient leaf - air	[-]
K_plantwater:	partition coefficient plant - water	[-]
Klw	: air-water partition coefficient	[(mol.m^{-3} air) /(mol.dm^{-1}water)]
Klw	= Vp/(S*R*T) or = Za/Zw	[-]
S	: solubility at soil temperature	[mol.m^{-3}]
R	: gas constant	[8.3144 Pa.m^{3}.mol^{-1}.K^{-1}]
T	: temperature	[283 K]
Za	: fugacity constant air	[mol.m^{-3}.Pa^{-1}]
Zw	: fugacity constant water	[mol.m^{-3}.Pa^{-1}]

- Tscf_1 =0.784*EXP((-(log_K_{ow}-1.78)^2)/2.44)

Tscf	: transpiration-stream concentration factor	[-]
Tscf_1	: according to Briggs et al. (1982)	[-]
K_{ow}	: octanol-water partition coefficient	[-]

- Tscf_2 =0.7*EXP((-(log(K_{ow})-3.07)^2)/2.78)

Tscf	: transpiration-stream concentration factor	[-]
Tscf_	2 : according to Hsu (et al 1991)	[-]
K_{ow}	: octanol-water partition coefficient	[-]

The highest result of both equations (Tscf_1,_2) will be used.

Elimination by plant

kelim_plant = kmetab_plant+kphoto_plant

kelim_plant: rate constant for total elimination in plants	[d^{-1}]
kmetab_plant: rate constant for metabolism in plants	[d^{-1}]
kphoto_plant: rate constant for photolysis in plants	[d^{-1}]

- ALPHA =(AREA_plant*g_plant)/(K_leafair*V_leaf)+kelim_plant+kgrowth_plant

ALPHA: sink term of differential equation	[d^{-1}]
AREA_plant: leaf surface plant	[5 m^2]
g_plant: conductivity plant	[80 $m.day^{-1}$]
K_leafair: partition coefficient leaf-air	[-]
V_leaf: leaf volume	[0.002 m^3]
kelim_plant: rate constant for total elimination in plants	[d^{-1}]
kgrowth_plant : rate constant for dilution by growth	[0.035 d^{-1}]

- BETA = C_porew*Tscf*Qtransp/V_leaf + (1-Fass_aer)*C_air*g_plant* AREA_plant/V_leaf

BETA : source term for differential equation for crops	[$kg.m^{-3}.day^{-1}$]
C_porew: concentration in soil moisture /1000 (Cpw/1000)	[$kg.m^{-3}$]
Tscf : transpiration stream concentration factor	[-]
Qtransp: transpiration stream	[0.001 $m^3.day^{-1}$]
V_leaf : leaf volume	[0.002 m^3]
Fass_aer: fraction of chemical associated with aerosol particles	[-]
C_air : the concentration in air outdoors – plant /1000 (Coap/1000)	[$kg.m^{-3}$]
g_plant: conductivity plant	[80 $m.day^{-1}$]
AREA_plant: leaf surface plant	[5 m^2]

- Fass_aer =CONjunge*SURF_aer/(VP_L+CONjunge*SURF_aer)

Fass_aer: fraction of chemical associated with aerosol particles	[-]
CONjunge: constant of junge	[0.4 -]
SURF_aer: surface area of aerosol particles	[0.00025 -]
VP_L : vapour pressure pure product	[Pa]

- BCFleafTM= (BETA/(ALPHA*RHO_plant))/Cpw

BCFleafTM= ratio BCFleaf/porewater wet weight	[($mg.kg^{-1}$ fw) /($mg.dm^{-3}$)]
BETA : source term for differential equation for crops	[$kg.m^{-3}.day^{-1}$]
ALPHA: sink term of differential equation	[d^{-1}]
RHO_plant: density plant tissue	[800 $kg.m^{-3}$]
Cpw : concentration in soil moisture	[$mg.dm^{-3}$]
BCFleaf: bioconcentration factor leaf	[($mg.kg^{-1}$ fw)/ ($mg.dm^{-3}$)]

♦ BCFrootTM= (K_rootwater*C_porew/RHO_root)/Cpw

BCFrootTM= ratio BCFroot/porewater wet weight	[(mg.kg^{-1} fw) /(mg.dm^{-3})]
K_rootwater: partition coefficient root-water	[-]
C_porew: concentration in soil moisture /1000 (Cpw/1000)	[kg.m^{-3}]
RHO_root: density root tissue	[1000 kg.m^{-3}]
Cpw : concentration in soil moisture	[mg.dm^{-3}]
BCF root: bioconcentration factor root	[(mg.kg^{-1} fw)/ (mg.dm^{-3})]

5.2 Concentration in crops

5.2.1 Organic compounds

♦ $Cpro_{org}$= Cpw*BCFroot

$Cpro_{org}$: amount in the root on basis of fresh weight (fw)	[mg.kg^{-1} fw]
Cpw : concentration in soil moisture	[mg.dm^{-3}]
BCF root: bioconcentration factor root	[(mg.kg^{-1} fw)/ (mg.dm^{-3})]

♦ $Cpso_{org}$= Cpw*BCFleaf + Dpconst*Cs*Fdws

$Cpso_{org}$: concentration in the leaves on basis of fresh weight (fw)	[mg.kg^{-1} fw]
Cpw : concentration in soil moisture	[mg.dm^{-3}]
BCFleaf: bioconcentration factor leaf	[(mg.kg^{-1} fw)/ (mg.dm^{-3})]
Dpconst: deposition constant	[0.01 -]
Cs : initial soil concentration (total concentration in gas-, water- and solid phase)	[mg.kg^{-1}]
Fdws : fraction dry matter leaf	[0.098 kg dw. kg^{-1} fw]

Concentration in crops due to local deposition

♦ Cpdep = Dpconst*Cs*Fdws [mg.kg^{-1} fw]

Cpdep : concentration in leaf due to deposition	[mg.kg^{-1} fw]
Dpconst : deposition constant	[0.01 -]
Cs : initial soil concentration (total concentration in gas-, water- and solid phase)	[mg.kg^{-1}]
Fdws : fraction dry matter leafy crops	[0.098 kg dw.kg^{-1} fw]

5.2.2 Inorganic compounds

♦ $Cpro_{in}$ = Cpw*(1-Fdwr)

$Cpro_{in}$: concentration in the root on basis of fresh weight (fw)	[mg.kg^{-1} fw]
Cpw : concentration in the soil moisture	[mg.dm^{-3}]
Fdwr : dry matter fraction in root crops	[0.167 kg dw.kg^{-1} fw]

♦ $Cpso_{in}$ = Cpw*(1-Fdws)+Dpconst*Cs*Fdws)

$Cpso_{in}$	: concentration in leaves on basis of fresh weight (fw)	[mg.kg^{-1} fw]
Cpw	: concentration in the soil moisture	[mg.dm^{-3}]
Fdws	: dry matter fraction in root crops	[0.098 kg dw.kg^{-1} fw]
Dpconst	: deposition constant	[0.01 -]
Cs	: initial soil concentration (total concentration in gas-, water- and solid phase)	[mg.kg^{-1}]

5.2.3 Metals

♦ Cpr1 = Cs*BCFrme

Cpr1	: average consumption in crops	[mg.kg^{-1}dw]
Cs	: initial soil concentration (total concentration in gas-, water- and solid phase)	[mg.kg^{-1}]
BCFrme	: BCF average consumption (metals)	[-]

NB: The average consumption BCF for metals is based on empirical data for which it is supposed that the contribution due to local deposition is included.

5.3 Exposure via consumption of crops

5.3.1 Organic compounds

CHILD

♦ VIc_{org} = (QK_c*Cpro*fvk + QB_c*Cpso*fvb)*Fa/BWc)

VIc_{org}	: exposure via ingestion of crops – child	[mg.kg^{-1} bw.d^{-1}]
QK_c	: consumption root crops - child	[0.0595 kg fw.d^{-1}]
Cpro	: concentration in root crops	[mg.kg^{-1} fw]
fvk	: fraction contaminated root crops	[0.1 -]
QB_c	: consumption leafy crops - child	[0.0583 kg fw.d^{-1}]
Cpso	: concentration in leafy crops (incl. deposition)	[mg.kg^{-1} fw]
fvb	: fraction contaminated root crops	[0.1 -]
Fa	: relative sorption factor	[-]
BWc	: bodyweight child	[15 kg]

ADULT

♦ VIa_{org} = (QK_A*Cpro*fvk+QB_a*Cpso*fvb)*Fa/BWa)

VIa_{org}	: exposure via ingestion of crops – adult	[mg.kg^{-1} bw.d^{-1}]
QK_a	: consumption root crops - adult	[0.122 kg fw.d^{-1}]
Cpro	: concentration in root crops	[mg.kg^{-1} fw]
fvk	: fraction contaminated root crop	[0.1 -]
QB_a	: consumption of leafy crops – adult	[0.139 kg fw.d^{-1}]
Cpso	: concentration in leafy crops (incl. deposition)	[mg/kg fw]
fvb	: fraction contaminated leafy crops	[0.1 -]
Fa	: relative sorption factor	[-]
BWa	: bodyweight adult	[70 kg]

LIFELONG AVERAGE

♦ VIL_{org} = $(6*VIc_{org}+64*VIa_{org})/70$

VIL_{org}	= exposure via ingestion of crops lifelong average	[$mg.kg^{-1}$ $bw.d^{-1}$]
VIc_{org}	: exposure via ingestion of crops - child	[$mg.kg^{-1}$ $bw.d^{-1}$]
VIa_{org}	: exposure via ingestion crops - adult	[$mg.kg^{-1}$ $bw.d^{-1}$]

5.3.2 Metals

CHILD

♦ VIc_{met} = (B146*Cpr1)*Fa/BWc

VIc_{met}	: exposure via ingestion of crops – child	[$mg.kg^{-1}$ $bw.d^{-1}$]
DCCc	: daily consumption crops – child	[kg $dw.d^{-1}$]
Cpr1	: consumption average amount in crop	[$mg.kg^{-1}$ ds]
Fa	: relative sorption factor	[-]
BWc	: bodyweight child	[15 kg]

DCCc = (QK_c*Fdwr*fvk)+(QB_c*Fdws*fvb)

QK_c	: root crop consumption – child	[0.0595 kg $fw.d^{-1}$]
Fdwr	: dry matter content root crops	[0.167 kg dw kg^{-1} fw]
fvk	: fraction contaminated root crop	[0.1 -]
QB_c	: leafy crop consumption - child	[0.0583 kg $fw.d^{-1}$]
Fdws	: dry matter content leafy crop	[0.098 kg dw. kg^{-1} fw]
fvb	: fraction contaminated leafy crops	[0.1 -]

ADULT

♦ VIa_{met} = (C146*Cpr1)*Fa/BWa

VIa_{met}	: exposure via ingestion of crop – adult	[$mg.kg^{-1}$ $bw.d^{-1}$]
DCCa	:daily consumption of crop – adult	[kg $dw.d^{-1}$]
Cpr1	: consumption average amount in crop	[$mg.kg^{-1}$ dw]
Fa	: relative sorption factor	[-]
BWa	: bodyweight adult	[70 kg]

DCCa = (QK_a*Fdwr*fvk)+(QB_a*Fdws*fvb)

QK_a	: root crop consumption – adult	[0.122 kg $fw.d^{-1}$]
Fdwr	: dry matter content root crops	[0.167 kg dw. kg^{-1} fw]
fvk	: fraction contaminated root crop	[0.1 -]
QB_a	: leafy crop consumption – adult	[0.139 kg $fw.d^{-1}$]
Fdws	: dry matter content leafy crops	[0.098 kg dw. kg^{-1} fw]
fvb	: fraction contaminated crops	[0.1 -]

LIFELONG AVERAGE

- $VIL_{met} = (6*VIc_{met}+64*VIa_{met})/70$

VIL_{met}	: exposure via ingestion of crops lifelong average	$[mg.kg^{-1}\ bw.d^{-1}]$
VIc_{met}	: exposure via ingestion of crops – child	$[mg.kg^{-1}\ bw.d^{-1}]$
VIa_{met}	: exposure via ingestion of crops – adult	$[mg.kg^{-1}\ bw.d^{-1}]$

Appendix 6: Equations to calculate total exposure

6.1 Total exposure via inhalation

Child

- SUMac = IPc + IVci+ IVco +IVWc

SUMac: total exposure via inhalation – child [mg.kg^{-1} bw.d^{-1}]
IPc : exposure via inhalation of soil particles – child [mg.kg^{-1} bw.d^{-1}]
IVci : exposure via inhalation of indoor air – child [mg.kg^{-1} bw.d^{-1}]
IVco : exposure via inhalation of outdoor air – child [mg.kg^{-1} bw.d^{-1}]
IVWc : exposure via inhalation of vapours during showering – child[mg.kg^{-1} bw.d^{-1}]

Adult

- SUMao = IPa + IVai + IVao + IVWa

SUMao: total exposure via inhalation - adult [mg.kg^{-1} bw.d^{-1}]
IPa : exposure via inhalation of soil particles – adult [mg.kg^{-1} bw.d^{-1}]
IVai : exposure via inhalation of indoor air – adult [mg.kg^{-1} bw.d^{-1}]
IVao : exposure via inhalation of outdoor air – adult [mg.kg^{-1} bw.d^{-1}]
IVWa : exposure via inhalation of vapour during showering - adult[mg.kg^{-1} bw.d^{-1}]

Lifelong average

- SUMAL = (6*SUMac+64*SUMao)/70

SUMAL: total exposure via inhalation lifelong average [mg.kg^{-1} bw.d^{-1}]
SUMac: total exposure via inhalation – child [mg.kg^{-1} bw.d^{-1}]
SUMao: total exposure via inhalation – adult [mg.kg^{-1} bw.d^{-1}]

6.2 Total exposure oral and dermal

Child

- SUMOc = DIc + DAci + DAco +Vic + DIWc + DAWc

SUMOc: total exposure oral and dermal – child [mg.kg^{-1} bw.d^{-1}]
DIc : exposure via ingestion of soil – child [mg.kg^{-1} bw.d^{-1}]
DAci : exposure via dermal contact indoors – child [mg.kg^{-1} bw.d^{-1}]
DAco : exposure via dermal contact soil outdoors – child [mg.kg^{-1} bw.d^{-1}]
VIc : exposure via ingestion of crops – child [mg.kg^{-1} bw.d^{-1}]
DIWc : exposure via permeation in drinking water – child [mg.kg^{-1} bw.d^{-1}]
DAWc : exposure via dermal uptake with drinking water during showering – child [mg.kg^{-1} bw.d^{-1}]

Adult

- SUMOo = DIa + DAai + DAao + Via + DIWa + DAWa

SUMOo: total exposure oral and dermal – adult [mg.kg^{-1} bw.d^{-1}]
DIa : exposure via ingestion of soil – adult [mg.kg^{-1} bw.d^{-1}]
DAai : exposure via dermal contact soil indoors – adult [mg.kg^{-1} bw.d^{-1}]

DAao : exposure via dermal contact outdoors – adult [$mg.kg^{-1}$ $bw.d^{-1}$]
VIa : exposure via ingestion of crops – adult [$mg.kg^{-1}$ $bw.d^{-1}$]
DIWa : exposure via permeation of drinking water – adult [$mg.kg^{-1}$ $bw.d^{-1}$]
DAWa : exposure via dermal contact with drinking water during showering – adult [$mg.kg^{-1}bw.d^{-1}$]

LIFELONG AVERAGE

♦ SUMOL = (6*SUMOc+64*SUMOo)/70

SUMOL: total exposure oral and dermal lifelong average [$mg.kg^{-1}$ $bw.d^{-1}$]
SUMOc: total exposure oral and dermal – child [$mg.kg^{-1}$ $bw.d^{-1}$]
SUMOo: total exposure oral and dermal – adult [$mg.kg^{-1}$ $bw.d^{-1}$]

6.3 Total exposure inhalation, oral and dermal and the derivation of human risk

The MPR_{human} covers both oral and inhalation exposure (and if necessary also dermal exposure), and classical toxic risks as well as carcinogenic risks. The MPR_{human} can be expressed as a tolerable daily intake (TDI) or an excess carcinogenic risk via intake (CR_{oral}) ($mg.kg^{-1}$ $bw.d^{-1}$). The MPR_{human} can also be expressed as a tolerable concentration in air (TCA) or an excess carcinogenic risk via air (CR_{inhal}) ($\mu g.m^{-3}$) (Baars et al. 2001).
To prevent that both routes lead to exposure up to the risk limits, the exposures are added up. Therefore the TCA is converted to the MPR inhalation for a child and adult.
The total exposure for a child and adult is calculated from and 'weighted' summation.

In CSOIL 2000 the risk is defined as DOSE/MPR

CHILD

♦ Risk – child = SUMOc/MPR +SUMAc/MPR_Ac

SUMOc: total exposure oral and dermal child [$mg.kg^{-1}$ $bw.d^{-1}$]
MPR : maximum permissible risk [$mg.kg^{-1}$ $bw.d^{-1}$]
SUMAc: total exposure via inhalation – child [$mg.kg^{-1}$ $bw.d^{-1}$]
MPR_Ac: TDI inhalation child [$mg.kg^{-1}$ $bw.d^{-1}$]

ADULT

♦ Risk – adult = SUMOo/MPR +SUMAo/MPR_Aa

SUMOo: total exposure oral- and dermal – adult [$mg.kg^{-1}$ $bw.d^{-1}$]
MPR : maximum permissible risk [$mg.kg^{-1}$ $bw.d^{-1}$]
SUMAo: total exposure via inhalation – adult [$mg.kg^{-1}$ $bw.d^{-1}$]
MPR_Aa: TDI inhalation – adult [$mg.kg^{-1}$ $bw.d^{-1}$]

On basis of the above calculated weighted risk it is possible with MPR_AC and MPR_AA to calculate the corrected exposure for child (Tch) and adult (Tad).

With exposure = risk *MPR
Corrected exposure – child = (~~MPR~~*SUMOc/~~MPR)~~ +(MPR* SUMAc/MPR_AC)
Corrected exposure – adult = (~~MPR~~*SUMOo/~~MPR~~) +(MPR*SUMAo/MPR_AA)

CHILD

♦ Tch_{org} = SUMOc+(MPR/MPR_Ac)*SUMAc

Tch_{org}	: total exposure (dose) – child	[$mg.kg^{-1}$ $bw.d^{-1}$]
SUMOc	: total exposure oral and dermal child	[$mg.kg^{-1}$ $bw.d^{-1}$]
MPR	: maximum permissible risk	[$mg.kg^{-1}$ $bw.d^{-1}$]
SUMAc	: total exposure via inhalation – child	[$mg.kg^{-1}$ $bw.d^{-1}$]
MPR_Ac	: TDI inhalation child	[$mg.kg^{-1}$ $bw.d^{-1}$]

MPR_Ac = TCA*AVc*24/BWc

TCA	: acceptable concentration air	
AVc	: air volume – child	[0.317 $m^3.h^{-1}$]
BWc	: bodyweight child	[15 kg]

ADULT

♦ Tad_{org} = SUMOo+(MPR/MPR_Aa)*SUMAo

Tad_{org}	: total exposure (or dose) – adult	[$mg.kg^{-1}$ $bw.d^{-1}$]
SUMOo	: total exposure oral- and dermal – adult	[$mg.kg^{-1}$ $bw.d^{-1}$]
MPR	: maximal permissible risk	[$mg.kg^{-1}$ $bw.d^{-1}$]
SUMAo	: total exposure via inhalation – adult	[$mg.kg^{-1}$ $bw.d^{-1}$]
MPR_Aa	: TDI inhalation – adult	[$mg.kg^{-1}$ $bw.d^{-1}$]

MPR_Aa = TCA*AVa*24/BWa

TCA	: acceptable concentration air	
AVa	: air volume – adult	[0.833 $m^3.h^{-1}$]
BWa	: bodyweight adult	[70 kg]

LIFELONG AVERAGE

♦ DOSE = $(6*Tch_{org}+64*Tad_{org})/70$

DOSE	: total exposure (or dose) lifelong average	[$mg.kg^{-1}$ $bw.d^{-1}$]
Tch_{org}	: total exposure (or dose) – child	[$mg.kg^{-1}$ $bw.d^{-1}$]
Tad_{org}	: total exposure (or dose) – adult	[$mg.kg^{-1}$ $bw.d^{-1}$]

Appendix 7: Equation to calculate exposure via direct consumption of contaminated drinking water

7.1 Exposure via direct drinking of contaminated groundwater

♦ MPR = ((64*QDW_a/BWa)+(6*QDW_c/BWc))*1000/C_{max}*70

MPR	: maximal permissible risk	[$mg.kg^{-1}$ $bw.d^{-1}$]
QDW_a	: consumption of groundwater – adult	[2 $dm^3.d^{-1}$]
BWa	: bodyweight adult	[70 kg]
QDW_c	: consumption of groundwater – child	[1 $dm^3.d^{-1}$]
BWc	: bodyweight child	[15 kg]
Cmax	: concentration of compound in ground water	[$mg.dm^{-3}$]

This exposure does not contribute to the total human exposure calculated by CSOIL 2000.

Appendix 8: Previous CSOIL user scenarios

8.1 Introduction

This report has been written in a transition phase for the CSOIL model. The model used at the moment of writing, was CSOIL 2000. However at the same time, plans were present to make some adaptations on the CSOIL 2000 version. One of these adaptations is the change in user scenarios. The newer version will be called CSOIL 2000 (2006) in this Appendix.

The goal of this report was to describe the current CSOIL 2000, but because the adaptations will swiftly follow this publication, it was decided to describe the user scenarios of the CSOIL 2000 (2006) version. This appendix however will describe the CSOIL 2000 user scenarios. In the second part of the appendix the relation between the models CSOIL 2000 and CSOIL 2000 (2006) user scenarios will be described.

8.2 User scenarios CSOIL 2000

8.2.1 Residential with vegetable garden

The houses in this user scenario have a vegetable garden. This means that a large part of the consumed crops, originates from this garden. The exposure in this user scenario can take place via every described route. This user scenario is chosen when a large part of the crops is cultivated in this garden.

8.2.2 Residential with garden (standard scenario)

The houses in this user scenario have a garden. It is possible, that a part of the consumed crops originate from this garden. However the largest part of consumed crops originates from else where. The exposure in this user scenario can take place via every described route. This user scenario is chosen when it is unknown if the crops are cultivated in the garden or if this cultivation is limited. If a large part of the consumed crops originates from this garden the user scenario ‘Residential with vegetable garden’ should be chosen.

8.2.3 Residential without garden

The houses in this user scenario have no garden. It is therefore not possible to cultivate crops in a garden. Due to the absence of this garden, the ingestion frequency is lower, than with ‘Residential with garden or vegetable garden’. Except for soil ingestion, exposure is possible via every described route.

8.2.4 Infrastructure

In the user scenario infrastructure, exposure only takes place via outdoor exposure. The exposure via cultivation of crops and drinking water are however not possible. It is expected, that humans remain in this user scenario for one hour a day. The contact time with soil particles is lower than with ‘Residential with garden or vegetable garden’ and therefore the ingestion frequency is also lower. Exposure is only possible due to ingestion of soil, dermal contact with soil particles, inhalation of soil particles and inhalation of outdoor air.

8.2.5 Working and industry
In this user scenario crops are not grown and the people are only present during working hours (40 hour a week indoors and 7 hours outdoors). Children are not included in the model, if they are not present at the location. The contact time with soil particles is lower than with 'Residential with garden or vegetable garden' and therefore the ingestion frequency is also lower. Except for consumption of contaminated crops, exposure can take place via every described route.

8.2.6 Recreation
In this user scenario crops are not cultivated. The chance of direct contact with the soil is relatively high in this user scenario; therefore the ingestion frequency is similar to the frequency in 'Residential with garden or vegetable garden'. Except for exposure via consumption of contaminated crops every route of exposure is possible.

8.2.7 Social and cultural
This user scenario is similar to the scenario working and industry and includes theatres, libraries et cetera.

8.2.8 Nature, public greens and fallow ground
In this user scenario exposure only takes place outdoors. Exposure via the ingestion of contaminated crops and drinking water is not possible. It is assumed that people are present for one hour per day. The chance of direct contact with the soil is relatively high in this user scenario; therefore the ingestion frequency is similar to the frequency in 'Residential with garden or vegetable garden'. Exposure is possible via ingestion of soil particles, dermal contact with soil particles, inhalation of soil particles and inhalation of outdoor air .

8.3 Relations between old and new user scenarios CSOIL 2000

8.3.1 Residential with vegetable garden
For this soil user scenario only the name was changed into kitchen, -vegetable garden. The rest has not been changed in the latest CSOIL 2000 version.

8.3.2 Residential with garden
This user scenario has not been changed in the latest CSOIL 2000 version. It still is the standard user scenario.

8.3.3 Residential without garden
The user scenario 'Residential without garden' has not been included in the new CSOIL 2000 (2006). This scenario was used when there were housing sites without gardens, for example a block of flats. This scenario is now included under scenario 6 'Other greens, buildings, infrastructure and industry' of the CSOIL 2000 (2006) version.

8.3.4 Infrastructure
The user scenario infrastructure still exists in CSOIL 2000 (2006). However is has been extended with the scenarios other greens, buildings and industry. This scenario now not only includes roads, but also industrial areas, road sides and buildings without gardens. The new scenario is a combination of the previous scenarios infrastructure, working, industry, social and cultural.

8.3.5 Working, industry

As described in the previous paragraph working and industry are now included in the new infrastructure scenario. Therefore this user scenario does not exist anymore as such.

8.3.6 Nature, public green and fallow ground

This user scenario has also been divided over new scenarios. Nature is now a user scenario by itself, without any addition. Public green has become a part of the new scenario ‘Green with nature values -sports recreation and city parks’. Fallow ground is not placed in any specific new scenario; however it is possible to place it in the scenario ‘Other greens, buildings, infrastructure and industry’.

8.3.7 Recreation

The user scenario recreation is no longer a user scenario on its own, but has been included in the user scenario ‘Green with nature values –sports recreation and city parks’.

8.3.8 Social and cultural

The social and cultural scenario is implemented in the new scenario ‘Green with nature values -sports recreation and city parks’. Therefore this user scenario does not exist anymore as such.

8.3.9 New scenarios

In the CSOIL 2000 (2006) version there are two new scenarios that in the earlier model CSOIL 2000 did not exist: agriculture without farm (yard) and places where children play.

Agriculture without farm (yard)

In the earlier model CSOIL 2000 agriculture was included in the user scenario ‘Residential with vegetable garden’. Now it has become a solitaire user scenario that includes grassland, arable farming and crop farming.

Places where children play

In the earlier CSOIL 2000 children’s playgrounds and playing field were included in the standard user scenario. It was possible to select the option children for the contaminant lead. But otherwise this user scenario was related to the standard scenario.

Table 8.1 shows in which new user scenario, the previous scenarios (or part of it) are now located.

Table 8.1: The locations of the old user scenarios in the new user scenarios.

The model CSOIL 2000	The model CSOIL 2000 (2006)	Comments
1) Residential with vegetable garden	**1)** Kitchen, - vegetable garden	- Name change
2) Residential with garden (standard scenario)	**2)** Residential with garden (standard scenario)	- No change
3) Residential without garden	**7)** Other greens, buildings, infrastructure and industry	-Residential without garden → Buildings
4) Infrastructure	**7)** Other greens, buildings, infrastructure and industry	-Infrastructure → Infrastructure
5) Working and industry	**7)** Other greens, buildings, infrastructure and industry	-Working → Buildings -Industry → Industry
6) Recreation	**6)** Green with nature, sports recreation and city parks	-Recreation → Recreation
7) Social and cultural	**7)** Other greens, buildings, infrastructure and industry	-Social/cultural → Buildings
8) Nature, public green and fallow ground	**5)** Nature **6)** Green with nature, sports recreation and city parks **7)** Other greens, buildings, infrastructure and industry	-Nature → Nature -Public green → Green with nature -Fallow ground → Other greens
New scenarios		
Agriculture without farm (yard)	N/A	Was located under **1)** Residential with vegetable garden
Places where children play	N/A	Was located under **2)** Residential with garden (standard scenario)