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A human exposure model to calculate harmonized risk limits

Model description and analysis

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Rapport in het kort

Een humaan blootstellingsmodel om geharmonizeerde risicogrenzen te berekenen – modelbeschrijving en analyse

Het humane blootstellingsmodel zoals opgenomen in het Europese risicoschattingmodel EUSES mist een aantal blootstellingroutes via de bodem die wel zijn opgenomen in het Nederlandse blootstellingsmodel CSOIL. Dit rapport beschrijft hoe de twee modellen gecombineerd zijn tot een nieuw model. Dit blootstellingsmodel is ‘Humanex’ genoemd. Het heeft tot doel om concentraties in het milieu te berekenen die de mens beschermen tegen nadelige effecten van chemische stoffen die zich kunnen verspreiden in het milieu. Deze zogenaamde milieurisicogrenzen zijn gebaseerd op gelijktijdige blootstelling van de mens via water, bodem, lucht en het dieet. Het model werd geanalyseerd aan de hand van proefberekeningen met 17 stoffen. De stofeigenschappen bepalen welke van deze routes het meest bijdragen aan de totale blootstelling. De modelanalyse liet tevens zien welke modelonderdelen nog verder kunnen worden verbeterd.

Trefwoorden: mens, blootstelling, model, chemische stoffen, normstelling

Abstract

A human exposure model to calculate harmonized risk limits - model description and analysis

The human exposure model, as integrated in the European risk assessment tool EUSES, lacks several exposure routes to contaminated soil that are part of the Dutch model CSOIL. This report describes how the two models are combined into a new model, called ‘Humanex’. This new model is aimed at calculating environmental concentrations for the protection of humans against hazardous effects of chemicals that can disperse into the environment. These concentrations, or so-called environmental risk limits, are based on a cumulative exposure of humans by way of water, soil, air and the diet. The model was analysed in a study on 17 compounds. Analysis showed that substance properties determine which of the potential exposure routes are most important for the total exposure. The study also revealed wich model components could still be improved.

Keywords: humans, exposure, model, chemicals, quality objectives

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Samenvatting

Dit rapport beschrijft het humane blootstellingsmodel Humanex. Humanex is ontwikkeld om milieurisicogrenzen (MRG's) af te leiden voor de effecten van stoffen op mens. MRG's zijn uitgedrukt als concentraties in lucht, water, bodem en sediment die overeenstemmen met bepaalde beschermingsniveaus voor de mens of het milieu. MRG's worden afgeleid in het project '(Inter)nationale normstelling stoffen (INS). MRG's met het Humanex model zijn zodanig berekend dat de gecombineerde blootstelling door middel van voedsel, inhalatie, bodemcontact et cetera niet mag leiden tot overschrijding van humaan-toxicologische grenswaarden. Dit rapport beschrijft hoe het model is opgebouwd en bevat tevens een nauwkeurige analyse van de onderdelen ervan. Hierdoor konden kritische blootstellingroutes en modelelementen geïdentificeerd worden. De modelanalyse laat zien dat een model nodig is om MRG's te berekenen, vanwege de complexe interactie tussen stofeigenschappen en het grote aantal (potentiële) blootstellingsroutes.

Een van de doelen van de milieukwaliteitsnormen die de overheid vaststelt is het uitsluiten van ongewenste effecten van stoffen op de mens of het ecosysteem. Voor risico's van vluchtige stoffen voor de mens werd vaak aangenomen dat de blootstelling via inademing de belangrijkste rol speelt. Eerdere studies hebben echter laten zien dat de totale blootstelling ook via andere routes verloopt. Daarom zijn directe en indirecte routes gecombineerd in het Humanex model, gebaseerd op twee bestaande modellen: EUSES en CSOIL.

De Europese Unie heeft het computer programma EUSES ontwikkeld (European Union System for the Evaluation of Substances). EUSES bevat een multi-media blootstellingsmodel dat concentraties van stoffen kan voorspellen in het milieu, gebaseerd op (schattingen van) stofeigenschappen, productievolume en emissies. Het CSOIL model is ontwikkeld in Nederland om de blootstelling van mensen die leven of werken op verontreinigde grond Dit model bevat een aantal blootstellingsroutes die afwezig zijn in EUSES.

Humanex combineert CSOIL en EUSES in een gecombineerd blootstellingsmodel. De volgende routes worden in aanmerking genomen: blootstelling via gewassen, vlees, melk en vis, bodemingestie, inademing van stof, huidcontact met bodemstof, inademing, drinkwater, permeatie van stoffen uit de bodem in drinkwater en douchen. De invoer voor het model begint met milieuconcentraties, die berekend worden met EUSES op basis van fysisch-chemische stofeigenschappen en emissiekarakteristieken.Vervolgens worden deze gecombineerd met gegevens over de humane blootstelling. Met behulp van een set vergelijkingen worden de concentraties in het milieu vertaald naar directe en indirecte blootstelling. De laatste stap vergelijkt de totale blootstelling met toxicologische grenswaarden, waarna het maximaal toelaatbaar risico (MTR_{humaan}) in de milieucompartimenten wordt berekend.

Summary

This report describes the multi-compartment exposure model Humanex. Humanex is developed to calculate environmental risk limits (ERLs) for human exposure to chemicals. ERLs are expressed as concentrations in air, water, soil and sediment that are associated with defined levels of protection for man or environment. ERLs are derived in the project '(Inter)National Environmental Quality Standards (INS)'. ERLs calculated by the Humanex model are such that the combined exposure by way of food, inhalation, soil contact et cetera does not exceed human-toxicological standards. This report contains a detailed description of the Humanex model and a model analysis to identify dominant exposure routes and model elements. Model analysis shows that the combined model is needed to calculate the ERLs due to the complex interaction between properties of chemicals and the multitude of potential exposure routes.

One of the objectives of environmental quality standards set by the government is that exposure to substances should not result in adverse effects on man and ecosystems. For volatile substances it is assumed that inhalation is the predominant route of exposure for man. Previous studies have shown that this underestimates total exposure, therefore direct and indirect exposure of man was combined in the Humanex model. The Humanex model is based on two existing models, EUSES and CSOIL.

The European Union has developed the computer program EUSES (European Union System for the Evaluation of Substances) to assess the exposure of Europeans to contaminants in the environment. EUSES contains a multi-media exposure model that can predict concentrations of substances in the environment, based on estimates for production volume, compound properties and emission.
The CSOIL model was developed in the Netherlands to estimate the exposure of humans who live on contaminated sites. The model includes several exposure routes not present in EUSES.

Humanex combines the CSOIL and EUSES model into a comprehensive model for human exposure. The following routes are considered: exposure from crops, meat milk and fish, soil ingestion, dust inhalation, dermal exposure to dust, inhalation of contaminant, drinking water, permeation of contaminant from the pore water into the drinking water and the exposure from showering with polluted drinking water.
The model needs input concentrations in the environment, calculated with EUSES. This requires physico-chemical properties of substances and production information. Subsequently, these are combined with data on human exposure into a set of equations tot calculate exposure by way of fish, cattle, drinking water, air, soil, crops and dust. These contaminant concentrations in human exposure media are subsequently used to calculate direct and indirect human exposure. The model contains a final procedure to calculate maximum permissible concentrations (MPC_{human}), based on a comparison of estimated total human exposure and toxicological threshold values.

1. Introduction

The ‘Project Setting (Inter)National Environmental Quality Standards (INS)’ exists since 1989. The aim of the project is to derive environmental risk limits (ERLs) for air, water, sediment and soil for selected substances. ERLs (Table 1) have been derived for a large number of substances [41] and serve as advisory values to set environmental quality standards (EQS, Table 1) by the government for various policy purposes [42]. The most important policy goals are:

- Develop source-orientated policy and policies to further reduce and control emissions to meet the general basis of the overall environmental policy, which is sustainable development [42,43]. Sustainable development means that the quality of the environment is guaranteed for the next generation and beyond. Exposure to substances should not result in adverse effects on *man and ecosystems.*
- Systematically evaluate the environmental quality with national, regional and local monitoring programs that measure the concentration of substances in the environment.

Table 1. Environmental Risk Limits (ERLs) and the related Environmental Quality Standards (EQS) that are set by the Dutch government in The Netherlands for the protection of ecosystems.

NC *Negligible Concentration*
MPC *Maximum Permissible Concentration*
SRC_{eco} *Serious Risk Concentration for the ecosystem*

Description	ERL	EQS
The NC represents a value causing negligible effects to ecosystems. The NC is derived from the MPC by dividing it by 100. This factor is applied to take into account possible combined effects.	NC (for air, water, soil, groundwater and sediment)	Target Value (for air, water, soil, groundwater and sediment)
The MPC is a concentration of a substance in air, water, soil or sediment that should protect all species in ecosystems from adverse effects of that substance. A cut-off value is set at the fifth percentile if a species sensitivity distribution of NOECs is used. This is the Hazardous Concentration for 5% of the species, the HC_5^{NOEC}.	MPC (for air, water, soil, groundwater and sediment)	MPC (for air, water, sediment and air)
The SRC_{eco} is a concentration of a substance in the soil, sediment or groundwater at which functions in these compartments will be seriously affected or are threatened to be negatively affected. This is assumed to occur when 50% of the species and/or 50% of the microbial and enzymatic processes are possibly affected.	SRC_{eco} (for water, soil, groundwater and sediment)	Intervention Value (for soil, sediment and groundwater)

Since the EQSs are supposed to protect both ecosystems *and* man, special attention has been paid to substances that are volatile and can be expected to expose man by inhalation of contaminated air [44]. For volatile substances it is assumed that inhalation through air is the predominant route of exposure for man. A previous study showed that this is not always true

[18]. Calculating the exposure to man only from the air compartment was found to underestimate total exposure.
In 1995 the Committee on Setting Integrated Environmental Quality Objectives (Stuurgroep Integrale Normstelling Stoffen) concluded that multiple routes of exposure should be taken into account when calculating MPCs so no relevant route of exposure would be ignored. The committee also confirmed that it was necessary to take the partitioning of substances into account when setting maximum permissible risk concentrations for water, sediment, soil and air [10]. This partitioning of substances is formalised in the concept of multi-media exposure models [17,30]. Multi-media exposure models [17] as implemented in EUSES [23] can predict concentrations of substances in the environment. To protect humans from multi-compartimental exposure, environmental quality standards should be based on human exposure through multiple pathways. It is assumed that chemicals may partition from one compartment to another, driven by thermodynamic gradients between the compartments. The present report describes the multi-compartment exposure model Humanex that was developed to meet this goal.

1.1 Exposure models

When a contaminant is produced for some time it may accumulate in the ecosystem and eventually enter the human food chain. To assess the exposure of a person through food one has to actually measure the concentration of the contaminant for every single item of food and measure total food intake. This is not feasible for the purpose of general risk assessment and a model is needed. The model consists of mathematical equations describing the exposure of humans to contaminants, using information on diet, behaviour and contaminant properties. Exposure assessment is based on an average person. Different models are already available for exposure assessment. The two most important ones for the present purpose are briefly described.

The European Union has developed the computer program EUSES (European Union System for the Evaluation of Substances) to assess the exposure of Europeans to contaminants in the environment. With estimates for production volume, compound properties and emission, the model calculates concentrations in the environment. These predicted environmental concentrations (PECs) are then used to calculate the exposure of humans through air, drinking water, meat, milk, fish and crops.
The CSOILmodel was developed in the Netherlands to estimate the exposure of humans who live on contaminated sites. The model includes routes not present in EUSES: exposure from home grown crops, soil ingestion, dust inhalation, dermal exposure to dust, inhalation of contaminant evaporated from the soil or ground water, permeation of contaminant from the pore water into the drinking water and the exposure from showering with polluted drinking water.
By combining the CSOIL and EUSES model a comprehensive model can be built to describe multi-media exposure. This new multi-media exposure model should be in agreement with the INS-concept of partitioning of substances and calculates human exposure and is named INS-Humanex.
The ERLs calculated by Humanex are meant to protect humans from exposure to chemicals at background levels due to diffuse(non-local) emissions. This is obviously a different goal than the current Intervention Values, which are based on local exposure due to soil pollution. The exposure scenario in CSOIL for humans that are exposed to polluted soil, whether direct or indirect, is different from the one used in this study.

1.2 INS-Humanex model

In this report a new procedure to derive MPCs for humans is presented. Well-documented exposure routes of humans were combined. This effectively gave rise to a new model named Humanex and it is programmed in Excel. It needs the input concentrations for the four compartments soil, surface water, air and pore water.

Humanex combines human exposure routes from CSOIL and EUSES. This approach is based on the predicted environmental concentrations (PECs) produced by EUSES. To calculated PECs physico-chemical properties of substances and production information is needed. The PECs, substance properties, and data about human exposure are combined into a set of equations (Chapter 2). A thorough analysis of the model was performed in the form of a sensitivity analysis (Chapter 3). Humanex calculates contaminant concentrations in e.g.: fish, cattle, drinking water, air, crops and dust. These contaminant concentrations in human exposure media are subsequently used to calculate the direct and indirect human exposure (Chapter 4). Then, total human exposure is compared to toxicological threshold values. Based on this comparison 'safe' environmental levels are calculated (Chapter 5). The influence of physico-chemical properties and predicted environmental concentrations on the main route of exposure were studied (Chapter 6). The use and validity of the Humanex model is discussed and suggestions for improved are made in the final section (Chapter 7).

2. Description of the Humanex model

2.1 The Humanex-model

The purpose of this project is to calculate human risk limits, maximum permissible concentrations (MPC_{human}), for exposure to chemicals from non-local sources. The Humanex model predicts the relative and absolute exposure of a man to a single substance. It is possible to calculate the MPC_{human} for all compartments if the tolerable daily intake (TDI) is also known. First, contaminant concentrations in all human exposure media need to be calculated. The EUSES program [23] is used to calculate predicted environmental concentrations for the regional scale (PEC_{reg} values). These PECreg values are subsequently used to calculate the direct and indirect human exposure. From this exposure the estimated total exposure (ETE) for humans is calculated. The ETE is compared to the TDI after which the maximum permissible concentrations in the environment are calculated. This procedure is explained in Chapter 5. First, the model itself is discussed in the next sections.

The Humanex model combines the EUSES routes with the CSOIL routes of exposure. Because CSOIL and EUSES use different scenarios for assessing exposure, the models are very complementary in a combined model (see Figure 1 and Table 2). Overlap is only observed for exposure through crops (Table 3). All exposure routes in the combined Humanex model use the same environmental concentrations as input. These are for the compartments surface water, air, pore water (groundwater) and soil. The formulas and parameter values are derived from the most recent CSOIL-update and the EUSES manual (Table 4).
Compartments are assumed to be at steady-state concentrations when using the predicted concentrations of the regional scale (PECreg) as input for the Humanex calculations. When routes were both modelled by EUSES and Coil, such as the exposure through crops, then the parameter values used are specifically stated in Appendix II. In this project EUSES is used to predict environmental concentrations of most of the substances, for other compounds the PECs are from EU-RAR-reports that are based on expert use of EUSES.

Table 2. The Humanex model combines routes of exposure from EUSES and from CSOIL into a new model.

EUSES-model	CSOIL-model	Humanex-model
Air	Air	Air
n.i.	Inhalation of contaminant evaporated from the soil	n.i.
	Differentiation between inside and outside air.	n.i.
Meat[1]	n.i.	Meat
Milk[2]	n.i.	Milk
Fish	n.i.	Fish
Crops: root, leaf	Home grown crops: root, leaf	Crops: root, leaf
Drinking water purification	n.i.	Drinking water purification
n.i.	Permeation of contaminant from the soil into the drinking water	Permeation of contaminant from the soil into the drinking water
n.i.	Showering with drinking water	Showering with drinking water
n.i.	Soil ingestion	Soil ingestion
n.i.	Dust inhalation	Dust inhalation
n.i.	Dermal exposure to dust	Dermal exposure to dust

n.i. = not implemented, [1] Meat = all meat sources, [2] Milk = all diary products

The last group of chemicals are veterinary drugs [35].

Unless special precaution is taken, Humanex can only be used for calculations with non-dissociating organic compounds and not for other compounds such as metals.

Table 3. Used compounds.

Nr.	Compound	CAS	data from:	Nr.	Compound	CAS	data from:
1	triethanolamine	102-71-6	EPIWIN	17	acrylaldehylde	107-02-8	RAR EUR 19728 EN
2	diethylene glycol	111-46-6	EPIWIN	18	cumene	98-82-8	RAR EUR 19726 EN
3	ethylene glycol	107-21-1	EPIWIN	19	bis-pentabromo-phenyl ether	1163-19-5	RAR EUR 20402 EN
4	methanol	67-56-1	EPIWIN	20	ethyl acetoacetate	141-97-9	RAR EUR 30396 EN
5	tribromomethane	75-25-2	EPIWIN	21	linear alkylbenzenes	67774-74-7	RAR EUR 19011 EN
6	tetrahydriothiophene	110-01-1	EPIWIN	22	methacrylic acid	79-41-4	RAR I.01.36
7	butyl acetate	123-86-4	EPIWIN	23	pentabromodiphenylether	32534-81-9	RAR EUR 19730 EN
8	butanol	71-36-3	EPIWIN	24	chlorocresol	1570-64-5	RAR EUR 19757 EN
9	methyl tert-butyl ether	1634-04-4	EPIWIN	25	methylene dianaline	101-77-9	RAR EUR 19727 EN
10	methyl ethyl ketone	78-93-3	EPIWIN	26	biphenylol	90-43-7	Art. [35]
11	cyclohexylamine	108-91-8	EPIWIN	27	4-chloro-m-cresol	59-50-7	Art. [35]
12	ethyl acetate	141-78-6	EPIWIN	28	Ibuprofen	15687-27-1	Art. [35]
13	dodecylbenzene	123-01-3	EPIWIN	29	Ivermectin	70288-86-7	Art. [35]
14	hexachlorobutadiene	87-68-3	EPIWIN	30	Oxytetracycline	79-57-2	Art. [35]
15	nonylphenol	84852-15-3	RAR EUR 20387 EN	31	Triclosan	3380-34-5	Art. [35]
16	chloro-alkanene	85535-84-8	RAR EUR 19010 EN				

RAR: European Union Risk Assessment Report produced via the Institute for Health and Consumer Protection by the European Chemicals Bureau. RAR documents available via internet: http://ecb.jrc.it/

Table 4. Origin of formulas and parameter values.

Origin of EUSES exposure formulas	EUSES manual [7].
Origin of CSOIL exposure formulas	Appendix 6 of RIVM report nr. 711701022.
Origin of EUSES parameter values	EUSES manual [7].
Origin of CSOIL parameter values	Revised CSOIL 200 dataset in RIVM report 711701021
Used Parameter values are given in Appendix II: Parameter values.	

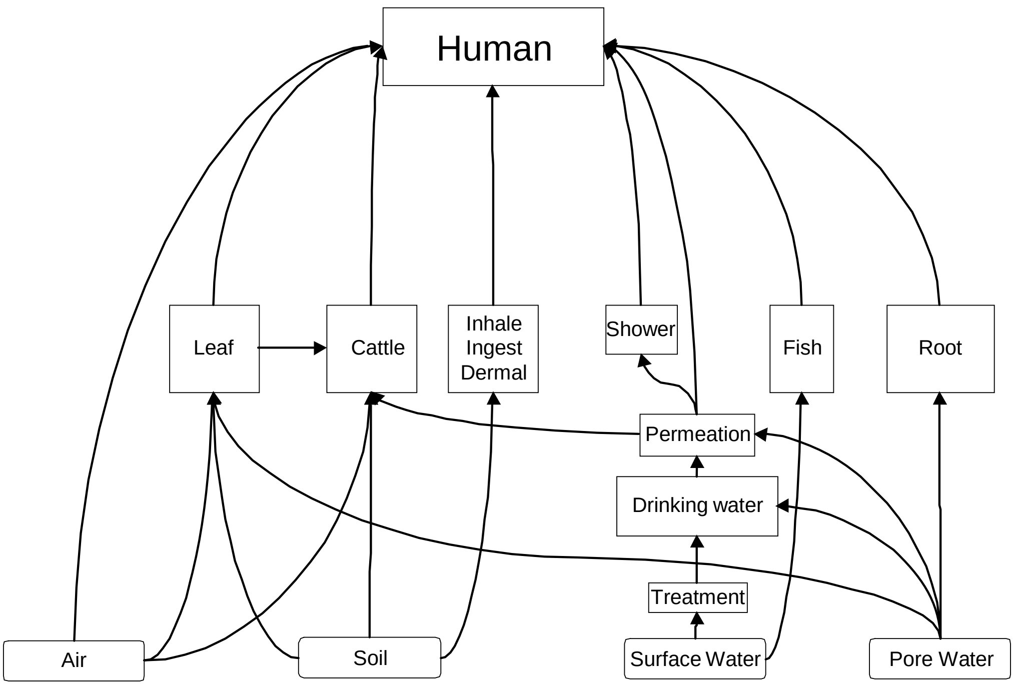

Figure 1. All routes of exposure in the Humanex model. Cattle includes meat and milk

In the following paragraphs brief descriptions are given about the models from which the building blocks for Humanex are derived and how the building blocks function. In the end of this chapter strengths and weaknesses of the modules are reviewed.

‘EUSES facilitates the quantitative assessment of the risks posed by new and existing substances and the environment’ [7]. EUSES is capable of assessing risk to man, consumers, workers, sewage treatment plants micro-organisms populations and certain ecosystems. It is capable of predicting environmental concentrations on all scales, with the scale of a country being named the regional scale (PECregs).
These PECregs represent concentrations in the soil, air, pore water and surface water. PECregs are the predicted environmental concentrations on the scale of one country. The prediction is based on the mostly factual way of production and usage of the product of concern. This means that if the way of production or usage changes than the PECregs will change to. Any calculation based on PECregs is only valid as long as the entered data is still a representation of the reality. When the amount of produced chemical is increased than the PECregs should increase proportional. If increased production volumes mean a change in the type of production than PECregs have become invalid and new PECregs must be calculated based on the new way of production.
The exposure to a given compound can be calculated using production volumes, compound properties and emission estimates. Routes of exposure in EUSES for humans are air, drinking water, meat, milk, fish and crops (Figure 2).

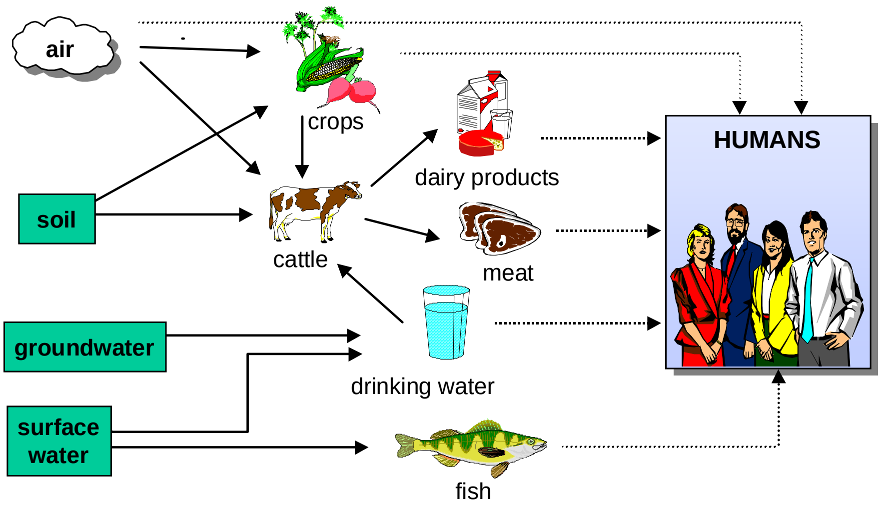

Figure 2. All routes of exposure in the EUSES model

‘The CSOIL model is developed to calculate the serious risk concentrations (SRC) at which human toxicological maximum permissible risk limits (MPR or TDI) is exceeded. The model is used to quantify the human exposure to soil pollutants for a residential situation at a local scale’[22].
CSOIL does not use estimates of concentrations for the compartment soil data must be entered derived from measurements from which concentrations in soil solids, soil air and pore water are calculated. From there on concentrations in the contact media are calculated. The following routes of exposure are present in CSOIL: exposure from home grown crops, soil ingestion, dust inhalation, dermal exposure to dust, inhalation of contaminant evaporated from the soil, permeation of contaminant from the pore water into the drinking water and the exposure from showering with polluted drinking water (Figure 3).

Humanex is based on multi-media exposure pathways. Just like EUSES it is a generic model and assumptions are made on the distributions of the contaminants over the compartments and the compartments are assumed to be homogenous and well mixed; e.g. there is no spatial difference within one compartment.

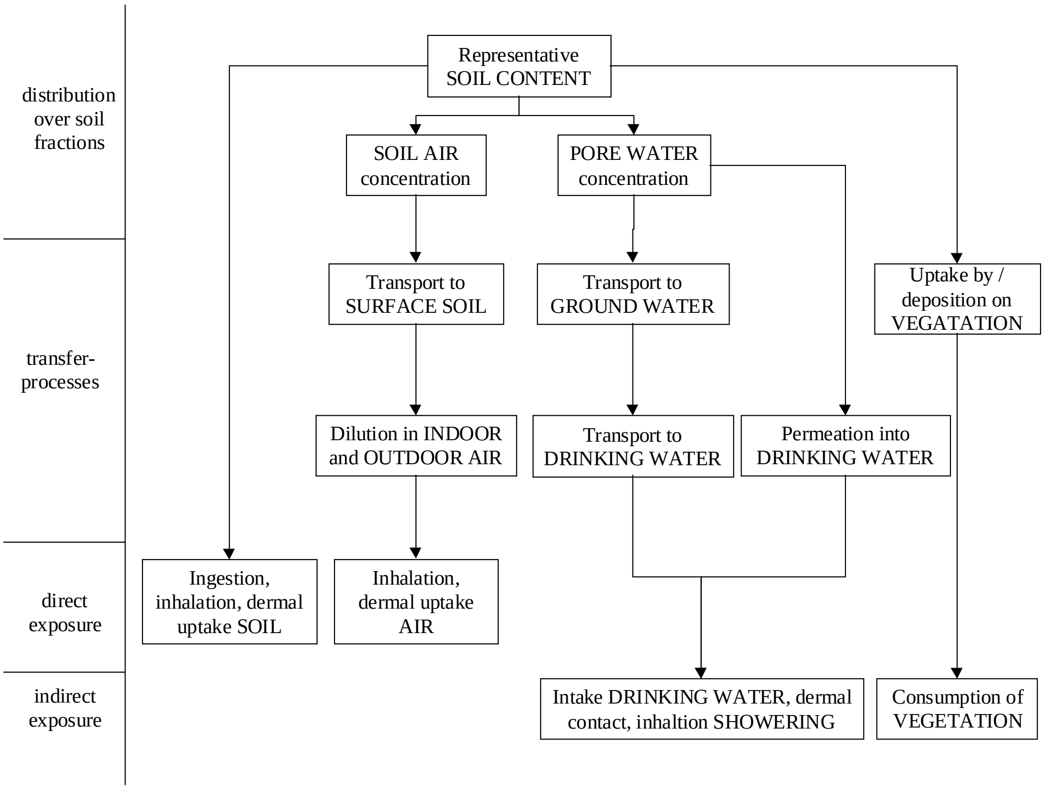

Figure 3. All routes of exposure in the CSOIL model

2.2 Model Description

The Humanex model is implemented in an Excel file with several work sheets. One work sheet contains the compound data such as K_{ow}, solubility, Henry's law constant, molecular weight, PECregs et cetera. The Input sheet contains default values for the formulas. Default values can always be altered, if no value is entered the default is used. Each route of exposure has a separate work sheet in which the formulas are implemented; the data needed for these formulas is gained from the input sheet with default values. The Input sheet also has a table in which routes of exposure can be toggled on and off. The Output sheet which calculates overall exposure, calculates maximum permissible concentrations and generates tables which show the absolute exposure and the absolute and relative importance of each route of exposure, and from which compartment the exposure originates. The Output sheet also checks for improper solubility and vapour pressures at input concentrations and MPCs.

Below follows a summary of each module. Parameter values are listed in Appendix II and the exact formulas are in the Appendix III. The following section gives a brief description of the processes in the exposure routes and are meant to point out any possible difference between EUSES, CSOIL, and Humanex formula implementation. The summary also gives the limitations of each module.

2.2.1 Fish module

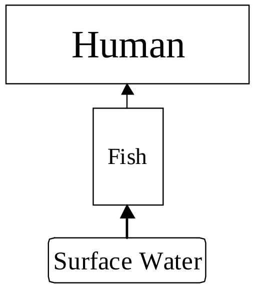

Figure 4. Route of exposure through fish.

Used compartments: surface water (Figure 4).
Processes: The fish module is the same as in EUSES and consists of only one formula to calculate the concentration of contaminants in fish, for this a bioconcentration factor (BCF) is used. This BCF predicts the ratio between the concentration in fish and the predicted environmental concentration in the surface water.
Limitations:
1. Molecular weight must be less then 700 g/mol
2. Used Log K_{ow} must be between 1 and 10
3. The QSAR on which the BCF is based is based on a limited amount of data-points and near the outer limits of log K_{ow} 1 and 10 the estimation becomes less reliable. Also, the BCF is only valid for the neutral fraction of dissociating compounds [24].
4. Only freshwater fish is consumed which may over-estimate exposure, as mainly sea fish is consumed [13].

2.2.2 Air module

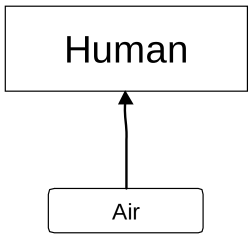

Figure 5. Route of exposure through air.

Used compartments: Air (Figure 5).
Processes: Formulas are from EUSES, and only direct exposure to air is modelled in this module. Concentrations in air are equal to the PECreg air. The same air concentrations are assumed for indoors, outdoors and at work.
Optional: It is possible to activate a module in which contaminant evaporates from soil into the outdoor air and in to the basement as in CSOIL. There will the contaminant accumulation in the basement and diffusion into the house will occur. Extended descriptions of this route of exposure are available [19,22,37,40]. All data and conclusions presented in this report are based on module settings in which this option was not activated. SimpleBox calculates the concentrations of the PEC being in steady state, all transport between soil and air compartment has been taken into account. To model this soil to air evaporation would mean abandoning the assumption that the calculated concentrations are in steady state.
Limitations:
1. No basement accumulation was modelled.
2. No differentiation in indoor, outdoor and work air concentrations was modelled for reasons of simplicity.

2.2.3 Root Module

Used compartments: pore water (Figure 6).
Processes: The root module is the same as in EUSES and CSOIL, but CSOIL parameter values are used. The root consists of a water fraction and a lipid fraction. The water fraction is considered to be in equilibrium with the pore water and has the same concentration as the pore water. The lipid fraction is assumed to behave like octanol. Depending on the lipophilicity, expressed as the K_{ow} of the neutral organic compound, the root lipids will reach equilibrium with the pore water surrounding the root. The source of all contaminant is the pore water; the PECreg, agricultural pore-water.

According to the verification in Rikken *et al*. [22] the concentration in the roots is realistic worst case, because the model is used for thick roots but is based on fine roots. Fine roots reach equilibrium more quickly with the surrounding pore water. Potatoes and carrots are thicker and thus the inside of these thicker root products could not be in equilibrium with the centre of the root.

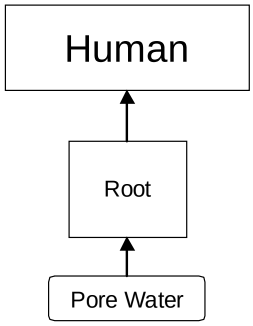

Figure 6. Route of exposure through root.

Limitations:
The root concentration factor is based on measurements done on barley ($r^2 = 0.96$), but the number of 7 data-points is very low and only based on a few compounds [2].
A validation study has been done in Rikken *et al*. [22] in which 27 sources for BCFs from literature are compared with the BCFs predicted with the Trapp and Matthies model. This comparison concludes that the BCF can reasonably be estimated for the fine roots and that more experiments, model modification and parameterisation is needed for further use.

2.2.4 Plant module

The formulas in the Humanex plant module is based on the PLANTX model of Trapp and Matthies [28]. The same model is used in EUSES and CSOIL. The parameters have been taken from the latest CSOIL edition.
Used compartments: The plant takes up contaminant from a number of compartments: air, soil and pore water (Figure 7).

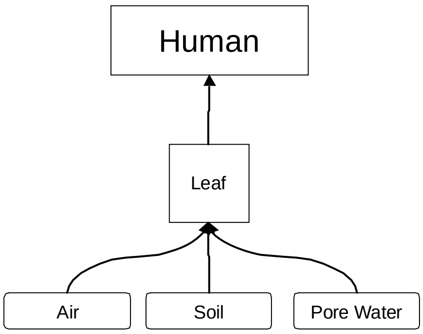

Figure 7. Route of exposure through stem and leaves

Transport from pore water to the plant
The plant evaporates water and thus creates a flux (mass transport) of water towards the xylem of the plant; this stream is called the transpiration stream. The flux of water originates in the pore water and can contain contaminants. These contaminants travel with the water in the xylem and into the leaves. The transpiration stream concentration factor (TSCF) is calculated with the method of Briggs *et al.* [2] and with the method of Hsu *et al.* [47]. In Humanex and in CSOIL the highest value of these are chosen as the TSCF. In EUSES only the method of Briggs is used with a minimum and a maximum log K_{ow}. The TSCF always has a minimum value of 0.04 in Humanex and in CSOIL.
Transport from air to the plant
A flux is calculated based on a partitioning coefficient of the contaminant between water and air and the partitioning coefficient between plant and water. This latter partitioning coefficient is likewise calculated as the concentration ratio between root and pore water. The fraction bound to aerosols is taken into account in Humanex as in EUSES; this is not done in CSOIL. If the concentration in the plant is higher than in the air than the flux is negative, thus reducing the amount of contaminant in the plant. Otherwise the concentration increases.
Concentration in the plant
The above water flux and air flux are added and together form a constant rate of input of contaminant. (Although it is possible to have evaporation of contaminant out of the plant.) The input flux can be countered by photo-degradation, the metabolism of the plant and the

growth rate of the plant. The growth rate of the plant can by default cause a lower end concentration in the plant by growth dilution. Many elimination and metabolism rates are unknown and are set at zero as a worst case scenario. In EUSES, CSOIL and in Humanex photo-degradation rate and the metabolism rate of the plant are zero.

Soil particle resuspension / deposition

Transport from the soil to leaf can take the form of small soil particles, which splash up against the stems and leaves of plants when it rains or when the wind blows. These particles are part of the dirt on the outside of the plant, which are washed of mostly before consumption. The concept is taken from the CSOIL2000R model and is now part of Humanex. This process is not implemented in EUSES.

Final concentration in stem and leaves

The concentration in plant is calculated by adding the concentration in plants together with the contamination from deposition and is expresses as kg contaminant per kg fresh weight plant.

Limitations: Points of limitation are in Rikken *et al.* [22], and summarised below:

1. The calculation of the TSCF is only valid in the range of log K_{ow} minus 0.5 to plus 4.5. Outside this range a minimum value of 0.04 for the TSCF is used.
2. This model is only valid for non-dissociating (neutral) organic compounds.
3. The model generates the concentration of contaminants in a plant, which is an abstraction of real plants. This model is used to predict the concentration in grass for cattle, and to predict the concentration in the leafy plants humans eat. Fruit, seeds and stems are not modelled in this way and non-leafy parts are expected to be less contaminated than the xylem. This means using this model to predict the concentration in fruit, seeds and stems is a worst-case scenario.
4. The model assumes continues exponential growth. This means the model only applies to plants that are eaten before they stop growing. This is correct for grass and lettuce. But many plant parts slow their growth towards the end of the growth season.
5. The empirical parameters for TSCF and the ‘b’-value for the conversion of plant lipids to octanol are derived from a small amount of experiments.
6. There are no experimental data available for substances with a high log K_{ow}.
7. It would be good to have specific parameter values for grass so the exposure through grass for cattle can be assessed more precisely. Currently cattle and humans eat the same generic vegetable fodder.

The predictions of the BCF calculated with the Trapp and Matthies PLANTX-model are compared with at least 6 groups of compound [22]. The calculated BCFs deviated log units above and below the measured BCFs. The main point of concern is that only one set of equations (or PLANTX-model) is used to simulate all type of consumed plant types using default parameters [27]. These parameters are not incorrect by default because many plants behave likely but validation is limited. The predicted concentration in the plant has an uncertainty of at least one log unit [22].

2.2.5 Drinking water

Used compartments: Surface water, pore water (Figure 8).

Processes: Drinking water is either produced from groundwater or from purified surface water. Drinking water is transported through the network of the supplier to the households. Contaminant in soil can permeate through

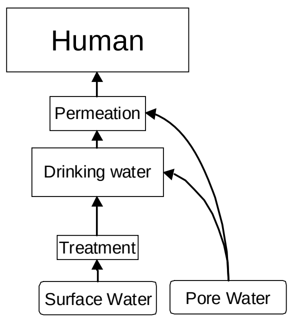

Figure 8. Route of exposure through drinking water.

the pipes into the drinking water close to the buildings where pipes are assumed to be made of PE or PUC and permeable. During the last part of the transport of the drinking water to the households permeation of the contaminants through a low-density polyethylene tube, as worst-case scenario, into the water supply can occur. This is modelled using CSOIL formulas. The speed in which the tube is infiltrated by the compound is expressed with the permeation coefficient (m^2/d). As a default this value was set as $1.4*10^{-6}$ m^2/d for all compounds used in this report. The production of drinking water is modelled through the use of EUSES formulas. A purification factor for surface water is derived from a table from Hrubec and Toet using physicochemical properties, such as Henry coefficient, log K_{ow}, purification system and biodegradability of the compound [12]. As a worst-case scenario the most contaminated source for the drinking water is used: either unpurified groundwater or purified surface water.

Limitations:

1. The derivation of an accurate purification factor is quite difficult. The table used in EUSES is based on a preliminary assessment of the removal percentage of organic chemicals by the diverse treatment systems [12]. This table has not been validated with new and more recent data. The worst-case scenario to use the most contaminated water as source for drinking water can cause a great over-estimation of the exposure through drinking water. Improving the estimation of the purification factor can only reduce this. Jager *et al*. proposes to use a fixed uniform purification factor of 0.15 based on 8 pesticides as worst-case situation [14].
2. The permeation model is based on experiments with a limited amount of compounds. The permeability coefficients of other compounds have to be estimated [36,39].
3. The permeation model is obsolete (paragraph 7.2.4).

2.2.6 Meat and Milk

Used compartments:

All four compartments: Air, soil, pore water and. surface water (Figure 9 next page).

Processes: All calculations are based on EUSES formulas. Cattle is exposed through grass fodder, air, drinking water and soil particles on the grass. The exposure of cattle is totalled to a daily average expressed in the units kg/d. An experimental derived bio transfer coefficient (BTF) with units d/kg is used together with the contaminants log K_{ow} to calculate the concentration of contaminant in meat and milk. A BTF is in general similar to a BCF.

Limitations:

1. The BTF for meat is derived from a data set with compounds with a range of 1.5 to 6.5 [29]. Outside this range the BTF should not be calculated, but if the contaminants log K_{ow} is outside this range it is set to 1.5 or 6.5 [7].
2. The BTF for milk is derived from a data set with compounds with a range of 3 to 6.5 [29]. Outside this range the BTF should not be calculated, but if the contaminants log K_{ow} is outside this range it is set to 3 or 6.5 [7].
3. The drinking water for cattle is the same as human drinking water in Humanex. Cattle are not modelled in CSOIL and in EUSES cattle drink the same water as humans.
4. Outside the previous mentioned range of log K_{ow} the BTFs should not be estimated.
5. The predicting formulas should only be used to predict BTFs for the type of substances on which the formula is derived from, i.e. lipophilic, non-metabolisable narcotic substances.
6. The BTFs are based on data from 1988. Measurements are based on a limited number of data points on a limited number of compounds and limited explained variance [29]. (For BTF_{meat} n=36, r^2 = 0.66, and for BTF_{milk} n =29, r^2 = 0.53.)
7. Only cattle is used for BTF measurements, other meat sources such as pork and chicken are ignored.

8. All dairy products in the EUSES model are lumped together and a BTF for milk is used to calculate the concentration in this dairy. Milk is less fat than cheese and butter. Thus the calculated concentrations for the diary is an underestimation because fat has the tendency to accumulate compounds for which the BTF is used [24]. A future solution can be found by considering the exposure to milk-fat instead of exposure to milk and diary, since it is this fat that contains the lipophilic substances and is used in many food items.

More experiments would be welcome to decrease the uncertainty in the relationship between log K_{ow} and BTF, to increase the range in which the relation is valid more species should be used when doing this.

2.2.7 Shower

Used compartments: surface water and pore water (Figure 10).
(**Processes:** Drinking water is used to take a shower. While showering, contaminant from the water can be absorbed through the skin. Droplet formation of the water will increase the surface-volume ratio and will increase the evaporation rate of the contaminant from water to air. An increased temperature of the water also increases the rate of evaporation. The dermal and inhaled exposure is calculated using the physic-chemical parameters: Henry, molecular mass and K_{ow}. All formulas are based on CSOIL. More information in Otte *et al.* [19].

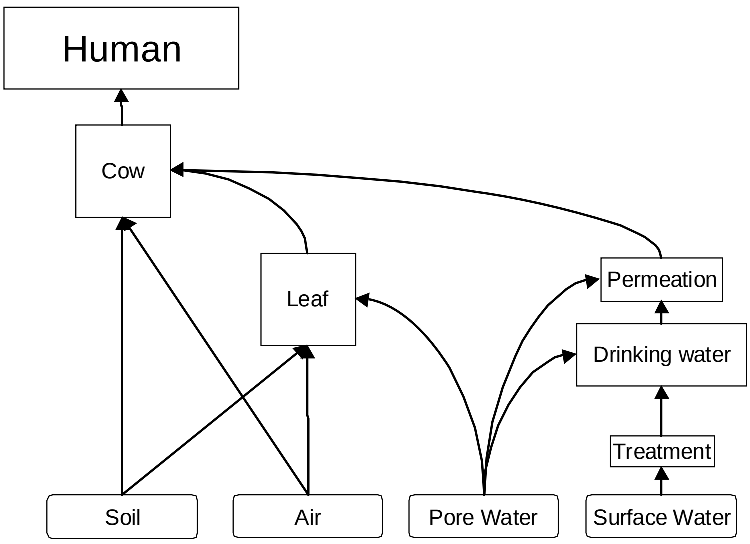

Figure 10. Route of exposures through the cow derived products meat and milk.

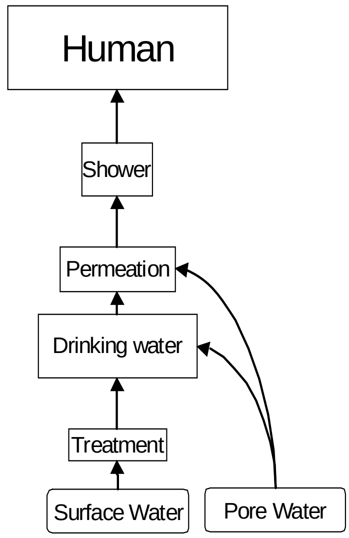

Figure 10. Route of exposures through showering.

Soil and Dust

Used compartments: soil (Figure 11).
Soil ingestion: Adults and especially children ingest soil on purpose and by accident. This soil is then digested and the contaminant is released partly into the digestive tract after which the chemical can be absorbed into the body. For some compounds this the main route of exposure in CSOIL. The parameters involved in this route have been revised and updated [16,19].

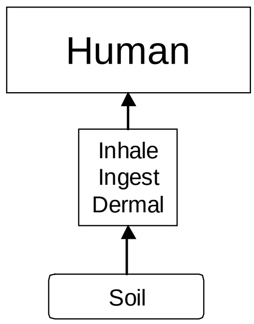

Figure 11. Route of exposures through inhalation, dermal absorption and ingestion.

Dust inhalation: When breathing air dust is also inhaled, with a different exposure regime for indoors and outdoors. Dust particles are composed partly of soil. 75% of all inhaled particles is considered to be retained in the longs. Outdoors the concentration of dust particles is higher but the fraction of soil in these particles is lower. Indoors the concentration of dust particles is lower but the soil content is higher in each particle. The concept of this exposure route has not been evaluated because it is a minor contributor to the overall exposure in CSOIL [22].

Dermal exposure to dust and soil: Particles contact the skin after which the contaminant in the soil fraction can absorb through the skin into the body. The amount of exposed surface area (skin) is higher outdoors and lower indoors. The amount of particles per square meter skin is higher outdoors and lower indoors. The concept of this exposure route has not been evaluated because it is a minor contributor to the overall exposure in CSOIL [22].

Limitations:

1. While dust inhalation and dust exposure are both routes of exposure in CSOIL each route uses different amounts of dust per particle even when comparing outside situation with outside situations.
2. According to the model all compounds behave the same. Molecular size or weight or hydrophobicity has no effect on the dermal absorption speed, but dermal absorption speed should be compound dependent.
3. All ingested contaminant is considered to be absorbed into the body in the same amount as was the case in the toxicology study for that compound on which the TDI is based. This means that the relative absorption for soil compared to the relative absorption food is equal but should be less. Generally an overestimation of the exposure will be the result because soil is expected to release it contaminant less easily than food but compound specific data is lacking, except for lead.

2.3 Reviewing the limitations

An overall limitation of the input is whether or not the concentrations in water are below the solubility of a compound. This was checked for input and output concentrations in the compartments pore water and surface water. For the maximum concentrations in pore air and the air compartment the Henry-coefficients were used to compare with the maximum possible concentrations. CSOIL was developed for volatile and persistent compounds. EUSES-modules are based on predictive formulas that are based on relative hydrophobic and persistent compounds. This would make the Humanex model only usable for persistent compounds in theory.

If all the module limitations and requirements would be taken in to account than the EUSES and thus Humanex model would have a small confined range of applicability.

Only a small K_{ow} range has a valid regression range in all QSARs. The joint regression ranges of log K_{ow} 3 to 4.5 is valid for all modules in EUSES (Figure 12) [7].

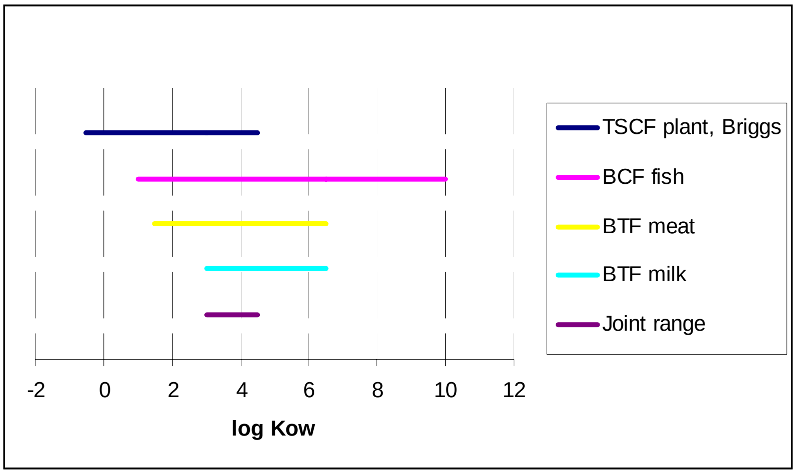

Figure 12. All regression ranges in the EUSES equations have a small overlap from log K_{ow} 3 to 4.5. After a figure of Schwatz [24].

This limited range of applicability needs careful consideration. When only a few percent of the total exposure goes through a route which is outside the regression range of the compound then this can be ignored. Problems arise if tens of percents of the total exposure is derived through routes which are used outside their range of application. Then the predicted exposure is very uncertain. For all compounds it has been checked that if the exposure through a route is 5% or more of the total exposure, the log K_{ow} does indeed fall within the range of application of the corresponding QSAR for that route of exposure.
For methanol with log K_{ow} of –0.8 the exposure is 86% through air, 8% through fish and 7% of the total exposure is through leafy products. The QSAR for the leaf model is log K_{ow} 0.5 to 4.5. Thus the exposure through leaf could be underestimated with an unknown magnitude, therefore expected exposure pattern for methanol can not stated.
For dodecyl benzene with log K_{ow} of 8.7 the exposure is 78% through root, 9% through fish and 5 percent through meat and 5 percent through milk. The QSAR for the meat module is log K_{ow} 1.5 to 6.5, and for the exposure through milk the QSAR is valid from log K_{ow} 3.0 to 6.5. Large molecules can have a high log K_{ow} but a large molecule is less easily resorbed than smaller molecules. Exposure can differ 2 orders of magnitude because the model does not consider a reduced resorption. This means the exposure through milk and meat can combine to a total exposure of 100% or be less than 0.1 %. The deviation can be either way and is unknown.
The log K_{ow} of pentabromodiphenylether is 6.6 and 22 percent of the exposure is through meat and also 22 percent of the exposure is through milk. Both QSARs for milk and meat have an upper limit of log K_{ow} of 6.5. This small difference is ignored.

All formulas in EUSES and CSOIL are meant for neutral non-ionising organic chemicals. While this is the case for most chemicals tested in EUSES and in the RAR reports this not the case for all 31 compounds used in this report.

3. Sensitivity analysis of Humanex

To learn how the model reacts to its input, a sensitivity analysis was done. A sensitivity analysis is performed to find the most sensitive parameters. These parameters must be the most accurate parameter to get accurate output from the relevant routes of exposure. A diverse set of compounds, of which half of them are volatile, was used for this analysis. The results of the sensitivity analysis are presented in the following sections based on 17 substances that are in realistic (relative) concentrations in the environment (Table 5).

3.1 Introduction to sensitivity analysis

The output of a model will respond to its input, e.g.: doubling the concentration of a contaminant in the surface water will cause a twofold increase in exposure from this compartment. A model is very sensitive to a specific parameter if a small change in the value of that parameter results in a large change in the output value. A model is insensitive to a parameter if a large change in the input parameter result in an unnoticeable change of the output value. The Humanex model has 198 input parameters, and some are sensitive and most are not sensitive.

To find out how the Humanex model reacts to its input a sensitivity analysis was done. This was done by multiplying all input parameters with a value chosen randomly between 0.9 and 1.1. This deviation was set as a uniform distribution (Figure 13) with a maximum of 1.1 and a minimum of 0.9 (average 1.0).

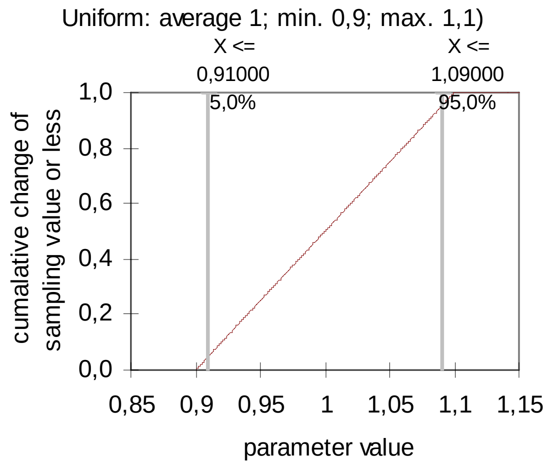

Figure 13. Uniform distibution with an average of 1 and a 10% variation.

3.2 Monte Carlo-Latin Hypercube

The Monte Carlo–Latin Hypercube method was use for randomly assigning values to parameters, and rerunning the model with these parameter sets. The next step in the sensitivity analysis is to relate the varied input with the corresponding output. For this Standardised Regression Coefficients (SRC) were calculated by the @RISK programme [1].

An SRC of one or minus one between an input parameter and an output value means that the output is completely dependent upon these input parameters.

Most coefficients that will be found are low and in the range of minus 0.4 to plus 0.4.
SRC values bigger than minus 0.4 and plus 0.4 are interesting and SRC values of +/- 0.7 are considered sensitive and should be determined with more precision (Figure 14).

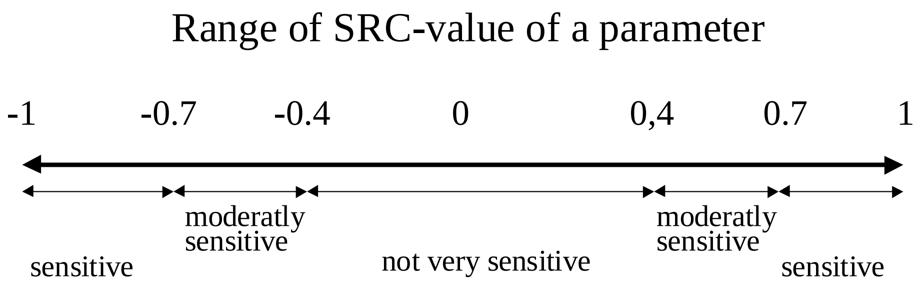

Figure 14. The arbitrary set range for interpreting the sensitivity for parameters. The range in which a parameter is interesting or sensitive seems large but a few parameters per module utmost are expected to be sensitive. When all parameters in a module are equally important than the SRC-values of these parameters will be the same but low.

A parameter value that depends on other altered parameter values was not altered. This would otherwise cause a doubling of the effect of the first distribution.
When fractions were altered such as the time at work, the time outside, and the time at home which always add up to 24 hours total than the largest parameter was more dependent on the smaller parameter values. E.g. T_{indoor} = 24 -new value of T_{work} – new value of $T_{outdoors}$. Thus T_{indoor} was not altered directly with 10% percent (or less) but is dependent upon its smaller complementing fractions. The same method was used for other fraction (F) that together add up to one, e.g. Fair, Fwater and Fsolids in soil add to one.
Calculated output values were automatically recorded and regressed on the input by the @RISK program.

3.3 Used compounds for the sensitivity analysis

For all compounds used in the sensitivity analysis (Table 5) a summary of the compound data is in Appendix V: Correlation data.

Table 5. Substances used for the sensitivity analysis.

Substance	CAS	Substance	CAS
bis-pentabromophenyl-ether	1163-19-5	Ivermectin	70288-86-7
butanol	71-36-3	methanol	67-56-1
butylacetate	123-86-4	methylethylketone	78-93-3
cyclohexylamine	108-91-8	methyl-tert-butyl ether	1634-04-4
diethylene glycol	111-46-6	pentabromodiphenylether	32534-81-9
ethylacetate	141-78-6	tetrahydriothiophene	110-01-1
ethylene glycol	107-21-1	tribromomethane	75-25-2
hexachlorobutadiene	87-68-3	triethanolamine	102-71-6
Ibuprofen	15687-27-1		

3.4 Summary of the sensitivity analysis results

As explained in the introduction to sensitivity analysis a high value of the SRC near minus or plus one means a highly sensitive parameter. Changing this parameter in value will cause a great change in the output of the model.

Some parameters are always sensitive such as: body weight, intake rates of media (food, air, water, and soil) and predicted environmental concentrations. These parameters are not taken into account in the evaluation of the effects of the compounds on the sensitivity of the Humanex model for parameter values. Parameters that are always sensitive are listed in Table 6.

Table 6. The predictable sensitive parameter values.

PECregionals:	Human physiology:	Consumption rates:
Surface water Pore water of agricultural soil Agricultural soil Air	Body weight	Intake leaf Intake root Intake drinking water Intake fish Intake air Intake soil

Body weight (BW) has an SRC of –0.6 to –0.7 on the total exposure with 15 compounds. In the cases of Ivermectin and bis-pentabromophenyl-ether BW has a real low SRC of less than -0.2. This is because the root lipid to octanol conversion factor (b-value) is highly sensitive in these cases. SRCs for intake rates differ according to the importance of the corresponding route of exposure. Where air is the main route of exposure the SRC IHair is up to 0.57. When drinking water is the main route of exposure the SRC IHdrw is up to 0.58. Where fish is the 65 % of the main route of exposure the SRC IHfish is up to 0.47 (hexachlorobutadiene).

3.4.1 Sensitivity analysis results per route of exposure

The highest relative exposure is given for each module. As compounds behave differently, a different compound is expected to be most important per module (Table 7).

Fish Module

The highest exposure through fish is 65.2 % with hexachlorobutadiene. The SRC for the K_{ow} parameter over total exposure is 0.41, that is moderately sensitive.

Air Module

The exposure to tetrahydrothiophene is for 93 % through air. The sensitive parameters are the intake rates of air (SRC of 0.56) and body weight (SRC of –0.59).

Root Module

The highest exposure through root is 47 % with the veterinary drug Ivermectin. The SRC for b-value is 0.92, that is highly sensitive. Even when the exposure via root is only 20 percent, as with bis-pentabromophenyl-ether than the SRC is still 0.78.

Plant Module

Exposure to diethylene glycol is mainly through drinking water. But the exposure to leafy plant products is the highest with DEG, that is 35.6 % with an SRC of –0.23 for the density of plant tissue and SRC of –0.13 for the volume of the leaf. None of these SRCs are sensitive.

Drinking Water Module

The highest exposure through drinking water is 98.3 % with ethylene glycol. The SRC for body weight and intake rate of drinking water are sensitive but no other parameters are sensitive.

Meat and Milk Module

The indirect exposure of humans to bis-pentabromophenyl-ether is for 30.8 % through meat and 30.7 % through milk. Cattle take the contaminant up by eating soil particles attached to the grass. These particles contain the contaminant. This explains the SRC of 0.16 for the RHOsolid-parameter value and SRC of 0.15 for the dry weight soil-parameter value. K_{ow} has an SRC of 0.26. K_{ow} is used in the BTF calculations. All three parameters are insensitive.

Table 7. Sensitivity analysis results per route of exposure.

Module/ route	highest relative exposure %	with the compound	SRC	for the parameter	sensitivity
Fish	65	hexachlorobutadiene	0.41	K_{ow}	moderately
Air	93	tetrahydrothiophene	0.56 -0.59	intake rate of air bodyweight	sensitive sensitive
Root	47	Ivermectin	0.92	root-lipid to octanol conversion parameter	highly sensitive
Plant	36	diethylene glycol	-0.23	plant tissue density	not sensitive
Drinking water	98	ethylene glycol	-0.66 0.40	bodyweight intake rate of water	sensitive sensitive
Meat and Milk	61	bis-pentabromo-phenyl-ether	0.16 0.15 0.26	density of solids in the ground dry weight soil K_{ow}	not sensitive not sensitive not sensitive
Soil ingestion	1	bis-pentabromo-phenyl-ether		no sensitive parameter	
Shower	38	Ibuprofen	-0.57 0.33	molecular weight K_{ow}	sensitive less sensitive
Soil and Dust	0.15	bis-pentabromo-phenyl-ether		no sensitive parameter	

Soil Ingestion Module

Soil ingestion is at most relevant for one percent with bis-pentabromophenyl-ether and no parameter corresponding to this route has an SRC outside the minus 0.1 to plus 0.1 range.

Shower Module

The highest exposure through showering is with Ibuprofen for 38 %. The sensitive parameter is molecular weight with SRC of –0.57 and less sensitive K_{ow} with SRC of 0.30. Molecular weight is related to K_{ow} and size. The more hydrophobic and larger a molecule is the more difficult the molecule diffuses into the skin of man, hence the negative related SRC of –0.57.

Soil and Dust Module

The exposure to soil through dust inhalation and dermal exposure to soil particles is of minor importance and total together at maximum 0.15 percent. The total exposure is not sensitive for the parameters in these routes.

3.5 Conclusions from the sensitivity analysis

Parameters are either from the physico-chemical properties, module-formulas, human-descriptive-parameters or PECregs. For the physico-chemical properties K_{ow} and molecular weight are sensitive. For the module formulas the b-value value for root-lipid to octanol conversion parameter was highly sensitive. Parameters describing the exposure through soil

eaten by cattle are not unimportant. Human descriptive parameters, such as intake rates, for the corresponding main route of exposure are always sensitive. PECregs are also sensitive.
The uncertainty in the above parameters must be the low to run the model to create precise output. It is more useful to estimate the uncertainty in the parameters from Table 6, K_{ow}, molecular weight and the b-value than estimating the uncertainty in other compound parameters or in the model parameters.

Above conclusions are based on the results of the sensitivity analysis which is not an uncertainty analysis in which the uncertainty in the output parameters is established. What must be kept in mind is that a less sensitive parameter with a big uncertainty can have more effect on the total uncertainty than a highly sensitive parameter with a low uncertainty. Thus it is still needed to improve the modules to remove the uncertainty in a main route of exposure.
E.g. for linear alkylbenzenes the main route of exposure is through root but with a K_{ow} of 9.12 the BCF is quite uncertain. The BCF is even more uncertain than the uncertainty in the intake rate of root products by humans.

4. Detecting important routes and modules

All 31 compounds behave different due to their compound properties and thus have different routes of exposing adult humans. For each route the minimum and maximum relative exposure is listed in Table 8. The compound causing the relative highest or lowest exposure through a specific route is also shown. That each compound has different PECregs and different absolute exposure does not matter because all calculated exposure is relative.

Table 8. Minimum and maximum percentile of the total exposure per route.

Compound	CAS	min %	Route		max %	Compound	CAS
cumene	98-82-8	2.5E-2	Drinking water	Both	98.3	ethylene glycol	107-21-1
acrylaldehylde	107-02-8	3.4E-3	Fish	EUSES	81.4	hexachlorobutadiene	87-68-3
methylene dianaline	101-77-9	5.3E-6	Stem and leaves	Both	35.6	diethylene glycol	111-46-6
methylene dianaline	101-77-9	1.3E-7	Root	Both	85.1	Linear Alkylbenzenes	67774-74-7
methyl-tert-butyl ether	1634-04-4	8.4E-5	Meat	EUSES	30.8	bis(pentabromophenyl) ether	1163-19-5
tetrahydriothiophene	110-01-1	2.2E-3	milk	EUSES	30.7	bis(pentabromophenyl) ether	1163-19-5
Linear Alkylbenzenes	67774-74-7	0.0E+0	Air	EUSES	99.7	cumene	98-82-8
methylene dianaline	101-77-9	9.9E-12	Soil ingestion	CSOIL	0.5	bis(pentabromophenyl) ether	1163-19-5
diethylene glycol	111-46-6	2.9E-2	Shower	CSOIL	51.1	nonylphenol	84852-15-3
methylene dianaline	101-77-9	1.2E-13	Soil inhalation	CSOIL	0.01	bis(pentabromophenyl) ether	1163-19-5
methylene dianaline	101-77-9	2.6E-12	Soil contact	CSOIL	0.1	bis(pentabromophenyl) ether	1163-19-5

EUSES: route is modelled according to EUSES formulas and parameter values.
Both: route is modelled according to EUSES and CSOIL formulas and parameter values, Stem and leaves and Root module are very similar in EUSES and CSOIL.
CSOIL: route is modelled according to CSOIL formulas and parameter values.
Permeation from the pore water in to the drinking water is modelled with CSOIL formulas.
More compound data can be found in Appendix V: Correlation data.

Table 8 shows the maximum and minimum percentile participation of a route to the total exposure. The table clearly shows that routes that are from the CSOIL model do not influence the total exposure much. The routes soil ingestion, soil inhalation and soil contact hardly contribute to the total exposure, with at most 0.5 % for soil ingestion. The exception is showering which can contribute to 51 % to the total exposure to Ibuprofen.
Drinking water can contribute up to 98 % of the total exposure but the permeation part in the drinking water module has no influence on the total exposure as predicted in the review of the limitations of the permeation concept in paragraph 2.2.5 above.
When the soil contains an amount of contaminant at background concentration than the soil compartment plays no role in the total exposure. From this can be concluded that direct soil contact routes have little importance for the INS concept of calculating exposure from background concentrations, for the studied compounds.
The most important routes measured in maximum contribution to the exposure are the four routes: air (100 %), drinking water (98 %), root (85 %) and fish (81 %). The routes stem and leaves (36 %), meat (31 %) and milk (31 %) are also important, (Table 10). The total maximal exposure from bovine products is 62 %.
Deposition of rain splash is not an important route but can be included. The permeation model is by definition unnecessary in the Humanex concept (paragraph 2.2.5). The CSOIL exposure routes soil ingestion, dust inhalation and dermal exposure to dust are unnecessary for the calculation of the possible exposure in the Humanex concept. The shower exposure route (maximum 51 %) from CSOIL is needed. Evaporation from the soil was not modelled during the sensitivity analysis because it violates the assumption of steady state between the compartments.

Direct soil contact is not very important for exposure to background concentrations, contrary to the CSOIL scenario of living on contaminated soil. Soil consumption by children can be quite high therefore it is better to keep the direct soil contact routes in Humanex. Thus, Humanex needs routes of exposure from both EUSES and CSOIL.

Table 9. Contribution of deposition to total exposure.

Compound	total exposure through deposition in %	total exposure through leaves in %
bis-pentabromophenyl-ether	3.74	4.1
chloro-alkanene	1.38	1.4
Biphenylol	0.80	30.2
Triclosan	0.36	3.9
Nonylphenol	0.26	0.5
Dodecylbenzene	0.07	1.9
Hexachlorobutadiene	0.03	0.2

Only compounds with relative much exposure through deposition are shown.

Table 10. The importance of each route in descending order. (Data from Table 8).

Route	max %	Origin	Comment
Air	100	EUSES	
Drinking water	98	Both	possible without permeation than EUSES formulas only
Root	85	Both	possible with EUSES only
Fish	81	EUSES	
Shower	51	CSOIL	
Stem and leaves	36	Both	possible without deposition than EUSES formulas only
Meat	31	EUSES	
milk	31	EUSES	
Soil ingestion	0.5	CSOIL	
Soil contact	0.1	CSOIL	
Soil inhalation	0.01	CSOIL	

5. Calculating Maximum Permissible Concentrations with Humanex

5.1 MPC formulae and example calculations

With the Humanex model that predicts the relative and absolute exposure of a man to one compound at a time it is possible to calculate maximal permissible concentrations for all used compartments if the maximum permissible risk (MPR) or tolerable daily intake (TDI) is also known. First, with the Humanex model, contaminant concentrations in all human exposure media can be calculated. These contaminant concentrations can subsequently be used to calculate the direct and indirect human exposure. From this exposure the Estimated Total Exposure (ETE) for humans is calculated (Figure 15).

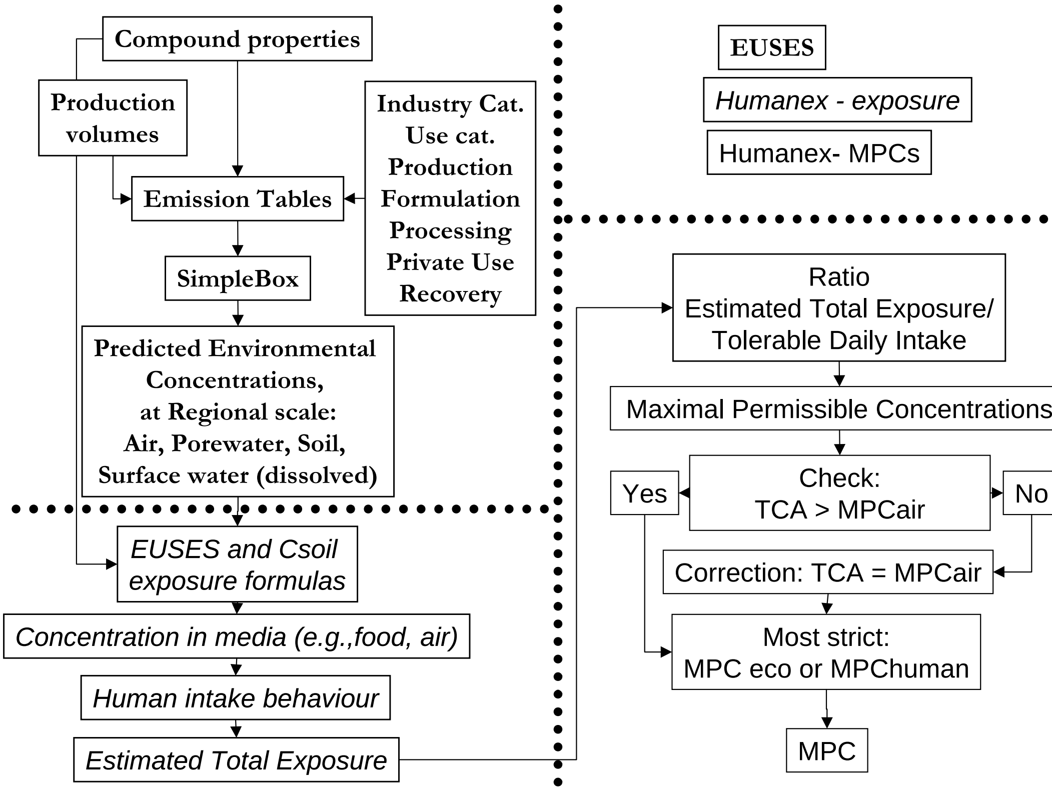

Figure 15. Steps taken to calculate the MPChuman. Information needed to calculate a MPChuman: compound properties, production information, use and application information, human behaviour data, human toxicological data and the program EUSES to calculate the PECregs and Humanex.

Second, the ETE is compared with the Tolerable Daily Intake (TDI). If the ETE divided by the TDI is higher than 1 than the PECs (mg/kg of mg/m3) must be proportionally lowered until the ETE is equal to the TDI otherwise humans are at risk of adverse effects. When the ETE is equal to the TDI, the adjusted PECs represent MPC_{human} for each compartment. An ETE/TDI with a value of less than one indicates that the exposure is lower than allowed and no risk ensues.

Finally, the MPCs (mg/kg of mg/m3) are calculated:

$MPC_{soil} = PECreg_{soil}*TDI/ETE$

$MPC_{air} = PECreg_{air}*TDI/ETE$

$MPC_{surface\ water} = PECreg_{surface\ water}*TDI/ETE$

$MPC_{pore\ water} = PECreg_{pore\ water}*TDI/ETE$

For the substances tetrahydrothiophene and tribromomethane example calculations of the MPChuman based on the tolerable daily intake (TDI) are presented (Table 11).

Table 11. Example MPC_{human} calculation for tetrahydrothiophene and tribromomethane.

EUSES derived PECregs for the compartments	PECreg of the compartment	Tetrahydro-thiophene	Tribromo-methane	Units
Water	Surface water	1.15E-04	8.04E+00	µg/L
Air	Air	2.08E-04	3.65E+00	µg/m3
Agricultural soil	Soil	5.44E-06	7.12E-01	µg/kg dwt
Agricultural pore water	Pore water	5.63E-06	2.63E-01	µg/L
Estimated Total Exposure	ETE	6.39E-05	1.34E+00	µg /kg bw/d
Tolerable Daily Intake	TDI	6.50E-01	2.00E-02	µg /kg bw/d
	TDI/ETE	1.02E+04	1.50E-02	-/-
Maximum Permissible Concentrations for adults	$MPC_{surface\ water}$	1E+03	1E+02	µg/L
	MPC_{air}	2E+03	5E+01	µg/m3
	MPC_{soil}	6E+01	1E+01	µg/kg dwt
	$MPC_{pore\ water}$	6E+01	4E+00	µg/L

5.1.1 Correction for the TCA

The tolerable concentration for air (TCA) is also taken into account by calculating a similar ratio of the TCA through air divided by the MPCair. If this ratio is less than one, the previous calculated MPCs is reduced with this ratio. The MPCair for the air compartment can not be reduced solely the concept of steady state between the compartments will be violated. All MPCs are reduced proportionally to the ratio of maximum permissible exposure through air divided by the calculated exposure through air as shown in Table 12.

Correction for the TCA if MPCair/TCA is greater than one:

$\text{Corrected } MPC_{soil} = MPC_{soil\ based\ on\ TDI}*(TCA/\ MPC_{air\ based\ on\ TDI})$

$\text{Corrected } MPC_{air} = MPC_{air\ based\ on\ TDI}*(TCA/\ MPC_{air\ based\ on\ TDI}) = TCA$

$\text{Corrected } MPC_{surface\ water} = MPC_{surface\ water\ based\ on\ TDI}*(TCA/\ MPC_{air\ based\ on\ TDI})$

$\text{Corrected } MPC_{pore\ water} = MPC_{pore\ water\ based\ on\ TDI}*(TCA/\ MPC_{air\ based\ on\ TDI})$

Table 12. Correction for when MPCair higher than the TCA.

		Tetrahydro-thiophene	Tribromo-methane	Units
Maximum Permissible Concentrations for adult humans	$MPC_{surface\ water}$	1E+3	1E+2	ug/L
	MPC_{air}	2E+3	5E+1	ug/m3
	MPC_{soil}	6E+1	1E+1	ug/kg dwt
	$MPC_{pore\ water}$	6E+1	4E+0	ug/L
Maximum Permissible Concentrations in Air		1.8E+2	1.0E+2	ug/m3
MPCair higher than TCA?		yes	no	-/-
Ratio TCA/MPCair		8.5E-02	-/-	-/-
correction because TCA lower than MPCair	$MPC_{surface\ water}$	1.0E+2	not needed	ug/L
	MPC_{air}	1.8E+2	not needed	ug/m3
	MPC_{soil}	5.5E-2	not needed	ug/kg dwt
	$MPC_{pore\ water}$	4.9E+0	not needed	ug/L

With adjustment in the set of parameter values according to CSOIL, the exposure of children can be calculated and a MPC for a specific life-stage can be calculated. This is not demonstrated in this report.

The next and final step is to derive a general MPC that protects both humans and eco-systems. This last step depends on decision rules to take the uncertainty in the calculated MPCs into account [44].

6. Predicting routes of exposure

The sensitivity analysis suggested many relations between physico-chemical properties and route of exposure, e.g. a high K_{ow} causes exposure through bovine products, fish and plants. An attempt has been made to correlate physico-chemical parameters such as solubility, octanol-water partitioning coefficient et cetera, and emission patterns (PECregs), to routes of exposure.

PECregs were used in adjusted concentrations so the exposure from all compounds was equal and could be compared. Exposure was expressed as percent per route. All information was ordered in one table and a correlation analysis was performed (Appendix V: Correlation data).

6.1 Substance physico-chemical parameters

First relations between physico-chemical parameters were evaluated. Correlation values of less than 0.5 are omitted from Table 13.

Table 13. Correlations between compound parameters.

	MW	*log Kow*	*log K_{oc}*	*log SOL*	*T. Melt C.*	*T. Boil C.*	*log VP*	*log Henry*
MW	1.00							
log K_{ow}		1.00						
log K_{oc}	0.55	0.94	1.00					
log SOL	-0.71	-0.92	-0.90	1.00				
T. Melt C.	0.66				1.00			
T. Boil C.	0.67				0.79	1.00		
log VP				0.59	-0.64	-0.63	1.00	
log Henry						-0.59	0.83	1.00

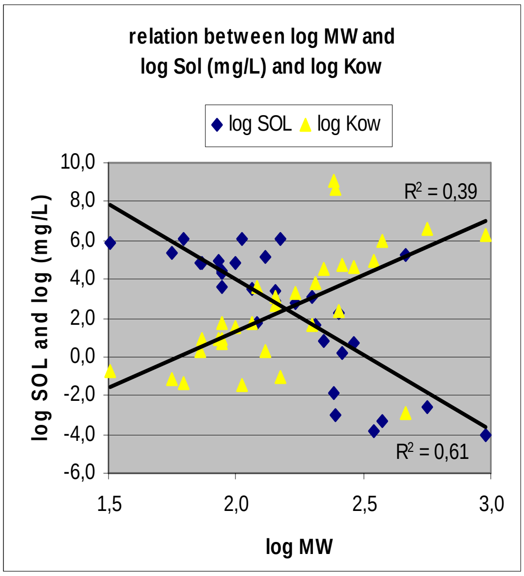

Figure 16. The relation between log Sol (mg/L) and log Kow with MW.

Substance properties are often estimated from other properties; K_{oc} is usually estimated based on log K_{ow} and molecular structure and the Henry coefficient is calculated from vapour pressure, solubility and molecular weight. Many other substance properties are evidently inversely correlated such as solubility and K_{ow} (Figure 16) To facilitate interpretation of the Humanex predictions, the most obvious relations are listed below:

- log solubility is inversely correlated with log vapour pressure,
- log solubility is inversely correlated with log K_{ow},
- log solubility is inversely correlated with molecular weight,
- molecular weight is positively correlated with log K_{ow}.

6.2 Relation between physico-chemical properties and PECregs

The predicted environmental concentrations for a region/country are calculated in EUSES with emission routes and substance properties as model input. It is expected that the type of use and production and the relevant emission factors are important. Due to continued release to the soil compartment the concentration in the soil will reach a higher steady state than when the substance only reaches the soil by partitioning from other compartments. Likewise, an emission to the surface water will cause a higher steady state concentration than would be reached solely due to equilibrium partitioning from other compartments. The physico-chemical properties below (Table 14) were subsequently correlated to calculated PECregs.

Table 14. Correlations between physico-chemical properties and PECregs.

Predicted Environmental Concentrations on a Regional Scale		MW	log K_{ow}	log K_{oc}	log SOL	T. Melt C.	T. Boil C.	log VP	log Henry
PECreg-water	(dissolved mg/L)		-0.53		0.59				
PECreg- air	(mg/m3)					-0.53			
PECreg- agric, soil	(mg/kg wwt)	0.85		0.51	-0.56				
PECreg- agric, porew.	(mg/L)								

Only 6 correlations higher than 0.5 have been found. The correlation of 0.85 between molecular weight and the concentration in agricultural soil is the most prominent. Other relevant parameters are the K_{ow}, solubility and melting point. The conclusion from this table is that not only substance properties but also emission patterns substantially influence the PECregs.

6.3 Relation between PECregs and the route of exposure

Table 15 Correlation between Predicted Environmental Concentrations and the route of exposure.

		PECreg-water (dissolved) (mg/L)	PECreg- air (mg/m3)	PECreg-agric, soil (mg/kg$_{wwt}$)	PECreg-agric, porew (mg/L)
Route of exposure	Drinking water	0.88	-0.39		
	Fish	-0.28	-0.32		
	Leaf				0.37
	Root	-0.42	-0.34		
	Meat	-0.28		0.91	
	Milk	-0.28		0.91	
	air	-0.31	1.00		
	soil ingestion	-0.28		1.00	
	Shower		-0.33		
	Soil inhalation.	-0.28		1.00	
	Soil contact.	-0.28		1.00	
Indirect source of exposure	Surface water	0.77	-0.53		
	Pore water.	-0.49	-0.40		0.34
	Air	-0.30	0.99		-0.25
	Soil	-0.26		0.95	

Highly correlated combinations between PECregs and routes of exposure are observed (Table 15). The high correlation with the soil compartment for the routes of exposure from soil ingestion, soil inhalation and soil contact is no surprise because the concentration of contaminant is modelled as a linear dependence of concentrations in the soil.
The air compartment contributes to four routes: meat, milk (cattle module), vegetable (leaf) products, and breathing air (Table 16). Only the route of exposure through air is highly correlated to the concentration in the air compartment (Figure 17). The other three routes are less correlated to the concentration in the air compartment (see Appendix VI: Correlation analysis results). Only when the concentrations in the air and surface water compartment are low, exposure from the pore water compartment will result because exposure from pore water is negatively correlated to the compartments surface water and air.

Figure 17. The exposure from the air compartment is linearly related to the concentration in this compartment. Four data points (3 visible due to overlap) are not on the trendline, explainded on the next page.

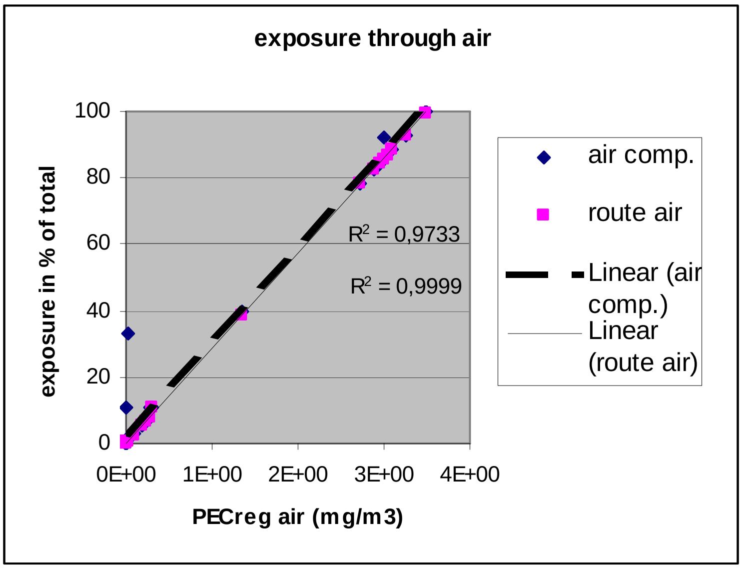

Table 16. Contribution of the air compartment to four dependent routes of exposure: air, meat and milk, and leaf.

		Source (% exposure)	Route (exposure in % of total)				Contribution of the air compartment in % of total exposure to the route of:		
Compound	PECreg- air (mg/m3)	Air comp.	air	meat	milk	leaf	meat	milk	leaf
Pentabromodiphenyl ether	4.25E-03	10.8	0.1	22.4	22.3	3.2	4.4	4.4	1.9
dodecyl benzene	1.07E-02	10.6	0.7	5.2	5.2	1.9	4.2	4.2	1.8
diethylene glycol	1.59E-02	32.9	0.5	0.0	0.0	35.6	0.0	0.0	32.5
methanol	2.99E+00	92.2	85.5	0.0	0.0	6.6	0.0	0.0	6.6

Cattle and plants take up contaminates from the air. If these food products are highly contaminated compared to other sources than the exposure from the air compartment is not only derived through breathing but also derived from indirect exposure through eating leaf or bovine products. Exposure to dodecyl benzene from the air compartment is for only 0.7% gained directly through breathing. The routes meat, milk and leaf contribute almost 10% to the exposure originating from the air compartment. With methanol for instance, all contaminant taken up by the plant originates from the air (6-4), which totals the direct and indirect exposure to methanol derived from the air compartment to 92.2% of the total exposure.
Exposure from surface water is less predictable due to the indirect routes by way of fish and showering (Figure 18). These two routes depend upon the K_{ow}. A high K_{ow} will increase the exposure from that compartment through fish. The exposure through showering is also dependent upon K_{ow} and on molecular weight. The direct exposure can be predicted for three out of four compartments. Indirect exposure is difficult to trace back to the compartments.

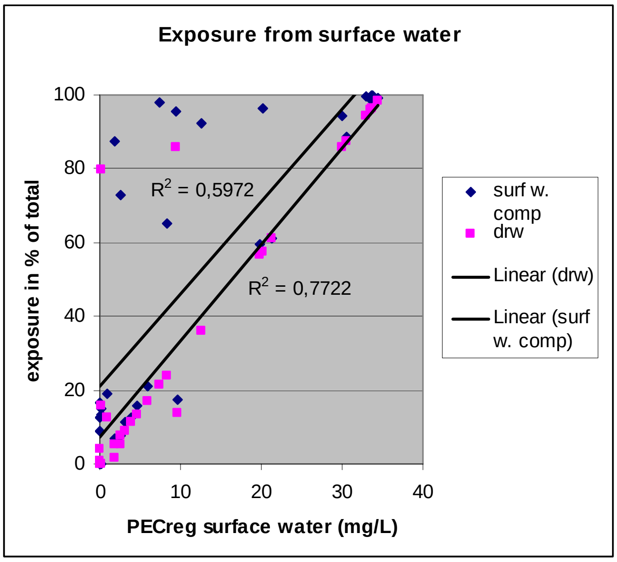

Figure 18. The total exposure from the compartment is higher than the direct exposure, similar to the exposure from air in figure 6.7. The exposure through drinking water (drw) is lineary related to the PECreg surface water.

Other routes depending on the PECreg surface water, such as showering and fish, lead to deviations that cannot be directly predicted from the surface water compartment.

6.4 Relation between physico-chemical properties and the route of exposure

The correlations between physico-chemical properties and the routes of exposure are presented in Table 17. The most significant parameters are again MW, K_{oc}, K_{ow}, solubility and melting point, which already became apparent in section 6.1.2.

Table 17. Correlation between compound parameters and the route of exposure.

		MW	log K_{ow}	log K_{oc}	log SOL	T. Melt C.	T. Boil C.	log VP	log Henry
Route of exposure	Drinking water		-0.67	-0.65	0.64				
	Fish								
	Leaf								
	Root		**0.75**	0.62	**-0.77**				
	Meat	**0.86**		0.52	-0.59				
	Milk	**0.86**		0.52	-0.58				
	Air					-0.53			
	Soil ingestion	**0.85**		0.51	-0.57				
	Shower								
	Soil inhalation.	**0.85**		0.51	-0.57				
	Soil contact.	**0.85**		0.51	-0.57				
Indirect source of exposure	Surface water								
	Pore water.		0.56		-0.63				
	Air					-0.54			
	Soil	**0.86**			-0.55				

Molecular weight is an important parameter in relation to several soil routes (bold in Table 18). As can be seen in Table 14, a high molecular weight is correlated with a high PECreg soil. As shown in paragraph 6.2 a high MW is correlated with a high soil concentration. This in turn leads to a positive correlation with exposure through meat, milk, soil ingestion, soil inhalation and soil contact. In the case of bis-pentabromophenyl-ether, 65% of the exposure originates from the soil compartment through root, meat and milk (soil ingestion by cattle) but almost nothing through human direct exposure to dust and soil ingestion.

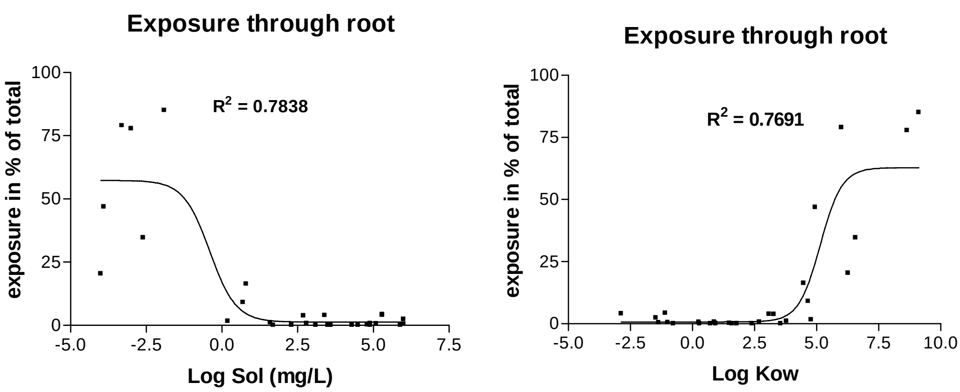

Figure 19a (left) and Figure 19b (right): the log solubility and log Kow are inversely correlated. The watery part of the root has the same contaminant concentration as the pore water. The lipid part of the root can have orders of magnitude higher concentrations of contaminant than the watery part if the Kow is high. Thus a high Kow will strongly increase the root concentration and root consumption will make up for an important route of exposure.

A logical dependence is observed in Figure 19a and Figure 19b. Exposure through root mainly depends on the K_{ow} and the solubility. When the solubility increases, the fraction of root exposure decreases (Figure 19a). This is related to the inverse relation with lipophilicity of a compound, which leads to a strong increase of root uptake at low solubility and high lipophilicity (Figure 19b).

6.5 Combining the origin of exposure and physico-chemical properties

Six groups where found on basis of the origin of exposure:

- Group 1 with 80 percent of total exposure derived from the surface water compartment,
- Group 2 with at least 20 percent of total exposure derived from the surface water compartment and 20 percent derived from the pore water compartment,
- Group 3 with at least 20 percent derived from the surface water compartment and 20 percent derived from the air compartment,
- Group 4 with 80 percent of total exposure derived from the air compartment,
- Group 5 with 80 percent of total exposure derived from the pore compartment,
- Group 6 with at least 20 percent derived from the pore water compartment and 20 percent derived from the soil compartment.

The groups based on the origin of the exposure were compared to physico-chemical properties and group characteristics were established (Table 18). An index to the substances is given in Table 19.

From Table 18 it can be concluded that compounds with high solubility will expose man mainly via water (drinking water). Compounds with high vapour pressure and low solubility will expose man mainly via the air (breathing) and substances with high K_{ow} (that equals low solubility) and low vapour pressure will expose man mainly via the pore water (root products). Due to complex relations between substance properties, emission patterns and the resulting exposure, no exact quantitative relation can be given.

Table 18. Compound groups and group characteristics.

Group	Source Compartment	Substances	Characteristics
1	Surface water	1, 3, 11, 14, 20, 22, 24, 25, 27, 28, 30	High Sol
2	Surface and pore water	15, 26, 31	None
3	Surface water and air	2, 5, 8	High Sol
4	Air	4, 6, 7, 9, 10, 12, 18	High Vp and low Sol
5	Pore water	13, 17, 21, 29	High K_{ow} and low Vp
6	Pore water and soil	16, 19, 23	High K_{ow}, high MW and low Vp

MW = molecular weight, Sol = solubility, Vp = vapour pressure

Table 19. Index to clustering.

Nr	Compound	CAS
1	triethanolamine	102-71-6
2	diethylene glycol	111-46-6
3	ethylene glycol	107-21-1
4	methanol	67-56-1
5	tribromomethane	75-25-2
6	tetrahydriothiophene	110-01-1
7	butylacetate	123-86-4
8	butanol	71-36-3
9	methyl-*tert*-butyl ether	1634-04-4
10	methylethyl ketone	78-93-3

Nr	Compound	CAS
11	cyclohexylamine	108-91-8
12	ethylacetate	141-78-6
13	dodecylbenzene	123-01-3
14	hexachlorobutadiene	87-68-3
15	nonylphenol	84852-15-3
16	chloro-alkanene	85535-84-8
17	acrylaldehylde	107-02-8
18	cumene	98-82-8
19	bis-pentabromophenyl-ether	1163-19-5
20	ethyl acetoacetate	141-97-9
21	linear alkylbenzenes	67774-74-7
22	methacrylic acid	79-41-4
23	pentabromo-diphenylether	32534-81-9
24	chlorocresol	1570-64-5
25	methylene dianaline	101-77-9
26	biphenylol	90-43-7
27	4-chloro-m-cresol	59-50-7
28	Ibuprofen	15687-27-1
29	Ivermectin	70288-86-7
30	Oxytetracycline	79-57-2
31	Triclosan	3380-34-5

6.6 Conclusions

While all combinations of physico-chemical properties, PECregs and relative importance of each route have been correlated no truly quantitative predications can be given. All these factors influence each other in a complicated way. Nevertheless important qualitative relations have been found:

- A higher MW leads to higher soil concentrations
- A higher soil concentration means more exposure through root, meat and milk.
- A higher K_{ow} and lower solubility means more exposure through fish, root, meat and milk.
- Compounds with high solubility will expose man mainly via (drinking) water.
- Compounds with high vapour pressure and low solubility will expose man via the air (breathing).
- Only when the concentrations in the air and surface water compartment are low, exposure from the pore water compartment can be significant.
- Direct exposure of man to soil is relative unimportant due to relatively low soil concentrations at steady-state levels.

The general guideline is that a high concentration in the compartment that is directly ‘consumed’ such as air, drinking water or soil ingestion leads to a strong correlation between the PECreg and the exposure. This was also shown with the sensitivity analysis and was predictable by normal deduction from the formula: exposure = $IH_{medium}*C_{medium}/BW$.

(With IH_{medium} is consumption rate of product, C_{medium} is concentration of contaminant in product and BW is body weight.)

The previous analysis has shown that the relation between substance properties and exposure is complicated. This is mainly due to the interaction between emission, emission scenario’s and substance properties. Model validation should point the way to improved accuracy of the Humanex model.

7. Discussion and Conclusions

7.1 Discussion and general conclusions

In 1995 the Committee on Setting Integrated Environmental Quality Objectives (Stuurgroep Integrale Normstelling Stoffen) concluded that multiple routes of exposure should be taken into account when calculating MPCs so no relevant route of exposure would be ignored. The committee also confirmed that it was necessary to take the partitioning of substances into account when setting maximum permissible risk concentrations for water, sediment, soil and air [10].
The Humanex model greatest strength is that it is capable of calculation maximum permissible concentrations for the compound of interest based on the most likely distribution pattern over the environment. This distribution can be estimated based on the physico-chemical properties of the chemical and characteristics of the compartments. Here, by default, the dimensions and properties of the Netherlands are used for the regional scale of EUSES. By application of the multi-media model concept, the calculation of integrated environmental quality standards is safeguarded as required (see chapter 1).

The model and its parameter values can easily be edited or updated due to its implementation in a standard MS Excel® spreadsheet. If a new relevant route of exposure is developed or new insights warrant revision of a route than this can be implemented easily. When probabilistic exposure assessment and MPC derivation is an accepted method in the environmental policy, this is easily accommodated with add-on programs such as Crystal Ball or @Risk. This makes Humanex flexible and adaptive to future needs and insights. As concluded in paragraph 6.6, the Humanex model works with relative simple relationships based on a few parameters per relationship to predict exposure, main routes of exposure and the resulting MPCs. Although the output of the Humanex model is related to the type of substance (paragraph 6.5), the number of possible routes of exposure and relationships that are different for each substance makes a model necessary.

7.2 Recommendations for module improvements

Improvement of nearly all modules is needed, together with a new consumption pattern for humans. Most of these improvements are necessitated by new scientific insights, or just that the availability of data has increased since the EUSES model was built.

7.2.1 Fish module

The fish module was not used outside its intended range. Improvements however, can be made. A future distinction could be made between marine fish, fresh water fish and fat fish such as eel [24]. New insights in accumulation and biomagnification [45] can be added to the fish model, which is somewhat outdated.

7.2.2 Air module

Indoor and outdoor air concentrations

The modelled air concentrations apply to both indoor and outdoor air, as long as the assumption of steady state is taken into account. Indoor concentrations can be different than outdoor concentrations due to lack of diffusion between indoor and outdoor air, and by the presence of (local) contamination in the subsoil. The CSOIL concept is meant for local soil contamination, whereas the INS framework is meant for regional (diffuse) contamination at background levels. A separate indoor air module is therefore considered not appropriate.

TCA

The tolerable concentration in air (TCA) expressed in mg/m^3 is a quality objective that prevents humans to be exposed by inhalation above threshold concentrations. Although the concentration in air is then known, it is unknown what the precise exposure is. A translation step must be made from amount of inhaled contaminant (mg/m3/day) to absorbed amount of contaminant (mg/kg bodyweight/day). As a worst-case scenario it is assumed that all inhaled contaminate is absorbed [7,19]. It is not unlikely that only a fraction is absorbed. This fraction is conceivably dependent upon compound properties such as solubility, partitioning between octanol and water (Koa) and molecular size [46]. The current worst-case assumption probably over-estimates pulmonary uptake for many compounds, leading to a too strict MPCair and related compartments.

7.2.3 Root module and Plant module

It has been proposed to use a 150 days growth period for roots and plants [26]. This could mean that towards the centre of thick roots, the lipophilic compounds may not yet have diffused into the root to reach equilibrium. All contaminant reaching the core of the thick root is brought there with the transpiration stream, caused by the evaporation of water in the leaves. If this process is implemented, the new model assumptions would implicate a decrease of the concentration of contaminant in the thick root, especially if the root is peeled before consumption. This model for thick roots is not valid for potatoes because the potatoes receive their nourishment from the phloem and not from the transpiration stream [26]. The model has been tested with a small number of compounds. This model is invalid for potatoes, which are a staple diet product for humans, and another model with parameters for the potato is needed. Such models are now being developed (Trapp, personal communication).
Currently in CSOIL and EUSES, it is assumed that the stem and leave compartments are in equilibrium with their surroundings at the moment of harvest. To accomplish this, an indefinite growth season is modelled. Introduction of a growth period will probably lower the predicted concentrations in the stem and leaves for lipophilic compounds.

Dowdy and McKone (1997) [5] have refitted the data from Briggs of 1982 [2], data from Travis and Arms of 1988 [29] and data from Paterson of 1991 [21]in new regression equations. They used a molecular connectivity index, K_{ow} and K_{oa} (octanol-air partitioning) as predictive parameters of the *soil-to-root* concentration ratio and the *soil-to-above ground plant parts* concentration ratio and *the air-to-above ground plant parts* ratio. The underlying data sets were not changed or expanded but the predictive formulas are improved by using not only the K_{ow} but also more compound descriptive parameters.
The *soil-to-root* concentration ratio was predicted with the log K_{ow} with a fraction of explained variance (r^2) of 0.89 in Briggs and decreased to r^2 of 0.84 in Dowdy and McKone. The *soil-to-above ground plant parts* concentration ratio was predicted with the log K_{ow} with a r^2 of 0.53 in Travis and Arms and greatly improved r^2 to 0.83 in Dowdy and McKone. The *air-to-above ground plant parts* concentration ratio was predicted with the log K_{ow} with an r^2 of 0.74 and K_{oa} with an r^2 of 0.73 in Paterson and was slightly improved to a r^2 of 0.78 in Dowdy and McKone. This shows that the incorporation of a molecular connectivity index can enhance the predictive properties of regressions equations. These improved relationships can be built into an updated Humanex.

7.2.4 Drinking water module

Permeation formula

Humanex and EUSES work with two polluted drinking water sources namely surface water or pore water. These two sources are, by model definition, equal to or more polluted than the pore water. Combined with the worst case assumption that the most polluted source will be used as a source of drinking water, this leads to the conclusion that drinking water is always equal to or more contaminated than the pore water. Permeation is only important when the concentration in the pore water (groundwater) is higher than the concentration in the drinking water. Therefore, permeation into the drinking water will not occur. If the concentration in drinking water is higher than the concentration in pore water permeation out of the drinking water pipe system should occur with as result cleaner drinking water. The permeation module as derived from CSOIL is not compatible with EUSES formulations. Permeation can be removed from the Humanex model if the drinking water assumptions are unchanged. Only when the drinking water module is improved, permeation may still be a relevant process.

Drinking water purification

The concentration of substances in drinking water is dependent upon several factors.
First, the predicted environmental concentrations in the surface water and the pore water. These PECregs are dependent upon the emission tables in EUSES and substance properties.
Second, the purification factor is based on the log K_{ow}, Henry-coefficient, and biodegradability. Biodegradability is set at zero as default. Based on these three parameters, a purification factor is selected based on dune-recharge or storage in open reservoirs. Subsequently, the least purifying system is chosen as a worst-case scenario.
Third, the amount of purification of the surface water plays a major part in the calculation of the concentration of contaminants in the drinking water as the drinking water is either made of purified surface water or unpurified pore water. The compartment that has the highest concentration after purification will be the source for the drinking water as a worst-case scenario. This last worst-case scenario seems a good choice because 61% of the drinking water in the Netherlands is produced from purified surface water and the remaining 39% from ground water (data 2000 [38]).
Due to the above worst-case scenarios humans are assumed to be drinking purified surface water that still contains 100 percent of the original contaminant, as is the case for 19 of the 31 compounds (Table 20). While all these worst-case scenarios are understandable in view of protection goals, it is unlikely that purification is this inefficient. Jager *et al.* [14] proposed to use a fixed uniform purification factor of 85% removal (from the original concentration) based on 8 pesticides as worst-case situation [14]. A choice for one of these two methods of calculating concentrations in drinking water is arbitrary. An improvement of this EUSES-module thus seems necessary.

An attempt has been made to compare measured input concentrations in surface and pore water with measured output concentrations after purification of the drinking water per compound type per purification system with Dutch data from 2001. More analysis must be done before conclusion can be drawn from the data set because many compounds are below detection levels. It is expected that such an analysis will lead to an increase in the modelled removal efficiency. Then, the exposure through drinking water would be considerably less then currently used in Humanex and EUSES.

Table 20. Frequency of calculated purification factors.

purification factor (percent of total amount left after purification)	number of substances
100	19
50	6
25	4
12.5	2

7.2.5 Meat and Milk Module

The bio-transfer factors (BTF) are based on data of Travis and Arms from 1988 [29]. Recently a new QSAR model has been proposed for these BTF values. This fit is done with a molecular connectivity index as stated in Dowdy et al [6]. This new correlation causes an improvement in the regression fit of r^2 = 0.55 to r^2 = 0.89 for milk and r^2 = 0.66 to r^2 = 0.90 for meat [34]. The range of the QSAR remains the same. This new fit would be an improvement of the current QSAR and should be built into Humanex.

7.2.6 Shower Module

The shower model is based on articles of 1989 [3,9]. A recent article of 2002 has formalised a QSAR to predict the speed at which the substance permeates in to the skin with a measure of correlation of r^2 = 0.90 with 143 data points. This QSAR is based on the parameters log K_{ow}, molecular weight, absolute charge on the oxygen and nitrogen atoms, and on the sum of the rotation freedom (E-indices) for methyl groups [20]. Implementing of this formula for the dermal absorption velocity will be an improvement for the Humanex model.

7.2.7 Soil and Dust Module

The exposure through soil and dust is minimal and no improvement is needed for the assessment of the human exposure. For lipophilic compounds, the amount of soil particles on the grass eaten by cattle is relevant for the indirect exposure for humans.

7.3 Emission tables in EUSES

The emission tables in EUSES determine part of the input for the multi-compartment model and contribute to uncertainty in the predicted environmental concentrations. The MPCs derived in this document are based on the PECregs and thus uncertainty in the MPCs is partly due to the emission tables. Uncertainty was quantified previously in the form of triangular distribution for a limited number of instances and remains unclear [8]. With probabilistic risk assessment this distribution could be taken into account. More defined emission tables with included estimated uncertainty could help to calculate a likely emission pattern with better-known uncertainty in the predicted environmental concentrations.
An example of the effect of varying the emission patterns and the subsequent predicted environmental concentrations is tribromomethane in Table 21.

Table 21. Effect of changing the emission pattern of tribromomethane.

emission of 1000 kg/d total to the compartments:				
surface water	100	700	0	kg/d
air	700	100	100	kg/d
agricultural soil	0	0	700	kg/d
waste water	200	200	200	kg/d
PEC surface water	9.0E-05	5.0E-04	2.4E-05	mg/L
PEC air	3.6E-05	3.5E-05	3.6E-05	mg/m3
PEC agricultural soil	2.6E-06	5.5E-06	1.7E-03	mg/kg wwt
PEC agricultural pore water	2.6E-06	2.6E-06	8.1E-04	mg/L

The concentrations in air are nearly constant for the three emissions types and are independent from the emission to air. The concentrations in soil are variable with the emission to the soil. The concentration in surface water is variable with the emission to surface water. As long as the exposure derived from the soil and pore water is limited compared to the exposure derived from the air compartment, then the exposure pattern will not change much. The exposure derived from the soil and pore water will increase dramatically in the case of emission of 700 k/d to the soil compartment, consequently the main route of exposure will no longer be breathing air but through crops and cattle. The exposure pattern for other compounds will change in a manner linked to their respective emission patterns and compound properties. In conclusion, emission patterns are important for the calculation of the MPChuman. It may be advisable to collect additional data on emissions instead of solely relying on the default EUSES emission scenarios.

7.4 Biodegradability

Biodegradability was not taken into account for in the calculation of the predicted environmental concentrations even though a number of compounds such as methanol are easily degraded. Methanol is readily metabolised into aldehydes. As the biodegradability of a compound is difficult to assess and to apply without comprehensive knowledge of that compound it was decided not to parameterise biodegradability. The inclusion of biodegradation will have a compound specific effect on the equilibrium of the compartments air, soil, pore and surface water.

Hertwich and McKone have investigated the effect of biodegradability (and other parameters) on the estimation of the potential dose for humans to a number of compounds. The calculated potential dose (or exposure) has a variance of typically one to two orders of magnitude with biodegradability being responsible for 10% to 92% of the variance [11]. The assessment of biodegradability rates must be done with care. An example of the difficulty to derive a correct half-life for a compound is the study of the degradation of Triclosan in surface water. Degradation rates of 2 days to 5.5 years were found, depending on the circumstances [25]. This stresses the importance of implementing biodegradability in models.

7.5 Children

The exposure for children can be incorporated into Humanex with an adjustment to the set of parameter values. In that case, exposure for this specific risk category can be taken into account. Compared to CSOIL, typical behaviour of children such as high soil contact due to playing and ingestion are not expected to contribute much to the Humanex risk estimate. Soil routes play a much smaller role in the low contamination situation for which Humanex is developed than in the 'contaminated site' situation for which CSOIL was developed. In addition, the TDI estimate is based on a life-time averaged exposure and is based on extrapolation factors that take sensitive sub-populations into account. Therefore, it is advised to use the default risk scenario of Humanex to derive generic MPCs to protect humans.

References

1. @RISK, Professional Edition, Version 4.0.5, 2000 Palisade Corporation, Newfield, NY, USA.
2. Briggs G, Bromilow R, Evans A. 1982. Relationship between lipophilicity and root uptake and translocation of non-ionised chemicals in barley. Pestic Sci 13: 495-504.
3. Brown S, Rossi J. 1989. A simple method for estimating dermal absorption of chemicals in water. Chemosphere 19: 1989-2001.
4. Ciarelli S, Posthumus R, Traas T. 2005. Environmental Risk Limits for several volatile compounds for water, soil and sediment. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 601501016.
5. Dowdy D, McKone T. 1997. Predicting plant uptake of organic chemicals from soil or air using octanol/water and octanol/air partition ratios and a molecular connectivity index. Environ Toxicol Chem 16: 2448-2456.
6. Dowdy DL, McKone TE, Hsieh DPH. 1996. Prediction of chemical biotransfer of organic chemicals from cattle diet into beef and milk using the molecular connectivity index. Environ Sci Technol 30: 984-989.
7. EC (1996). 1996. EUSES, the European Union System for the Evaluation of Substances. Institute for Public Health and the Environment (RIVM), the Netherlands: European Chemicals Bureau (EC/JRC), Ispra, Italy.
8. Etienne RS, Ragas A, Van de Meent D. 1997. Operational Uncertainties in SimpleBox. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 719101031.
9. Fiserova-Bergerova V, Pierce J. 1989. Biological monitoring. V: Dermal absorption. Appl. Ind. Hyg. 4: F14-F21.
10. Gezondheidsraad: Commissie Integrale Normstelling Stoffen. 1995. Het Project Integrale Normstelling Stoffen. Den Haag, Nederland: ISBN: 90-5549-076-8. Report no. 1995/07. 116 pp.
11. Hertwich E, McKone T, Pease W. 1999. Parameter uncertainty and variability in evaluative fate and exposure models. Risk Analysis 19: 1193-1203.
12. Hrubec J, Toet C. 1992. Predictability of the removal of organic compounds by drinking water treatment. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 714301007.
13. Jager T. 1998. Evaluation of EUSES: inventory of experiences and validation activities. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 679102048.
14. Jager T, Rikken MGJ, Poel P. 1997. Uncertainty analysis of EUSES: Improving risk management by probabilistic risk assessment. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 679102039.
15. Janssen PHM, Heuberger PSC, Sanders R. 1994. UNCSAM: a tool for automating sensitivity and uncertainty analysis. Environ Software 9: 1-11.
16. Lijzen J, Baars A, Otte P, Rikken M, Swartjes F, Verbruggen E, Wezel A. 2001. Technical evaluation of the Intervention Values for Soil/sediment and Groundwater. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 711701023.
17. Mackay, D. (1991) Multimedia Environmental Models: The Fugacity Approach, Lewis Publishers, Chelsea, Michigan, USA, , ISBN 0-87371-242-0.
18. Mennes WC, Van den Hout KD, Van de Plassche EJ. 1995. Characterisation of human exposure patterns to environmental contaminants: possibilities of the USES approach. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 679101021.

19. Otte PF, Lijzen JPA, Otte JG, Swartjes FA, Versluijs CW. 2001. Evaluation and revision of the CSOIL parameter set. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 711701021.
20. Patel H, Ten Berge W, Cronin W. 2002. Quantitative structure-activity relationships (QSARs) for the prediction of skin permeation of exogenous chemicals. Chemosphere 48: 603-613.
21. Paterson S, Mackay D, Bacci E, Calamari D. 1991. Correlation of the equilibrium and kinetics of leaf-air exchange of hydrophobic organic chemicals. Environ Sci Technol 25: 866-871.
22. Rikken MGJ, Lijzen JPA, Cornelese AA. 2001. Evaluation for updating the most relevant exposure routes of CSOIL. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 711701022.
23. RIVM, VROM, WVC. 1994. Uniform System for the evaluation of substances (USES) version 1.0. The Hague, Ministry of Housing, Spatial Planning and the Environment (VROM): National Institute for Public Health and Environmental Protection (RIVM), Ministry of Housing, Spatial Planning and the Environment (VROM), Ministry of Welfare, Health and Cultural Affairs (WVC). Report no. 11144/150.
24. Schwartz S, Trapp S, Matthies M. 2000. Validation of Environmental Exposure Models and Parameters: Part I. Osnabruck, Deutschland: Institute for Environmental System Research, University Osnabruck. Report no. FKZ29667075. 164 pp.
25. Tixier C, Singer HP, Canonica S, Muller SR. 2002. Phototransformation of Triclosan in surface water: a relevant elimination process for this widely used biocide. Environ Sci Technol 26: 3482-3489.
26. Trapp S. 2002. Dynamic root uptake model for neutral lipophilic organics. Environ Toxicol Chem 21: 203-206.
27. Trapp S, McFarlane C, Mathies M. 1994. Model for uptake of xenobiotics into plants: validation with bromacil experiments. Environ Toxicol 13: 413-422.
28. Trapp, S. and Matthies, M. (1998) Chemodynamics and Environmental Modelling: An Introduction, Springer-Verlag Berlin Heidelberg, Berlin, Germany.
29. Travis C, Arms A. 1988. Bioconcentration of organics in beef, milk and vegetation. Environ Sci Technol 22: 271-274.
30. Van de Meent D. 1993. SimpleBox: a generic multimedia fate evaluation model. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 672720001.
31. Van de Meent D, Aldenberg T, Canton J.H., Van Gestel CAM, Sloof W. 1990. Desire for levels. Background study for the policy document 'Setting integrated environmental quality objectives for water and soil'. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 670101002. 147 pp.
33. Van der Kooij LA, Van de Meent D, Van Leeuwen CJ, Bruggeman WA. 1991. Deriving quality criteria for water and sediment from the results of aquatic toxicity tests and product standards: application of the equilibrium partitioning method. Wat. Res. 25: 679-705.
34. Van Wezel A, De Vries W, Beek M, and others. Bodemgebruikswaarden voor de functies landbouw, natuur en waterbodem. VROM/DGM/Directie Bodem, Water en Landelijk Gebied, in het kader van project 711701, 'Risico's in relatie tot bodemkwaliteit'. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 711701031.
35. Van Wezel A, Jager T. 2000. Comparison of two screening level risk assessment approaches for six disinfectants and pharmaceuticals. Chemosphere 1113-1128.

36. Veenendaal G, Verheijen LAHM, Vonk MW. 1985. Waterleidingen in vervuilde bodem: de invloed van bodemverontreiniging en leidingmateriaal op de drinkwaterkwaliteit 'een samenvatting'. KIWA Nieuwegein Mededeling nummer 87 RLIT0154:
37. Versluijs CW, Koops R, Kreule P, Waitz MFW. 1998. The accumulation of soil contaminants in crops, location-specific calculation based on the CSOIL-module. Part 1 Evaluation and suggestions for model development. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 711701008.
38. VEWIN, Vereniging van drinkwater bedrijven in Nederland. 2001. Benchmark2000 - Water in zicht 2000: Een bedrijfsvergelijking. internet: http://www.vewin.nl/
39. Vonk M. 1985. Permeatie en drinkwaterleidingen: permeatie van organische verbindingen door leidingmateriaal. KIWA Nieuwegein Mededeling nummer 85 RLIT0153:
40. Waitz MFW, Freijer JI, Kreule P, Swartjes FA. 1996. The VOLASOIL risk assessment model based on CSOIL for soils contaminated with volatile compounds. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 715810014.
41. Crommentuijn T, Sijm D, De Bruijn J, Van Leeuwen K, Van de Plassche E (2000). Maximum permissible and negligible concentrations for some organic substances and pesticides. J Environ Management 58: 297-312.
42. VROM. 1989. Premises for risk management. Risk limits in the context of environmental policy. Second chamber, session 198801989, 21137, no.5
43. VROM. 1994. Ministry of Housing, Spatial Planning and Environment. Environmental Quality Objectives in the Netherlands. VROM The Hague, the Netherlands.
44. Van de Plassche EJ, Bockting GJM. 1993. Towards integrated environmental quality objectives for several volatile compounds. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 679101011.
45. Jager DT, Hamers T. 1997. Estimation methods for bioaccumulation in risk assessment of organic chemicals. Bilthoven, the Netherlands: National Institute for Public Health and the Environment (RIVM). Report no. 679102013.
46. Kelly BC, Gobas FAPC. 2003. An arctic terrestrial food-chain bioaccumulation model for persistent organic pollutants. Environ Sci Technol 37: 2966, 2974.
47 Hsu *et al*. 1991. Study of root uptake and xylem translocation of cinmethyl and related compounds in detopped soybean roots using a pressure chamber technique, Plant Physiol 93: 1573-1578.

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Appendix I: EUSES settings for calculations of PECregs

EUSES version 1.00 was used with all settings on default, unless stated otherwise. Production volumes for all compounds are assumed to be 1e5 ton/year, unless stated otherwise. Regional production volume of substance was assumed to be 10% of total production volume of the chemical in the EU, unless stated otherwise. Screen shots were taken as a way of archiving the used compound specific settings EUSES input files were saved to disk and archived for easy access of all EUSES settings. [Bontje, M.Sc. Report, IRAS, RUU Utrecht].

Appendix II: Parameter values

"idem" means same values as one column to the left.

Intake rates of humans and bioavailability

Module	parameter	description of parameter	USES 1.0 #	CSOIL2000 Data from 71170102	CSOIL _BGW _programme	EUSES default	parameter values for sensitivity analysis	parameter values used for comparison with CSOIL scenario 'residential with garden'	units
Intake Human	air	consumption rate of air	20	20	20	20	20	idem	[m3.d-1]
Intake Human	drw	consumption rate of drinking water	2	2	2	2	2	idem	[l.d-1]
Intake Human	fish	consumption rate of fish products	11	n/a	n/a	115	11	idem	[g.d-1]
Intake Human	leaf	consumption rate of fresh leafy products	349	139	13.9	1200	349	13.9	[g.d-1]
Intake Human	root	consumption rate of fresh root products	129	122	12.2	384	129	12.2	[g.d-1]
Intake Human	meat	consumption rate of meat products	120	n/a	n/a	301	120	idem	[g.d-1]
Intake Human	milk	consumption rate of dairy products	378	n/a	n/a	561	378	idem	[g.d-1]
Intake Human	AID	soil ingestion rate of adults (dry weight)	50	50	50	n/a	50	idem	[mg dwt/d]
Intake Human	BW	body weight		70	70	70	70	idem	[kg]
Intake Human	**BIOinh**	**bio availability after inhalation**		1	1	0.75	0.75	1	[-]
HUMAN	BIOoral	bio availability after oral uptake			1	1	1	idem	[-]
HUMAN	**Fresp**	**bio availability after inhalation**					1	idem	[-]

see reference [23]
"idem" means same values as one column to the left.

Cow module

Module	parameter	description of parameter	EUSES default	parameter values for sensitivity analysis	parameter values used for comparison with CSOIL scenario 'residential with garden'	units
Intake Cow	dwtgrass	consumption rate of dry weight grass	16.90	16.90	idem	[kgdwt.d-1]
Intake Cow	dwtsoil	consumption rate of dry weight soil	0.41	0.41	idem	[kgdwt.d-1]
Intake Cow	air	consumption rate of air	122.00	122.00	idem	[m3.d-1]
Intake Cow	drw	consumption rate of water	55.00	55.00	idem	[l.d-1]
Intake Cow	CONVgrass	conversion rate from dry weight grass to fresh weight grass	4.00	5.00	idem	[kgwwt.kgdwt-1]

An evaluation has set CONVgrass to 1/0.2 = 5 thus 5 is used [19].

Physical constants

Module	parameter	description of parameter	CSOIL2000 Data from 711701021	CSOIL _BGW _programme	EUSES default	parameter values for sensitivity analysis	parameter values used for comparison with CSOIL scenario 'residential with garden'	units
Phys. Cons.	R gas constant	gas constant	8.3144	8.3144	8.3144	8.314	idem	[Pa.m3.mol^{-1}.K^{-1}]
Phys. Cons.	TEMPenv	environmental temperature	n/a	n/a	12	10	idem	[deg. C]
Phys. Cons.	TEMPsoil	environmental soil temperature	10	10	12	10	idem	[deg C]
Phys. Cons.	TEMP shower	temperature of shower water	40	40	n/a	40	idem	[deg C]
Phys. Cons.	CONjunge* SURFaer	product of the constant of Junge and surface area of aerosols			1.00E-04	1.00E-04	idem	[Pa]

Plant module (Leaf and Stem)

Module	parameter	description of parameter	CSOIL2000 Data from 711701022	EUSES default	parameter values for sensitivity analysis	parameter values used for comparison with CSOIL scenario 'residential with garden'	units
plant	Fwater	fraction water in plant		0.65	0.65	idem	[m3.m-3]
plant	Flipid	fraction lipid in plant		0.01	0.01	idem	[m3.m-3]
plant	b	correction factor for plant lipid to octanol for leafy plant parts		0.95	0.95	idem	[-]
plant	Qtransport	transpiration stream		0.001	0.001	idem	[m3.d-1]
plant	AREA	total surface of all leafs above one square meter of soil		5	5	idem	[m2]
plant	Vleaf	volume of all leafs above one square meter of soil		0.002	0.002	idem	[m3]
plant	k growth	growth rate of plant		0.035	0.035	idem	[d-1]
plant	Fair	fraction of air in plant		0.3	0.3	idem	[-]
plant	k metab	metabolism rate in plant		0	0	idem	[d-1]
plant	k photo	photo-degradation rate in plant		0	0	idem	[d-1]
plant	g	air conductance of leaf	80	86.4	80	idem	[m.d-1]

Root module

Module	parameter	description of parameter	CSOIL2000 Data from 711701022	CSOIL_BGW_ programme	EUSES default	Para-meter values for sensi-tivity analysis	parameter values used for comparison with CSOIL scenario 'residential with garden'	units
root	FDWR	fraction dry weight in root	0.167	0.167	n/a	0.167	idem	[-]
root	b	correction factor for root lipid to octanol for root plant parts	0.8		0.95	0.8	idem	[-]
root	RHOroot	specific density of fresh root	1000		700	1000	idem	[kg wwt.m-3]
root	Flipid	fraction of lipid in root	0.005		0.01	0.005	idem	[-]
plant	RHOplant	specific density of fresh leafy plant parts	800		700	800	idem	[kg.m-3]
Plant	Vfp	dilution velocity plant (needed for evaporation calculations)	84	84	n/a	84	idem	[m/h]
Plant	FDWS	fraction dry weight shoot	0.098		n/a	0.098	idem	[-]
Plant	dep. cons.	deposition constant	0.01	0.01	n/a	0.01	idem	[-]

Drinking water – permeation module

Module	parameter	Description of parameter	CSOIL2000 Data from 711701022	EUSES default	parameter values for sensitivity analysis	parameter values used for comparison with CSOIL scenario 'residential with garden'	units
Permeation	t	Stagnation time	0.33	n/a	0.33	idem	[d]
Permeation	L	Pipe length	100	n/a	100	idem	[m]
Permeation	r	Pipe radius	0.0098	n/a	0.0098	idem	[m]
Permeation	d	Pipe thickness	0.0027	n/a	0.0027	idem	[m]
Permeation	Qwd	Water consumption per residence	0.5	n/a	0.5	idem	[m3/d]

Soil

Module	parameter	Description of parameter	CSOIL 2000 data from 711701 021	CSOIL_ BGW_p rogram me	EUSES default	parameter values for sensitivity analysis	parameter values used for comparison with CSOIL scenario 'residential with garden'	units
Soil	Fair	Volume fraction of air in soil	0.2	0.2	0.20	0.2	idem	[-]
Soil	Fwater	Volume fraction of water in soil	0.3	0.3	0.20	0.3	idem	[-]
Soil	Fsolid_soil	Volume fraction of solids in soil	0.5	0.5	0.60	0.5	idem	[-]
Soil	Foc_soil	Volume fraction of organic carbon is soil	0.058	0.058	0.02	0.058	idem	[-]
Soil	RHOsolid	Specific density of soil solids			2500	2500	idem	[kg/m3]
Soil	RHOwater	Specific density of water			1000	1000	idem	[kg/m3]
Soil	RHOair	Specific density of air			1.3	1.3	idem	[kg/m3]
Soil	RHOsoil_dwt	Specific density of dry weight soil	1200	1200	n/a	1200	idem	[kg/m3 dwt]

House-module

Module	parameter	description of parameter	CSOIL2000	Ref.	CSOIL_BGW_programme	EUSES default	parameter values for sensitivity analysis	parameter values used for comparison with CSOIL scenario 'residential with garden'	units
house	dc	below soil surface crawlspace depth	0.5	A	0.5	n/a	0.5	idem	[m]
house	Fbi	percentage crawlspace air in indoor air	0.1	A	0.1	n/a	0.1	idem	[-]
house	deltapcs	air pressure difference between soil and crawlspace	1	A	1	n/a	1	idem	[Pa]
house	eta	dynamic viscosity of air	6.0E-09	A	5E-09	n/a	5.0E-09	idem	[Pa.h]
house	dg	depth groundwater table	1.75	B	1.75	n/a	1.75	idem	[m]
house	vvc	air-exchange rate crawl space	1.1	B	1.1	n/a	1.1	idem	[h-1]
house	z	height capillary. transition bound	0.5	B	0.5	n/a	0.5	idem	[m]
house	kappa	air permeability soil	1.0E-11	B	1.0E-11	n/a	1.0E-11	idem	[m2]
outside air	Lp	diameter contaminated area	100	C	100	n/a	100	idem	[m]
outside air	dp	mean depth of contamination	1.25	C	1.25	n/a	1.25	idem	[m]
outside air	Z	breathing height	1.5	C		n/a	1.5	idem	m
outside air	V10	speed of wind at 10 meters high	1800	C		n/a	18000	idem	[m/h]
outside air	k	Von Karman constant	0.4	C		n/a	0.4	idem	[-]
outside air	Zo	surface roughness constant	1	C		n/a	1	idem	-

outside air	Z10	height of 10 meters	10	C	n/a	10	idem	[m]

Footnote: a is reference to 711701022 [22], b is reference to 711701021 [19], and c to 715810014 [40].

Dermal exposure module

Module	parameter	description of parameter	CSOIL2000 Data from 711701022	CSOIL _BGW _programme	EUSES default	parameter values for sensitivity analysis	parameter values used for comparison with CSOIL scenario 'residential with garden'	units
dermal	Atota	adult total skin surface	1.8	1.8	n/a	1.8	idem	[m2]
dermal	Aexpai	exposed skin surface outside	0.09	0.09	n/a	0.09	idem	[m2]
dermal	Aexpao	exposed skin surface inside	0.17	0.17	n/a	0.17	idem	[m2]
dermal	DAEai	amount of soil contact per kg soil per m2 skin indoor	5.60E-04	5.60E-04	n/a	5.60E-04	idem	[kg grond/m2]
dermal	DAEao	amount of soil contact per kg soil per m2 skin outdoor	3.75E-02	3.75E-02	n/a	3.75E-02	idem	[kg grond/m2]
dermal	DARd	dermal absorption speed adult	0.005	0.005	n/a	5.00E-03	idem	[1/h]

Time table to calculate duration of exposures

Module	parameter	description of parameter	CSOIL _BGW _programme	Parameter values for sensitivity analysis	parameter values used for comparison with CSOIL scenario 'residential with garden'	units
time table	Tind wd	duration of stay indoors during week days	n/a	14	n/a	[h/d]
time table	Toutd wd	duration of stay outdoors during week days	n/a	2	n/a	[h/d]
time table	Twork	duration of stay at work during week days	n/a	8	n/a	[h/d]
time table	Tind wkd	duration of stay indoors during weekend days	n/a	20	n/a	[h/d]
time table	Toutd wkd	duration of stay outdoors during weekend days	n/a	4	n/a	[h/d]
time table	Tavg in	average duration of stay indoors	22.9	n/a	22.9	[h/d]
time table	Tavg out	average duration of stay outdoors	1.14	n/a	1.1	[h/d]
time table	Tavg wrk	average duration of stay at work	n/a	n/a	0	[h/d]

During the sensitivity analysis Tind wd is 24 minus Toutd wd minus Twork. And Tind wkd is 24 minus Toutd wkd. The values of Toutd wd, Twork, and Toutd wkd were varied within the uniform 10% distribution range.

Soil and Dust Module parameters

Module	parameter	description of parameter	CSOIL2000 711701022	CSOIL_BGW_ programme	EUSES default	parameter values for sensitivity analysis	parameter values used for comparison with CSOIL scenario 'residential with garden'	units
soil&dust	fr	retention factor of particles in longs	0.75	0.75	n/a	0.75	idem	[-]
soil&dust	TSPo	total dust concentration outdoor air	70		n/a	7.00E+01	idem	[ug/m3]
soil&dust	frso	fraction soil particles in outdoor dust	0.5	0.5	n/a	0.5	idem	[-]
soil&dust	frsi	fraction soil particles in indoor dust	0.8	0.8	n/a	0.8	idem	[-]
soil&dust	fm	matrix factor dermal absorption	0.15	0.15	n/a	0.15	idem	[-]

Shower module

Module	parameter	description of parameter	CSOIL2000 (711701022)	CSOIL_BGW _programme	EUSES default	parameter values for sensitivity analysis	parameter values used for comparison with CSOIL scenario 'residential with garden'	units
shower	fexp	fraction exposed skin during showering	0.4	0.4	n/a	0.4	idem	[-]
shower	tdc	duration of showering	0.25	0.25	n/a	0.25	idem	[h/d]
shower	td	duration of stay in bathroom	0.5	0.5	n/a	0.5	idem	[h]
shower	Kl	liquid phase exchange velocity	0.2		n/a	0.2	idem	[m/h]
shower	Kg	gas phase mass transport coefficient	29.88		n/a	29.88	idem	[m/h]
shower	tf	dropping time of drop			n/a	1	idem	[s]
shower	r	radius of drop	5.E-04		n/a	5.E-04	idem	[m]
shower	Vwb	water consumption per shower	0.15		n/a	0.15	idem	[m3]
shower	Vbk	volume of bathroom	15		n/a	15	idem	[m3]

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Appendix III: Model Formulas

Generic formulas

Estimation of solubility

Origin of formula is unknown but all used compounds have a known solubility.
So this formula was never used

$Sol = (MOLW*1000000)*10^{(LOG(K_{ow})*-1,214+0,85)}$

Input

MOLW	molecular weight	kg/mol
K_{ow}	octanol-water partition coefficient	m3/m3

Output

Sol	water solubility	kg/m3

Estimation of Henry coefficient and air-water partition coefficient

EC: III-21: formula 22 and 23

Henry = (VP*MOLW)/SOL

$K_{air\text{-}water}$ = Henry/(R*TEMPenv)

Input

VP	vapour pressure	Pa
MOLW	molecular weight	kg/mol
SOL	water solubility	kg/m3
R	gas constant	8.3144 Pa*m3/mol/K
TEMPenv	environmental temperature	K

Output

Henry	Henry’s law constant	Pa*m3/mol
$K_{air\text{-}water}$	air-water partition coefficient	m3/m3

Fish Module

Bioconcentration factor for fish

Calculations as in EC: III-60: formula 86,87

If K_{ow} <= 6

Log BCFfish = 0.85 * log K_{ow} – 0.070 –3

If K_{ow} > 6

Log BCFfish = -0.20 * $(\log K_{ow})^2$ + 2.74 * logK_{ow} – 4.72 –3

Input

K_{ow}	octanol-water partition coefficient	m3/m3

Output

BCFfish	bioconcentration factor for wet (life) fish	$m3/kg_{wwt}$

Concentration in fish

Calculations as in EC: III-64: formula 92

Cfish = BCFfish*Cwater

Input

BCFfish	bioconcentration factor for fish on wet weight basis	$m3/kg_{wwt}$
Cwater	concentration in surface water (dissolved)	kg/m3

Output

Cfish	concentration in wet fish	kg/kg_{wwt}

Exposure from fish

Calculations as in EC: III-74: formula 116,117,118
Self defined variable
Expfish = IHfish*Cfish/BW

Input

IHfish	daily consumption of fish (wwt)	kg_{wwt}/d
Cfish	concentration in wet fish	kg/kg_{wwt}
BW	human body weight	kg

Output

Expfish	daily exposure from fish consumption	$kg/kg_{bw}/d$

Air Module

Calculation of air flux (CSOIL) outdoors. These are only used for comparison CSOIL-Humanex, but not included in the Humanex final model.
Formulas as in Waitz et al, 715810014 appendix 5.5-5.2

Formulas fugacity calculations

Fugacity capacity constant air

RIVM 715810014p144
Za = 1/(R*T)

Input

R	gas constant	8.3144	Pa*m3/mol/K
T	temperature		Kelvin

Output

Za	fugacity capacity constant air	mol/m3/Pa

Fugacity constant water

RIVM 715810014p144
Zw = S/Vp

Input

S	water solubility	mol/m3
Vp	vapour pressure substance	Pa

Output

Zw	fugacity constant water	mol/m3/pa

Fugacity capacity constant soil

RIVM 715810014p144
Zs = K_d*SD*Zw/Vs

Input

K_d	distribution coefficient soil-water	$(mol/kg_{dwt})/(mol/dm3)$
SD	mass volume of the dry soil	kg dry soil/dm3 humid soil
Vs	volume fraction solid phase	-/-

Output

Zs	Fugacity capacity constant soil	mol/m3/Pa

Volume fraction solid phase

RIVM 715810014p144

Vs = 1 – porosity = 1- Va -Vw

Input

Va	volume fraction air in soil	-/-
Vw	volume fraction water in soil	-/-

Output

Vs	volume fraction solid phase	-/-

Distribution coefficient soil-water

RIVM 715810014p144

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

Input

K_{oc}	distribution coefficient soil-water corrected for organic carbon	(mol/kg organic carbon) /(mol/dm3)
F_{oc}	fraction organic carbon	kg organic carbon/kg dry soil

Output

K_d	distribution coefficient soil-water	(mol/kg$_{dwt}$)/(mol/dm3)

Fraction organic carbon

This is the Humanex default (RIVM 715810014p145). The program however allows overriding the default with experimental K_{oc} values or K_{oc} estimates from other regressions.

$K_{oc} = 0.411 * K_{ow}$

Or

$\text{Log } K_{oc} = 0.989 * \log K_{ow} - 0.346$

Input

K_{ow}	octanol-water distribution coefficient	(mol/dm3)/(mol/dm3)

Output

K_{oc}	distribution coefficient soil-water corrected for organic carbon	(mol/kg organic carbon) /(mol/dm3)

Air-water distribution coefficient

RIVM 715810014p145

Klw = Za/Zw = Vp/(S*R*T)

Input

Za	fugacity capacity constant air		mol/m3/Pa
Zw	fugacity constant water		mol/m3/pa
Vp	vapour pressure substance		Pa
S	water solubility		mol/m3
R	gas constant	8.3144	Pa*m3/mol/K
T	temperature		Kelvin

Output

Klw	air-water distribution coefficient	(mol/m3 air)/(mol/m3 water)

Calculation mass fractions

RIVM 715810014p145

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)

Input

Za	fugacity capacity constant air	mol/m3/Pa
Zw	fugacity constant water	mol/m3/pa
Va	volume fraction air in soil	-/-
Vw	volume fraction water in soil	-/-
Zs	Fugacity capacity constant soil	mol/m3/Pa
Vs	volume fraction solid phase	-/-

Output

Pa	mass fraction in soil air	-/-
Pw	mass fraction in soil moisture	-/-
Ps	mass fraction in solid phase	-/-

Formulas air flux calculations – outdoor

Diffusion coefficient in the soil-gas phase

RIVM 715810014p147

Dsa = (Va^(10/3))*Da/((1-Vs)^2)

With Da = 0.036*((76/M)^(1/2))

Input

Da	diffusion coefficient in the soil-gas- phase	m2/h
M	molecular mass	g/mol

Output

Dsa	diffusion coefficient in the soil-gas phase	m2/h

Diffusion coefficient in the soil-water phase

RIVM 715810014p147

Dsw = (Vw^(10/3))*Dw/((1-Vs)^2)

With Dw = 3.6e-6*((76/M)^(1/2))

Input

Dw	diffusion coefficient in the free water phase	m2/h
M	molecular mass	g/mol

Output

Dsw	diffusion coefficient in the soil-water phase	m2/h

Mean depth of the contaminant

RIVM 715810014p60

dp = dg – z

Input

dg	depth ground water table	m
z	height capill. trans. Boundary	m

Output

dp	mean depth of the contaminant	m

Diffusion coefficient in the soil

RIVM 715810014p147

Du = (Pa*Dsa/Va) + (Pw*Dsw/Vw)

Input

Pa	mass fraction in soil air	-/-
Dsa	diffusion coefficient in the soil-gas phase	m2/h

Va	volume fraction air in soil	-/-
Pw	mass fraction in soil moisture	-/-
Dsw	diffusion coefficient in the soil-water phase	m2/h
Vw	volume fraction water in soil	-/-

Output

Du	diffusion coefficient in the soil	m2/h

Total flux outdoor

RIVM 715810014p147

Jo = Joutdoor = J4 = Du*PECreg, agriCSOIL*SD/dp

Input

Du	diffusion coefficient in the soil	m2/h
PECreg, agriCSOIL	concentration contaminant in wwt soil	kg/kg_{wwt}
SD	mass volume of the dry soil	kg dry soil/m3 humid soil
dp	mean depth of the contaminant	m

Output

Jo	diffusion flux water-soil to surface level	kg/m2/h

Outdoor air concentration

Generic dilution velocity

RIVM 715810014p149

Vf = Vg*Sz/Lp

Input

Vg	mean wind velocity	m/h
Sz	vertical Pasquill dispersion coefficient, related to Pasquill weather stability class D	m/h
Lp	diameter contaminated area	m

Output

Vf	generic dilution velocity	m/h

Mean wind velocity

RIVM 715810014p149

Vg = (Vx + V')/2

Input

Vx	wind velocity at x m altitude	m/h
V'	friction velocity	m/h

Output

Vg	mean wind velocity	m/h

Wind velocity at x m altitude

RIVM 715810014p149

Vx = (ln(Z/Zo))*V'/k

Input

Z	breathing altitude	m
Zo	roughness of the surface area (resident area)	-/-
V'	friction velocity	m/h
k	von Karman constant	-/-

Output

Vx	wind velocity at x m altitude	m/h

Friction velocity

RIVM 715810014p149

V' = k*V10/ln(Z10/Zo)

Input

k	von Karman constant	-/-
V10	wind velocity at 10 m altitude	m
Z10	altitude	m
Zo	roughness of the surface area (resident area)	-/-

Output

V'	friction velocity	m/h

Vertical Pasquill dispersion coefficient, related to Pasquill weather stability class D

RIVM 715810014p149

Sz = Co*0.20*(Lp^0.76)

Input

Co	correction factor for the roughness length	-/-
Lp	diameter contaminated area	m

Output

Sz	vertical Pasquill dispersion coefficient, related to Pasquill weather stability class D	m/h

Correction factor for the roughness length

RIVM 715810014p149

Co = (10*Zo)^(0.53*(Lp^-0.22))

Input

Zo	roughness of the surface area (resident area)	-/-
Lp	diameter contaminated area	m

Output

Co	correction factor for the roughness length	-/-

Dilution velocity adult

RIVM 715810014p147

Is calculated as the generic dilution velocity but with the specific parameters

Vf = Vfa, dilution velocity adult

Z = breathing altitude adult

Va = wind velocity at breathing altitude adult

Dilution velocity plant

Is calculated as the generic dilution velocity but with the specific parameters

Vf = Vfp

Vfp is a fixed parameter value

Concentration addition to the outdoor air for humans

Coaa = Jo/Vfa

Input

Jo	diffusion flux water-soil to surface level	kg/m2/h
Vfa	dilution velocity adult	m/h

Output

Coaa	concentration addition to the outdoor air for humans	kg/m3

Outdoor air concentration for humans

Cair, outdoor = PECreg, air + Coaa

Input

PECreg, air	predicted environmental concentration of air	kg/m3
Coaa	concentration addition to the outdoor air for humans	kg/m3

Output

Cair, outdoor	outdoor air concentration for humans	kg/m3

Concentration addition to the outdoor air for plants

Coaa = Jo/Vfp

Input

Jo	diffusion flux water-soil to surface level	kg/m2/h
Vfa	dilution velocity adult	m/h

Output

Coaplant	concentration addition to the outdoor air for plants	kg/m3

Outdoor air concentration for plants

Cair, plant = PECreg, air + Coaplant

Input

PECreg, air	predicted environmental concentration of air	kg/m3
Coaplant	concentration addition to the air for plants	kg/m3

Output

Cair, plant	air concentration for plants	kg/m3

Formulas air flux calculations – indoor

(CSOIL, not used in Humanex)

Length of soil column

RIVM 715810014p60

Ls = Max((dp-dc);0.01)

Maximalisation from CSOIL2000: length of soil column at least 1 cm.

Input

Dp	average depth of contaminant	m
Dc	depth of crawl space beneath soil surface	m

Output

Ls	length of soil column	m

Air conductivity of soil

RIVM 715810014p64

Ks = kappa/etta

Input

kappa	air permeability of soil	m2
etta	dynamic viscosity of air	Pa*h

Output

Ks	air conductivity of soil	m2/Pa/h

Air flux from soil to crawl space

RIVM 715810014p64

Fsc = Ks*ΔPcs/Ls

Input

Ks	air conductivity of soil	m2/Pa/h
ΔPcs	air pressure difference between crawl space and soil	Pa
Ls	length of soil column	m

Output

Fsc	Air flux from soil to crawl space	m/h

Concentration of pore air

RIVM 715810014p146

Csa = PECreg,agriCSOIL*RHOsoil$_{wwt}$*Pa/Va

Input

PECreg, agriCSOIL	concentration contaminant in wwt soil	kg/kg$_{wwt}$
RHOsoil$_{wwt}$		
Pa	mass fraction in soil air	-/-
Va	volume fraction air in soil	-/-

Output

Csa	concentration of pore air	kg/m3

Total contaminant flux from soil to crawl space

RIVM 715810014p69

J1 = (-Fsc*Csa)/(exp(-Fsc*Ls/Dsa)-1)

Input

Fsc	Air flux from soil to crawl space	m/h
Csa	concentration of pore air	kg/m3
Ls	length of soil column	m
Dsa	diffusion coefficient in the soil-gas phase	m2/h

Output

J1	total contaminant flux from soil to crawl space	kg/m2/h

Concentration of basement air

RIVM 715810014p151

Cba = J1/(dc*vvc)

With dc = Bv/Bo = 25/50 = 0.5 m

Input

J1	total contaminant flux from soil to crawl space	kg/m2/h
dc	depth of crawl space beneath soil surface	m
vvc	air-exchange rate crawl space	h^{-1}
Bv	volume of the crawl space	m3
Bo	surface of the crawl space	m2

Output

Cba	concentration of basement air	kg/m3

Concentration addition to the indoor air

Based on RIVM 715810014p151

DeltaCindoor = fbi*Cba

Input

Cba	concentration of basement air	kg/m3
Fbi	contribution of the crawl space air to the indoor air as fraction	-/-

Output

deltaCindoor	concentration addition to the indoor air	kg/m3

Indoor air concentration at home

Cindoor = Cair + deltaCindoor
With Cair = PECreg,air

Input

Cair	predicted environmental air concentration	kg/m3
deltaCindoor	concentration addition to the indoor air	kg/m3

Output

Cindoor	indoor air concentration for adults at home	kg/m3

Indoor air concentration at work

Cair, work = Cindoor

Input

Cindoor	indoor air concentration for adults at home	kg/m3

Output

Cair, work	indoor air concentration for adults at work	kg/m3

Calculation of the average air concentration for humans

RIVM 715810014p186-188
Cair, average = (1/24)*(Tind*Cair, indoor + Toutd*Cair, outdoor + Twork*Cair, work)

Input

Tind	weekly average of time spend indoor	hours/day
Cindoor	indoor air concentration for adults at home	kg/m3
Toutd	weekly average of time spend outdoor	hours/day
Cair, outdoor	outdoor air concentration for humans	kg/m3
Twork	weekly average of time spend at work	hours/day
Cair, work	indoor air concentration for adults at work	kg/m3

Output

Cair, average	average concentration of air for humans	kg/m3

Example calculation:

		Hours	Days	Product
Week day	Indoor	14	5	70
	Outdoor	2	5	10
	Work	8	5	40
Weekend	Indoor	20	2	40
	Outdoor	4	2	8
	Work	0	2	0
	Total	24	7	168

Weekly	average hours/day
Indoor	15,7
Outdoor	2,6
Work	5,7
Total	24

Cair, average (example) = based on average indoor, outdoor and work duration
= (1/24)*(15.7* Cair, indoor + 2.6*Cair, outdoor + 5.7*Cair, work)

Calculation of the average air concentration for cows

Cair, cow = Cair average

Input

Cair, average	average concentration of air for humans	kg/m3

Output

Cair, cow	average concentration of air for cows	kg/m3

Exposure for humans from air

Self defined variable

Expair = IHair*Cair, average/BW

Input

IHair	daily consumption of air	m3/d
Cair, average	average concentration of air for humans	kg/m3
BW	human body weight	kg

Output

Expair	daily exposure from air	$kg/kg_{bw}/d$

Root Module

Fraction water in root tissue

Partition coefficient between root tissue and water

Calculations as in EC: III-66: formula 93

Kroot-pore water = $Fwater_{plant} + Flipid_{plant} * (K_{ow}{}^{b})$

Input

$Fwater_{plant}$	volume fraction of water in plant tissue	m3/m3
$Flipid_{plant}$	volume fraction of lipids in plant tissue	m3/m3
K_{ow}	octanol-water partition coefficient	-/-
b	correction for differences between plant lipids and octanol	-/-

Output

Kroot-pore water	partition coefficient between root tissue and water	m3/m3

Concentration in root tissue

Calculations as in EC: III-66: formula 94

Croot = Kroot-pore water*Cagric, porew/RHOplant

Input

Kroot-pore water	partition coefficient between root tissue and water	m3/m3
Cagric, porew	concentration in agraric pore water	kg/m3
RHOplant	bulk density of root tissue (wet weight)	$kg_{ww}t/m3$

Output

Croot	concentration in root tissue of plant	kg/kg_{wwt}

Concentration in agraric pore water

Cagric, porew = PECreg, agric pore

Input

PECreg, agric pore	predicted env. concentration in agraric pore water	kg/m3

Output

Cagric, porew	concentration in agraric pore water	kg/m3

Exposure from root products

Self defined variable

Exproot = IHroot*Croot/BW

Input

IHroot	daily human consumption of root (wwt)	kg_{wwt}/d
Croot	concentration in root tissue of plant	kg/kg_{wwt}
BW	human body weight	kg

Output

Exproot	daily exposure form root products	$kg/kg_{bw}/d$

Plant Module

Partitioning coefficient between water and plant tissue

EC: III-66: formula 93

$K_{plant\text{-}water} = Fwater_{plant} + Flipid_{plant} * K_{ow}^{bplant}$

Input

$K_{plant\text{-}water}$

$Fwater_{plant}$	volume fraction of water in plant tissue	-/-
K_{ow}	octanol-water partition coefficient	-/-
bplant	correction factor for differences between plant lipids and octanol	-/-

Output

$K_{plant\text{-}water}$	partition coefficient between plant and water	-/-

Partition coefficient between plant leaves and air

EC: III-67: formula 96

$K_{leaf\text{-}air} = Fair_{plant} + (K_{plant\text{-}water}/Kaw)$

Input

$Fair_{plant}$	volume fraction of air in plant tissue	-/-
$K_{plant\text{-}water}$	partition coefficient between plant and water	-/-
Kaw	air-water partition coefficient	-/-

Output

$K_{leaf\text{-}air}$	partition coefficient between leaves and air	-/-

Transpiration stream concentration factor EUSES

EUSES-method: based on Briggs *et al.* [2]

EC: III-66: formula 95

$TSCF = 0.784 * \exp((-(\log K_{ow} - 1.78)^2)/2.44)$

If $\log K_{ow}$ is < -0.5 then a TSCF corresponding to $\log K_{ow}$ of –0.5 is used.

If $\log K_{ow}$ is > 4.5 then a TSCF corresponding to $\log K_{ow}$ of 4.5 is used.

Input

K_{ow}	octanol-water partition coefficient	-/-

Output

TSCF	transpiration stream concentration factor	-/-

Transpiration stream concentration factor CSOIL 2000

CSOIL2000-methode: based on Hsu and Briggs.

$TSCF_1 = 0.784 * \exp((-(\log K_{ow} - 1.78)^2)/2.44)$

If $TSCF_1 < 0.04$ than $TSCF_1 = 0.04$

$TSCF_2 = 0.7*\exp(-((\log K_{ow} - 3.07)^2)/2.78)$

If $TSCF_2 < 0.04$ than $TSCF_2 = 0.04$

$TSCF = \max(TSCF_1;TSCF_2)$

Input

K_{ow}	octanol-water partition coefficient	-/-

Output

TSCF	transpiration stream concentration factor	-/-

Transpiration stream concentration factor Humanex

HUMANEX-method

TSCF = as calculated with the CSOIL2000- method

Input

K_{ow}	octanol-water partition coefficient	-/-

Output

TSCF	TSCF used in HUMANEX model	-/-

Factor2

Self defined variable

Fact2 = Qtrans/Vleaf

Input

Qtrans	transpiration stream	m3/d
Vleaf	shoot volume	m3

Output

Fact2	source term from pore water	d^{-1}

Factor3

Self defined variable

Fact3 = (1 – Fass-aer)*g_{plant}*AREAplant*(1/Vleaf)

Input

Fass-aer	fraction of substance absorbed to aerosol	-/-
g_{plant}	conductance	m/d
AREAplant	leaf surface area	m2
Vleaf	shoot volume	m3

Output

Fact3	source term form air	d^{-1}

$Fass_{ear}$: fraction of chemical associated with aerosol particles

EC: III-20: formulas 19, 20 and 21 are added together into the below formula for Humanex:

$Fass_{aer}$=IF(TEMPmelt<=TEMPenv;CONjungexSURFaer/(VP+CONjungexSURFaer);CONjungexSURFaer/(CONjungexSURFaer+(VP/(EXP(6,79*(1-(TEMPmelt/TEMPenv))))))

Input:

CONjungexSURFaer	constant of Junge * surface area of aerosol particles	Pa
VP	vapour pressure	Pa
TEMPenv	environmental temperature	K
TEMPmelt	melting point of substance	K

Output

$Fass_{aer}$	fraction of chemical associated with aerosol particles	-/-

ALPHA sink term of differential equation

EC: III-67: formula 98

ALPHA = $ratio_{surf/vol}$* g_{plant}*(1/Kleaf-air) + kphotoplant – kmetabplant
+ kgrowth-plant

Input

$ratio_{surf/vol}$	ratio leaf surface area / shoot volume	m
g_{plant}	conductance	m/d
Kleaf-air	partition coeff. between leaves and air	-/-
Kphotoplant	rate constant for metabolism in plants	d^{-1}
Kmetabplant	rate constant for photolysis in plants	d^{-1}
kgrowth-plant	rate constant for dilution by growth	d^{-1}
Output		
ALPHA	sink term of differential equation	d^{-1}

Factor4

Self defined variable

Fact4 = ALPHA*RHOplant

Input

ALPHA	sink term of differential equation	d^{-1}
RHOplant	bulk density of root tissue (wet weight)	$kg_{ww}t/m3$
Output		
Fact4	self defined variable	$kg_{ww}t/m3/d$

Ratio leaf surface area / shoot volume

self defined variable

$ratio_{surf/vol}$ = AREAplant/Vleaf;

Input

AREAplant	leaf surface area	m2
Vleaf	shoot volume	m3
Output		
$ratio_{surf/vol}$	ratio leaf surface area / shoot volume	m

BETAagric source term for differential equation for crops

Based on EC: III-68: formula 99

BETAagric = Cagric, porew*TSCF*Fact2 + Cair, plant*Fact3

Input

Cagric, porew	concentration in agraric pore water	kg/m3
TSCF	transpiration stream concentration factor	-/-
Fact2	source term from pore water	d^{-1}
Cair, plant	air concentration for plants	kg/m3
Fact3	source term form air	d^{-1}
Output		
BETAagric	source term for differential equation for crops	kg/m3/d

Deposition of resuspended particles / rainsplash

CSOIL2000-program and RIVM 711701022p90 (not p129)

Cdep = Cagric, soil*CONVsoil*dpconst*fdws

Input

Cagric, soil	concentration in agricultural soil	kg/kg_{wwt}
CONVsoil	wwt dry weight conversion for soil	kg_{wwt}/kg_{dwt}
Dpconst	deposition constant	-/-

fdws	fraction dry matter leafy crops	-/-
Output		
Cdep	concentration in leafs caused by deposition	kg/kg_{wwt}

Concentration in leaf

Based on EC: III-68: formula 101

Cleaf = BETAagric/Fact4 + Cdep

Input		
BETAagric	source term for differential equation for crops	kg/m3/d
Fact4	self defined variable	kg_{wwt}/m3/d
Cdep	concentration in leafs caused by deposition	kg/kg_{wwt}
Output		
Cleaf	concentration of contaminant in plant leafs (wwt)	kg/kg_{wwt}

Exposure for humans from leaf products

Self defined variable

Expleaf = IHleaf*Cleaf/BW

Input		
IHleaf	daily intake of leaf products	kg_{wwt}/d
Cleaf	concentration of contaminant in plant leafs (wwt)	kg/kg_{wwt}
BW	human body weight	kg
Output		
Expleaf	Exposure for humans from leaf products	kg/kg_{bw}/d

Drinking water module

Purification of surface water module

Rate constants and half-lives for biodegradation in bulk-surface water

EC: III-28: table III-6

Data dependent on compound properties.

In the Humanex model biodegradation can be used in the assessment of purification of drinking water but all compounds were considered not biodegradable. In some cases this might have caused an over estimation of a factor four in the concentration in drinking water.

Table III-1	Rate constant (d^{-1})	Half-live (d)
$DT50bio_{water} = ln(2)/kbio_{water}$	$kbio_{water}$	$DT50bio_{water}$
Readily biodegradable	$4.6*10^{-2}$	15
Readily biodegradable, but failing 10 day window	1.4*10-2	50
Inherently biodegradable	$4.6*10^{-3}$	150
Not biodegradable	0	$1*10^{20}$ T
T normally infinite long, but to make calculations possible DT50 is max $1*10^{20}$ days.This a modification for Humanex, not a EUSES default.		

Calculation of Fpur

EC: III-72: formula 114

Fpur = max(Fsys1pur, Fsys2pur)

Table for derivation of Fsys1pur, Fsys2pur							
Treatment process	Log K_{ow}			Henry's law constant (Pa*m3/mol)		Aerobic Biodegradation rate DT50biowater (days)	
	=<4	4 –5	>5	=< 100	> 100	> 10	=< 10
System 1	1	¼	1/16	1	½	1	1
System 2	1	½	¼	1	½	1	¼

See EC III-72 for details

Input

K_{ow}	octanol-water partition coefficient	m3/m3
Henry	Henry's law constant	Pa*m3/mol
DT50biowater	half-life for biodegradation in bulk surface water	d
Fsys1pur	purification factor for system 1	-/-
Fsys2pur	purification factor for system 2	-/-

Output

Fpur	purification factor for surface water	-/-

Concentration in drinking water before permeation

EC: III-73: formula 115

Cwater = max (Csurface water*fpur; Cground water)

Input

Csurface water	concentration in surface water	kg/m3
Fpur	purification factor for surface water	-/-
Cground water	concentration in ground water	kg/m3

Output

Cwater	concentration in drinking water before permeation	kg/m3

Concentration in surface water and ground water

Csurface water = PECreg, surf w

Cground water = PECreg, agric porew

Input

PECreg, surf w
predicted environmental concentration surface water (dissolved) kg/m3

PECreg, agric porew
predicted environmental concentration in agricultural pore water kg/m3

Output

Csurface water	concentration in surface water	kg/m3
Cground water	concentration in ground water	kg/m3

Permeation module

Max. concentration in the drinking water after stagnation

RIVM 711701022p131

Cmax = Cpw*2*Dpe*t/(r*d)

Input

Cpw	concentration in pore water	kg/m3
Dpe	permeation coefficient	m2/d
t	time of water stagnation	d
r	radius of the pipe	m
d	thickness of pipe wall	m

Output

Cmax max. concentration in the drinking water after t days of stagnation kg/m3

Concentration in pore water

Cpw = PECreg, agric porew

Input

PECreg, agric porew

predicted environmental concentration in agricultural pore water kg/m3

Output

Cpw	concentration in pore water	kg/m3

Mean drinking water concentration after stagnation

RIVM 711701022p131

$Cdrw = Cmax*3*pi*r^2*L/Qwd + Cwater$

Input

Cmax max. concentration in the drinking water after t days of stagnation kg/m3

Pi		3.141593
r	radius of the pipe	m
L	length of the pipe along which permeation can occur	m
Qwd	mean daily water consumption of a household	m3/d
Cwater	concentration in drinking water before permeation	kg/m3

Output

Cdrw	concentration in drinking water	kg/m3

Concentration in human drinking water

$Cdrw_{human} = Cdrw$

Input

Cdrw	concentration in drinking water	kg/m3

Output

$Cdrw_{human}$	Concentration in human drinking water	kg/m3

Concentration in bovine drinking water

$Cdrw_{cow} = Cdrw$

Input

Cdrw	concentration in drinking water	kg/m3

Output

$Cdrw_{cow}$	Concentration in bovine drinking water	kg/m3

Exposure for humans from drinking water

Self defined variable
Expdrw = IHwater*Cdrw/BW

Input

IHwater	daily intake of drinking water	m3/d
Cdrw	concentration in drinking water	kg/m3
BW	human body weight	kg

Output

Expdrw	daily exposure from drinking water	kg/kgbw/d

Cow Module

Cow exposure module

Conversion of dwt product to wwt product

EC: III-71:formula 109 and 110
ICgrass = ICdwtgras*CONVgrass
ICSOIL = ICdwtsoil*CONVsoil

Input

ICdwtgras	daily intake of grass (dwt)	kg_{dwt}/d
CONVgrass	conversion factor grass from dry to wet weight	kg_{wwt}/kg_{dwt}
ICdwtsoil	daily intake of soil (dwt)	kg_{dwt}/d
CONVsoil	conversion factor soil from dry to wet weight	kg_{wwt}/kg_{dwt}

Output

ICgrass	daily intake of grass (wwt)	kg_{wwt}/d
ICSOIL	daily intake of grass (wwt)	kg_{wwt}/d

Exposure from grass

EC: III-71
Excgrass = ICgrass*Cleaf

Input

ICgrass	daily intake of grass (wwt)	kg_{wwt}/d
Cleaf	concentration of contaminant in plant leafs (wwt)	kg/kg_{wwt}

Output

Excgrass	exposure from grass consumption	kg/d

Exposure from grassland soil

EC: III-71
Exsoil = ICSOIL*Cgrassland

Input

ICSOIL	daily intake of grass (wwt)	kg_{wwt}/d
Cgrassland	concentration of contaminant in grassland soil(wwt)	kg/kg_{wwt}

Output

ExCSOIL	exposure from soil consumption	kg/d

Exposure from air

EC: III-71
Excair = ICair*Cair, cow

Input

ICair	daily intake of air	m3/d
Cair, cow	average concentration of air for cows	kg/m3

Output

Excair	exposure from air inhalation	kg/d

Exposure form drinking water

EC: III-71

$Excdrw = ICdrw*Cdrw_{cow}$

Input

ICdrw	daily intake of drinking water	m3/d
$Cdrw_{cow}$	concentration in bovine drinking water	kg/m3

Output

Excdrw	exposure from drinking water consumption	kg/d

Exposure of the cow

Exctot = Excgrass + ExCSOIL + Excair + Excdrw

Input

Excgrass	exposure from grass consumption	kg/d
ExCSOIL	exposure from soil consumption	kg/d
Excair	exposure from air inhalation	kg/d
Excdrw	exposure from drinking water consumption	kg/d

Output

Exctot	total exposure of the cow	kg/d

Bioaccumulation factors for meat and milk

BAF meat and milk

EC: III-70: formula 107 and 108

$BAFmeat = 10^{-7.6 + \log Kow}$

If log K_{ow} < 1.5 than a log K_{ow} of 1.5 is used

If log K_{ow} > 6.5 than a log K_{ow} of 6.5 is used

$BAFmilk = 10^{-8.1 + \log Kow}$

If log K_{ow} < 3.0 than a log K_{ow} of 3.0 is used

If log K_{ow} > 6.5 than a log K_{ow} of 6.5 is used

Input

K_{ow}	octanol-water partition coefficient	-/-

Output

BAFmeat	bioaccumulation factor for meat	d/kg
BAFmilk	bioaccumulation factor for milk	d/kg

Contaminant concentrations in meat and milk

EC: III-71: formula 111 and 112

Cmilk = BAFmilk*Extot

Cmeat = BAFmeat*Extot

Input

BAFmilk	bioaccumulation factor for milk	d/kg
Extot	total exposure of the cow	kg/d
BAFmeat	bioaccumulation factor for meat	d/kg

Output

Cmilk	contaminant concentration in milk (wwt)	kg/kg_{wwt}
Cmeat	contaminant concentration in meat (wwt)	kg/kg_{wwt}

Exposure for humans from meat or milk

Self defined variables
Expmeat = IHmeat*Cmeat/BW
Expmilk = IHmilk*Cmilk/BW

Input

IHmeat	daily intake of meat	kg/d
Cmeat	contaminant concentration in meat (wwt)	kg/kg_{wwt}
BW	human body weight	kg
IHmilk	daily intake of milk	kg/d
Cmilk	contaminant concentration in milk (wwt)	kg/kg_{wwt}

Output

Expmeat	daily exposure form meat consumption	$kg/kg_{bw}/d$
Expmilk	daily exposure form milk consumption	$kg/kg_{bw}/d$

Shower Module

Temperature correction for the Henry constant

RIVM 711701022p132
ln (Hsh) = LN(HENRY)+0,024*(Tsh-TEMPenv)

Input

Henry	Henry's law constant	Pa*m3/mol
Tsh	temperature of shower	K
TEMPenv	environmental temperature	K

Output

ln (Hsh)	natural log of Henry cons. at temp. of shower	K

Air-water partition coefficient at 313 Kelvin

Based on RIVM 711701022p132
Kaw_{313} = EXP(ln(Hsh))/(Gasconst*Tsh)

Input

ln (Hsh)	natural log of Henry cons. at temp. of shower	K
R	gas constant	8.3144 Pa*m3/mol/K
Tsh	temperature of shower	K

Output

Kaw_{313}	Air-water partition coefficient at 313 Kelvin	-/-

Mass transport coefficients

RIVM 711701022p132
$kL = Kl*(44/M)^{1/2}/3600$
$kG = Kg*(18/M)^{1/2}/3600$

Input

Kl	liquid phase exchange velocity	m/h
Kg	gas phase mass transport coefficient	m/h
M	molar mass of contaminant	g/mol

Output

kL	water mass transport coefficient	m/s
kg	vapour mass transport coefficient	m/s

Ratio area/volume drop

RIVM 711701022p132

Area of a drop = $4*pi*r^2$

Volume of a drop = $4/3*pi*r^3$

Ad/Vd = $3/r_{drop}$ with $(4*pi*r^2)/(4/3*pi*r^3) = 3/r$

Input

R_{drop}	radius of a drop	m

Output

Ad/Vd	ratio area/volume drop	m^{-1}

Degree of evaporation of the contaminant

RIVM 711701022p131

$Kwa = (tf*Ad/Vd*Kaw_{313}*kL*kG)/((Kaw_{313}*kG) + kL)$

Input

Tf	dropping time of drop	
Ad/Vd	ratio area/volume drop	m^{-1}
Kaw_{313}	Air-water partition coefficient at 313 Kelvin	-/-
kL	water mass transport coefficient	m/s
kg	vapour mass transport coefficient	m/s

Output

Kwa	degree of evaporation of the contaminant	-/-

Concentration in the bathroom air

RIVM 711701022p132

$Cbk = Kwa*Cdrw_{human}*5*10^{-3}$

Input

Kwa	degree of evaporation of the contaminant	-/-
$Cdrw_{human}$	concentration in human drinking water	kg/m3

Output

Cbk	concentration in bathroom air	kg/m3

Exposure from bathroom air

RIVM 711701022p135

$Exinhl_{shw} = Cbk*AV*td*fa_{inhl}/BW$

Input

Cbk	concentration in bathroom air	kg/m3
AV	breathing volume adult	m3/h
td	duration of stay in the bathroom	h
fa_{inhl}	relative absorption fraction, set at 1	-/-
BW	body weight adult	kg

Output

$Exinhl_{shw}$	exposure through vapours while showering	$kg/kg_{bw}/d$

Dermal absorption velocity
RIVM 711701022p136
DAR = (5*(38+153*K_{OW}))/(5+(38+153*K_{OW}))*(EXP(-0,016*M)/1,5)
Input

K_{ow}	octanol-water partition coefficient	-/-
M	molar mass of contaminant	g/mol

Output

DAR	dermal absorption velocity	((mg/m2)/(mg/dm3))/h

Uptake as a result of dermal contact during showering
RIVM 711701022p136
DAw = Atot*fexp*DAR*tdc*(1-kwa)*Cdrwhuman* fa_{derm}
Input

Atot	exposure surface adult	m2
Fexp	fraction exposed skin	-/-
DAR	dermal absorption velocity	((mg/m2)/(mg/dm3))/h
tdc	contact time = shower tome	h/d
(1-Kwa)	fraction substance remaining after evaporation	-/-
Cdrwhuman	concentration in human drinking water	kg/m3
fa_{derm}	relative absorption fraction, set at 1	-/-

Output

DAw	Uptake as a result of dermal contact during showering	kg/d

Exposure through dermal absorption while showering

$Exderm_{shw}$ = DAw/BW
Input

DAw	Uptake as a result of dermal contact during showering	kg/d
BW	human body weight	kg

Output

$Exderm_{shw}$	exposure through dermal uptake while showering	$kg/kg_{bw}/d$

Total exposure while showering

Exshw = $Exinhl_{shw}$ + $Exderm_{shw}$
Input

$Exinhl_{shw}$	exposure through vapours while showering	$kg/kg_{bw}/d$
$Exderm_{shw}$	exposure through dermal uptake while showering	$kg/kg_{bw}/d$

Output

Exshw	total daily exposure while showering	$kg/kg_{bw}/d$

Soil density formulas

CONVsoil: conversion factor for soil concentrations: wwt to dwt
Based on EC: III-19: formula 17
CONVsoil = RHOsoil_wwt/RHOsoil_dwt
Input

RHOsoil_wwt	wet bulk density of soil	$kg_{wwt}/m3$
RHOsoil_dwt	dry bulk density of soil	$kg_{dwt}/m3$

Output

CONVsoil	conversion factor for soil concentrations: wwt to dwt	kg_{wwt}/kg_{dwt}

(CONVsoil always > 1)

RHOsoil_wwt: wet bulk density of soil

EC: III-18: formula 14

RHOsoil_wwt = Fair_soil*RHOair+RHOwater*Fwater_soil+Fsolid_soil*RHOsolid

Input

Fair_soil	volume fraction of water in soil	m3/m3
RHOair	density of air phase	kg/m3
RHOwater	density of water phase	kg/m3
Fwater_soil	volume fraction of water in soil	m3/m3
Fsolid_soil	volume fraction of solids in soil	m3/m3
RHOsolid	density of solids phase	

Output

RHOsoil_wwt	wet bulk density of soil	$kg_{wwt}/m3$

RHOsoil_dwt: dry bulk density of soil

Based on EC: III-18: formula 14

adjusted formula due to replacement of water by air when drying wet ground into dry ground. Fwater is added to the Fair.

RHOsoil_dwt = (Fair_soil + Fwater_soil)*RHOair + Fsolid_soil*RHOsolid

Input

Fair_soil	volume fraction of water in soil	m3/m3
Fwater_soil	volume fraction of water in soil	m3/m3
RHOair	density of air phase	kg/m3
Fsolid_soil	volume fraction of solids in soil	m3/m3
Fsolid_soil	volume fraction of solids in soil	m3/m3

Output

RHOsoil_dwt	dry bulk density of soil	$kg_{dwt}/m3$

Concentration in soil

CSOILwwt = PECreg-agric, soil

Input

PECreg-agric, soil

predicted environmental concentration agricultural soil kg/kg_{wwt}

Output

$CSOIL_{wwt}$	concentration in wwt soil	kg/kg_{wwt}

Exposure from soil

Exposure from soil ingestion

RIVM 711701022p132

$Expsoil_{ingest} = CSOIL_{wwt}$*IHsoil* CONVsoil*BIOoral/BW

Input

CONVsoil	wwt dry weight conversion for soil	kg_{wwt}/kg_{dwt}
$CSOIL_{wwt}$	concentration in wwt soil	kg/kg_{wwt}
IHsoil	human daily consumption of soil (dwt)	kg_{dwt}/d
BIOoral	fraction absorbed by humans, set at 1	-/-
BW	human body weight	kg

Output

$Expsoil_{ingest}$	daily exposure from soil ingestion	$kg/kg_{bw}/d$

Amount of suspended particles indoor
RIVM 711701022p134
TSPw = TSPi = 0.75*TSPo
Input

TSPo	total dust concentration outdoor air	$kg_{dwt}/m3$

Output

TSPi	total dust concentration indoor air	$kg_{dwt}/m3$
TSPw	total dust concentration in work air	$kg_{dwt}/m3$

Soil fraction in particles in work air
self defined variable
frsw = frsi
Input

frsi	soil fraction in particles in indoor air	-/-

Output

frsw	soil fraction in particles in work air	-/-

Amount of inhaled soil (particles)
Based on RIVM 711701022p133
ITSP = (IHinh/24)*(Toutd*TSPo*frso + Tind*TSPi*frsi + Twork*TSPi*frsw
Input

IHinh	adult breathing volume	m3/d
Tind	weekly average of time spend indoor	hours/day
Toutd	weekly average of time spend outdoor	hours/day
Twork	weekly average of time spend at work	hours/day
	See exposure from air for calculation of weekly averages	
TSPo	total dust concentration outdoor air	$kg_{dwt}/m3$
TSPi	total dust concentration indoor air	$kg_{dwt}/m3$
TSPw	total dust concentration in work air	$kg_{dwt}/m3$
frso	soil fraction in particles in outdoor air	-/-
frsi	soil fraction in particles in indoor air	-/-
frsw	soil fraction in particles in work air	-/-

Output

ITSP	amount of inhaled soil particles	kg_{dwt}/d

Exposure from soil inhalation

$Expsoil_{inhl}$ = ITSP*CONVsoil*fr*$CSOIL_{wwt}$/BW
Input

ITSP	amount of inhaled soil particles	kg_{dwt}/d
CONVsoil	wwt dry weight conversion for soil	kg_{wwt}/kg_{dwt}
Fr	retention fraction of particles in the lung	-/-
BW	human body weight	kg
$CSOIL_{wwt}$	concentration in wwt soil	kg/kg_{wwt}

Output

$Expsoil_{inhl}$	exposure from inhaling dust/soil particles	$kg/kg_{bw}/d$

Dermal contact with soil and dust

Self defined variables for dermal exposure at work

Aexpaw = Aexpai
DAEaw = DEAai
frsw = frsi

Input

Aexpai	exposed surface area indoor	m2
DEAai	degree of coverage indoor	$kg_{soil}/m2_{skin}$
frsi	fraction soil in dust indoor	-/-

Output

Aexpaw	exposed surface area at work	m2
DEAaw	degree of coverage at work	$kg_{soil}/m2_{skin}$
frsw	fraction soil in dust at work	-/-

Total Daily Soil Contact

Based on RIVM 711701022p133

TDSC = Toutd*Aexpao*DAEao*1 + Tind*Aexpai*DAEai*frsi +
Twork*Aexpaw*DAEaw*frsw

Input

Toutd	weekly average of time spend outdoor	h/day
Aexpao	exposed surface area outdoor	m2
DAEao	degree of coverage outdoor	$kg_{soil}/m2_{skin}$
1	fraction soil in dust outdoor	-/-
Tind	weekly average of time spend indoor	h/day
Aexpai	exposed surface area indoor	m2
DEAai	degree of coverage indoor	$kg_{soil}/m2_{skin}$
frsi	fraction soil in dust indoor	-/-
Twork	weekly average of time spend at work	h/day
	See exposure from air for calculation of weekly averages	
Aexpaw	exposed surface area at work	m2
DEAaw	degree of coverage at work	$kg_{soil}/m2_{skin}$
frsw	fraction soil in dust at work	-/-

Output

TDSC	total daily soil (dwt) contact	kg_{dwt}/d

Exposure from dermal contact with soil (in dust)

Based on RIVM 711701022p133

$Expsoil_{derm}$ = TDSC*CONVsoil*fm*DARw/BW

Input

TDSC	total daily soil (dwt) contact	kg_{dwt}/d
CONVsoil	wwt dry weight conversion for soil	kg_{wwt}/kg_{dwt}
Fm	matrix factor	-/-
DARw	adult dermal absorption velocity	h^{-1}
BW	human body weight	kg

Output

$Expsoil_{derm}$	daily exposure from dermal contact with soil	$kg/kg_{bw}/d$

Total exposure form soil (in dust)

Self defined variable

$Expsoil = Expsoil_{ingest} + Expsoil_{inhl} + Expsoil_{derm}$

Input

$Expsoil_{ingest}$	daily exposure from soil ingestion	$kg/kg_{bw}/d$
$Expsoil_{inhl}$	exposure from inhaling dust/soil particles	$kg/kg_{bw}/d$
$Expsoil_{derm}$	daily exposure from dermal contact with soil	$kg/kg_{bw}/d$

Output

Expsoil	total daily exposure from soil (in dust)	$kg/kg_{bw}/d$

Total exposure for humans

Self defined variable

Exptot = Expfish + Expair + Exproot +Expleaf + Expdrw + Expmeat +Expmilk + Expshw + Expsoil

Input

Expfish	daily exposure from fish consumption	$kg/kg_{bw}/d$
Expair	daily exposure from air	$kg/kg_{bw}/d$
Exproot	daily exposure form root products	$kg/kg_{bw}/d$
Expleaf	daily exposure from leaf products	$kg/kg_{bw}/d$
Expdrw	daily exposure from drinking water	$kg/kg_{bw}/d$
Expmeat	daily exposure form meat consumption	$kg/kg_{bw}/d$
Expmilk	daily exposure form milk consumption	$kg/kg_{bw}/d$
Exshw	total daily exposure while showering	$kg/kg_{bw}/d$
Expsoil	total daily exposure from soil (in dust)	$kg/kg_{bw}/d$

Output

Exptot	total daily exposure of humans to a contaminant kg contaminant per kg body weight per day	$kg/kg_{bw}/d$

Appendix IV: Results of sensitivity analysis

The PECreg are sensitive but have been left out of the overviews. The predicted environmental concentrations consumption rates of food, air, water and soil are always sensitive as are if these routes are percentile imparted

Bis-pentabromophenyl ether

			primair	secon dair	tert	quart	source	source	source	source
	% contribution to exposure		30.8	30.7	20.4	12.7	12.7	21.2	1.2	64.9
type of parameter	***parameter name***	**total**	meat	milk	root	fish	surf water	pore water	air	soil
bis(pentabromophenyl)ether	*K_{ow}*	0.26	0.42	0.41		0.12	0.12		0.14	0.41
Intake Cow	*dwtsoil*	0.15	0.33	0.33						0.34
Intake Human	*BW*	-0.28	-0.41	-0.41		-0.53	-0.53			-0.44
Intake Human	*fish*					0.54	0.54			
Intake Human	*meat*		0.41							0.21
Intake Human	*milk*			0.41						0.20
plant	*b*								0.92	
root	*b*	0.78			0.93			0.93		
soil	*Fair*		-0.13	-0.13						-0.14
soil	*Fwater*		-0.12	-0.12						-0.13
soil	*RHOsolid*	0.16	0.33	0.33						0.36

Sensitive parameters which are important for the main routes of exposure

bis(pentabromophenyl)ether	*K_{ow}*
Intake Human	*BW*
Intake Human	*fish*
Intake Human	*meat*
Intake Human	*milk*
root	*b*

Butanol

			primair	secon dair	tert	source	source	source	source
	% contribution to exposure		56.8	38.46		59.4	0.8	39.7	0.0
type of parameter	***parameter name***	**total**	air	drw		surf. water	pore water	air	soil
1-butanol	*MOLW*								0.21
1-butanol	*SOL*								-0.22
1-butanol	*VP*								0.21
Intake Human	*air*	0.27		**0.59**				**0.58**	0.20
Intake Human	*BW*	**-0.71**	**-0.58**	**-0.60**		**-0.59**	**-0.51**	**-0.60**	-0.21
Intake Human	*drw*	**0.41**	**0.59**			**0.58**			
Intake Human	*root*						**0.50**		
Phys. Cons.	*R gas concstant*								-0.21
Phys. Cons.	*TEMPsoil*								-0.22
root	*density*						**-0.49**		
soil	*K_{oc}*								-0.22
soil	*RHOsolid*								0.17

sensitive parameters which are important for the main routes of exposure

Intake Human	*air*
Intake Human	*BW*
Intake Human	*drw*

Butyl acetate

type of parameter	parameter name	total	primair	secondair	tert	source	source	source	source
	% contribution to exposure		88.3	9.1		11.5	0.0	88.4	0.0
			air	drw		surf water	pore water	air	soil
1-butylaceteate	*MOLW*					-0.11			
Intake Human	*air*	0.54	0.57					0.56	
Intake Human	*BW*	-0.61	-0.57	-0.60		-0.61	-0.51	-0.57	-0.45
Intake Human	*drw*			0.60		0.49			
Intake Human	*leaf*								0.38
Intake Human	*root*						0.45		
Phys. Cons.	*TEMPenv*					-0.12			
Phys. Cons.	*TEMPshower*					0.12			
plant	*dep. cons.*								0.37
plant	*FDWS*								0.38
root	*b*						0.21		
root	*density*						-0.46		
soil	*Fair*								-0.15
soil	*Fwater*								-0.13

sensitive parameters which are important for the main routes of exposure

Intake Human	*air*
Intake Human	*BW*
Intake Human	*drw*

Cyclohexylamine

type of parameter	parameter name	totaal	primair	secondair	tert	source	source	source	source
	% contribution to exposure		85.8	6.8	5.2	94.3	0.2	5.4	0.0
			Drinking water	Shower	air	surf water	pore water	air	soil
cyclohexylamine	*K_{ow}*			0.19					
cyclohexylamine	*MOLW*			-0.36					
dermal	*Atota*			0.20					
Intake Human	*air*				0.59			0.57	
Intake Human	*BIOinh*			0.11					
Intake Human	*BW*	-0.62	-0.58	-0.30	-0.59	-0.59	-0.54	-0.60	-0.44
Intake Human	*drw*	0.53	0.58			0.54			
Intake Human	*leaf*								0.37
Intake Human	*root*						0.48		
Phys. Cons.	*TEMPenv*			-0.49					
Phys. Cons.	*TEMPshower*			0.47					
plant	*dep. cons.*								0.37
plant	*FDWS*								0.37
root	*b*						0.11		
root	*density*						-0.48		
shower	*fexp*			0.21					
shower	*td*			0.10					
shower	*tdc*			0.22					
soil	*Fair*								-0.14
soil	*Fwater*								-0.13
soil	*RHOsolid*								0.35

sensitive parameters which are important for the main routes of exposure

Intake Human	*BW*
Intake Human	*drw*
Phys. Cons.	*TEMPenv*
Phys. Cons.	*TEMPshower*

Diethylene Glycol

type of parameter	parameter name	Total	primair	secondair	tert	source	source	source	source
	% contribution to exposure		61.0	35.6		61.2	5.8	32.9	0.0
			Drw	leaf		surf water	pore water	air	soil
diethylene glycol	*Henry*	-0.10		-0.18			-0.12	-0.17	
Intake Human	*BW*	-0.66	-0.58	-0.41		-0.58	-0.49	-0.40	-0.43
Intake Human	*drw*	0.40	0.57			0.57			
Intake Human	*leaf*	0.23		0.41			0.28	0.40	0.37
Intake Human	*root*						0.21		
Phys. Cons.	*R gas concstant*			0.18			0.12	0.17	
Phys. Cons.	*TEMPenv*	0.10		0.18			0.11	0.18	
plant	*AREA*	0.12		0.21			-0.12	0.23	
plant	*density*	-0.23		-0.41			-0.28	-0.40	
plant	*dep. cons.*								0.36
plant	*FDWS*								0.36
plant	*Fwater*	0.10		0.18			0.12	0.18	
plant	*g*	0.11		0.20			-0.11	0.23	
plant	*k growht*	-0.13		-0.23			-0.16	-0.22	
plant	*Qtransport*						0.27		
plant	*Vleaf*	-0.13		-0.24			-0.16	-0.23	
root	*density*						-0.20		
soil	*Fair*								-0.14
soil	*Fwater*								-0.13
soil	*RHOsolid*								0.35

sensitive parameters which are important for the main routes of exposure

Intake Human	*BW*
plant	*density*

Ethylacetate

type of parameter	parameter name	total	primair	secondair	tert	source	source	source	source
	% contribution to exposure		84.1	13.4		15.8	0.0	84.2	0.0
			air	drw		surf. water	pore water	air	soil
ethylacetate	*MOLW*								0.22
ethylacetate	*SOL*								-0.19
ethylacetate	*VP*								0.22
Intake Human	*air*	**0.53**	**0.57**					**0.57**	0.22
Intake Human	*BW*	**-0.63**	**-0.57**	**-0.59**		**-0.60**	**-0.51**	**-0.57**	-0.21
Intake Human	*drw*			**0.59**		**0.59**			
Intake Human	*root*						**0.49**		
Phys. Cons.	*R gas concstant*								-0.20
Phys. Cons.	*TEMPsoil*								-0.21
root	*density*						**-0.49**		
root	*FDWR*						-0.10		
soil	*K_{oc}*								-0.22
soil	*RHOsolid*								0.17

sensitive parameters which are important for the main routes of exposure

Intake Human	*air*
Intake Human	*BW*
Intake Human	*drw*

Ethylene Glycol

			primair	secondair	tert	source	source	source	source
	% contribution to exposure		98.3			99.1	0.6	0.3	0.0
type of parameter	***parameter name***	**totaal**	drw			surf water	pore water	air	soil
ethylene glycol	*Henry*							-0.33	
Intake Human	*air*							0.12	
Intake Human	*BW*	-0.58	-0.58			-0.58	-0.55	-0.46	-0.44
Intake Human	*drw*	0.57	0.58			0.57			
Intake Human	*leaf*							0.32	0.37
Intake Human	*root*						0.47		
Phys. Cons.	*R gas concstant*							0.32	
Phys. Cons.	*TEMPenv*							0.33	
plant	*density*							-0.34	
plant	*dep. cons.*								0.37
plant	*FDWS*								0.38
plant	*Fwater*							0.32	
root	*density*						-0.46		
soil	*Fair*								-0.14
soil	*Fwater*								-0.13
soil	*RHOsolid*								0.35

sensitive parameters which are important for the main routes of exposure

Intake Human	*BW*
Intake Human	*drw*

Hexachlorobutadiene

			primair	secondair	tert	source	source	source	source
	% contribution to exposure		81.4	11.7	4.4	87.4	1.7	10.9	0.0
type of parameter	***parameter name***	**total**	fish	air	shower	surf water	pore water	air	soil
hexachlorobutadiene	*K_{ow}*	0.41	0.44			0.43			0.16
hexachlorobutadiene	*MOLW*				-0.83	-0.11			
dermal	*Atota*				0.22				
Intake Cow	*dwtsoil*								0.14
Intake Human	*BW*	-0.57	-0.52	-0.58	-0.22	-0.53	-0.11	-0.58	-0.51
Intake Human	*fish*	0.47	0.52			0.50			
Intake Human	*air*			0.58				0.56	
Intake Human	*leaf*								0.30
Intake Human	*root*						0.12		
plant	*b*							0.12	
plant	*FDWS*								0.32
plant	*dep. cons.*								0.33
root	*b*						0.92		
root	*density*						-0.12		
root	*Flipid*						0.12		
shower	*tdc*				0.20				
shower	*fexp*				0.20				
soil	*Fwater*								-0.14
soil	*Fair*								-0.17
soil	*RHOsolid*								0.41
soil	*RHOwater*								0.10

sensitive parameters which are important for the main routes of exposure

hexachlorobutadiene	*K_{ow}*
Intake Human	*BW*
Intake Human	*fish*
Intake Human	*air*

Ibuprofen

Ibuprofen			primair	secondair	tert	source	source	source	source
	% contribution to exposure		39.1	37.5	21.4	98.0	1.7	0.3	0.0
type of parameter	***parameter name***	**totaal**	fish	shower	drw	surf water	pore water	air	soil
dermal	*Atota*	0.18		0.25		0.18			
Ibuprofen	*K_{ow}*	0.30	0.45	0.20		0.30	0.14		
Ibuprofen	*MOLW*	-0.57		-0.79		-0.57		-0.11	
Ibuprofen	*SOL*							0.12	
Ibuprofen	*VP*							-0.11	
Intake Human	*BW*	-0.45	-0.53	-0.23	-0.59	-0.44	-0.21	-0.14	-0.46
Intake Human	*drw*				0.60				
Intake Human	*fish*	0.17	0.52			0.17			
Intake Human	*leaf*							0.13	0.37
Intake Human	*root*						0.11		
Phys. Cons.	*R gas concstant*							0.11	
Phys. Cons.	*TEMPenv*							0.12	
plant	*b*						0.46	0.90	
plant	*density*							-0.14	
plant	*dep. cons.*								0.37
plant	*FDWS*								0.37
plant	*Flipid*							0.10	
root	*b*						0.74		
root	*density*						-0.12		
root	*Flipid*						0.11		
shower	*fexp*	0.17		0.24		0.17			
shower	*tdc*	0.17		0.24		0.17			
soil	*Fair*								-0.14
soil	*Fwater*								-0.13
soil	*RHOsolid*								0.37

sensitive parameters which are important for the main routes of exposure

Intake Human	*BW*
Intake Human	*drw*
Ibuprofen	*K_{ow}*
Ibuprofen	*MOLW*

Ivermectin

			Primair	Secondair	Tert	Source	Source	Source	Source
	% contribution to exposure		46.9	15.7	13.4	134	86.5	0.0	0.2
Type of parameter	***Parameter name***	**Total**	Root	Drinking water	Fish	Surf water	Pore water	Air	Soil
Ivermectin	*K_{ow}*				**0.45**	**0.45**			0.17
Intake Cow	*Dwtsoil*								0.14
Intake Human	*BW*	-0.13	-0.11	**-0.59**	**-0.53**	**-0.53**	-0.12		**-0.50**
Intake Human	*Drw*			**0.59**					
Intake Human	*Fish*				**0.54**	**0.54**			
Intake Human	*Leaf*								0.22
Intake Human	*Root*	0.12	0.12				0.12		
Plant	*dep. cons.*								0.24
Plant	*FDWS*								0.25
Root	*b*	**0.92**	**0.92**				**0.92**		
Root	*Density*	-0.11	-0.11				-0.11		
Root	*Flipid*	0.11	0.12				0.12		
Soil	*Fair*								-0.16
Soil	*Fwater*								-0.14
Soil	*RHOsolid*								**0.40**

sensitive parameters which are important for the main routes of exposure

Intake Human	*BW*	-0.13	-0.11
Intake Human	*root*	0.12	0.12
root	*b*	**0.92**	**0.92**
root	*density*	-0.11	-0.11
root	*Flipid*	0.11	0.12

Methylethylketone

			primair	secondair	tert	source	source	source	source
	% contribution to exposure		86.9	11.3		12.5	0.1	87.4	0.0
type of parameter	***parameter name***	**total**	air	drw		surf. water	pore water	air	soil
methylethylketone	*MOLW*								0.23
methylethylketone	*SOL*								-0.24
methylethylketone	*VP*								0.23
Intake Human	*air*	**0.56**	**0.59**					**0.59**	0.24
Intake Human	*BW*	**-0.64**	**-0.59**	**-0.57**		**-0.57**	**-0.51**	**-0.59**	-0.23
Intake Human	*drw*			**0.57**		**0.56**			
Intake Human	*root*						**0.49**		
Phys. Cons.	*R gas concstant*								-0.24
Phys. Cons.	*TEMPsoil*								-0.22
root	*density*						**-0.49**		
soil	*K_{oc}*								-0.24
soil	*RHOsolid*								0.18

sensitive parameters which are important for the main routes of exposure

Intake Human	*air*
Intake Human	*BW*
Intake Human	*drw*

Methanol

			Primair	Secondair	Tert	Source	Source	Source	Source
	% contribution to exposure		85.5	7.6	6.6	7.8	0.1	92.2	0.0
Type of parameter	***Parameter name***	**Total**	Air	Drw	Leaf	surf. water	Pore water	Air	Soil
Methanol	*Henry*				-0.35				
Methanol	*MOLW*								0.17
Methanol	*SOL*								-0.15
Methanol	*VP*								0.16
Intake Human	*Air*	**0.53**	**0.58**					**0.55**	0.23
Intake Human	*BW*	**-0.62**	**-0.58**	**-0.58**	-0.34	**-0.58**	**-0.51**	**-0.59**	-0.24
Intake Human	*Drw*			**0.58**		**0.58**			
Intake Human	*Leaf*				0.35				
Intake Human	*Root*						**0.49**		
Phys. Cons.	*R gas concstant*				0.34				-0.16
Phys. Cons.	*TEMPenv*				0.35				
Phys. Cons.	*TEMPsoil*								-0.14
Plant	*Density*				-0.35				
Plant	*Fwater*				0.34				
Root	*Density*						**-0.50**		
Soil	*Fair*								-0.13
Soil	*Fwater*								-0.22

Soil	*RHOsolid*				0.18

Sensitive parameters which are important for the main routes of exposure

Intake Human	*Air*
Intake Human	*BW*
Intake Human	*Drw*

Methyl *tert*-butyl ether

			Primair	Secondair	Tert	Source	Source	Source	Source
	% contribution to exposure		82.7	13.7		17.3	0.0	82.7	0.0
Type of parameter	***Parameter name***	**Total**	Air	Drw		Surf. water	Pore water	Air	Soil
Methyl-tert-butyl-ether	*MOLW*								0.20
Methyl-tert-butyl-ether	*SOL*								-0.21
Methyl-tert-butyl-ether	*VP*								0.20
Intake Human	*air*	**0.53**	**0.56**					**0.56**	0.24
Intake Human	*BW*	**-0.62**	**-0.56**	**-0.59**		**-0.60**	**-0.48**	**-0.56**	-0.22
Intake Human	*drw*			**0.59**		**0.58**			
Intake Human	*root*						**0.46**		
Phys. Cons.	*R gas concstant*								-0.21
Phys. Cons.	*TEMPsoil*								-0.23
Root	*density*						**-0.46**		
Soil	*K_{oc}*								-0.21
Soil	*RHOsolid*								0.18

Sensitive parameters which are important for the main routes of exposure

Intake Human	*Air*
Intake Human	*BW*
Intake Human	*Drw*

Pentabromodiphenylether

			primair	secon dair	tetr	quart	source	source	source	source
	% contribution to exposure		34.6	22.4	22.3	16.5	16.5	35.7	10.8	36.9
type of parameter	***parameter name***	**totaal**	root	meat	milk	fish	surf water	pore water	air	soil
pentabromediphenylether	*TEMPmelt*								0.11	
Intake Cow	*CONVgrass*			0.12	0.12					
Intake Cow	*dwtgrass*			0.14	0.14				0.11	
Intake Cow	*dwtsoil*			0.23	0.22					0.38
Intake Human	*BW*	-0.22	-0.10	-0.36	-0.36	-0.56	-0.56	-0.10	-0.11	-0.47
Intake Human	*fish*					0.55	0.55			
Intake Human	*meat*			0.37						0.23
Intake Human	*milk*				0.35					0.23
Intake Human	*root*		0.10					0.10		
plant	*b*	0.21		0.60	0.61				0.92	
plant	*density*								-0.10	
root	*b*	0.87	0.93					0.93		
soil	*Fair*									-0.15
soil	*Fwater*									-0.14
soil	*RHOsolid*			0.21	0.21					0.38

sensitive parameters which are important for the main routes of exposure

root	*b*
plant	*b*
Intake Human	*BW*
Intake Human	*fish*

Tetrahydrothiophene

Type of parameter	Parameter name	Total	Primair	Secondair	Tert	Source	Source	Source	Source
	% contribution to exposure		93.0	5.1		6.9	0.0	93.0	0.0
Type of parameter	***Parameter name***	**Total**	Air	Drw		Surf. water	Pore water	Air	Soil
Tetrahydrothiophene	*MOLW*								0.22
Tetrahydrothiophene	*SOL*								-0.22
Tetrahydrothiophene	*VP*								0.22
Intake Human	*Air*	**0.56**	**0.57**					**0.57**	0.22
Intake Human	*BW*	**-0.59**	**-0.57**	**-0.59**		**-0.60**	**-0.49**	**-0.57**	-0.22
Intake Human	*Drw*			**0.59**		**0.57**			
Intake Human	*Root*						**0.47**		
Phys. Cons.	*R gas concstant*								-0.23
Phys. Cons.	*TEMPsoil*								-0.23
Root	*B*						0.23		
Root	*Density*						**-0.48**		
Soil	*K_{oc}*								-0.23
Soil	*RHOsolid*								0.19

Sensitive parameters which are important for the main routes of exposure

Intake Human	*Air*
Intake Human	*BW*
Intake Human	*Drw*

Tribromomethane

Type of parameter	Parameter name	Total	Primair	Secondair	Tert	Source	Source	Source	Source
	% contribution to exposure		78.1	17.1		21.0	0	78.5	0.5
Type of parameter	***Parameter name***	**Total**	Air	Drw		Surf. water	Pore water	Air	Soil
Tribromomethane	*K_{ow}*						0.12		
Tribromomethane	*MOLW*								0.21
Tribromomethane	*SOL*								-0.21
Tribromomethane	*VP*								0.20
Intake Human	*Air*	**0.54**	**0.60**					**0.60**	0.22
Intake Human	*BW*	**-0.68**	**-0.60**	**-0.59**		**-0.60**	-0.38	-0.61	-0.22
Intake Human	*Drw*	0.12		**0.58**		**0.53**			
Intake Human	*Root*						0.37		
Phys. Cons.	*R gas concstant*								-0.22
Phys. Cons.	*TEMPsoil*								-0.21
Root	*B*						**0.56**		
Root	*Density*						-0.38		
Root	*Flipid*						0.13		
Soil	*K_{oc}*								-0.20
Soil	*RHOsolid*								0.18

Sensitive parameters which are important for the main routes of exposure

Intake Human	*Air*
Intake Human	*BW*
Intake Human	*Drw*

Triethanolamine

			primair	secondair	tert	source	source	source	source
	% contribution to exposure		94.4	4.3		99.4	0.6	0.0	0.0
type of parameter	***parameter name***	**total**	drw	shower		surf water	pore water	air	soil
Intake Human	*air*			0.13				0.55	
Intake Human	*BIOinh*			0.14					
Intake Human	*BW*	-0.57	-0.57	-0.14		-0.57	-0.48	-0.57	-0.42
Intake Human	*drw*	0.53	0.56			0.53			
Intake Human	*leaf*								0.36
Intake Human	*root*						0.42		
Phys. Cons.	*TEMPenv*	-0.12		-0.62		-0.12			
Phys. Cons.	*TEMPshower*	0.12		0.59		0.12			
plant	*dep. cons.*								0.36
plant	*FDWS*								0.36
root	*density*						-0.42		
shower	*r*			-0.12					
shower	*td*			0.14					
shower	*tf*			0.13					
shower	*Vbk*			-0.12					
shower	*Vwb*			0.13					
soil	*Fair*								-0.14
soil	*Fwater*								-0.12
soil	*RHOsolid*								0.35

sensitive parameters which are important for the main routes of exposure

Intake Human	*BW*
Intake Human	*drw*
PECreg	*water*
Phys. Cons.	*TEMPenv*
Phys. Cons.	*TEMPshower*

Appendix V: Correlation data

(First half of table)

Compound	CAS	MW	log K_{ow}	log K_{oc}	SOL (mg/L)	log SOL	T. Melt C.	T. Boil C.	log VP	log Henry
triethanolamine	102-71-6	149.19	-1.00	1.00	1120000	6.0	83.32		-3.15	0.63
diethylene glycol	111-46-6	106.12	-1.47	-1.86	1118000	6.0	9	245	0.40	-3.70
ethylene glycol	107-21-1	62.07	-1.36	-1.75	1113000	6.0	-31.62	197	0.90	-1.89
methanol	67-56-1	32.04	-0.77	-1.16	793000	5.9	-101	650	4.72	-0.37
tribromomethane	75-25-2	252.73	2.4	1.55	204	2.3	-11.87	158	2.50	1.06
tetrahydriothiophene	110-01-1	88.17	1.79	1.95	3730	3.6	-48.82	84	3.59	1.79
1-butylacetate	123-86-4	116.16	1.78	1.32	3128	3.5	-56.83	125	3.21	1.62
1-butanol	71-36-3	74.12	0.88	0.39	76700	4.9	-62.33	117	3.11	0.00
methyl-tert-butyl ether	1634-04-4	88.15	0.94	0.72	19800	4.3	-94.3	55	4.66	2.31
methylethylketone	78-93-3	72.11	0.29	0.58	76100	4.9	-80.48	80	4.27	0.82
cyclohexylamine	108-91-8	99.18	1.49	1.61	63960	4.8	-27.11	134	2.83	0.15
ethylacetate	141-78-6	88.11	0.73	0.79	29930	4.5	-82.08	77	4.10	1.38
dodecylbenzene	123-01-3	246.44	8.65	5.37	0.001015	-3.0	60.83	331	-1.48	4.13
hexachlorobutadiene	87-68-3	260.76	4.78	3.00	1.71	0.2	-6.22	215	1.51	3.04
nonylphenol	84852-15-3	220.34	4.48	4.09	6	0.8	-8	295	-0.52	1.04
chloro-alkanene C12H20Cl6	85535-84-8	377	6	5.61	4.70E-04	-3.3	-30		-1.67	4.23
acrylaldehylde	107-02-8	56.06	-1.1	-1.49	208000	5.3	-87	53	4.47	0.90
cumene	98-82-8	120.19	3.55	3.16	50	1.7	-96	152	2.70	3.00
bis(pentabromophenyl) ether	1163-19-5	959.2	6.27	5.88	1.00E-04	-4.0	305		-5.33	1.65
ethyl acetoacetate	141-97-9	130.14	0.25	-0.14	1.25E+05	5.1	39	182	2.00	-0.98
Linear Alkylbenzenes	67774-74-7	241	9.12	4.34	0.014	-1.9	-70	296	1.11	1.98
Methacrylic Acid	79-41-4	86.09	0.93	0.54	89000	4.9	15	161	1.95	-1.06
pentaBrDiPhEther	32534-81-9	564.7	6.57	6.18	2.40E-03	-2.6	-5		-4.33	1.04
chlorocresol	1570-64-5	142.59	3.09	2.70	2300	3.4	50	231	1.43	0.22
methylene dianaline	101-77-9	198.3	1.59	1.20	1250	3.1	89	398	-5.54	-6.36
biphenylol	90-43-7	170.21	3.28	2.89	536	2.7	87	317	-2.09	-2.58
4-chloro-m-cresol	59-50-7	142.59	2.7	2.31	699	2.8	36	222	-1.40	-2.09
Ibuprofen	15687-27-1	206.29	3.79	3.40	41	1.6	94	323	-1.61	-0.90
Ivermectin	70288-86-7	350	4.95	4.56	1.40E-04	-3.9	350	943	-27.80	-21.40
Oxytetracycline	79-57-2	460.44	-2.87	-3.26	1.87E+05	5.3	344	782	5.27	2.66
Triclosan	3380-34-5	289.55	4.66	4.27	4.6	0.7	137	374	-3.23	-1.43

(Table continued)

compound	CAS	adj. PECreg-water (dissolved) mg/L	adj. PECreg- air mg/m3	adj. PECreg-agric.soil mg/kgwwt	adj. PECreg-agric.porew mg/L	drw	fish	leaf	root	meat	milk	air	soil ingestion	shower	soil inhalation	soil cont.act	surface water	pore water	air	soil
triethanolamine	102-71-6	3.30E+01	7.52E-07	4.03E-01	3.32E+00	94	1	0	1	0	0	0	0	4	0	0	99	1	0	0
diethylene glycol	111-46-6	2.13E+01	1.59E-02	1.86E+00	1.54E+01	61	0	36	2	0	0	0	0	0	0	0	61	6	33	0
ethylene glycol	107-21-1	3.44E+01	3.30E-03	3.79E-01	3.13E+00	98	1	0	0	0	0	0	0	0	0	0	99	1	0	0
methanol	67-56-1	2.65E+00	2.99E+00	4.93E-02	3.97E-01	8	0	7	0	0	0	86	0	0	0	0	8	0	92	0
tribromomethane	75-25-2	5.99E+00	2.72E+00	4.10E-01	1.96E-01	17	2	1	0	0	0	78	0	2	0	0	21	0	79	0
tetrahydriothiophene	110-01-1	1.80E+00	3.25E+00	6.58E-02	8.81E-02	5	0	0	0	0	0	93	0	2	0	0	7	0	93	0
butylacetate	123-86-4	3.17E+00	3.09E+00	1.68E-01	2.29E-01	9	0	0	0	0	0	88	0	2	0	0	12	0	88	0
butanol	71-36-3	1.98E+01	1.34E+00	1.07E+00	4.61E+00	57	0	1	1	0	0	38	0	2	0	0	59	1	40	0
methyl-tert-butyl ether	1634-04-4	9.59E+00	2.89E+00	1.43E-04	5.62E-02	14	0	0	0	0	0	83	0	3	0	0	17	0	83	0
methylethylketone	78-93-3	3.97E+00	3.04E+00	7.83E-02	5.01E-01	11	0	0	0	0	0	87	0	1	0	0	13	0	87	0
cyclohexylamine	108-91-8	3.00E+01	1.83E-01	6.22E-01	1.30E+00	86	2	0	0	0	0	5	0	7	0	0	94	0	5	0
ethylacetate	141-78-6	4.69E+00	2.94E+00	4.79E-02	2.33E-01	13	0	0	0	0	0	84	0	2	0	0	16	0	84	0
dodecylbenzene	123-01-3	5.53E-02	1.07E-02	1.06E+02	1.01E-02	0	9	2	78	5	5	1	0	0	0	0	9	78	11	2
hexachlorobutadiene	87-68-3	1.80E+00	3.00E-01	3.45E+01	2.08E-01	2	81	0	2	0	0	11	0	4	0	0	87	2	11	0
nonylphenol	84852-15-3	9.46E-01	4.95E-03	4.18E+02	4.42E+00	13	19	0	16	0	0	0	0	51	0	0	19	80	0	0
chloro-alkanene	85535-84-8	6.01E-05	2.18E-03	1.97E+03	1.22E+00	4	0	1	79	6	6	0	0	3	0	0	0	86	0	14
acrylaldehylde	107-02-8	1.54E-01	2.31E-01	1.54E-02	2.78E+01	80	0	0	4	0	0	7	0	9	0	0	0	93	7	0
cumene	98-82-8	1.50E-02	3.49E+00	1.35E-01	8.63E-03	0	0	0	0	0	0	100	0	0	0	0	0	0	100	0
bis-penta-bromo-phenyl-ether	1163-19-5	2.04E-02	1.16E-03	5.93E+03	2.13E-01	1	13	4	20	31	31	0	1	0	0	0	13	21	1	65
ethyl acetoacetate	141-97-9	3.06E+01	2.83E-01	1.38E+00	3.83E+00	88	1	3	1	0	0	8	0	0	0	0	89	1	11	0
linear alkyl benzenes	67774-74-7	1.78E-01	0.00E+00	1.65E+00	4.07E-03	0	14	0	85	0	0	0	0	1	0	0	15	85	0	0
methacrylic acid	79-41-4	3.36E+01	2.40E-02	7.20E-01	1.20E+00	96	1	0	0	0	0	1	0	2	0	0	99	0	1	0
penta-bromo-diphenyl-ether	32534-81-9	2.36E-02	4.25E-03	2.05E+03	2.08E-01	1	17	3	35	22	22	0	0	0	0	0	17	36	11	37
chlorocresol	1570-64-5	1.26E+01	8.77E-02	6.39E-02	9.00E+00	36	17	1	4	0	0	3	0	40	0	0	92	4	3	0
methylene dianaline	101-77-9	3.37E+01	1.55E-11	1.08E-07	7.74E-07	96	2	0	0	0	0	0	0	1	0	0	100	0	0	0
biphenylol	90-43-7	8.29E+00	2.05E-05	1.27E+03	6.99E+00	24	16	30	4	0	0	0	0	26	0	0	65	33	0	1
4-chloro-m-cresol	59-50-7	2.01E+01	8.52E-05	3.14E+01	2.45E+00	58	12	3	1	0	0	0	0	27	0	0	97	3	0	0
Ibuprofen	15687-27-1	7.48E+00	7.24E-04	6.61E-03	9.36E-01	21	39	1	1	0	0	0	0	38	0	0	98	2	0	0
Ivermectin	70288-86-7	2.65E-01	0.00E+00	1.25E+02	5.48E+00	16	13	10	47	1	1	0	0	13	0	0	13	86	0	0
Oxytetracycline	79-57-2	9.38E+00	1.51E-22	7.61E+00	4.16E+00	86	1	0	4	0	0	0	0	9	0	0	95	5	0	0
Triclosan	3380-34-5	2.54E+00	5.79E-05	5.77E+02	1.78E+00	5	73	4	9	0	0	0	0	9	0	0	73	26	0	1

Appendix VI: Correlation analysis results

	MW	log K_{ow}	log K_{oc}	log SOL	T. Melt C.	T. Boil C.	Log Vp	Log Henry	adj. PECreg-water (dissolved) mg/L	adj. PECreg- air mg/m3	adj. PECreg- agric.soil mg/kgwwt	adj. PECreg- agric.porew mg/L
MW	1											
log K_{ow}	0.50	1										
log K_{oc}	0.55	0.94	1									
log SOL	-0.71	-0.92	-0.90	1								
T. Melt C.	0.66	0.12	0.18	-0.36	1							
T. Boil C.	0.67	0.09	0.07	-0.37	0.79	1						
Log Vp	-0.41	-0.39	-0.49	0.59	-0.64	-0.63	1					
Log Henry	0.00	0.05	-0.01	0.11	-0.48	-0.59	0.83	1				
adj. PECreg-water (dissolved) mg/L	-0.35	-0.53	-0.49	0.59	0.00	-0.16	0.08	-0.18	1			
adj. PECreg- air mg/m3	-0.37	-0.25	-0.22	0.29	-0.53	-0.34	0.42	0.25	-0.30	1		
adj. PECreg- agric.soil mg/kgwwt	0.85	0.41	0.51	-0.56	0.39	0.15	-0.24	0.11	-0.28	-0.23	1	
adj. PECreg- agric.porew mg/L	-0.20	-0.36	-0.38	0.29	-0.01	-0.05	0.02	-0.17	0.03	-0.29	-0.12	1
drw	-0.30	-0.67	-0.65	0.64	0.12	-0.02	0.11	-0.18	0.88	-0.39	-0.30	0.36
fish	0.23	0.42	0.41	-0.36	0.22	0.14	-0.19	-0.01	-0.28	-0.32	0.07	-0.12
leaf	-0.01	-0.09	-0.09	0.06	0.16	0.19	-0.21	-0.34	0.03	-0.20	0.11	0.37
root	0.38	0.75	0.62	-0.77	0.13	0.32	-0.37	0.00	-0.42	-0.34	0.25	-0.13
meat	0.86	0.44	0.52	-0.59	0.33	0.16	-0.24	0.14	-0.28	-0.21	0.91	-0.16
milk	0.86	0.44	0.52	-0.58	0.33	0.16	-0.24	0.14	-0.28	-0.21	0.91	-0.16
air	-0.37	-0.24	-0.22	0.29	-0.53	-0.34	0.42	0.25	-0.31	1.00	-0.23	-0.29
soil ingest	0.85	0.41	0.51	-0.57	0.39	0.16	-0.24	0.12	-0.28	-0.24	**1.00**	-0.12
shower	-0.05	0.13	0.20	-0.06	0.18	0.14	-0.14	-0.13	-0.10	-0.33	-0.08	0.20
soil inhalation	0.85	0.41	0.51	-0.57	0.39	0.16	-0.24	0.12	-0.28	-0.24	**1.00**	-0.12
soil contact	0.85	0.41	0.51	-0.57	0.39	0.16	-0.24	0.12	-0.28	-0.24	**1.00**	-0.12
surface water	-0.15	-0.35	-0.32	0.41	0.29	0.08	0.02	-0.14	0.77	-0.53	-0.25	0.00
pore water	0.26	0.56	0.47	-0.63	0.13	0.29	-0.42	-0.15	-0.49	-0.40	0.19	0.34
air	-0.37	-0.26	-0.25	0.30	-0.54	-0.33	0.42	0.24	-0.30	0.99	-0.23	-0.25
soil	0.86	0.39	0.49	-0.55	0.34	0.12	-0.22	0.13	-0.26	-0.19	0.95	-0.15

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(Table continued)

	drw	fish	leaf	root	meat	milk	air	soil ingestion	shower	soil inhalation	soil contact	surface water	pore water	air	soil
drw	1														
fish	-0.34	1													
leaf	-0.01	-0.01	1												
root	-0.41	0.02	-0.04	1											
meat	-0.30	0.03	0.00	0.30	1										
milk	-0.30	0.03	0.00	0.30	1.00	1									
air	-0.40	-0.31	-0.20	-0.34	-0.21	-0.21	1								
soil ingestion	-0.30	0.07	0.11	0.27	0.91	0.91	-0.24	1							
shower	-0.05	0.28	0.06	-0.11	-0.19	-0.19	-0.33	-0.08	1						
soil inhalation	-0.30	0.07	0.11	0.27	0.91	0.91	-0.24	1	-0.08	1					
soil contact	-0.30	0.07	0.11	0.27	0.91	0.91	-0.24	1	-0.08	1	1				
surface water	0.70	0.26	0.04	-0.42	-0.28	-0.28	-0.53	-0.25	0.25	-0.25	-0.25	1			
pore water	-0.29	0.06	0.05	0.79	0.16	0.16	-0.40	0.20	0.18	0.20	0.20	-0.48	1		
air	-0.40	-0.33	-0.09	-0.33	-0.19	-0.19	0.99	-0.24	-0.37	-0.24	-0.24	-0.54	-0.41	1	
soil	-0.28	0.03	0.01	0.24	0.99	0.99	-0.19	0.95	-0.17	0.95	0.95	-0.26	0.12	-0.18	1

Appendix VII: Tolerable Daily Intakes and Tolerable Concentrations in Air

CAS	Compound	MTR		Reference:	Remark
		TDI[a]	TCA[b]		
75-25-2	Bromoform	20	100 (p)[c]	711701.004	
71-36-3	Butanol	125	550 (p)	715810.009	
123-86-4	Butylacetate	200 (p)	1000	715810.009	
108-91-8	Cyclohexylamine	11000	NA[d]	EU (1996)	miscible; basic
111-46-6	Diethylene glyol	400[e]	NA	715810.009	miscible
141-78-6	Ethyl acetate	900	4200 (p)	711701.004	
107-21-1	Ethylene glycol	400[e]	NA	715810.009	miscible
87-68-3	Hexachlorobutadiene	0.2	NA	WHO (1996)	
67-56-1	Methanol	500	1100	715810.009	miscible
1634-04-4	Methyl tert-butyl ether	300	800	MTBE-RAR (ECB, 2002)	
78-93-3	Methyl ethyl ketone	190 (p)	875	715810.009	
123-01-3	Dodecylbenzene	5	NA	715810.009	
102-71-6	Triethanolamine	12500[f]	5000[f]		miscible; basic
110-01-0	Tetrahydrothiophene	180 (p)	650	711701.025	

MTR = Maximum Tolerable Risk level
[a] TDI (Tolerable Daily Intake) in μg/kg bw/d
[b] TCA (Tolerable Concentration in Air) in $\mu g/m^3$
[c] p = provisional values
[d] NA = Not available
[e] Sum-TDI applicable for ethylene glycol and diethylene glycol
[f]Provisional data, from OECD SIDS (Triethanolamine)

References

ECB (2002). European Union Risk Assessment Report Tert-butyl methyl ether, Volume 19. Hansen, B. G., Munn, S. J., Pakalin, S., Musset, C., Luotamo, M., De Bruijn, J., Berthault, F., Vegro, S., Pellegrini, G., Allanou, R., and Scheer, S. eds. Luxemburg: Office for Official Publications of the European Communities. Report no. EUR 20417 EN. 282 pp.

EU (1996) Verslagen van het Wetenschapplijk Comite voor de Menselijke voeding (vijfendertigste reeks).

RIVM (1997) Herevaluatie MTRlucht van MTBE. Brief van W.H. Könemann aan H. Herremans d.d. 13 juni 1997 (briefnr. 1670/97 CSR HK/WM/pw).

WHO (1996) Guidelines for Drinking-Water Quality – Second edition volume 2.

Appendix VIII: Loadings of PCA

PCA was done with corrected input: all parameter values were divided by the average and expressed as a portion of the standard deviation.

Table VIII.1. Results of the Principal Components Analysis.

	MW	log K_{ow}	log Sol	T. Melt C.	log Vp
Standard deviation	1.772	1.054	0.767	0.363	0.157
Proportion of Variance	0.628	0.222	0.118	0.026	0.005
Cumulative Proportion	0.628	0.851	0.969	0.995	1.000

Table VIII.2. The loadings of the PCA.

	C_1 MW	C_2 log K_{ow}	C_3 log Sol	C_4 T. Melt C.	C_5 log Vp
MW	-0.469	0.123	-0.661	0.494	0.290
log K_{ow}	-0.430	-0.586		-0.456	0.508
log Sol	0.519	0.350			0.775
T. Melt C.	-0.382	0.658	-0.124	-0.628	-0.110
log Vp	0.424	-0.295	-0.736	-0.384	-0.213

The components molecular weight and log K_{ow} explain 85% of the total variance.

Appendix IX: Relative importance of the routes of exposure per substance

nr	CAS	substance	drw	fish	leaf	root	meat	milk	air	soil ingest	shower	soil inh.	soil cont.	surf w.	pore w.	air	soil	substance	nr
1	102-71-6	triethanolamine	94	1	0	1	0	0	0	0	4	0	0	99	1	0	0	triethanolamine	1
2	111-46-6	diethylene glycerol	61	0	36	2	0	0	0	0	0	0	0	61	6	33	0	diethylene glycerol	2
3	107-21-1	ethylene glycol	98	1	0	0	0	0	0	0	0	0	0	99	1	0	0	ethylene glycol	3
4	67-56-1	methanol	8	0	7	0	0	0	86	0	0	0	0	8	0	92	0	methanol	4
5	75-25-2	tribromomethane	17	2	1	0	0	0	78	0	2	0	0	21	0	79	0	tribromomethane	5
6	110-01-1	tetrahydriothiophene	5	0	0	0	0	0	93	0	2	0	0	7	0	93	0	tetrahydriothiophene	6
7	123-86-4	butylacetate	9	0	0	0	0	0	88	0	2	0	0	12	0	88	0	butylacetate	7
8	71-36-3	butanol	57	0	1	1	0	0	38	0	2	0	0	59	1	40	0	butanol	8
9	1634-04-4	methyl-tert-butyl ether	14	0	0	0	0	0	83	0	3	0	0	17	0	83	0	methyl-tert-butyl ether	9
10	78-93-3	methylethylketone	11	0	0	0	0	0	87	0	1	0	0	13	0	87	0	methylethylketone	10
11	108-91-8	cyclohexylamine	86	2	0	0	0	0	5	0	7	0	0	94	0	5	0	cyclohexylamine	11
12	141-78-6	ethylacetate	13	0	0	0	0	0	84	0	2	0	0	16	0	84	0	ethylacetate	12
13	123-01-3	dodecylbenzene	0	9	2	78	5	5	1	0	0	0	0	9	78	11	2	dodecylbenzene	13
14	87-68-3	hexachlorobutadiene	2	81	0	2	0	0	11	0	4	0	0	87	2	11	0	hexachlorobutadiene	14
15	84852-15-3	nonylphenol	13	19	0	16	0	0	0	0	51	0	0	19	80	0	0	nonylphenol	15
16	85535-84-8	chloro-alkanene	4	0	1	79	6	6	0	0	3	0	0	0	86	0	14	chloro-alkanene	16
17	107-02-8	acrylaldehylde	80	0	0	4	0	0	7	0	9	0	0	0	93	7	0	acrylaldehylde	17
18	98-82-8	cumene	0	0	0	0	0	0	100	0	0	0	0	0	0	100	0	cumene	18
19	1163-19-5	bis-pentabromophenyl-ether	1	13	4	20	31	31	0	1	0	0	0	13	21	1	65	bis-pentabromophenyl-ether	19
20	141-97-9	ethyl acetoacetate	88	1	3	1	0	0	8	0	0	0	0	89	1	11	0	ethyl acetoacetate	20
21	67774-74-7	linear alkylbenzenes	0	14	0	85	0	0	0	0	1	0	0	15	85	0	0	linear alkylbenzenes	21
22	79-41-4	methacrylic acid	96	1	0	0	0	0	1	0	2	0	0	99	0	1	0	methacrylic acid	22
23	32534-81-9	pentabromodiphenylether	1	17	3	35	22	22	0	0	0	0	0	17	36	11	37	pentabromodiphenylether	23
24	1570-64-5	chlorocresol	36	17	1	4	0	0	3	0	40	0	0	92	4	3	0	chlorocresol	24
25	101-77-9	methylene dianaline	96	2	0	0	0	0	0	0	1	0	0	100	0	0	0	methylene dianaline	25
26	90-43-7	biphenylol	24	16	30	4	0	0	0	0	26	0	0	65	33	0	1	biphenylol	26
27	59-50-7	4-chloro-m-cresol	58	12	3	1	0	0	0	0	27	0	0	97	3	0	0	4-chloro-m-cresol	27
28	15687-27-1	Ibuprofen	21	39	1	1	0	0	0	0	38	0	0	98	2	0	0	Ibuprofen	28
29	70288-86-7	Ivermectin	16	13	10	47	1	1	0	0	13	0	0	13	86	0	0	Ivermectin	29
30	79-57-2	Oxytetracycline	86	1	0	4	0	0	0	0	9	0	0	95	5	0	0	Oxytetracycline	30
31	3380-34-5	Triclosan	5	73	4	9	0	0	0	0	9	0	0	73	26	0	1	Triclosan	31

All exposure of more than 17 % is shaded.

Compound groups and group characteristics (see paragraph 6.5)

Group	Source Compartment	Substances	Characteristics
1	Surface water	1, 3, 11, 14, 20, 22, 24, 25, 27, 28, 30	High Sol
2	Surface and pore water	15, 26, 31	None
3	Surface water and air	2, 5, 8	High Sol
4	Air	4, 6, 7, 9, 10, 12, 18	High Vp and low Sol
5	Pore water	13, 17, 21, 29	High K_{ow} and low Vp
6	Pore water and soil	16, 19, 23	High K_{ow}, high MW and low Vp

MW = molecular weight, Sol = solubility, Vp = vapour pressure