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Variation in calculated human exposure
Comparison of calculations with seven European human exposure models

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This investigation has been performed for the account of the Ministry of Housing, Spatial Planning and the Environment of the Netherlands, Directorate General for the Environment (DGM), Directorate of Soil, Water and Rural Areas (BWL), within the framework of project 711701, Risk in relation to Soil Quality. This investigation was initiated by the concerted action CLARINET (Contaminated Land Rehabilitation Network), Working Group Human Health.

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Abstract

Twenty scenarios, differing with respect to land use, soil type and contaminant, formed the basis for calculating human exposure from soil contaminants with the use of models contributed by seven European countries (one model per country). Here, the human exposures to children and children calculated by each of the models are compared. All calculations were performed twice: once with a prescribed set of parameters and once with the default data used in the different countries. Exposure via the three major exposure pathways of soil ingestion, crop consumption and indoor air inhalation was calculated in each case. Relevant concentrations in contact media and the soil compartments were also calculated. Evaluation of variations in the calculated exposure for each major exposure pathway, and factors affecting the variation, have led to the following main conclusions:

- The variation in calculated exposure is large for exposure via indoor air inhalation, substantial for exposure via crop consumption and limited for exposure via soil ingestion.
- The variation in calculated exposure is mainly influenced by the choice of exposure model and, to a lesser extent, by the selection of contaminant and type of input parameter (standardised or default). The variation in calculated exposure is scarcely dependent on soil use and even less on soil type.
- Miscommunication is a source (difficult to avoid) for variation in calculated exposure.

Besides the above, characteristics of human exposure models and default values for the input parameters used in different countries have also been overviewed. One recommendation for the long term would be to construct a toolbox for use in the whole or part of Europe that would allow standardised assessment of human exposure, with the possibility of including flexible (country-specific) elements.

Preface

Recognising the value of a comparative study of human exposure models this project was initiated within the concerted actions CLARINET (Contaminated Land Rehabilitation Network), Working Group Human Health. As a result, a number of organisations directly or indirectly involved in the concerted action have begun a collaborative study based on the human exposure models that they have been responsible for developing. They are:

- the National Institute for Industrial Environment and Risks (*INERIS*), France;
- the National Environmental Protection Agency (*ANPA*), Italy;
- the Flemish Institute for Technological Research (*VITO*), Flanders, Belgium;
- Kemakta Konsult AB, Sweden;
- University of Nottingham, Land Quality Management (*LQM*), UK;
- DHI Water and Environment and Danish Toxicological Centre, Denmark;
- LABEIN Technological Centre, Basque Country, Spain;
- the National Institute of Public Health and the Environment (*RIVM*), the Netherlands.

Besides the NICOLE (Network on Contaminated Land) exposure factor dataset (ECETOC, 2001) has been included in this study.

The calculation were performed by the organisations mentioned above in the period 2000-2001.

Acknowledgement

In 1999 all participants were enthusiastic about the idea of a human exposure model comparison study. This was found something very useful and everybody agreed to participate, without hesitation. However, adapting the models and performing the calculations (40 scenarios!) was more work than most of us could expect. Moreover, nobody could foresee how many questions they got to answer during the course of the project and on how many chapters, tables and documents it was ask to comment. Realising that most of the work had to be done in between the daily routine (most of the participants did most of the work in time that was not planned or paid for) the author sincerely appreciates the efforts and many useful comments. Therefore, the author would like to thank Ms.dr. Francesca Quercia (the National Environmental Protection Agency (*ANPA)*, Italy), Ms.dr. Roseline Bonnart (the National Institute for Industrial Environment and Risks (*INERIS*), France), Ms. Christa Cornelis (the Flemish Institute of Technology and Development (*VITO*), Flanders, Belgium), Ms.dr. Naomi Earl and dr. Paul Nathanail (University of Nottingham, Land Quality Management (*LQM*), UK), Mr. Mark Elert (Kemakta Konsult AB, Sweden), Mr. Piet Otte (the National Institute of Public Health and the Environment (*RIVM*), the Netherlands), Ms. Dorte Rasmussen (DHI Water and Environment and Danish Toxicological Centre, Denmark), Ms.dr. Rosemary Zaleski (Exxon Biomedical Sciences, Inc.) and Ms.dr. Arantzazu Urzelai Azkune (LABEIN Technological Centre, Basque Country, Spain).
In the definition stage of the project RIVM colleague Mr. Leo Bouwmans proved to be a motivating sparring-partner. In the later stages of the project RIVM colleague Mr. Johannes Lijzen enriched the developments in the project with intellectual comments. Finally, the efforts of the RIVM colleagues Ms. Gea Stegen and Ms. Susan Sollie (editing data and text) and Mr. Dick de Zwart (reviewing the draft report) are appreciated.

Contents

Uitgebreide samenvatting

De betrouwbaarheid van berekening van de humane blootstelling aan contaminanten in de bodem is beperkt, als gevolg van onzekerheden in model concepten en input parameters. Het vergelijken van blootstelling berekend met verschillende blootstellingsmodellen en uitgaand van dezelfde uitgangspunten, kan een indruk geven van de mate van onbetrouwbaarheid. Met dit doel is de blootstelling berekend met zeven verschillende Europese modellen vergeleken. Uitwisseling van de benodigde informatie vond plaats op basis van een questionnaire en daaropvolgende email-communicatie. De volgende modellen participeerden in dit project:

- CETOX-human (Denemarken);
- CLEA D.D. (Verenigd Koninkrijk);
- CSOIL 8.0 (Nederland);
- ROME 01 (Italië);
- Vlier-humaan (Vlaanderen, België);
- een naamloos model uit Zweden;
- een naamloos model uit Frankrijk.

Er werd van het intensieve communicatienetwerk dat in dit project onstond geprofiteerd door toevoeging van de volgende activiteiten:

- Het geven van een overzicht van algemene karakteristieken van de blootstellingsmodellen.
- Het geven van een overzicht van standaard input parameters die in de verschillende procedures worden gebruikt.

Ten behoeve van beide activiteiten werd tevens het LUR blootstellingsmodel (Baskenland, Spanje) in beschouwing genomen. Voor de tweede activiteit werd de NICOLE dataset in het overzicht opgenomen.

Scenario's

Om de berekening van de humane blootstelling met elk van de zeven Europese modellen mogelijk te maken werden twintig scenario’s gedefinieerd. Deze verschillen voor wat betreft bodemgebruik (woonsituatie en industrieterrein), bodemtype (zand- en kleibodem) en type contaminant. De volgende vijf contaminanten, die verondersteld worden algemeen binnen Europa voor te komen en die verschillen voor wat betreft de blootstellings-karakterstieken, werden beschouwd: benzo(a)pyreen (PAK), cadmium (metalen), atrazine (pesticiden), benzeen (aromatische verbindingen) en trichloroetheen (vluchtige alifatische verbindingen). Alle blootstellingsberekeningen werden in tweevoud uitgevoerd: eenmaal met een voorgeschreven set van input parameters en eenmaal met de input parameters die worden gebruikt in de verschillende landen.

In elke berekening werd blootstelling voor kinderen en volwassenen via de drie belangrijkste blootstellingsroutes berekend, namelijk: via grondingestie, via gewasconsumptie en via inhalatie binnenlucht. Bovendien werden de concentraties in de contactmedia en in de bodemcompartimenten berekend.

Resultaten
In paragraaf 6.1.1 zijn conclusies getrokken over de karakteristieken van de Europese blootstellingsmodellen. Deze conclusies zijn gericht op de relatie tussen de verschillende Europese modellen onderling en op de opzet, mogelijkheden en wijze van gebruik van deze blootstellingsmodellen.

In paragraaf 4.2 is een overzicht gegeven van de relevante input parameters, welke in de zeven modelbenaderingen worden gebruikt. Bovendien worden in paragraaf 6.1.2 conclusies getrokken over de variatie in deze input parameters voor wat betreft humane karakteristieken en contaminant-specifieke input parameters, alsmede over de input parameters die specifiek worden gebruikt bij de berekening van de blootstelling via gewasopname, via inhalatie binnenlucht en via de overige blootstellingsroutes.

In paragraaf 6.1.3 zijn de 90% betrouwbaarheidsintervallen gegeven. De variatie in de berekende uitkomsten is als volg samengevat:

	Totale bl.stelling	Bl.stelling via grond-ingestie	Bl.stelling via gewas-consumptie	Bl.stelling via inhalatie binnenlucht	Conc. knol-gewassen	Conc. blad-gewassen	Conc. binnen-lucht	Conc. poriën-water	Conc. bodem-lucht
Beperkt		x							x
Aanzienlijk			x		x			x	
Groot	x			x		x	x		

De volgende (willekeurige) indeling is gebruikt:
- *Beperkte* variatie: De meerderheid van de uitkomsten ligt binnen een factor 5 hoger en een factor 5 lager dan de scenario-medianen.
- *Aanzienlijke* variatie: De meerderheid van de uitkomsten ligt binnen een factor 10 hoger en een factor 10 lager dan de scenario-medianen
- *Grote* variatie: De meerderheid van de uitkomsten ligt binnen een factor 100 hoger en een factor 100 lager dan de scenario-medianen.

Bovendien werden de volgende conclusies getrokken voor wat betreft de variatie in berekende blootstelling:
Inzicht in de variatie in berekende bloostelling:
- Voor *Totale blootstelling, Blootstelling via gewasconsumptie* en *Blootstelling via inhalatie binnenlucht* lijkt de variatie ten gevolge van de verschillen in modelconcepten te overheersen ten opzichte van verschillen door gebruik van verschillende input parameters. Alleen voor *Blootstelling via grondingestie* neemt de variatie duidelijk toe wanneer de land-specifieke input parameters in plaats van de gestandaardiseerde input parameters worden gebruikt. Voor alle typen blootstelling werden een aantal extreme waarden berekend, dat wil zeggen waarden die “sterk afwijken” van de mediane waarden. De meest extreme waarden werden berekend in de volgende afnemende volgorde: *Blootstelling via inhalatie binnenlucht* (hoge extremen) > *Totale blootstelling* (lage extremen) > *Blootstelling via gewasconsumptie* (hoge en lage extremen) > *Blootstelling via grondingestie* (lage extremen).

Verklaring van de variatie in berekende bloostelling:
- De meerderheid van de modellen dragen bij aan een grote variatie in de berekende blootstelling. Bovendien is de variatie in berekende blootstelling (*Totale blootstelling, Blootstelling via inhalatie binnenlucht* en met name *Blootstelling via gewasconsumptie*)

sterk afhankelijk van het type contaminant. Alleen voor *Blootstelling via grondingestie* is de variatie in de blootstelling nauwelijks afhankelijk van het type contaminant. De variatie in blootstelling is nauwelijks afhankelijk van bodemgebruik en nog minder van bodemtype.

- Er is een sterke relatie tussen *Blootstelling via inhalatie binnenlucht* en de variatie in *Concentratie in binnenlucht*. Dit suggereert dat de factoren die de variatie in *Concentratie in binnenlucht* bepalen, namelijk *Concentratie in de bodemlucht, Oppervlakte* en *volume van het huis of gebouw* en de *Ventilatiefrequentie*, tevens de variatie in *Blootstelling via inhalatie binnenlucht* bepalen.
- Daarentegen is er geen duidelijke relatie tussen de variatie in *Blootstelling via voedingsgewassen* en de variatie in *Concentratie in voedingsgewassen* (wortel- of bladgewassen). Dit suggereert dat de input parameters *Totale (wortel- en blad-)gewasconsumptie* en *Fractie van wortel- en bladgewassen uit eigen tuin* de variatie in *Blootstelling via gewasconsumptie* (mede) beïnvloeden.
- De variatie in *Concentratie in poriewater* is niet duidelijk gerelateerd aan de variatie in *Blootstelling via gewasconsumptie* of aan de variatie in *Concentratie in wortel- of bladgewassen.*
- De variatie in *Concentratie in de bodemlucht* is niet duidelijk gerelateerd aan de variatie in *Blootstelling via inhalatie binnenlucht* of aan de variatie in *Concentratie in de bodemlucht.*

Aanbevelingen

- Er dient nader onderzoek te worden verricht naar de variatie in berekende blootstelling. Hierbij zal de aandacht zich onder andere moeten richten op de invloed van de model-algoritmen op de variatie in berekende blootstelling. Om dit doel te verwezenlijken zullen internationale experts op het gebied van berekening van humane blootstelling actief moeten participeren in dit nader onderzoek.
- Op de langere termijn dient een *toolbox* te worden geconstrueerd voor gebruik op Europees niveau. Deze *toolbox* moet de volgende elementen bevatten:
  - Protocollen voor die elementen die te harmoniseren zijn ("gestandaardiseerde model *tools*" en "gestandaardiseerde input parameter *tools*");
  - flexibele elementen ("flexibel model *tools*" en "optionele parameter *tools*"), om tegemoet te kunnen komen aan land-specifieke (geografische, etnologische en politieke) elementen;
  - een methodiek die aangeeft hoe de humane blootstelling moet worden bepaald, inclusief een beschrijving van de gevoeligheden van de berekende blootstelling voor de input parameters en een richtlijn die aangeeft wanneer en hoe de concentraties in de contactmedia moeten worden gemeten.
  - Informatie over de onzekerheid/ betrouwbaarheid van de berekende blootstelling.

Extended summary

The reliability of calculated human exposure to contaminants in soil is limited because of uncertainties about model concepts and input parameters. A way to gain insight into the reliability of calculated exposure is to compare calculated exposures using different human exposure models. To this purpose, calculated outputs from seven European models have been compared. Information has been exchanged on the basis of a questionnaire and subsequent email communication. The following models participated in this project:

- CETOX-human (Denmark);
- CLEA D.D. (United Kingdom);
- CSOIL 8.0 (The Netherlands);
- ROME 01 (Italy);
- Vlier-humaan (Flanders, Belgium);
- an unnamed model from Sweden;
- an unnamed model from France.

Use was made of the intensive communication network that was developed within the project, which resulted in the following additional activities:

- Overviewing general information of human exposure models.
- Overviewing default values for the input parameters used in different approaches.

To these purposes also the LUR exposure model (Basque Country, Spain) has been included. To the second purpose the NICOLE dataset has been included in the overview.

Scenarios
To be able to calculate human exposure with each of the seven European models twenty scenarios have been defined. These scenarios differ in respect to land use (residential and industrial), soil type (sandy soil and clay soil), and type of contaminant. The five following contaminants, which have been assumed to be common throughout Europe and have different exposure characteristics, have been considered: benzo(a)pyrene (PAH), cadmium (metals), atrazine (pesticides), benzene (aromatic compounds) and trichloroethene (volatile aliphatic compounds). All exposure calculations have been performed twice for all twenty scenarios: once with a prescribed set of parameters and once with the data that is used in the different countries. In each calculation exposure to children and adults via the following three major exposure pathways is calculated: via soil ingestion, via crop consumption and via indoor air inhalation. Besides the relevant concentrations in contactmedia and in the soil compartments were calculated.

Results
In section 6.1.1 conclusions have been drawn about the characteristics of the European exposure models. These conclusions have been focused on mutual dependencies between the European exposure models and layout, possibilities and use of the European exposure models.

In section 4.2 an overview is given of all relevant input parameters that are used in the seven European model approaches. Conclusions have been drawn about the variation in these input parameters in section 6.1.2 for the human characteristics and contaminant-specific input

parameters, as well as for the input parameters that relate to exposure via crop consumption, exposure via indoor air inhalation and to exposure via other exposure pathways.

In section 6.1.3 the 90% confidence limits of the calculated outputs have been presented. The variation in the calculated outputs has been summarised as follows:

	Total exposure	Exp.via soil ingestion	Exp.via crop con-sumption	Exp.via indoor air inhalation	Conc.root vegetables	Conc. leafy vegetables	Conc. indoor air	Conc. pore water	Conc. soil air
Limited		x							x
Substantial			x		x			x	
Large	x			x		x	x		

The following (arbitrary) categorisation has been used:

- *Limited* variation: The majority of the outputs is within a factor of 5 higher and a factor of 5 lower than the scenario medians.
- *Substantial* variation: The majority of the outputs is in between a factor of 10 higher and a factor of 10 lower than the scenario medians: there is a "substantial variation" in the calculated human exposures.
- *Large* variation: The majority of the outputs is in between a factor of 100 higher and a factor of 100 lower than the scenario medians.
- *Huge* variation: The majority of the outputs is *not* in between a factor of 100 higher and a factor of 100 lower than the scenario medians.

Furthermore the following conclusions on the variation in calculated exposure have been drawn:

Insight in variation in exposure:

- For *Total exposure, Exposure via crop consumption,* and *Exposure via indoor air inhalation* the variation from different model concepts seems to dominate over the variation from using different input parameters. Only for *Exposure via soil ingestion* variation clearly increase when country-specific default parameters are used instead of standardised input parameters.
- For each type of exposure a few extreme values have been calculated, i.e. values that are “very different” from the median value. Most extreme values are calculated in the following decreasing order: *Exposure via indoor air inhalation* (high extremes) > *Total exposure* (low extremes) > *Exposure via crop consumption* (low and high extremes) > *Exposure via soil ingestion* (low extremes).

Understanding variation in exposure:

- The majority of the models contribute to large variation in calculated exposure. Besides, variation in calculated exposure (*Total exposure; Exposure via indoor air inhalation* and especially *Exposure via crop consumption*) is strongly dependent on the type of contaminant. Only for *Exposure via soil ingestion* the variation in calculated exposure is scarcely dependent on type of contaminant. The variation in exposures is scarcely dependent on soil use and even less on soil type.
- There is a strong relation between variation in *Exposure via indoor air inhalation* and variation in *Concentration in indoor air*. This suggests that the factors that control the variation in *Concentration in indoor air*, i.e. *Concentration in soil air*, *Surface* and

Volume of the house or building, *Ventilation frequency*, also control the variation in *Exposure via indoor air inhalation.*
- On the contrary there is no clear relation between the variation in *Exposure via crop consumption* and the variation in *Concentration in crop* (root or leafy vegetables). This suggests that the input parameters *Total (root and leafy) vegetable consumption* and *Fraction of root and leafy vegetables that is homegrown* (also) control the variation in *Exposure via crop consumption*.
- The variation in *Concentration in pore water* is not clearly related to the variation in *Exposure via crop consumption* or to the variation in *Concentration in leafy root or leafy vegetables.*
- The variation in *Concentration in soil air* is not clearly related to the variation in *Exposure via indoor air inhalation* or to the variation in *Concentration in indoor air.*

Recommendations
- The variation in calculated human exposure should be investigated in more detail. As part of this further research the differences in the model-algorithms on variation in exposure should be evaluated in more detail. To this purpose international human exposure model experts should participate actively in this further research.
- On the long term a toolbox should be constructed on an European level, including:
  - standardisation of the elements that are suitable for standardisation and harmonisation (“fixed model tools” and “fixed input parameter tools”);
  - flexible (country-specific) elements (“flexible model tools” and “optional parameter tools”) to account for country-specific (geographical, ethnological and political) elements;
  - a procedure on assessing human exposure, including documentation on the sensitivity of calculated human exposure to the input parameters and a guideline on when and how to measure concentrations in contactmedia;
  - information on the uncertainty/ reliability of the calculated human exposure.

1. Introduction

1.1 Background

The reliability of human exposure calculations is limited because of uncertainties about model concepts and input parameters, in particular:

- Uncertainties about model concepts, for example, there is lack of knowledge about model concepts that describe the relationship between contaminant concentration in groundwater and indoor air concentration, a major determinant of human exposure to volatile compounds (e.g. Waitz et al., 1994).
- Uncertainties about input parameters, for example, there is a lack of knowledge about the input parameters that describe human behaviour, such as the amounts of soil ingestion by humans (Stanek and Calabrese, 1995). In addition, there may be regional variations in input parameters, for example, in the organic matter content of the soil.

Variation in calculated exposure may also result from a limited understanding of how human exposure modelling is carried out by users of models and/or (subsequent) unintentional mis-use of human exposure models. For example, if an exposure model in which the transport of volatile contaminants usually is derived for homogeneous soils with an average soil temperature of around 10 degrees is used to assess the human exposure related to volatile contaminants at a waste dump site, where materials are heterogeneous and temperatures high. The consequences of the uncertainty around this type of mis-use are hard to assess, but they might become more widespread as a variety of commercial user-friendly software packages become available.
Some studies using with the same scenarios as staring point indicated rather large differences between calculated exposures, when using different models (Dor et al., 1998).

Human exposure models are in widespread use, both implicitly and explicitly. An example of implicit use is the comparison of measured contaminant concentrations with soil and groundwater quality standards derived from these exposure models. Explicit use is decision-making based on (site-specific) exposure calculations. Hence the impact of the uncertainties described above can have serious consequences for public health, if a site is incorrectly diagnosed as "safe". Otherwise can uncertainties about input parameters lead to the inclusions of high-end estimates, which can lead to compounded conservatism (e.g. Finley and Paustenbach, 1994; Paustenbach, 1995; Kissel et al., 1998). This could have adverse consequences for the social and financial situation of organisations and individuals, if a site is incorrectly diagnosed as "dangerous".

The combination of "limited reliability" and "major consequences" requires a better insight into the reliability of calculated exposure. This requirement can be most directly addressed by performing a validation study, i.e. comparing calculated exposure with measured exposure. However, measuring (long-term) exposure in the human body is difficult, both for ethical and technical reasons. Statistical procedures (like Monte Carlo techniques (e.g. Cullen, 1994; Kissel et al., 1998), can be used to deal with the influence of uncertain parameters, or uncertain model concepts. However, these procedures are relatively time-consuming.

Another way to gain insight into the reliability of calculated exposure is to compare calculation results using different human exposure models, for standard datasets and assumptions. Although such a comparison does not give a scientific proof, it does give a valuable insight into the variation in calculated human exposures.

1.2 Purpose

The present study has the following aims:
1. Gaining insight into the variation in calculated human exposure.
2. Understanding the variation in calculated human exposure.

Use was made of the intensive communication network that was developed within the study, which resulted in the following additional activities:
1. Overviewing default values for the input parameters used in different approaches.
2. Overviewing general information of human exposure models.

The results of this study are likely to be important to the evaluation of decision-making that uses soil quality standards based on human exposure calculations, and to indicate how to improve concepts and input parameters for existing exposure models. Its outputs could have a profound influence on future research and development in this area, and the study itself may be a precursor to a larger R&D proposal.

It should be noted that:
- this study is only focused on calculated exposure, not on critical exposure or on resulting soil quality standards;
- only exposure to one separate contaminant is considered, not the potentially synergistic or antagonistic effects of exposure to more than one contaminant;
- only exposure to soil contaminants is considered, exposure to contaminants in air, groundwater or surface water is not considered in this study;
- background exposure, i.e. exposure from other sources than contaminated soil, is not taken into consideration in this study.

2. Procedure

2.1 Collection of information

The needed information has been collected on the basis of a questionnaire and is categorised as follows:
- General information on the human exposure models (Chapter 3).
- Input parameters used as defaults in the different approaches (Chapter 4).
- Calculated outputs (Chapter 5).

During the project frequent additional communication, mainly using email, was found necessary with all participants.

2.2 Participating models

The models used in this human exposure comparison study are summarised in Table 2.1, which also provides an overview of each model developer, contact person and model applications.

Table 2.1. The models used in the human exposure comparison study, including developers, contact persons and model application.

MODEL	DEVELOPER	CONTACT	MODEL APPLICATIONS
CETOX-human	DHI Water and Environment and Danish Toxicological Centre	DHI Water and Environment, D. Rasmussen, Agern Allé 11, DK-2970 Hørsholm, Denmark	Management of risks from polluted soil. Advice is related to the specific polluting substance, land use and outlines how to minimise exposure to soil (e.g. which crops not to grow on the site)
CLEA D.D.	DEFRA & Environmental Agency	University of Nottingham, LQM, P. Nathanail, Nottingham, UK NG7 2RD	Derivation of soil guideline values
CSOIL 8.0	National Institute of Public Health and the Environment (*RIVM*)	*RIVM*, P. Otte, P.O. Box 1, 3720 BA Bilthoven, The Netherlands	Derivation of quality standards for deciding on remediation. Derivation of remediation objectives. Determination of remediation urgency (Dutch Soil Protection Act)
LUR	LABEIN Technological Centre	LABEIN, A. Urzelai, Cuesta de Olabeaga 16, 48013 Bilbao, Spain	Derivation of soil quality standards) in the framework of Contaminated Soil Policy in the Basque Country. Site-specific risk assessment
No name given	National Institute for Industrial Environment and Risks (*INERIS*)	*INERIS*, R. Bonnard, Parc Technologique Alata, BPno. 2, 60550 Verneuil-en-Halatte, France	Derivation of generic warning quality standards. Site-specific risk assessment, Help to identify remediation solutions
No name given	Kemakta Konsult AB	Kemakta Konsult AB, M. Elert, P.O. Box 12655, S-112 93 Stockholm, Sweden	Derivation of generic guidelines for contaminated soils. Used as a basis for the derivation of site-specific guidelines
ROME 01	National Environmental Protection Agency (*ANPA*)	*ANPA*, F. Quercia, Via V. Brancati 48, 00144 Rome, Italy	Derivation of generic screening values. Site-specific remediation objectives
Vlier-Humaan	Flemish Institute of Technology and Development (*VITO*)	*VITO*, C. Cornelis, Boeretang 200, B-2400 Mol, Belgium	Derivation of quality standards for deciding on remediation. Derivation of remediation objectives (Flemish legislation on soil remediation). Site-specific risk assessment

Note that

- the HESP model and the Risc human use the same algorithms and the same input parameter set as the CSOIL 8.0 model.
- The JAG model is similar, but not equal to the CETOX-human model and is used for different purposes as the CETOX-human model.

2.3 Activities

The following activities has been performed to conduct the human exposure comparison study":

1. Activity in relation to purpose 1 (*Gaining insight into the variation in calculated human exposure*):
   Comparison of calculated exposure via the different major exposure pathways, i.e. oral soil ingestion, crop consumption, inhalation of indoor air (inhalation of vapours only, excluding suspended particles in the air), using the different human exposure models ascertained from the questionnaires: a) by using the same prescribed input parameters and, b) by using the default input parameter that are used in different countries. The results of this activity have been described in chapter 5.
2. Activity in relation to purpose 2 (U*nderstanding the variation in calculated human exposure*):
   Evaluating the variation in calculated exposure on the basis of comparing the variation in exposure with the variation in other exposures and/or with variation in concentration in the contactmedia and in the soil compartments and the variation in input parameters. The results of this activity have also been described in chapter 5.
   Evaluating the variation in calculated exposure on the basis of the different model concepts is not part of this study, because this evaluation is difficult without direct participation of the human exposure model experts (workshop).
3. Activity in relation to additional activity 1 (*Overviewing default values for the input parameters used in different approaches*):
   Overviewing default values used for the major input parameters in the different approaches in the different countries ascertained from the questionnaires. The results of this activity have been described in chapter 4.
4. Activity in relation to additional activity 2 (*Overviewing general information of some European human exposure models*):
   Collecting general information of the European human exposure models. The results of this activity have been described in chapter 3.

3. General model information

On the basis of the questionnaires general model information was collected for all seven human exposure models. This information concerns:

- model characteristics (e.g. contact person);
- dependencies between the models and model applications;
- model layout (e.g. compartments and exposure pathways that are included);
- model possibilities (e.g. probabilistic application, acute exposure);
- model use (e.g. major applications, standard scenarios that have been included).

This information has been summarised in the following sections. The detailed general information on all seven human exposure models, as was derived from the questionnaires, is included in Appendix 2.

3.1 Dependencies between the models and model applications

In Table 3.1 the dependencies between the European models and default input parameters are indicated (see Appendix 2 for more detailed information).

Table 3.1: Dependencies between the models (before the slash) and between the default input parameters (after the slash); + = model concepts or input parameters are related.

MODEL: Model to which MODEL is related:	CETOX Human	CLEA D.D.	CSOIL 8.0	LUR	NoName France 2000[1]	NoName Sweden[1]	ROME 01	Vlier-Humaan
CETOXhuman			+ / +					
CLEA D.D.								
CSOIL 8.0	+ / +				+ / +	+ /		+ / +
LUR								
NoNameFrance 2000			+/ +					
NoNameSweden			+ /					
ROME 01								
Vlier-Humaan			+ / +					

[1] No official name is available for this model

The conclusion on the dependencies between the model and default input parameters is that the model concepts and the input parameters of the exposure models CETOX-human, NoNameFrance 2000, Vlier-Humaan and CSOIL 8.0 are related to each other. Besides, the model concept of the exposure model NoNameSweden is related to the four models mentioned and vice versa.

3.2 Model layout

In Table 3.2 information on the layout of the European models is summarised (see Appendix 2 for more detailed information).

Table 3.2: Information on the layout of the European human exposure models; x = incorporated in the model.

	CETOX-human	CLEA D.D.	CSOIL 8.0	LUR	NoName France 2000	NoName Sweden	ROME 01	Vlier-humaan
Compartments								
soil	x	x	x	x	x	x	x	x
groundwater unsaturated zone		x	x		x	x	x	
groundwater saturated zone						x	x	x
surface water						x		
air					x		x	x
Exposure pathways:								
soil ingestion	x	x	x	x	x	x	x	x
crop consumption	x	x	x	x	x	x		x
ingestion of particles attached to crops		x			x			
consumption of meat and milk products								x
fish consumption						x		
direct groundwater consumption			(x)			x	x	x
drinking water (contaminated by			x		x			x
inhalation of indoor air	x	x	x	x	x	x	x	x
inhalation outdoor air	x	x	x	x	x		x	x
inhalation dust/ soil particles, indoors	x	x	x	x	x	x	x	x
inhalation dust/ soil particles, outdoors	x	x	x	x	x	x	x	x
inhalation of bathroom air		x	x		x			x
inhalation of vapours from groundwater							x	
dermal uptake through soil, indoors	x	x	x		x	x		x
dermal uptake through soil, outdoors	x	x	x	x	x	x	x	x
dermal uptake during showering		x	x		x			x

Table 3.2: Information on the layout of the European models; x = incorporated in the model (continued).

	CETOX-Human	CLEA D.D.	CSOIL 8.0	LUR	NoName France 2000	NoName Sweden	ROME 01	Vlier-humaan
Principal basis model concepts (before the slash)/ input parameters (after the slash)								
worst case				x				x
realistic worst case	x						/x	
reasonable Maximal Exposure*1		x /x	/x	/x	x /x	x /x	x	/x
average case			x					
best case								
min, max, average	/x							
Starting point								
total soil content	x	x	x	x	x	x	x	x
groundwater concentration							x	
concentration contactmedia					x			(x)
How is the distribution of contaminants over the soil compartments calculated								
using the fugacifity theory		x	x					x
using partition coefficients	x	x		x	x	x	x	x

*1: Reasonable Maximal Exposure: best estimates in case of enough knowledge; upper bound estimate in case of doubt

The major conclusions on the layout of the European human exposure models are:

- The soil compartment and the unsaturated groundwater zone are included in most of the models; besides most models include several other compartments (air, surface water, saturated groundwater zone).
- The following exposure pathways are incorporated in all models: Soil ingestion, Crop consumption (except for ROME 01), Indoor air inhalation (inhalation of vapours only, excluding suspended particles in the air), Dermal uptake, Inhalation of dust/ soil particles. Besides most models include several other exposure pathways.
- All model concepts and default input parameters are based on Maximal Reasonable Exposure or (realistic) worst case.
- All models use the total soil content as starting point.
- The distribution of the contaminants over the soil compartments is mainly calculated on the basis of partition coefficients in some cases on the fugacitivity theory.

3.3 Model possibilities

In Table 3.3 information on the possibilities of the European models is summarised (see Appendix 2 for more detailed information).

Table 3.3: Possibilities of the European exposure models.

	CETOX-Human	CLEA D.D.	CSOIL 8.0	LUR	NoName France 2000	NoNameSweden	ROME 01	Vlier-humaan
Possibilities for probabilistic applications?	no	yes	no	no	yes	no	no	yes
Is background exposure taken into account?	yes	optional	no	yes	no	yes	no	yes
Standard age ranges (years)	1-3 20-60	year 0 to 6, 16-59, 59-70	0-6 (child) 6-70 (adult)	0-6 (child) 6-70 (adult)	0-6 (child) 6-70 (adult)	0-6 6-64	0-6 6-70	0-6 6-70
How is dealt with exposure to children and adults?								
calculated separately	x			x	x (non-carcino-gens)	x (non-car-cinogens)	x (non-car-cinogens)	x (non-carcino-gens)
summed up					x (carci-nogens)	x (carci-nogens)	x (carci-nogens)	x (carci-nogens)
calculated separately or summed up		x	x			x		x
Is the possibility for calculating acute exposure included in the model?	no	no	no	no	no	yes	no	no
Any kinetic (time dependent) processes in the model?	no	yes	no	no	yes	yes	no	no
Is degradation included in the model?	no	no	no	no	no	no	no	no
Any standards incorporate that limit concentrations in contactmedia?	no	no	yes	no	no	yes	yes	yes
Is exposure to mixtures included in the model?	no	no	no	no	no	yes	yes	no

The major conclusions on the possibilities of the European models are:
- Only part of the models include the possibility for probabilistic application, background exposure, kinetic processes, or standards that limit the concentration in contactmedia.
- Most models do not offer the possibility for acute exposure, degradation and exposure to a mixture of contaminants.

3.4 Model use

In Table 3.4 information on the use of the European models is summarised (see Appendix 2 for more detailed information).

Table 3.4: Information on the use of the European exposure models.

	CETOX-human	CLEA D.D.	CSOIL 8.0	LUR	NoName France 2000	NoName Sweden	ROME 01	Vlier-humaan
The models is used for								
deriving soil quality standards	yes	yes	yes	yes	yes	yes	(yes)*1	yes
standardised risk assessment	yes		yes		yes			
deriving remediation goals		(yes)	yes		yes		yes	yes
site-specific exposure assessment		(yes)	yes	yes	yes	yes	yes	
Is the model available for third parties	no	yes	(yes)	no	no	no	yes	no
In the model in general use?	no	yes	yes	yes	no	yes	yes	yes
What standard scenario's are included								
residential with garden(s)	(yes)	yes	yes	yes	yes	yes	yes	yes
residential without garden(s)		yes	yes		yes	yes	yes	
industrial	(yes)	yes	yes	yes	yes	yes	yes	yes
vegetable garden (allotments)	yes	yes	yes			(yes)	no	
kindergarten	yes					(yes)	(yes)	
children playground				yes		(yes)	(yes)	
sport fields	yes						(yes)	
parks	yes		yes	yes		(yes)	yes	yes
garden	yes	yes					yes	
recreation			yes		yes	(yes)	yes	yes
parks, playing fields and open spaces		no	yes				yes	
nature reserves						(yes)	no	
agriculture						(yes)	no	yes
less sensitive land-use, but with						(yes)		
infrastructure			yes			(yes)		
consolidated areas	yes							

*1: no formalised standards

Table 3.4: Information on the use the European exposure models (continued).

	CETOX-human	CLEA D.D.	CSOIL 8.0	LUR	NoName France 2000	NoName Sweden	ROME 01	Vlier-humaan
Any guidelines for selection of input parameters?	no	yes	yes	yes	yes	no	yes	(yes)
Any recommendation or guidelines for measurements in contactmedia?	no	no	yes	no	no	yes	yes	no
Is phytotoxicity (a maximal concentration in crops) included?	no	(no)	no	no	no	no	no	no
Is site-specific calculation of the Concentration in crops possible?	yes	yes	no	no	no	no	no	no
Is site-specific calculation of the concentration in indoor air possible?	yes	yes	(yes)	yes	yes	yes	yes	(yes)

The major conclusions on the use of the European models are:

- All models are used for the derivation of soil quality standards. Besides all models are used for at least one additional purpose.
- The soil uses Residential site and Industrial site are incorporated in all models; besides all models includes several other soil uses.
- No model includes phytotoxicity (a maximal concentration in the crop, above which the crop will show adverse effects).
- Most models do include guidelines for selection of input parameters; most models do not include recommendations or guidelines for measurements in contactmedia.
- All models offer the possibility for the site-specific calculation of the concentration in the indoor air. However, only two models offer the possibility for the site-specific calculation of the concentration in crops.

4. Overviewing input parameters

In this chapter an overview is given of the (variation in) default input parameters used in different model approaches. The overview of default parameters enables model users to select data (additional activity 1, i.e. *Overviewing default values for the input parameters used in different approaches*). For policy makers it could be interesting to have insight into the *variation* in default input parameters. Besides the *variation* in the default input parameters is used in relation to purpose 2, i.e. *Understanding the variation in calculated human exposure*: variation in exposure or variation in concentration in contactmedia can possibly or in soil compartments be related to variations in relevant input parameters, in Chapter 5.

Because developments in the use of human exposure models and the derivation of soil quality standards are quick, several elements changed since the start of the project. Major revisions of models and input parameters were performed in

- Italy: ROME 2.0, available from www.sinanet.anpa.it (addition of exposure pathway via surface water, extension of database on contaminants, update of toxicological and chemical data, independent screening and site-specific levels, possibility for comparison of observed concentration with both legal limits and risk-based screening values).
- The Netherlands: CSOIL2000 (Rikken et al., 2001: model concepts; Otte et al., 2001: input parameters).
- The United Kingdom: CLEA2002, available from www.environment-agency.gov.uk or www.defra.gov.uk.

The data presented in this chapter relate to the available models and default input parameters available in the year 2000. These data also are the basis for the calculations using country-specific default input parameters in Chapter 5.

4.1 Data organisation

The default input parameters are categorised in the following categories:

- human characteristics;
- parameters that relate to the Exposure via crop consumption;
- parameters that relate to the Exposure via inhalation of indoor air;
- parameters that relate to other exposure pathways;
- contaminant-specific input parameters.

A "practical format" has been used: scientific format for most parameters and normal format (number between 0 and 1) for fractions.

To facilitate comparison, bar charts are presented in Figure 4.1, which enable visual interpretation of the variation in the default input parameters. Note that when input parameters have a value of 0, “0” has been added in the graphs. When “0” or any other number is lacking this input parameter is note used in the model.

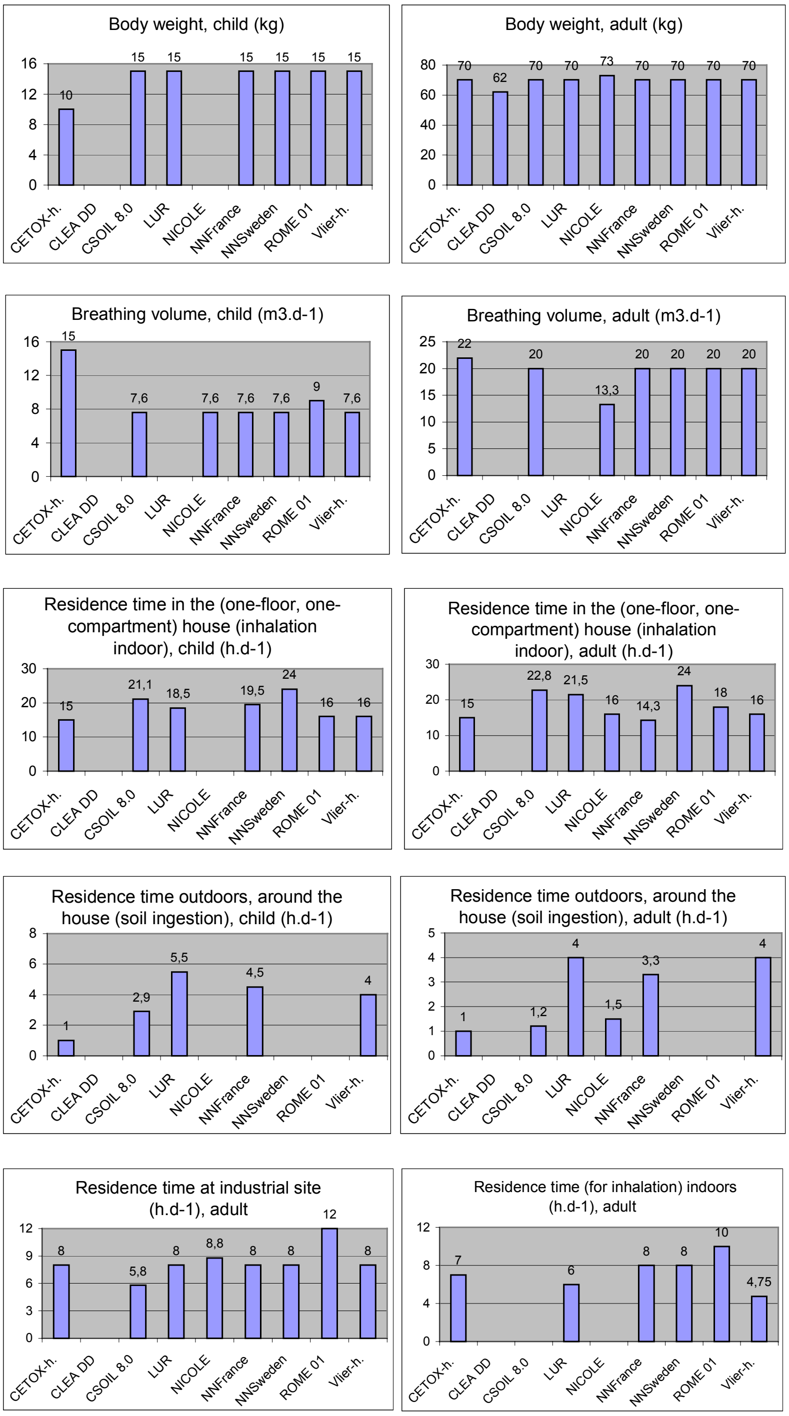

Figure 4.1: Bar charts of the default input parameters: Human Characteristics.
When "0" or any other number is lacking this input parameter is not used in the model; for CLEA D.D. several input parameters have been given in a probabilistic format, no value given in the bar charts.

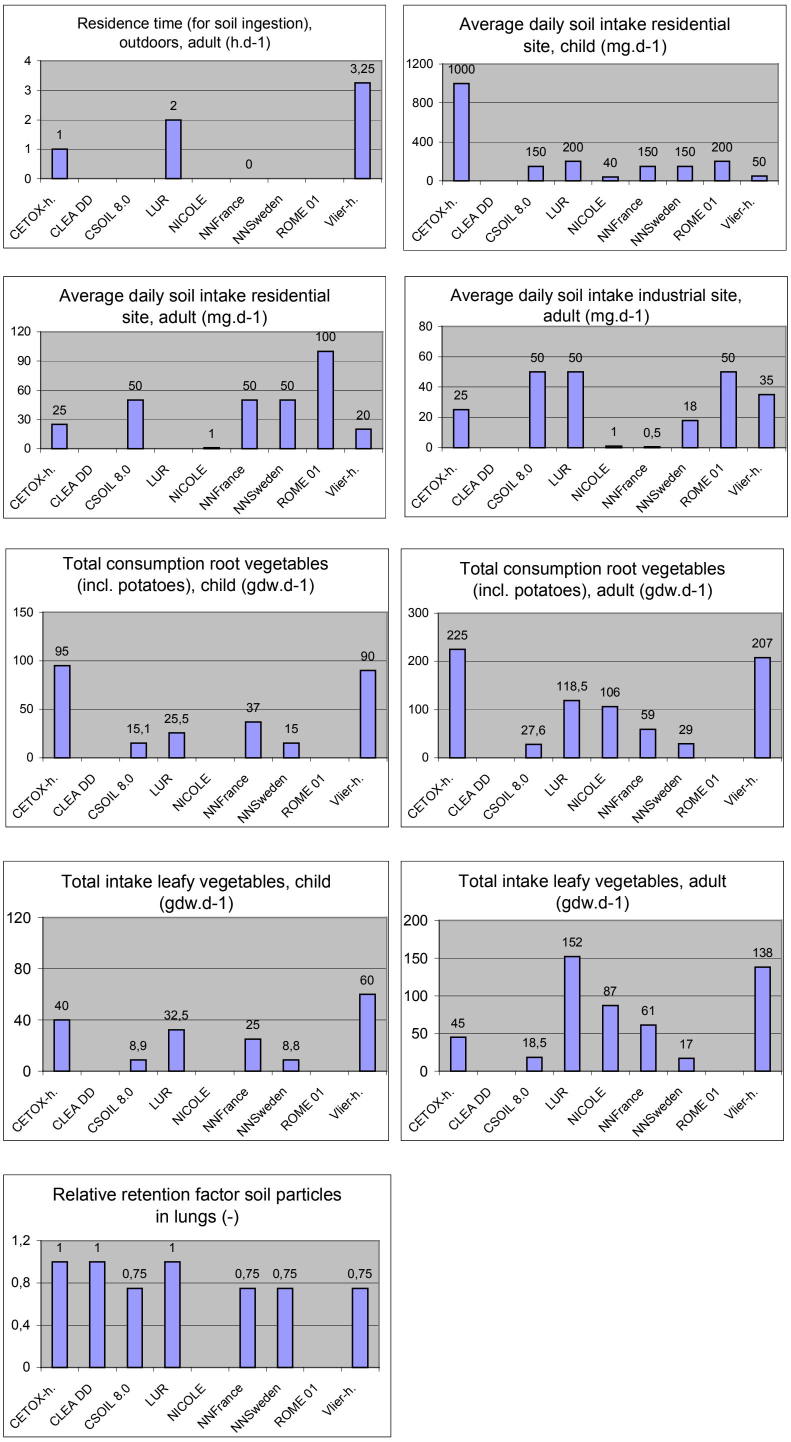

Figure 4.1 (continued): Bar charts of the default input parameters: Human Characteristics.
When "0" or any other number is lacking this input parameter is not used in the model; for CLEA D.D. several input parameters have been given in a probabilistic format, no value given in the bar charts.

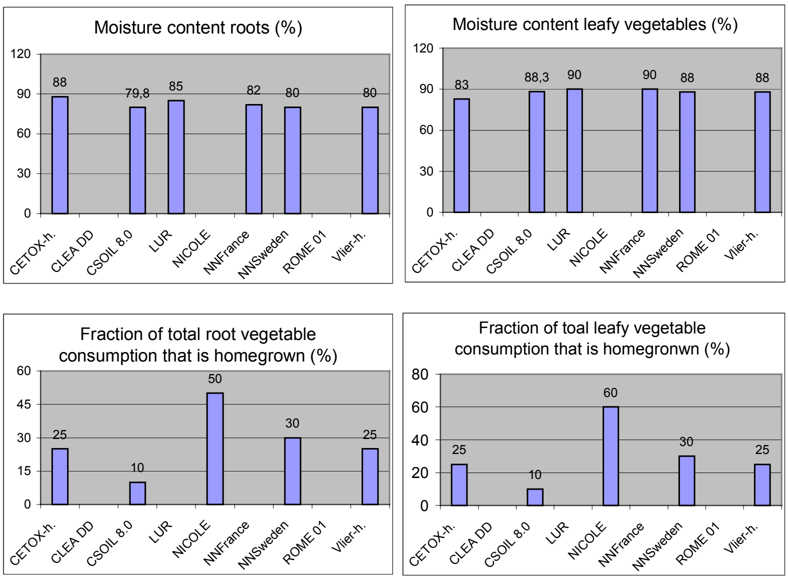

Figure 4.1 (continued): Bar charts of the default input parameters: Exposure due to crop consumption.
When "0" or any other number is lacking this input parameter is not used in the model.

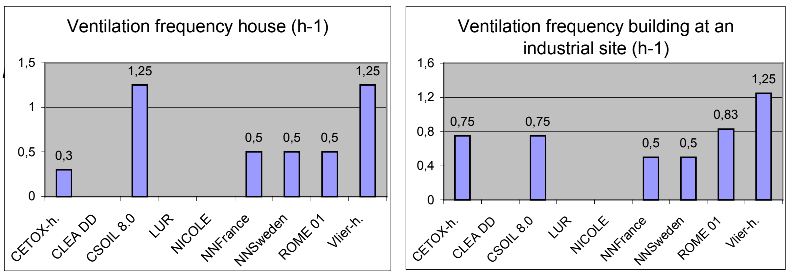

Figure 4.1 (continued): Bar charts of the default input parameters: Exposure due to inhalation.
When "0" or any other number is lacking this input parameter is not used in the model.

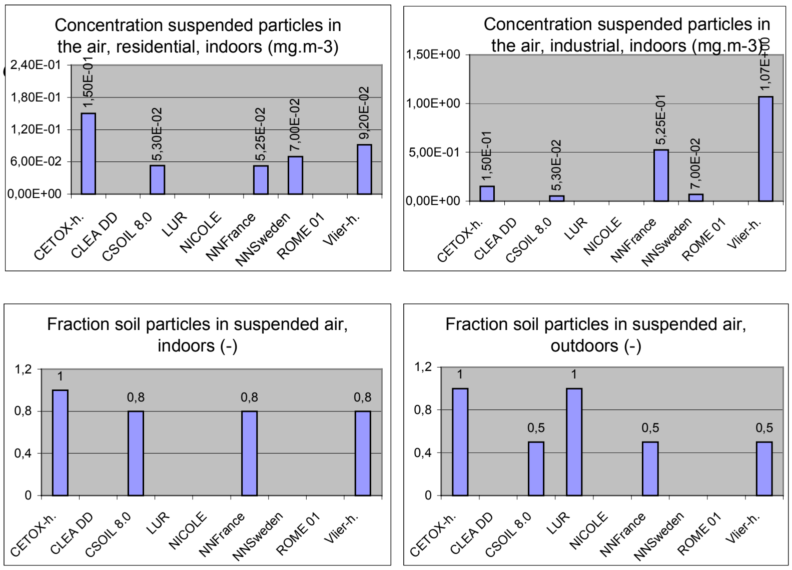

Figure 4.1 (continued): Bar charts of the default input parameters: Other exposure pathways. When "0" or any other number is lacking this input parameter is not used in the model.

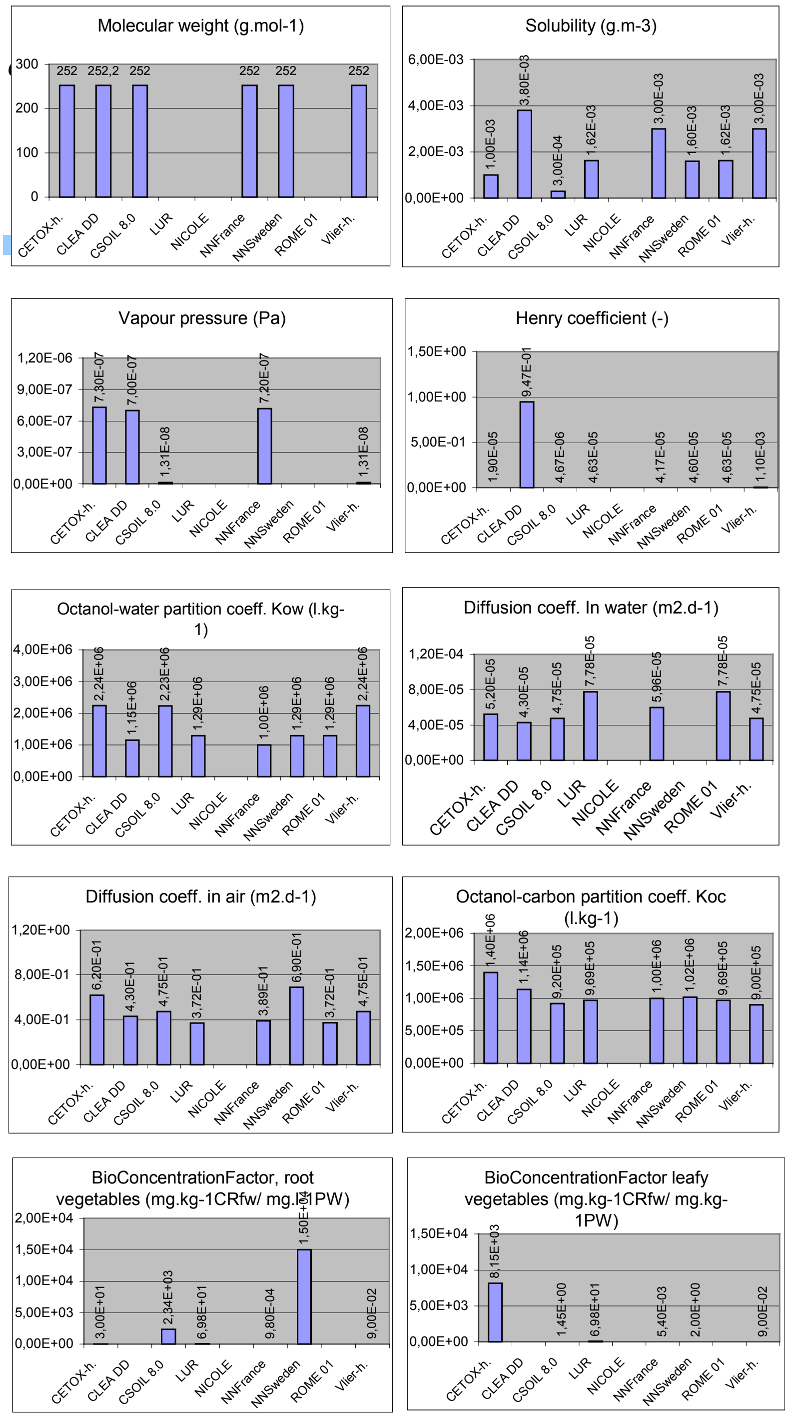

Figure 4.1 (continued): Bar charts of the default input parameters: B(a)P-specific input parameters.
When "0" or any other number is lacking this input parameter is not used in the model.

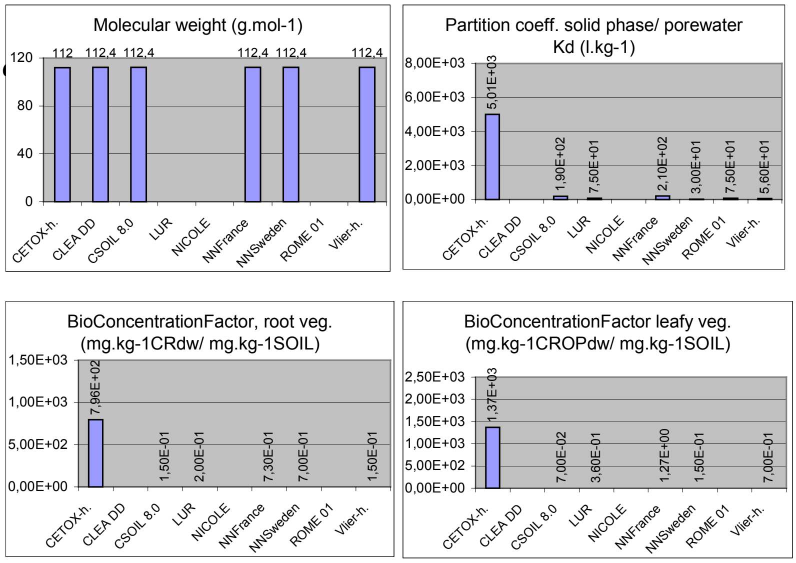

Figure 4.1 (continued): Bar charts of the default input parameters: cadmium-specific input parameters.

When "0" or any other number is lacking this input parameter is not used in the model.

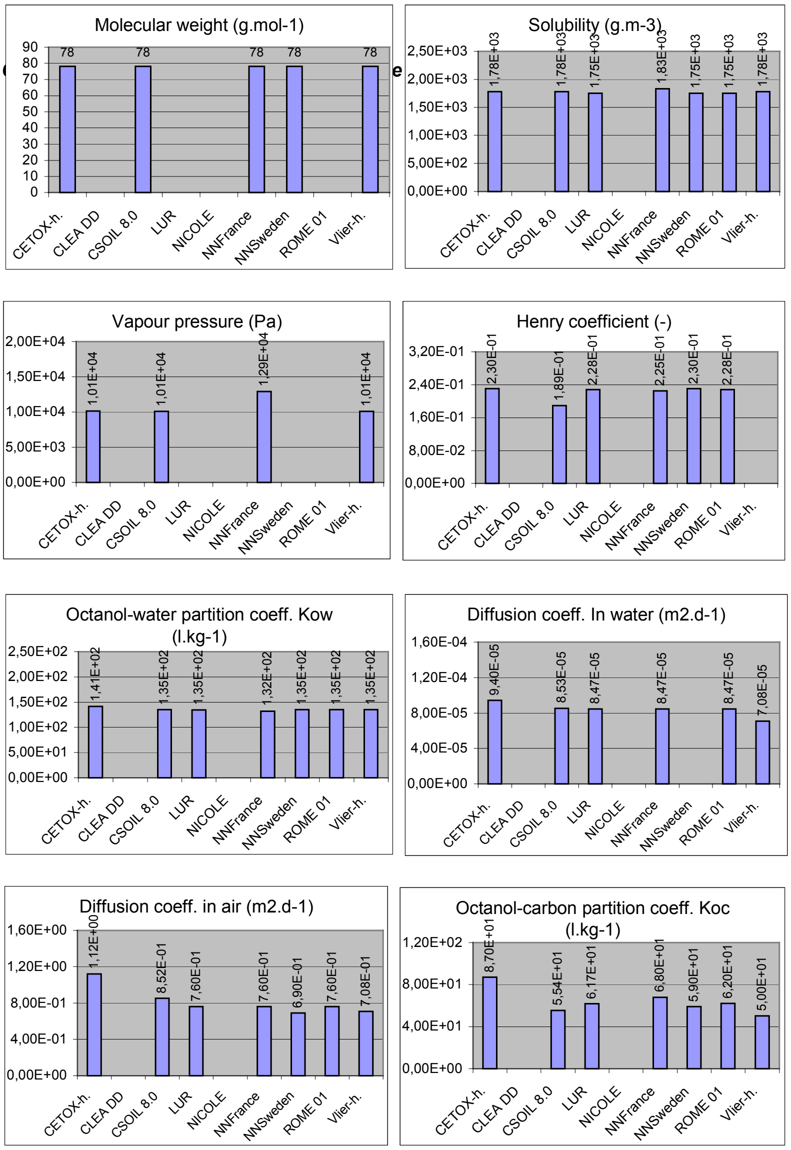

Figure 4.1 (continued): Bar charts of the default input parameters: benzene-specific input parameters.

When "0" or any other number is lacking this input parameter is not used in the model.

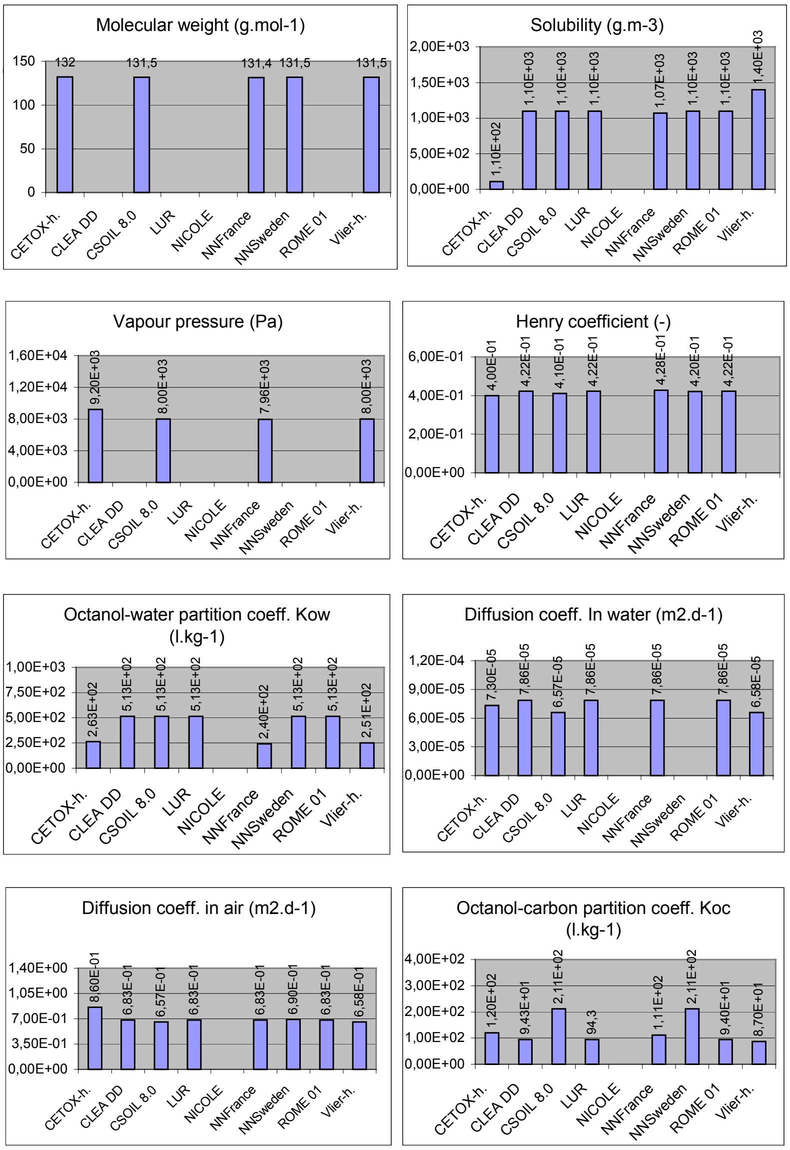

Figure 4.1 (continued): Bar charts of the default input parameters: trichloroethene-specific input parameters.

When "0" or any other number is lacking this input parameter is not used in the model.

4.2 Conclusions

In the following sections the major conclusions are drawn about the variation in default input parameters used in different approaches. To this purpose the following (arbitrary) categorisation has been used:

- The difference between the extreme values is within a factor of 2: default input parameters are "similar".
- The difference between the extreme values is in between a factor of 2 and 10: there is a "substantial variation" in the default input parameters.
- The difference between the extreme values is in between a factor of 10 and 100: there is a "large variation" in the default input parameters.
- The difference between the extreme values is more than a factor of 100: there is a "huge variation" in the default input parameters.

The conclusions are drawn in the order of increasing variation in the default input parameters.

4.2.1 Human characteristics

- The *Body weight* is similar for all approaches, although in the CETOX-human approach a lower *Body weight* for children is used.
- The *Breathing volume* is similar for all approaches, although in the CETOX-human approach a relatively high *Breathing volume* for children and in the NICOLE approach a relatively low *Breathing volume* for adults is used.
- There is a substantial variation in most *Residence times* between the approaches. In all approaches the *Residence time at an industrial site for children* is zero, except for the NoNameSweden approach where this is 8 hours.
- There is a substantial variation in the *Amount of total consumption of root vegetables* for children (from 15 g_{dw}/day in the CSOIL 8.0 and NoNameSweden approaches up to 95 g_{dw}/day in the CETOX-human approach) and for adults (from 28 g_{dw}/day in the CSOIL 8.0 approach up to 225 g_{dw}/day in the CETOX-human approach). The same trend is found for the *Amount of total consumption of leafy vegetables*.
- There is a substantial variation in the *Average daily soil intake at a residential site* for adults (from 1 mg/day in the NICOLE approach up to 100 mg/day in the ROME 01 approach) and a large variation in the *Average daily soil intake at a residential site* for children (from 40 mg/day in the NICOLE approach up to 1000 mg/day in the Danish approach). The same trend is found for the *Average daily soil intake at an industrial site* adults.

4.2.2 Input parameters in relation to Exposure via crop consumption

- The *Moisture content of root and leafy vegetables* is similar for all approaches.
- There is a substantial variation in the *Fraction of total root and leafy vegetable consumption that is homegrown* (from 10% for the CSOIL 8.0 approach up to 50% (for *root vegetables*) and 60% (for *leafy vegetables*) for the NICOLE approach).

4.2.3 Input parameters in relation to Exposure via inhalation of indoor air

- There is a substantial variation in the *Ventilation frequency of a house* (from 0.3 1/h for the CETOX-human approach up to 1.25 1/h for Vlier-humaan and the CSOIL 8.0 approaches). The same trend is found for the *Ventilation frequency of a building at an industrial site*.

The *Surface of a house*, the *Surface of a building at an industrial site,* the *Volume of a house* and the *Volume of a building at an industrial site* has not been compared, because of differences in building construction types in different countries. In some approaches transport of volatile contaminants from the soil to a crawl space, having a different surface and volume, is considered.

4.2.4 Input parameters related to other exposure pathways

- The *Fraction soil particles in suspended air, indoors* and the *Fraction soil particles in suspended air, outdoors* is similar in all approaches.
- There is a substantial variation in the *Concentration in suspended particles in the air at a residential site, indoors* (from 0.05 mg/m^3 for the NoNameFrance 2000 and the CSOIL 8.0 approaches up to 0.15 mg/m^3 for the CETOX-human approach). There is a large variation in the *Concentration in suspended particles in the air at an industrial site, indoors* (from 0.05 mg/m^3 for the CSOIL 8.0 approach up to 1.07 mg/m^3 for the Vlier-humaan approach).

4.2.5 Contaminant-specific input parameters

Conclusions are only drawn for benzo(a)pyrene, cadmium, benzene and trichloroethene, not for atrazine because of lack of data from the questionnaires.

- The *Molecular weight* is similar for all contaminants in all approaches.
- The *Solubility* is similar for benzene in all approaches; however, there is a large variation in the *Solubility* for benzo(a)pyrene and trichloroethene.
- The *Vapour pressure* is similar for benzene and trichloroethene for all approaches; however, there is a large variation in the *vapour pressure* for benzo(a)pyrene.
- The *Henry coefficient* is similar for benzene and trichloroethene for all approaches; however, there is a large variation in the *Henry coefficient for* benzo(a)pyrene.
- The *Octanol-water partition coefficient Kow* is similar for benzene for all approaches; however, there is a substantial variation in the *Octanol-water partition coefficient Kow* for benzo(a)pyrene and trichloroethene.
- The *Diffusion coefficient in water* is similar for benzene, trichloroethene and, to a lesser extent, for benzo(a)pyrene for all approaches. The same trend is found for *Diffusion coefficient in air*.
- The *Octanol-carbon partition coefficient Koc* is similar for benzo(a)pyrene and for benzene for all approaches; however there is a substantial variation for the *Octanol-carbon*

partition coefficient Koc for trichloroethene. There is a huge variation in the *Partition coefficient solid phase/ pore water* for cadmium (from 75 l/kg for the LUR approach up to 5010 l/kg for the CETOX-human approach).

- There is a huge variation in the *BioConcentrationFactor for root and leafy vegetables* for benzo(a)pyrene (root vegetables: from 0.00098 mg/kg-crop$_{fw}$: mg/l$_{pore\ water}$ for the NoNameFrance 2000 approach up to 15000 mg/kg-crop$_{fw}$: mg/l$_{pore\ water}$ for the NoNameSweden approach; leafy vegetables: (from 0.054 mg/kg-crop$_{fw}$: mg/l$_{pore\ water}$ for the NoNameFrance 2000 approach up to 8150 mg/kg-crop$_{fw}$: mg/l$_{pore\ water}$ for the CETOX-human approach). There also is a huge variation in the *BioConcentrationFactor for root and leafy vegetables* for cadmium (root vegetables: from 0.15 mg/kg-crop$_{dw}$: mg/kg$_{soil}$ for the CSOIL 8.0 and the Vlier-Humaan approach up to 796 mg/kg-crop$_{dw}$: mg/kg$_{soil}$ for the CETOX-human approach; leafy vegetables: (from 0.07 mg/kg-crop$_{dw}$: mg/kg$_{soil}$ for the CSOIL 8.0 approach up to 137 mg/kg-crop$_{dw}$: mg/kg$_{soil}$ for the CETOX-human approach. Note that some of the *BioConcentrationFactors* have been based on measured data, while others have been calculated.
- Half of the models use a *Relative retention factor for soil particles in lungs* of 0.75, while the other half of the models use a *Relative retention factor for soil particles in lungs* of 1.0.

5. Comparison of calculated exposure

For practical purposes policy makers and model users are usually interested in absolute values of exposure, because these absolute exposures are directly related to human risks. However, the purpose of this study is focused on *variation* in exposure. No attention has been given to (giving insight into/ evaluating) absolute values of exposure.

For at least two reasons high or low variations in calculated exposures or in concentrations of contactmedia or in soil compartments, are not necessarily criteria for "good" or "bad" calculations or models:

- Because of differences in geographical and ethnological conditions within Europe exposure from the same source and under the same conditions is not necessarily equal. These differences might be revealed more clearly in calculated exposure when country-specific default parameters are used. However, calculated exposure from the same source and under the same conditions will also be different when standardised input parameters are used, because many model concepts contain "country-specific/ region-specific" elements. There is no insight into actual differences in exposures in the several countries for which models are participating.
- When testing the accuracy of models often a comparison between calculated and measured outputs is made. With the purpose to quantify this accuracy of models many statistical model indicators are available which quantify the degree of approximation (or misfit) between calculated and measured data, see for example Janssen and Heuberger (1995). However, no measured data on human exposure are available, which implies that the "correct exposure" is not known, and the accuracy of calculated exposures or the quality of the participating models can not be tested in this study.

As a consequence comparison of calculated exposure does not give information about the accuracy of model calculations, but only can be used to describe the variation between separate model calculations.

5.1 Scenarios

To be able to calculate human exposure with each of the seven European models hypothetical scenarios have been defined. These scenarios differ in respect to two land uses (residential and industrial), two soil types, and five different contaminants. This results in twenty hypothetical scenarios.

The soil types are described as follows:

- Sandy soil, with an "average" organic matter content: 0% clay, 10% silt, 90% sand; porosity 40% (20% air; 20% pore water); groundwater table at 1.25 m below surface; average soil temperature of 10 °C; 5% organic matter content; dry bulk density of 1.5 $kg.l^{-1}$.

- Clay soil, with a "high" organic matter content: 60% clay, 20% silt, 20% sand; porosity 50% (10% air; 40% pore water); groundwater table at 1.25 m below surface; average soil temperature of 10 °C; 10% organic matter content; dry bulk density of 1.2 $kg.l^{-1}$.

The five contaminants, which are considered to be common throughout Europe, have different exposure characteristics:
- benzo(a)pyrene (PAH); major exposure pathway: soil ingestion and, to a lesser extent, crop consumption;
- cadmium (metals); major exposure pathway: soil ingestion and, to a lesser extent, crop consumption;
- atrazine (pesticides); major exposure pathways: soil ingestion and crop consumption;
- benzene (aromatic compounds); major exposure pathway: inhalation of indoor air;
- trichloroethene (volatile aliphatic compounds); major exposure pathway: inhalation of indoor air.

The following assumptions have been defined:
- Average soil content, homogeneously distributed over the site (spatial distribution) and the unsaturated zone of the soil (depth distribution):
  - benzo(a)pyrene: 40 $mg.kg_{dw}^{-1}$;
  - cadmium: 12 $mg.kg_{dw}^{-1}$;
  - atrazine: 6 $mg.kg_{dw}^{-1}$;
  - benzene: 1 $mg.kg_{dw}^{-1}$;
  - trichloroethene: 60 $mg.kg_{dw}^{-1}$.

  These concentrations are equal to the Dutch Intervention Values (Ministry of VROM, 1994).
- Age ranges (average daily exposure over the time period given [$mg.kg_{body\ weight}^{-1}.d^{-1}$]):
  - child (0-6 years);
  - adult (20-70 years);
  - lifelong (0-70 years).

5.2 Outputs

All exposure calculations have been performed twice for all twenty scenarios:
- once with a prescribed set of parameters (*standardised input parameters*) derived from the data set that was used to derive the Dutch soil quality standards (Swartjes 1999), but with the elimination of some typical Dutch features (e.g. construction of a house, including a crawl space). Furthermore, several parameters have been schematised, such as a homogeneous depth distribution of the contaminants in the unsaturated zone.
- once with the data that is used in different countries (*country-specific default input parameters*). In some cases these input parameters can be considered as "national" input parameters.

In each calculation exposure via the following three major exposure pathways is calculated:
- exposure via soil ingestion;
- exposure via crop consumption;
- exposure via indoor air inhalation.

Total exposure via all exposure pathways combined is also calculated.

Eighteen different outputs have been defined for each calculation (see Figure 5.1):
- lifelong exposure and exposure to children and adults via the three major exposure pathways (soil ingestion, crop consumption, indoor air inhalation),
- lifelong exposure and exposure to children and adults via all exposure pathways combined,
- concentrations in contactmedia (root vegetables, leafy vegetables (due to root uptake and due to deposition), indoor air), and
- concentrations in the soil compartments (pore water, soil air).

Also the remaining exposure via to other exposure pathways has been calculated (lifelong, to children and adults), by subtracting exposure via the three major exposure pathways from total exposure (see also Figure 5.1).

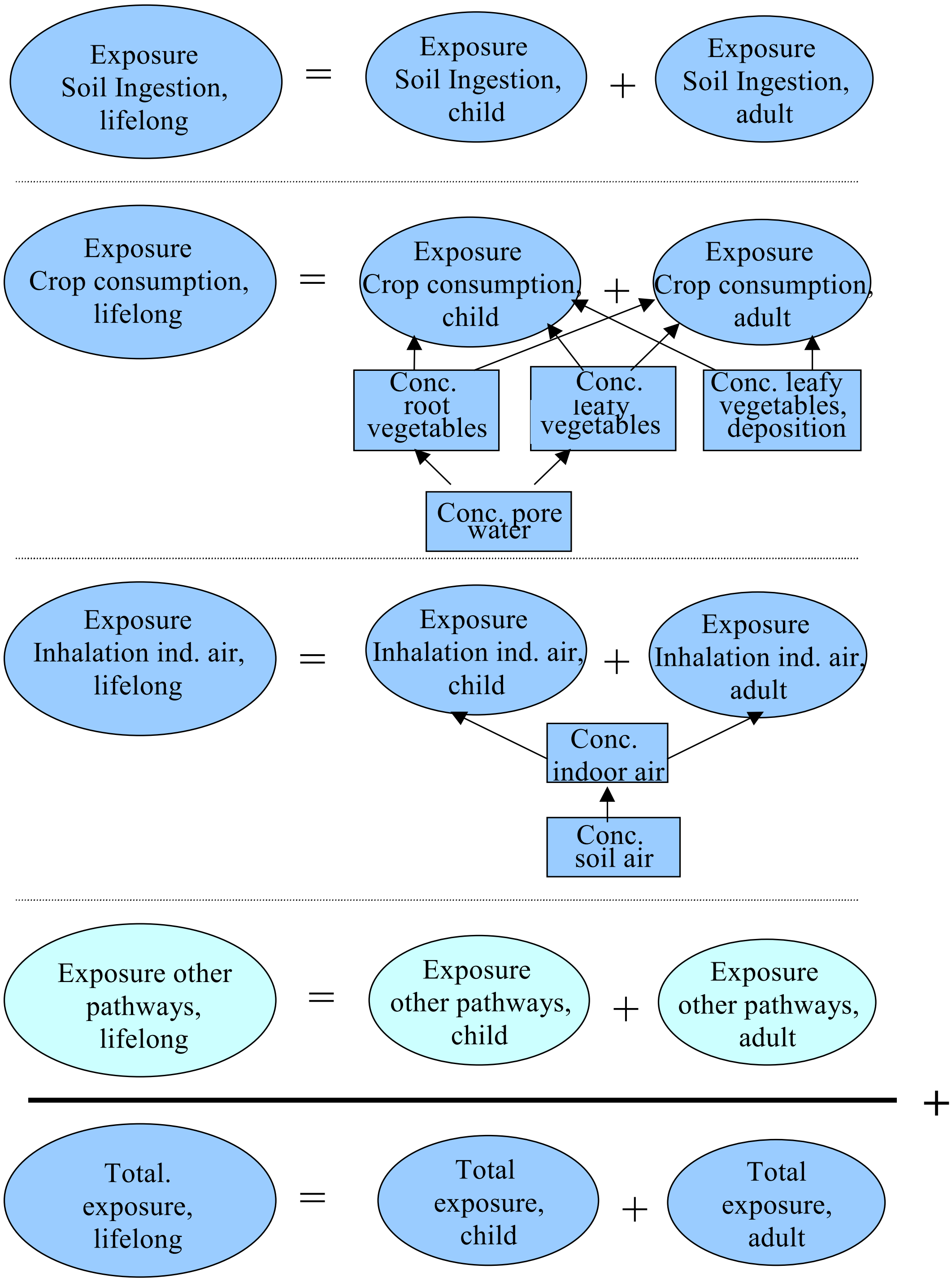

Figure 5.1: Outputs calculated in this study (in blue) and their interactions; ovals represent exposure, boxes represent concentrations in contactmedia and soil compartments.

As has been presented in Figure 5.1, there is an interaction between several outputs.

5.3 Definitions

Definitions were formulated for use in all of the participating human exposure models. These definitions are as follows:
Input parameters:

- Standardised input parameters: a prescribed set of parameters derived from the data set that was used to derive the Dutch soil quality standards (*Swartjes, 1999*), but with the elimination of some typical Dutch features. Furthermore, several parameters have been schematised, such as a homogeneous depth distribution of the contaminants in the unsaturated zone.
- Country-specific default input parameters: input parameters used for the derivation of soil quality standards, in risk assessment procedures and/or described or listed in manuals in the different countries.

Exposure:

- Exposure: amount of a contaminant expressed in [$mg.kg_{bw}^{-1}.day^{-1}$] that enters the blood or target organ (internal doses) of an average human being due to soil contamination (not to groundwater contamination). Sensitive groups like children showing pica behaviour or pregnant women are not considered in this study.
- Potential exposure: exposure representative of the soil use (i.e. residential, industrial), can be seen as the average exposure for a large number of sites with that particular type of soil use.
- Exposure via soil ingestion: potential exposure due to unintentional oral intake of soil particles (i.e. not including inhalative intake of suspended soil particles or dust).
- Exposure via crop consumption: potential exposure due to oral intake of contaminated homegrown crops from a “standard garden” (i.e. not a vegetable garden at a location other than the residential environment). Contamination of crops can be caused by root uptake and/or deposition (“deposition” means here the deposition of soil particles adhering to the crops originating from the contaminated site); no contamination of crops from vapours is considered.
    - Root vegetables: the part of the crop growing under the soil surface, including potatoes.
    - leafy vegetables: the part of the crop growing above the soil surface.
- Exposure via indoor air inhalation: potential exposure due to unconscious inhalative intake of contaminated indoor air (vapours, excluding suspended particles), originating from contaminated soil (not from contaminated groundwater), in a house or building; consider a house or building as a one-storey, one-compartment structure, directly situated above the soil surface.

Soil use:

- Residential site: site where living is the main function; house and garden are included; garden crops are consumed as vegetables, although crop consumption is not the main function of the garden.
- Industrial site: site where industrial activity is the main function; crop cultivation is excluded.

5.4 Procedure

Outputs were investigated in the following ways:

- Statistical interpretation of outputs. The influence of the different variables on exposure has been investigated and confidence limits have been determined using the REML (Residual Maximal Likelihood) method (GenStat statistical package). A severe limitation of this tool is caused by gaps in calculated outputs, which results in an asymmetric data set.
- Visual interpretation of variation in outputs.

Visual interpretation was found the most functional and efficient way to evaluate variation in calculated outputs. Therefore, the results from this procedure have been described in this report.

5.4.1 Visual interpretation

In general the formulae used to calculate exposure to children or to adults are similar. Besides many input parameters for the calculation of exposure to children and adults are similar. Therefore in depth visual evaluation of the lifelong exposures on the basis of comparing its variation with the variation in the respective exposures to children and adults is considered less important. Exposure to adults yielded the most extended data set. Therefore, only the variation in exposure to adults has been investigated in this study. As a consequence, the following questions are considered less important and left out of this study[2]:

- How does the variation in *Total lifelong exposure* relate to the variation in *Total exposure, child* and *Total exposure, adult*?
- How does the variation in the lifelong exposure via separate exposure pathways relate to the variation in the lifelong exposure to children and adults via these separate exposure pathways?
- How does the variation in *Total lifelong exposure* and the variation in the Total *exposure indoor air, child* relate to the variation in the concentration in the contactmedia (*Concentration root vegetables, Concentration leafy vegetables*), to the variation of the *Concentration in the pore water*, respectively *Concentration in soil air*, and to the variation in the input parameters?

It is assumed that the statistical distribution of calculated exposures and concentrations in contactmedia and in the soil compartments are unknown at forehand. Because of the limited number of “replies” of each calculated exposure and each calculated concentration in contactmedia (i.e. maximal seven) it is not meaningful to determinate the statistical distributions. Therefore the *median value* has been considered as representative figure for each output. This does not mean that the median value has been considered as *the correct* figure for the ideal human exposure or concentration in contactmedia or in the soil compartments, it simply serves a reference value to assess the variation.

[2] Calculated outputs and input parameters that has been compared in Chapter 4 and are used in this chapter for evaluation of the variation in exposures are presented *in italics*.

To be able to visually assess the variation in calculated outputs all calculated outputs are indexed according to the median value of the respective scenario. To this purpose the following index is used:

Relative deviation from the scenario-medians (RD).

To derive this RDs for a specific scenario, each of the seven individual model results is divided by the median value of these seven individual model results. In Figure 5.2 an example of the derivation of RDs for *Total exposure, adult* has been given. At the left hand-site of this figure absolute exposures are shown, calculated with the seven European models, for two different scenarios. At the right hand-site the RDs are shown for the same scenarios, which have been calculated simply by dividing each individual model result by the respective scenario median value.

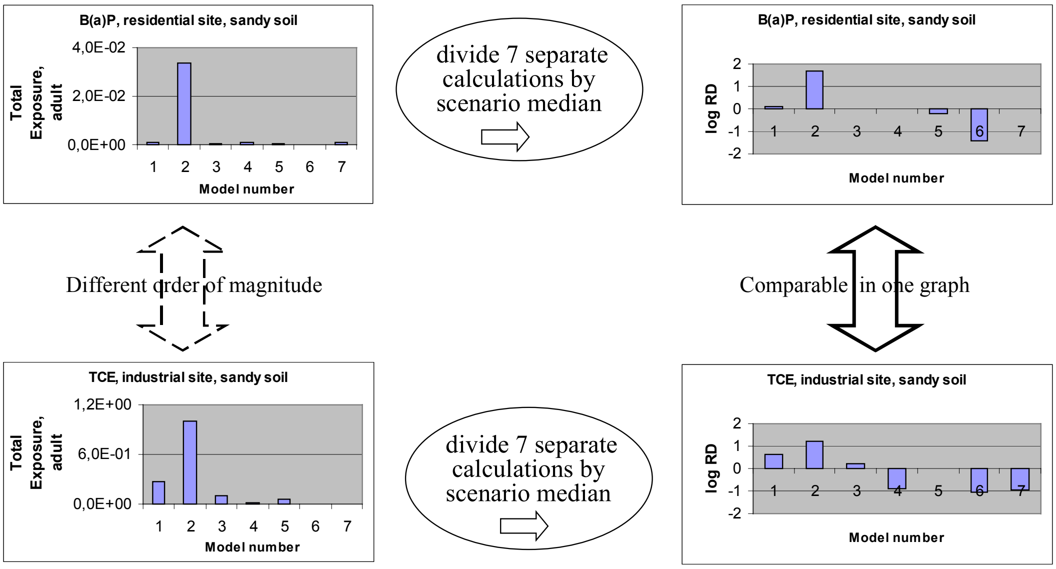

Figure 5.2: Example of calculated exposures (left side of the picture) and illustration of derivation of RDs (relative deviation from the scenario-medians) (right side of the picture). The numbers at the x-axes represent individual calculated outputs of the seven European models.

The resulting index represents a “factor x higher”, or “a factor y lower” than the median value of that specific scenario, for each specific output. The index enables mutual comparison of variation between a calculated output in different scenario’s, although absolute values of this output might be of a different order of magnitude. See Figure 5.2, for example, in which *Total exposure, adult* to benzo(a)pyrene on a residential site, sandy soil is compared with *Total* *exposure, adult* to trichloroethene on an industrial site, clay soil. The absolute exposures for these two scenarios are of another order of magnitude. Nevertheless, the RDs for both scenarios could be combined in one graph, resulting in 14 data points for this particular example.

As was mentioned at the beginning of this chapter high or low variations in calculated exposures or in concentrations in contactmedia or in the soil compartments, and hence high or low RDs (big or small deviations from scenario medians), are not necessarily criteria for “good” or “bad” calculations or models.

The following (arbitrary) categorisation has been used:
- The majority of the outputs is within a factor of 5 higher and a factor of 5 lower than the scenario medians: there is a "limited variation" in the calculated human exposures.
- The majority of the outputs is in between a factor of 10 higher and a factor of 10 lower than the scenario medians: there is a "substantial variation" in the calculated human exposures.
- The majority of the outputs is in between a factor of 100 higher and a factor of 100 lower than the scenario medians: there is a "large variation" in the calculated human exposures.
- The majority of the outputs is *not* in between a factor of 100 higher and a factor of 100 lower than the scenario medians: there is a "huge variation" in the calculated human exposures.

Besides, the 90%-confidence intervals were calculated under the assumption that the variation in RDs can be characterised by a log-normal distribution, although this assumption is debatable.

5.5 Contribution of separate exposure pathways to total exposure

Although the absolute exposures are not relevant for this study, the contribution of the separate exposure pathways to total exposure, adult might be important for the evaluation of variation in exposure. Therefore, for all five contaminants the *average* contribution of the separate exposure pathways (averaged for all scenarios and all calculated exposures with the seven European models) to Total exposure, adult is presented in Figure 5.3.

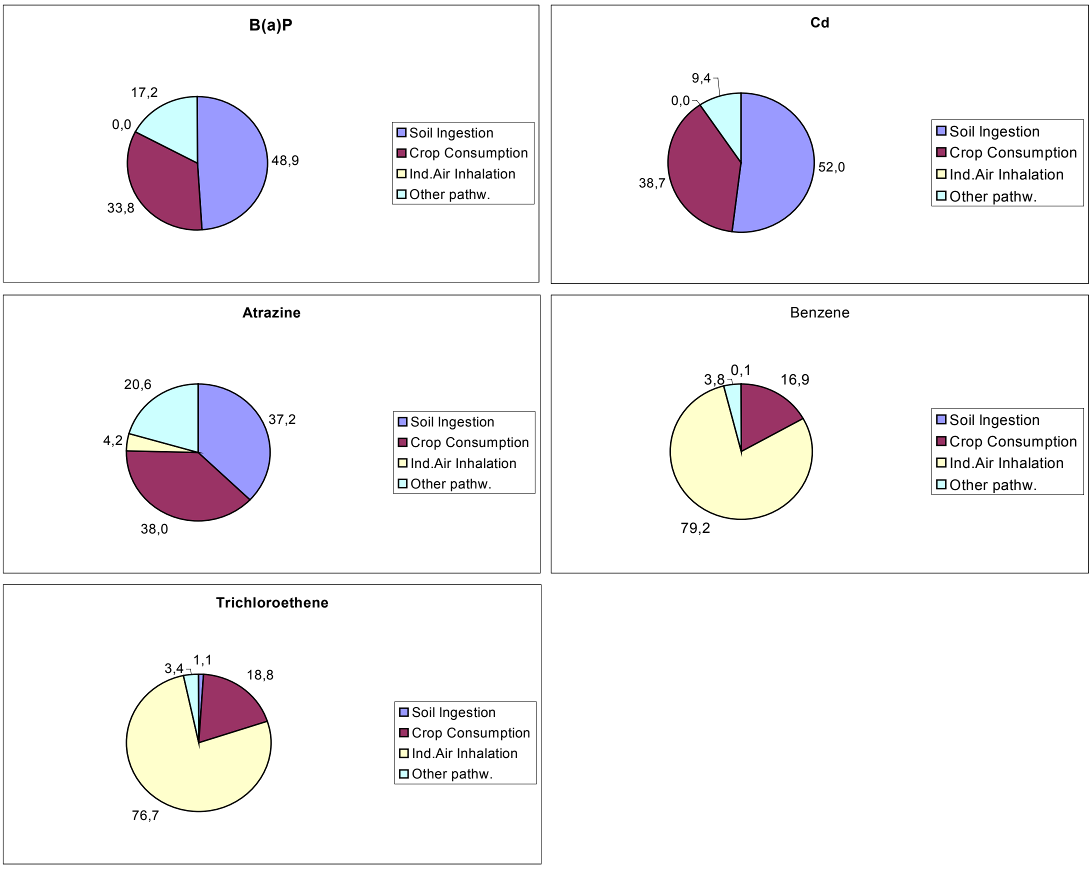

Figure 5.3: Contribution of the separate exposure pathways to total exposure, adult: average value (averaged for all scenarios and all calculated exposures with the seven European models) (%).

The variation in contribution of the separate exposure pathways between the different scenarios and models is substantial, see Table 5.1 in which, except for the average values, the standard deviation and coefficients of variation are presented. Nevertheless, these average contributions give an indication of the importance of the exposure pathways.

Table 5.1: Contribution of the separate exposure pathways to total exposure, adult (%); the values are average, standard deviation and coefficients of variation of all individual calculations, for all scenarios and all model calculations.

Exposure via soil ingestion	Exposure via crop consumption	Exposure via indoor air inhalation	Exposure via other pathways
48,92	33,83	0,04	17,21
42,73	42,73	0,10	27,12
0,87	1,26	2,33	1,58
51,97	38,67	na	9,36
46,72	47,48	na	22,98
0,90	1,23	na	2,45
37,19	37,96	4,23	20,61
46,27	48,31	18,25	41,28
1,24	1,27	4,31	2,00
0,14	16,86	79,23	3,77
0,27	29,40	30,03	10,24
2,00	1,74	0,38	2,72
1,11	18,83	76,65	3,40
6,67	32,47	32,87	9,56
6,00	1,72	0,43	2,81

From Figure 5.3 the following can be concluded:

- For benzo(a)pyrene and cadmium exposure via soil ingestion is the most important exposure pathway (contribution to total exposure, adult is circa $^1/_2$). Besides exposure via crop consumption is an important exposure pathway (contribution to total exposure, adult is circa $^1/_3$). Exposure via indoor air inhalation is not a relevant exposure pathway (contribution to total exposure, adult is less than 1% for benzo(a)pyrene and 0 for cadmium).
- For atrazine exposure via soil ingestion and exposure via crop consumption are the most important exposure pathways (contribution to total exposure, adult is circa $^1/_3$ for both exposure pathways). Exposure via indoor air inhalation is a minor exposure pathway (contribution to total exposure, adult is 4%).
- For benzene and trichloroethene exposure via indoor air inhalation is the dominant exposure pathway (contribution to total exposure, adult is circa $^4/_5$). Besides exposure via crop consumption plays a role (contribution to total exposure, adult is circa $^1/_5$). Exposure

via soil ingestion is not a relevant exposure pathway (contribution to total exposure, adult is 0.1; respectively 1%).

It should be noted that the contribution of the separate exposure pathways to total exposure should not necessarily represent the risk, because contaminants have different toxicity for oral or inhalative exposure. Exposure to benzo(a)pyrene, for example, is almost 100% orally, but is much more toxic by inhalative exposure. However, because no risk assessment is considered in this study, only variation in exposure, this is not a relevant issue in this human exposure comparison study.
In the evaluation of variation in exposures and concentrations in contactmedia (Section 5.6) all calculated outputs have been incorporated, unless the contribution of a specific exposure pathway is 0 (like for example exposure via indoor air inhalation for cadmium). The reason for this it that is has been assumed that the advantage of having more data available carries more weight then the disadvantage of the fact that the absolute value of exposure is low and hence the calculation would be less valuable. Even in case that the contribution to total exposure is low, a calculation of exposure via a specific exposure pathway can be assumed as another "reply" for a calculation according to that specific model concept, and using that specific input data, of the specific exposure pathway.

5.6 Results

5.6.1 Insight in the variation in calculated human exposure

5.6.1.1Total exposure, adult

Purpose 1 of the Human Exposure Comparison Study is: *Gaining insight into the variation in calculated human exposure*. This purpose serves policy makers, who are interested in the power and reliability of soil quality assessments in which exposure models are used, explicitly (site-specific calculation of exposure) or implicitly (using soil quality standards derived from exposure calculations). Besides, this purpose is interesting for individuals who manage and use exposure models. These target groups can learn about the correct use of models and improve (part of the) models to serve their specific purposes. As mentioned in Section 5.4.1, only the variation in exposure to adults, which is assumed to be representative for the variation in calculated human exposure in general, has been investigated.

The following key questions are important, for both target groups (i.e. policy makers and individuals who manage and develop models):

- How is the variation in *Total exposure, adult* when standardised input parameters are used (insight into variation due to different model concepts)?
- How is the variation in *Total exposure, adult* when country-specific default input parameters are used (insight in variation due to different model concepts and different input parameters)?

In Figure 5.4 the RDs for the *Total exposure, adult* have been presented as a function of type of input parameters, contaminant, model, soil use and soil type (260 calculated outputs). Each data point is this figure represents the RD for an individual calculation. In the figures the RDs for all scenarios have been combined. As a consequence the number of data points equals maximal 7 (number of models) x 20 (number of scenarios) x 2 (standardised input parameters versus own defaults) = 280. Note that the RDs (y-axes) are presented on a log scale.

From the graphs in Figure 5.4 the following can be concluded:

- In general, variation in *Total exposure, adult* is large: the majority of the individual calculations of the *Total exposure, adult* are in the range from a factor of 100 lower up to a factor of 100 higher than the scenario medians.
  The 90%-confidence interval ranges from a factor of 20 lower up to a factor of 21 higher than the scenario medians.
- A few individual calculations of the *Total exposure, adult* are more than a factor of 100 lower than the scenario medians (up to a factor of 600). These individual calculations were exposure to atrazine, calculated with the ROME 01 model, for a residential site. The reason for this is that one of the major exposure pathways, i.e. exposure via crop consumption, has not been incorporated in the ROME 01 model.
- Most variation in *Total exposure, adult* can be attributed to:
    - variation in exposure to atrazine (from a factor of 600 lower up to a factor of 10 higher than the scenario medians);
    - the ROME 01 model (from a factor of 600 lower than the scenario medians up to a factor of 2 higher than the scenario medians); again the reason for this is that one of the major exposure pathways, i.e. exposure via crop consumption, has not been incorporated in the ROME 01 model, which explains the relatively low values for these scenarios for which exposure via crop consumption is an important pathways in calculations with the other six models.
- In general, there is no clear influence from type of input parameters on the variation in *Total exposure, adult.* This suggests that the variation due to selection of input parameters does not yield an additional variation to *Total exposure, adult* over the variation due to model concepts.
- In general, there is no clear influence from soil use or soil type on the variation in *Total exposure, adult.*

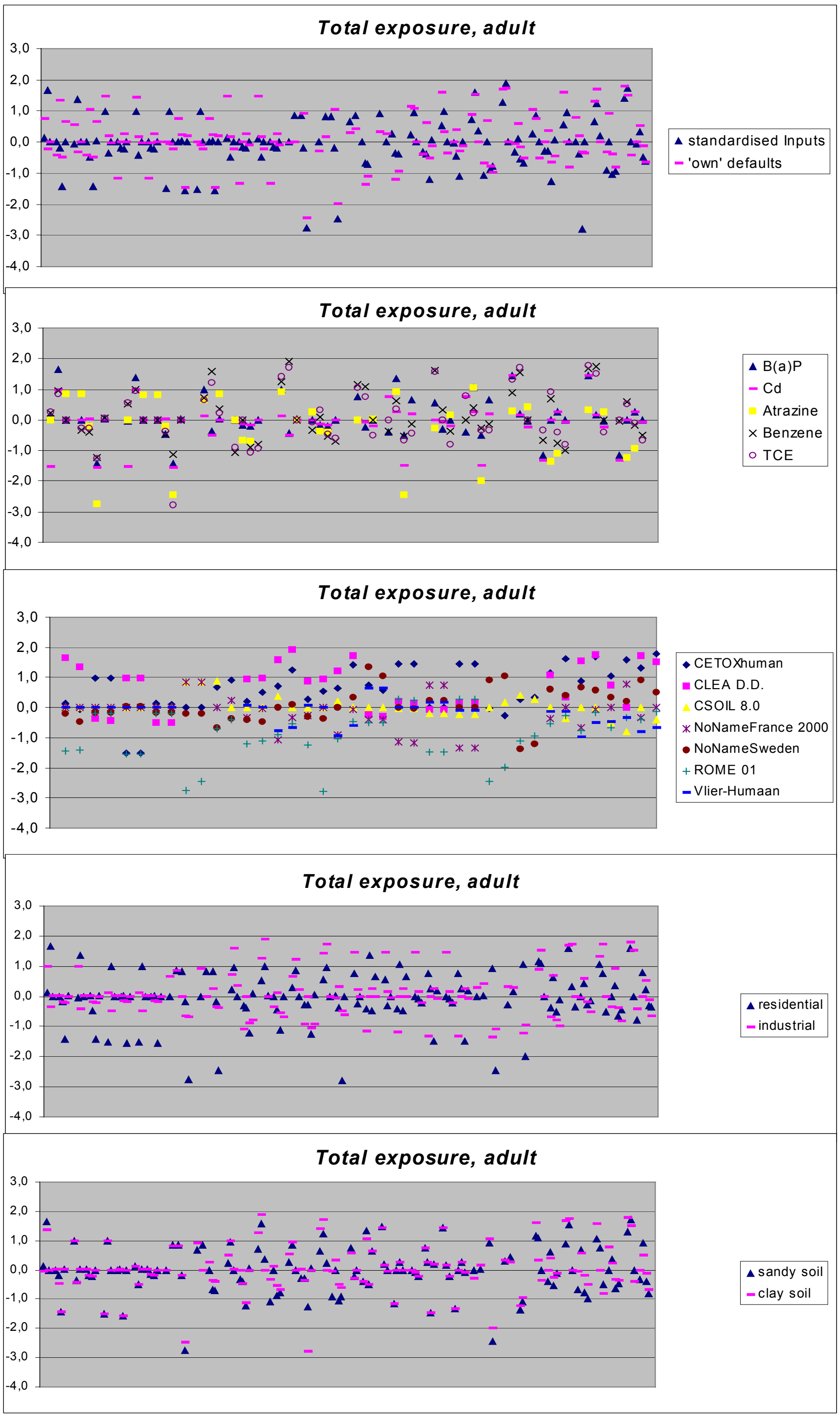

Figure 5.4: RDs (relative deviation from the scenario-medians) for the *Total exposure, adult* as a function of type of input parameters, contaminant, model, soil use and soil type.
RDs at log scale. Each symbol represents an individual model calculation. Note that exposure via crop consumption, has not been incorporated in the ROME 01 model.

5.6.1.2 Exposure via separate exposure pathways

Not every exposure pathway is relevant for each contaminated site. Besides, not every exposure pathway is included in every model. For these reasons it is important to have insight into the variation in exposure for the separate exposure pathways (*Exposure via soil ingestion, Exposure via crop consumption* and *Exposure via indoor air inhalation)*. It is also important how the variation in *Total exposure* relates to the variation in calculated exposure via the separate exposure pathways. In this perspective the following questions are important for both target groups (i.e. policy makers and individuals who manage and develop models):

- How is the variation in calculated exposure via the separate exposure pathways for adults *(*i.e. *Exposure via soil ingestion, Exposure via crop consumption, Exposure via indoor air inhalation)* when standardised input parameters are used (insight into variation due to different model concepts)?
- How is the variation in calculated exposure via the separate exposure pathways for adults *(*i.e. *Exposure via soil ingestion, Exposure via crop consumption, Exposure via indoor air inhalation)* when country-specific default input parameters are used (insight into variation due to different model concepts and different input parameters)?

The relation between *Total exposure, adult* and calculated exposure to adults via the separate pathways has been illustrated in Figure 5.5.

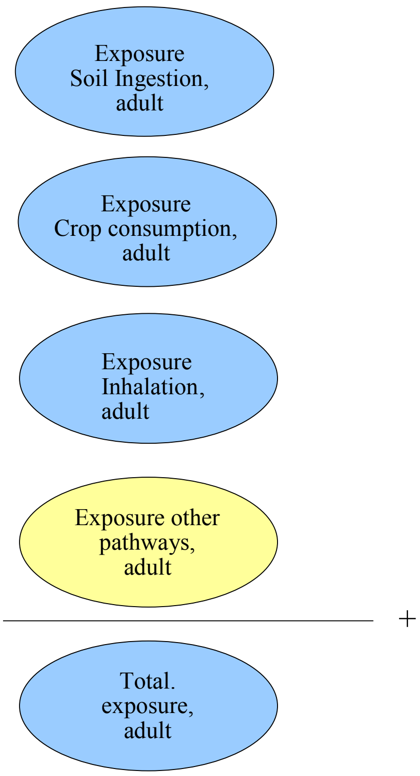

Figure 5.5: Relation between Total exposure, adult and the exposures to adults via separate pathways (dark shaded parts outputs has been evaluated in this study).

In Figure 5.6 the RDs have been presented for the *Total exposure, adult* (260 calculated outputs) and for the calculated exposure via the separate exposure pathways for adults, i.e. *Exposure via soil ingestion, adult* (260 calculated outputs), *Exposure via crop consumption, adult* (110 calculated outputs) and *Exposure via indoor air inhalation, adult* (204 calculated outputs), as a function of type of input parameters.

From the graphs in Figure 5.6 the following can be concluded:

- In general, variation in *Exposure via soil ingestion, adult* is limited: the majority of the individual calculations of *Exposure via soil ingestion, adult* is equal to the scenario medians or within the range from a factor of 5 lower up to a factor of 2 higher than the scenario medians.
  The 90%-confidence interval ranges from a factor of 5 lower up to a factor of 3 higher than the scenario medians.
- In general, variation in *Exposure via crop consumption, adult* is substantial: the majority of the individual calculations of *Exposure via crop consumption, adult* are in the range from a factor of 10 lower up to a factor of 10 higher than the scenario medians. The 90%-confidence interval ranges from a factor of 13 lower up to a factor of 11 higher than the scenario medians.
- In general, variation in *Exposure via indoor air inhalation, adult* is large: the majority of the individual calculations of the *Exposure via Indoor air inhalation, adult* are in the range from a factor of 100 lower up to a factor of 100 higher than the scenario medians. The 90%-confidence interval ranges from a factor of 27 lower up to a factor of 71 higher than the scenario medians.

More details in variation in exposure via the separate exposure pathways are given in Section 5.6.1.3.

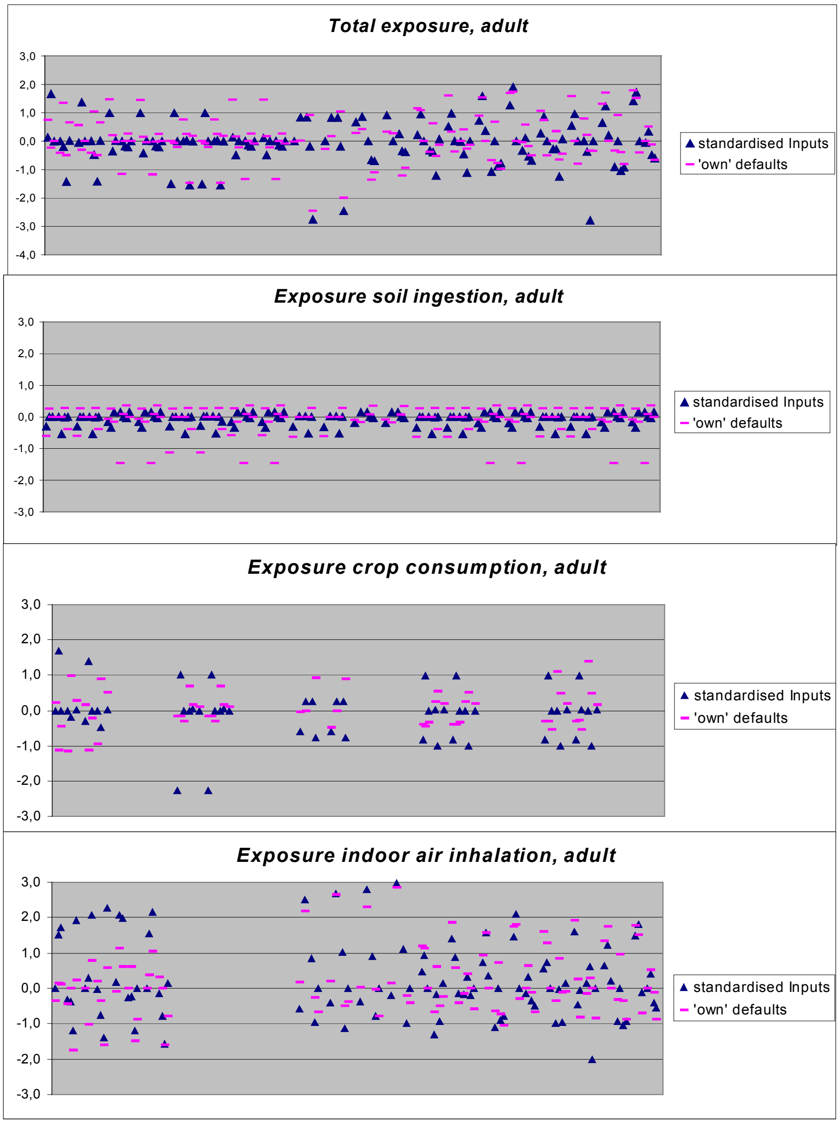

Figure 5.6: RDs (relative deviation from the scenario-medians) for Total exposure, adult and for Exposure via soil ingestion, adult; Exposure via crop consumption, adult and Exposure via indoor air inhalation, adult, as a function of type of input parameters.
RDs at log scale. Each symbol represents an individual model calculation.

5.6.1.3 The influence of site characteristics on exposure via separate exposure pathways

It is also important to have insight into the influence of site characteristics (type of contaminant, soil use and soil type) and the influence of type of model on the variation in exposure for the separate exposure pathways (*Exposure via soil ingestion, adult; Exposure via crop consumption, adult* and *Exposure via indoor air inhalation, adult)*. In this perspective the following questions are important for both target groups (i.e. policy makers and individuals who manage and develop models):

- How is the variation in calculated exposure to adults via the separate exposure pathways (i.e. *Exposure via soil ingestion, adult; Exposure via crop consumption, adult; Exposure via indoor air inhalation, adult)* related to contaminant, soil use, soil type and model when standardised input parameters are used (insight into variation due to different model concepts for the separate exposure pathways)?
- How is the variation in calculated exposure to adults via the separate exposure pathways (i.e. *Exposure via soil ingestion, adult; Exposure via crop consumption, adult* and *Exposure via indoor air inhalation, adult)* related to contaminant, soil use, soil type and model when country-specific default input parameters are used (insight into variation due to different model concepts and different input parameters for the separate exposure pathways)?

Exposure via soil ingestion

In Figure 5.7 the RDs for *Exposure via soil ingestion, adult* have been presented as a function of type of input parameters, contaminant, model, soil use and soil type (260 calculated outputs).

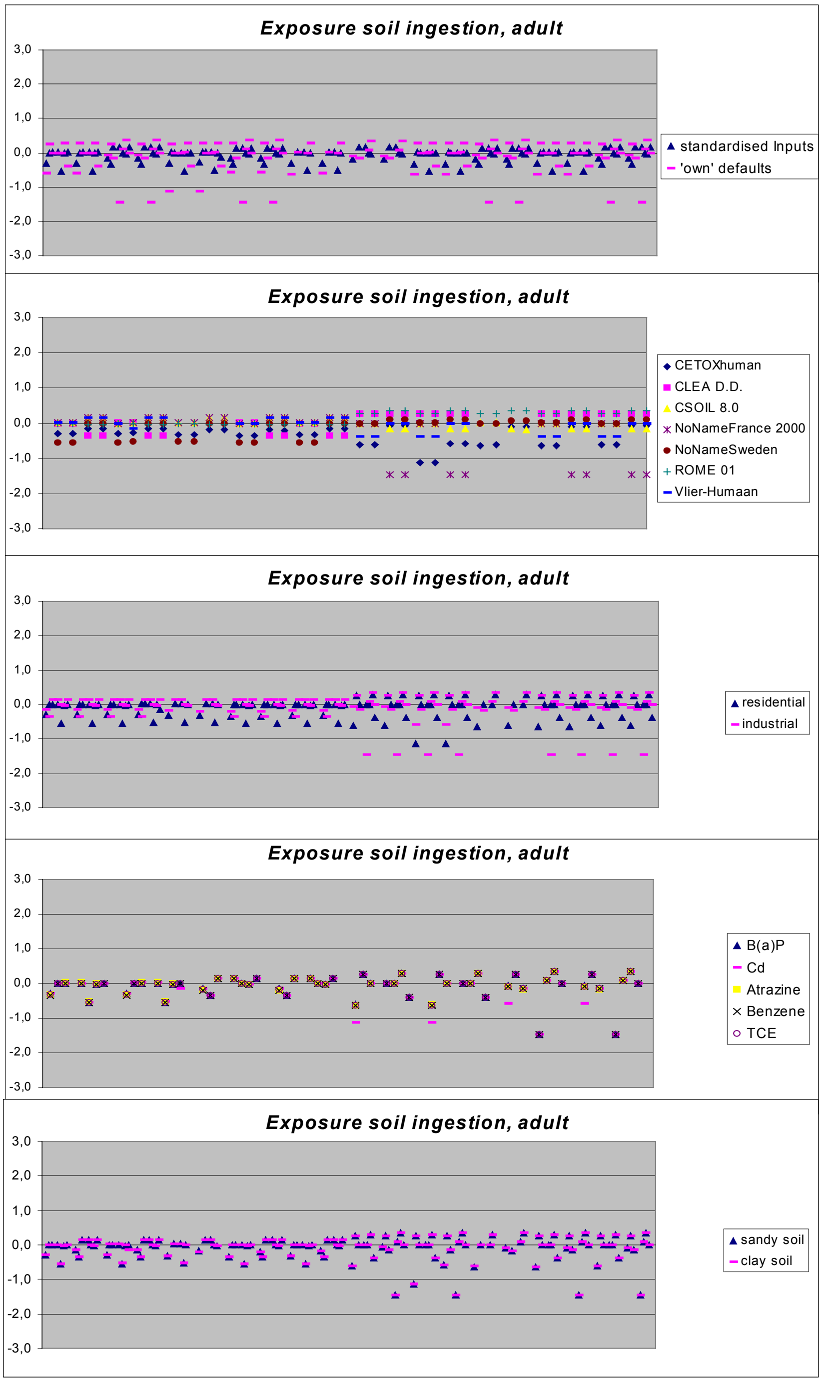

Figure 5.7: RDs (relative deviation from the scenario-medians) for the Exposure via soil ingestion, adult, as a function of type of input parameters, contaminant, model, soil use and soil type.

RDs at log scale. Each symbol represents an individual model calculation.

It was already concluded that in general variation in *Exposure via soil ingestion, adult* is limited. Besides from the graphs in Figure 5.7 the following can be concluded:

- A few individual calculations of the *Exposure via soil ingestion, adult* are more than a factor of 10 lower than the scenario medians (up to a factor of 30). These individual calculations concern exposure calculated with the NoNameFrance 2000 model, using country-specific default parameters, for industrial sites. This suggests that for these calculations the selection of input parameters yields additional variation in *Exposure via soil ingestion, adult.*
- In general, variation in *Exposure via soil ingestion, adult* is much larger when country-specific default input parameters are used. This suggests that in general the variation due to selection of input parameters does seem to yield an additional variation to *Total exposure, adult* over the variation due to model concepts.
- In general *Exposure via soil ingestion, adult* on a residential site gives slightly larger variation than *Exposure via soil ingestion, adult* on an industrial site.
- In general there is no clear influence from contaminant, model, or soil type on the variation in *Exposure via soil ingestion, adult.*

<u>Exposure via crop consumption</u>

In Figure 5.8 the RDs for *Exposure via crop consumption, adult* have been presented as a function of type of input parameters, contaminant, model, soil use and soil type (110 calculated outputs).

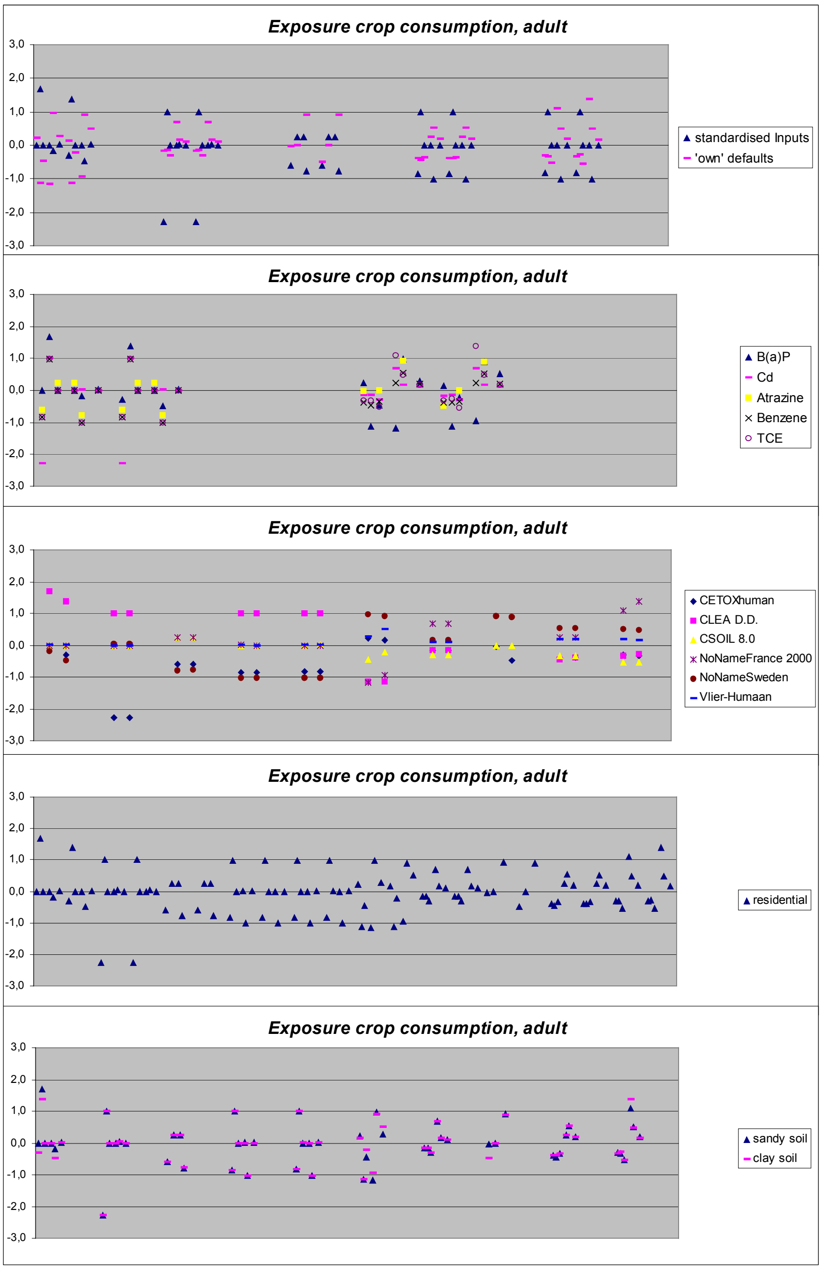

Figure 5.8: RDs (relative deviation from the scenario-medians) for the Exposure via crop consumption, adult, as a function of type of input parameters, contaminant, model, soil use and soil type.
RDs at log scale. Each symbol represents an individual model calculation.

It was already concluded that in general, variation in *Exposure via crop consumption, adult* is substantial. Besides, from the graphs in Figure 5.8 the following can be concluded:

- A few individual calculations of the *Exposure via crop consumption, adult* are more than a factor of 10 lower than the scenario medians (up to a factor of 200). These individual calculations were exposures to cadmium, calculated with the CETOX-human model, using standardised parameters, for residential sites.
- A few individual calculations of the *Exposure via crop consumption, adult* are more than a factor of 10 higher than the scenario medians (up to a factor of 50). These individual calculations were exposures to benzo(a)pyrene, calculated with the CLEA D.D. model and exposure to trichloroethene, calculated with the NoNameFrance 2000 model.
- Most variation in *Exposure via crop consumption, adult* can be attributed to:
    - variation in exposure to cadmium (from a factor of 200 lower up to a factor of 10 higher than the scenario medians) and to a lesser extent to the variation in exposure to benzo(a)pyrene (from a factor of 15 lower up to a factor of 50 higher than the scenario medians) and to the variation in exposure to trichloroethene (from a factor of 10 lower up to a factor of 25 higher than the scenario medians);
    - calculation with the CLEA D.D. model (from a factor of 15 lower up to a factor of 50 higher than the scenario medians).
- In case standardised input parameters are used more calculations of *Exposure via crop consumption, adult* give values close to the scenario medians. However, also large deviations from the scenario medians are found when standardised input parameters are used. This suggests that only in some cases the selection of input parameters does yield an additional variation to *Exposure via crop consumption, adult* over the variation due to model concepts.
- In general, there is no clear influence from soil type on the variation in *Exposure via crop consumption, adult.*

The pathway exposure via crop consumption on industrial sites was excluded in this study, and hence the influence of soil use on *Exposure via crop consumption, adult*, has not been investigated.

<u>Exposure via indoor air inhalation</u>

In Figure 5.9 the RDs for *Exposure via indoor air inhalation, adult* have been presented as a function of type of input parameters, contaminant, model, soil use and soil type (204 calculated outputs).

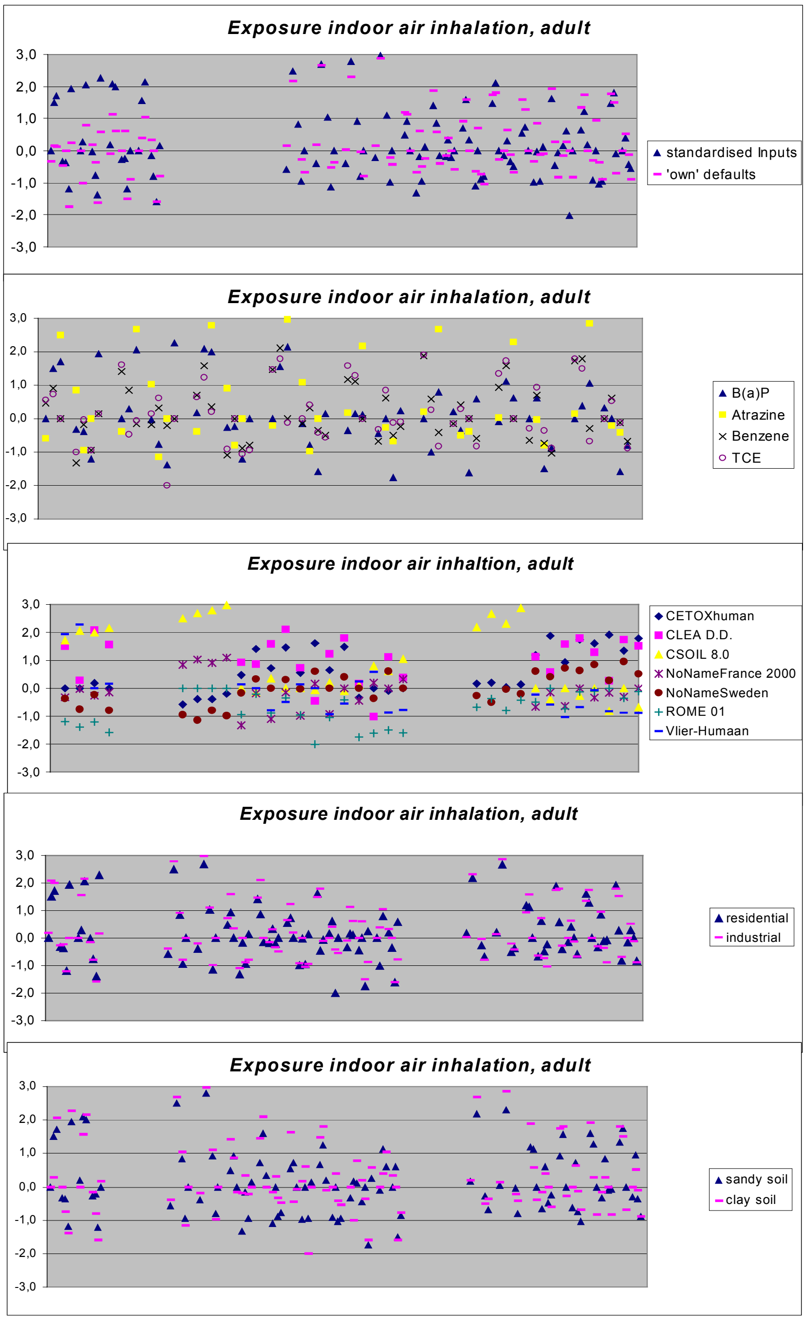

Figure 5.9: RDs (relative deviation from the scenario-medians) for the Exposure via indoor air inhalation, adult, as a function of type of input parameters, contaminant, model, soil use and soil type.

RDs at log scale. Each symbol represents an individual model calculation.

It was already concluded that variation in *Exposure via indoor air inhalation, adult* is large. Besides, from the graphs in Figure 5.9 the following can be concluded:

- A number of individual calculations of the *Exposure via indoor air inhalation, adult* give exposures that are more than a factor of 100 higher than the scenario medians (up to a factor of 900). These individual calculations were mainly exposures to atrazine (low contribution of exposure via indoor air inhalation to total exposure), calculated with the CSOIL 8.0 model.
- Most variation in *Exposure via indoor air inhalation, adult* can be attributed to:
    - variation in exposure to atrazine (from a factor of 15 lower up to a factor of 900 higher than the scenario medians) and to a lesser extent to the variation in exposure to benzo(a)pyrene (from a factor of 60 lower up to a factor of 190 higher than the scenario medians; low contribution to total exposure);
    - calculation with the CSOIL 8.0 model (from a factor of 10 lower up to a factor of 1000 higher than the scenario medians) and to a lesser extent calculation with the CETOX-human model (from a factor of 5 lower up to a factor of 900 higher than the scenario medians) and calculation with the ROME 01 model (from a factor of 100 lower up to values equal to the scenario medians); however, for all models variation in *Exposure via indoor air inhalation, adult* is large.
- In general, there is no clear influence from type of input parameters on the variation in *Exposure via indoor air inhalation, adult.* This suggests that the variation due to selection of input parameters does not yield an additional variation to *Exposure via indoor air inhalation, adult* over the variation due to model concepts.
- In general, there is no clear influence from soil use, or soil type on the variation in *Exposure via indoor air inhalation, adult.*

5.6.2 Understanding the variation in calculated human exposure

A second purpose of this human exposure comparison study is: *Understanding the variation in calculated human exposure*. This purpose is important for the individuals who manage and use exposure models and in fact need to understand all details of the model. For this purpose an extensive number of questions is relevant, among others focused on the relation between variation in exposures and in concentration in contactmedia, the relation between variation in exposures and in concentration in soil compartments, and the relation between variation in concentration in contactmedia and concentration in soil compartments. The most important questions for the individuals who manage and use exposure models are of the format:

- How does the variation in exposure via a specific exposure pathway relate to the variation in the concentration in the related contactmedia, to the variation in the concentrations in the relevant soil compartments, and to the variation in the relevant input parameters?

And hence:

- How does the variation in concentration in the contactmedia relate to the variation in the concentration in the related soil compartments and to the variation in the relevant input parameters?
- How does the variation in the concentration in the soil compartments relate to the variation in the relevant input parameters?

In regard to the influence of the variation in the relevant input parameters on the variation in exposure and concentrations in contactmedia and soil compartments attention was focussed on:

- the most sensitive input parameters in relation to exposure via the specific exposure pathways (*Vissenberg and Swartjes, 1996*);
- additional input parameters that are typically for a specific exposure pathway (generic input-parameters); the relation between relevant input parameters that are contaminant-specific versus exposures or concentrations in contactmedia were not investigated in this study, because only conclusions could be drawn for calculations for specific contaminants, not for all calculated outputs. Besides, exposures and concentrations in contactmedia are influenced by a combination of these contaminant-specific input parameters.

The question “how does variation in total exposure, or in exposure via a specific exposure pathway, relate to the model concepts” can not be answered within the scope of this study. To this purpose detailed knowledge of all model concepts would be necessary. Therefore this question only could be answered with participation of all participants, i.e. in an international project.

5.6.2.1 Exposure via soil ingestion

For the calculation of *Exposure via soil ingestion* using the CSOIL 8.0 model the following generic input parameters were found the most sensitive (Vissenberg and Swartjes, 1996): *average daily soil intake, child* > *average daily soil intake, adult* > *relative absorption factor*. It has been assumed that this series include all generic input parameters that are typically for *Exposure via soil ingestion*.

The relation between *Exposure via soil ingestion, adult* and the relevant input parameters is presented in Figure 5.10.

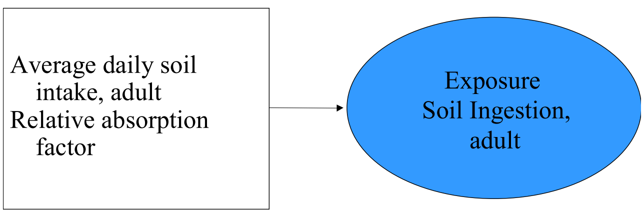

Figure 5.10: Relation between Exposure via soil ingestion, adult and relevant input parameters, which variations are compared.

Note that no contactmedia are involved in this exposure pathway, except for the soil itself.

In relation to this exposure pathway the most important question for the individuals who manage and use exposure models implies (see Figure 5.10):

- How does the variation in *Exposure via soil ingestion, adult* relate to the variation in *average daily soil intake, adult* and in *relative absorption factor*?

In Figure 5.7 the RDs for *Exposure via soil ingestion, adult* were presented as a function of type of input parameters, contaminant, model, soil use and soil type. In Figure 4.1 the input parameters were presented.

From the graphs in Figure 4.1 and 5.7 the following can be concluded[3]:

- There is a substantial variation in *average daily soil intake residential site, adult* between the approaches (from 20 up to 100 mg/d) and a large variation in *average daily soil intake industrial site, adult* (from 0.5 up to 50 mg/d). There is a clear relation between the differences in the input parameters and the variation in *Exposure via soil ingestion, adult* when country-specific default input parameters are used.
    - For the CETOX-human and the Vlier-humaan models, for which the *average daily soil intake residential site, adult* and *average daily soil intake industrial site, adult* are relatively low, *Exposure via soil ingestion, adult* is lower when country-specific default input parameters are used.
    - For the NoNameFrance2000 model, for which the *average daily soil intake industrial site, adult* is relatively very low, *Exposure via soil ingestion, adult* on an industrial site is substantially lower when country-specific default input parameters are used.
    - For the ROME 01 model, for which the *average daily soil intake residential site, adult* is relatively high, *Exposure via soil ingestion, adult* on a residential site is higher when country-specific default input parameters are used.

Relative absorption factors are similar for all models, so that the influence of variation in this input parameter on *Exposure via soil ingestion, adult* could not be investigated in this study.

5.6.2.2 Exposure via crop consumption

For the calculation of *Exposure via crop consumption, adult* using the CSOIL 8.0 model, the following generic input parameters were found the most sensitive (Vissenberg and Swartjes, 1996): *fraction of total root vegetable consumption that is homegrown* ≅ *fraction of total leafy vegetable consumption that is homegrown* ≈ *organic matter content* > *relative absorption factor*. Besides, *total crop consumption* is assumed to be a generic input parameter that is typically for *Exposure via crop consumption, adult*.
The organic matter content is a site-specific input parameter. A very important input parameter in relation to *Exposure via crop consumption, adult* (or more directly: in relation to the *Concentration in the root vegetables* and *Concentration in leafy vegetables*) is the *BioConcentrationFactors crop/ soil* (*BCFs*). However, this input parameter is model and

[3] For (arbitrary) catagorisation of the input parameters, see section 4.2)

contaminant specific and suffers from lack of data in this human exposure comparison study. For these reasons, the influence of these parameters could not be investigated.

The relation between *Exposure via crop consumption*, *adult*, concentrations in relevant contactmedia, concentrations in relevant soil compartments and the relevant input parameters is presented in Figure 5.11.

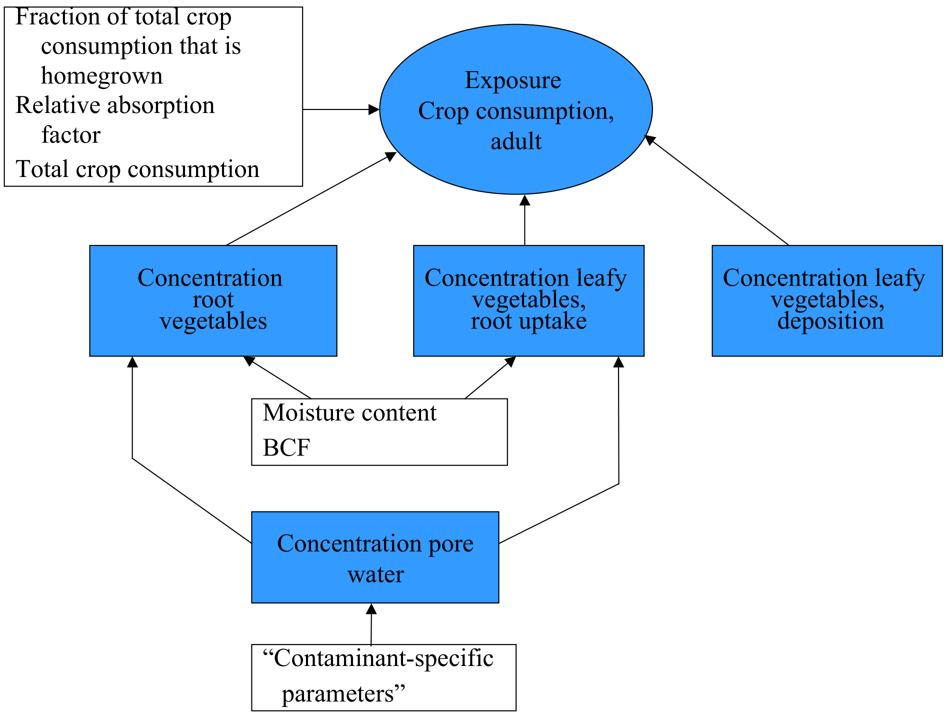

Figure 5.11: Relation between Exposure via crop consumption, adult, concentrations in relevant contactmedia, concentrations in relevant soil compartments, and relevant input parameters, which variations are compared.

In relation to *Exposure via crop consumption, adult* the most important questions for the individuals who manage and use exposure models imply (see Figure 5.11):

- How does the variation in *Exposure via crop consumption, adult* relate to the variation in *Concentration in root vegetables/ Concentration in leafy vegetables* (due to root uptake), to the variation in *Concentration in the pore water* and to the variation in *fraction of total root and leafy vegetable consumption that is homegrown, relative absorption factor* and *total crop consumption*? The influence of the *Concentration leafy vegetables, deposition* on *Exposure via crop consumption, adult has* not been investigated because of limited number of calculated outputs in this comparison study. In Figure 4.1 the input parameters were presented.
- How does the variation in *Concentration in root vegetables* and the variation in the *Concentration in leafy vegetables* (due to root uptake) relate to the variation in the *Concentration in pore water* and to *moisture content*?

The *Concentration in pore water* is influenced by several contaminant-specific input parameters. Therefore, the relation between *Concentration in pore water* and input parameters could not be investigated in this study.

In Figure 5.8 the RDs for the *Exposure via crop consumption, adult* were presented, as a function of type of input parameters, contaminant, model, soil use and soil type. In Figure 5.12 the RDs for the *Exposure via crop consumption, adult* (110 calculated outputs), *Concentration in root vegetables* (110 calculated outputs), *Concentration in leafy vegetables* (110 calculated outputs) and *Concentration in pore water* (232 calculated outputs) have been presented as a function of type of input parameters.

Note that:
- the *Exposure via crop consumption, adult* has not been calculated for the soil use industrial site, because this is not a relevant pathway for this soil use;
- the *Exposure via crop consumption, adult has* not been included in the model ROME 01.

From the graphs in Figure 4.1, 5.8 and 5.12 the following can be concluded:
- The variation in *Exposure via crop consumption, adult* shows a different pattern than the variation in *Concentration in root vegetables* and *Concentration in leafy vegetables*, for both types of input parameters. This is more clearly illustrated in Figure 5.13, in which the quotients between the RDs for *Exposure via crop consumption, adult* versus the RDs for *Concentration in root vegetables* and *Concentration in leafy vegetables* have been presented. In case there would be a strong relation between these two outputs, the quotients will be close to 1. However, Figure 5.13 shows that deviations from the scenario medians for Exposure via crop consumption, adult follow a quite different pattern than deviations from the scenario medians for both Concentration in root vegetables and Concentration in leafy vegetables, for both type of input parameters (i.e. standardised and country-specific default input parameters). These differences are more pronounced (highest deviations from 1) for the calculation in which country-specific default parameters have been used.
  In general, variation in both *Concentration in root vegetables* and *Concentration in leafy vegetables* is substantial: the majority of the individual calculations of *Concentration in root vegetables* and *Concentration in leafy vegetables* is within the range from a factor of 10 lower up to a factor of 10 higher than the scenario medians. The 90%-confidence interval for *Concentration in root vegetables* and *Concentration in leafy vegetables* ranges from a factor of a factor 21 lower up to a factor of 8 higher than the scenario medians, respectively from a factor of a factor 26 lower up to a factor of 10 higher than the scenario medians. (The 90%-confidence interval for *Exposure via crop consumption*, adult ranges from a factor of 13 lower up to a factor of 11 higher than the scenario medians).

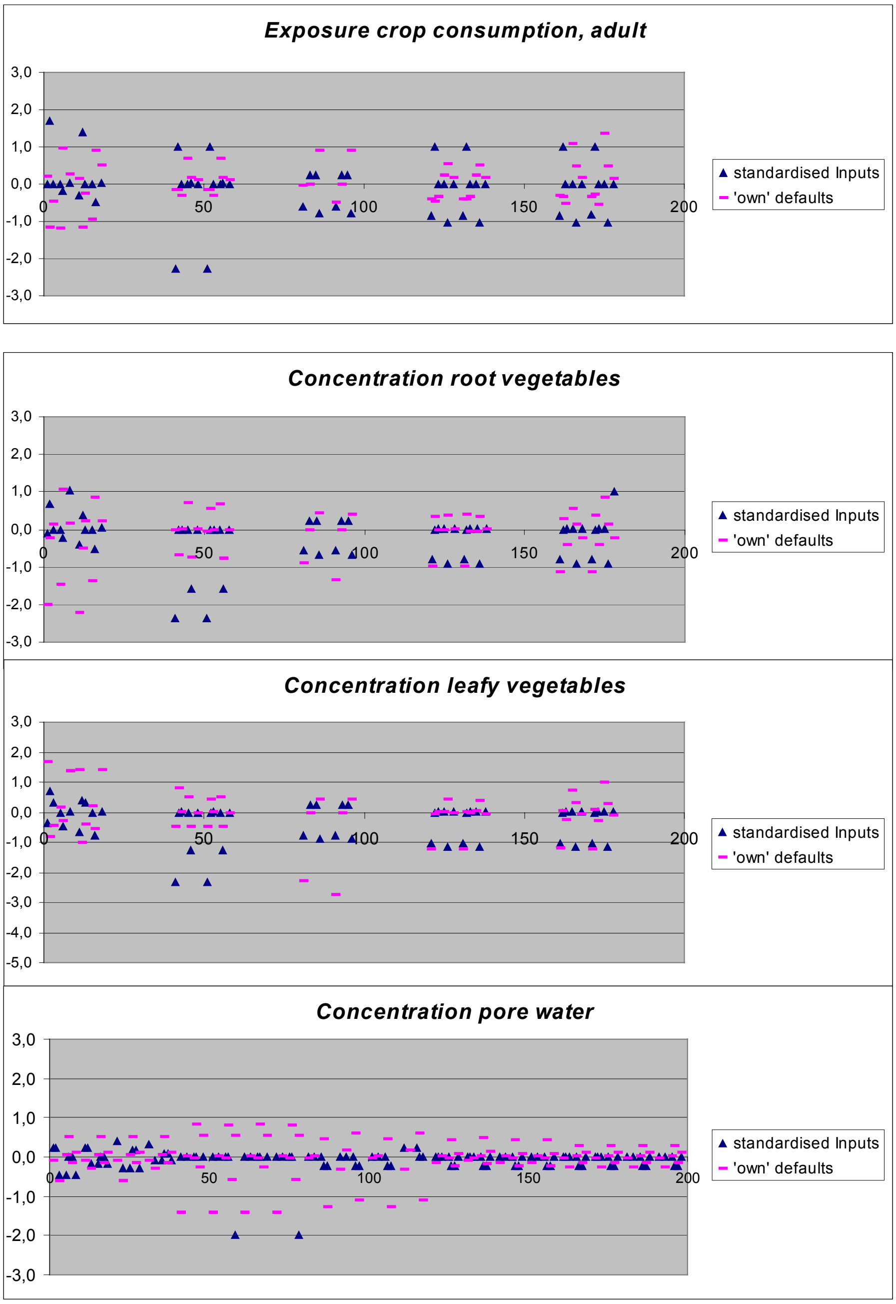

Figure 5.12: RDs (relative deviation from the scenario-medians) for the Exposure via crop consumption, adult; Concentration in root vegetables, Concentration in leafy vegetables and Concentration in pore water as a function of type of input parameters.
RDs at log scale. Each symbol represents an individual model calculation.

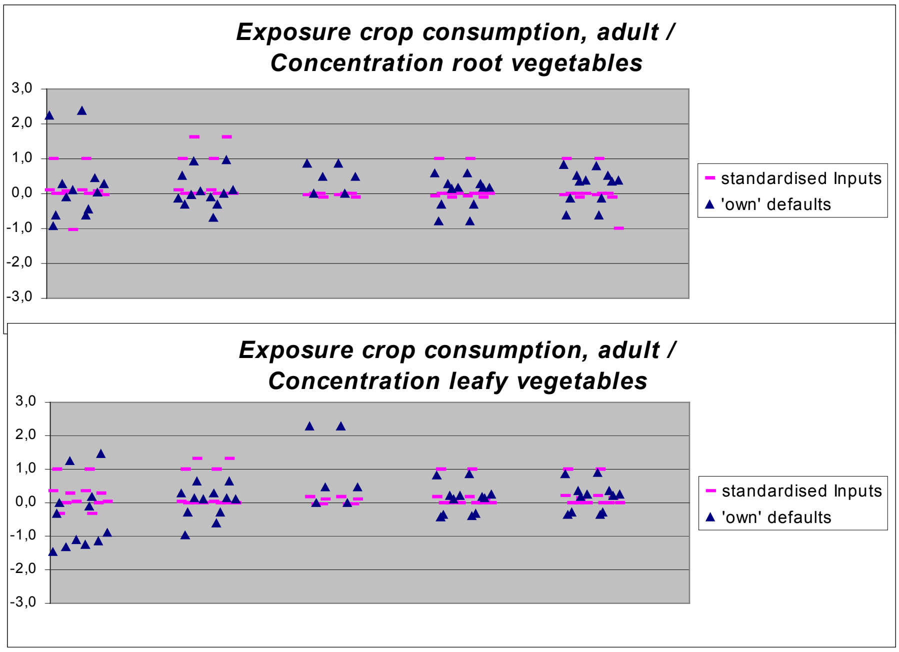

Figure 5.13: Quotients between the RDs (relative deviation from scenario medians) for Exposure via crop consumption, adult versus the RDs for Concentration in root vegetables and *Concentration in leafy vegetables.*
Quotients between RDs at log scale. Each symbol represents an individual model calculation.

- However, the variation pattern of *Exposure via crop consumption, adult* versus the variation pattern of *Concentration in root vegetables* and *Concentration in leafy vegetables* is similar for exposure to atrazine when standardised input parameters are used and, to as lesser extent, for exposure to benzene when standardised input parameters are use (not separately shown in the graphs). Besides the variation pattern of *Exposure via crop consumption, adult* versus the variation pattern of *Concentration in root vegetables* and *Concentration in leafy vegetables* is similar for the NoNameFrance 2000, NoNameSweden and, to a lesser extent and CSOIL 8.0 models.
- The variation in *Exposure via crop consumption, adult* shows a different pattern than the variation in *Concentration in pore water*, for both types of input parameters. This is more clearly illustrated in Figure 5.14, in which the quotients between the RDs for *Exposure via crop consumption, adult* versus the RDs for *Concentration in pore water* have been presented. In case there would be a strong relation between these two outputs, the quotients will be close to 1. However, Figure 5.14 shows that deviations from the scenario medians for *Exposure via crop consumption, adult* follow a quite different pattern than deviations from the scenario medians for *Concentration in pore water*, for both type of input parameters (i.e. standardised and country-specific default input parameters).
  In general, variation in both *Concentration in pore water* is limited: the majority of the individual calculations of *Concentration in pore water* is within the range from a factor of 3 lower up to a factor of 3 higher than the scenario medians. The 90%-confidence interval for *Concentration in pore water* ranges from a factor of 12 lower up to a factor of 9 higher than the scenario medians. (The 90%-confidence interval for *Exposure via crop*

consumption, adult ranges from a factor of 13 lower up to a factor of 11 higher than the scenario medians).

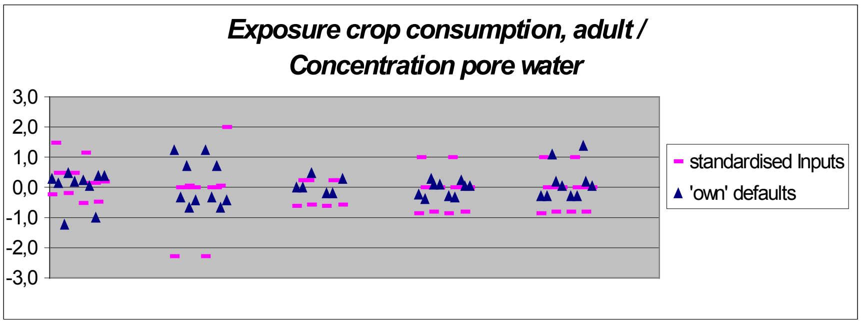

Figure 5.14: Quotients between the RDs (relative deviation from scenario medians) for Exposure via crop consumption, adult versus the RDs for Concentration in pore water.
Quotients between RDs at log scale. Each symbol represents an individual model calculation.

- *Total consumption root vegetables, adult* shows two different clusters of values, i.e. one cluster of high values (from 207 up to 225 g_{dw}/d) and one cluster of low values (from 28 up to 119 g_{dw}/d). *Total consumption leafy vegetables, adult* also shows two different clusters of values, i.e. two high values (138 g_{dw}/d and 152 g_{dw}/d) and one cluster of low values (from 17 up to 61 g_{dw}/d). *Fraction of total root and leafy vegetable consumption that is homegrown* vary substantially (both input parameters from 10 up to 50% (root vegetables, respectively 60% (leafy vegetables)). There is a relation between these variations and the *Exposure via crop consumption, adult.* For the CETOX-human and Vlier-humaan models, for which the product of total consumption and fraction of total consumption that is homegrown is relatively high, *Exposure via crop consumption, adult* is higher when country-specific default input parameters are used. For the CSOIL 8.0 model, for which the product between of total consumption and fraction of total consumption that is homegrown is relatively low, *Exposure via crop consumption, adult* is lower when "own default" parameters are used.

The *Relative absorption factor* is similar for all models and *moisture content root vegetables* and *moisture content leafy vegetables* are almost similar for all models, so that the influence of variation in these input parameter on *Exposure via crop consumption, adult* is absent, respectively negligible.

- The variation in *Concentration in root vegetables* and *Concentration in leafy vegetables* is different than the variation in *Pore water concentration*, for both types of input parameters. This is more clearly illustrated in Figure 5.15, in which the quotients between the RDs for *Concentration in root vegetables* and *Concentration in leafy vegetables* versus the RDs for *Pore water concentration* are presented. Figure 5.15 shows that deviations from the scenario medians for *Concentration in root vegetables* and *Concentration in leafy vegetables* follow a quite different pattern than deviations from the scenario medians for *Pore water concentration*, for both type of input parameters.

(The 90%-confidence interval for *Concentration in pore water* ranges from a factor of 12 lower up to a factor of 9 higher than the scenario medians. The 90%-confidence interval for *Concentration in root vegetables* and *Concentration in leafy vegetables* ranges from a factor of a factor 21 lower up to a factor of 8 higher than the scenario medians, respectively from a factor of a factor 34 lower up to a factor of 1750 higher than the scenario medians).

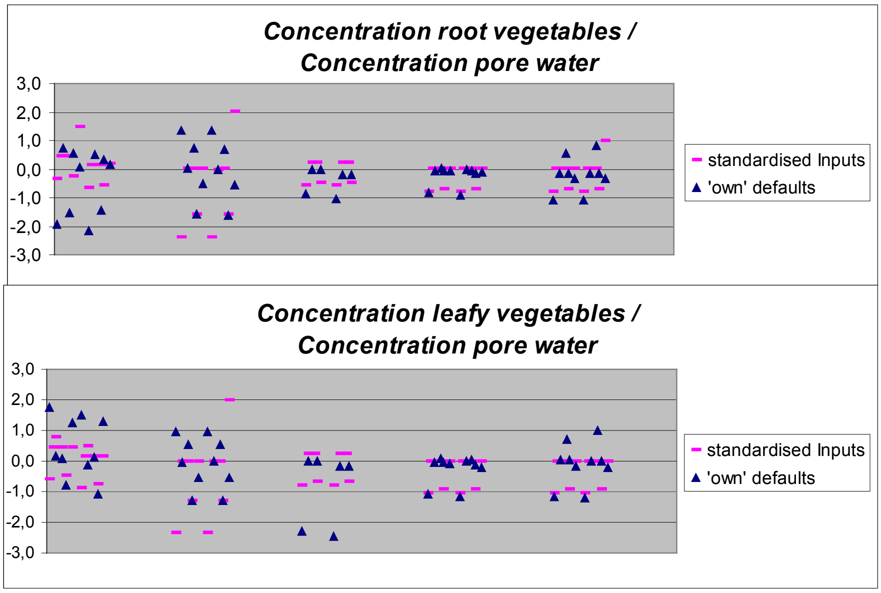

Figure 5.15: Quotients between the RDs (relative deviation from scenario medians) for Concentration in root vegetables and Concentration in leafy vegetables versus the RDs for Pore water concentration
Quotients between RDs at log scale. Each symbol represents an individual model calculation.

5.6.2.3 Exposure via indoor air inhalation

For the calculation of *Exposure via indoor air inhalation* using the CSOIL 8.0 model no specific input parameters were found the most sensitive. *Exposure via indoor air inhalation* is rather influenced by a whole range of input-parameters (Vissenberg and Swartjes, 1996). However, *breathing volume, residence time, surface of the building, volume of the building* and *ventilation frequency* are assumed to be generic input parameters that are typically for *Exposure via indoor air inhalation*.

The relation between *Exposure via indoor air inhalation*, *adult,* concentrations in relevant contactmedia, concentration in relevant soil compartments and the input parameters is presented in Figure 5.16.

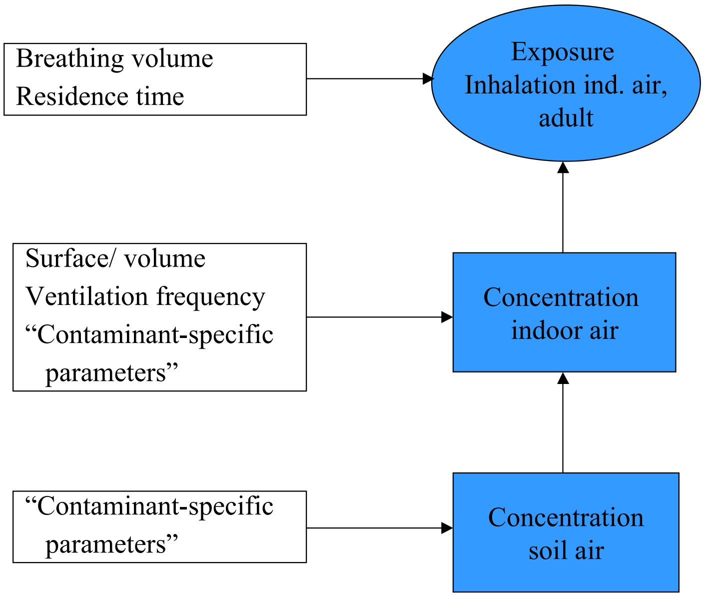

Figure 5.16: Relation between Exposure via indoor air inhalation, adult, concentrations in relevant contactmedia, concentrations in relevant soil compartments, and input parameters, which variations are compared.

In relation to *Exposure via indoor air inhalation, adult* the most important questions for the individuals who manage and use exposure models imply (see Figure 5.16):

- How does the variation in *Exposure via indoor air inhalation, adult* relate to the variation in *Concentration in the indoor air*, the variation in *Concentration in soil air* and to the variation in *breathing volume, residence time, surface of the building, volume of the building* and *ventilation frequency*?
- How does the variation in *Concentration in the indoor air* relate to the variation in *Concentration in soil air* and to the variation in *breathing volume, residence time, surface of the building, volume of the building* and *ventilation frequency*?

From Figure 5.16 it can be concluded that the relation between *Concentration in soil air* and relevant input-parameters could not be investigated in this study, because all relevant input parameters are contaminant-specific.

In Figure 5.9 the RDs for the *Exposure via indoor air inhalation, adult* were presented, as a function of type of input parameters, contaminant, model, soil use and soil type. In Figure 5.17 the RDs (relative deviation from the scenario-medians) for *Exposure via indoor air inhalation, adult*, *Concentration in the indoor air* and *Concentration in soil air* have been presented as a function of type of input parameters. In Figure 4.1 the input parameters were presented.

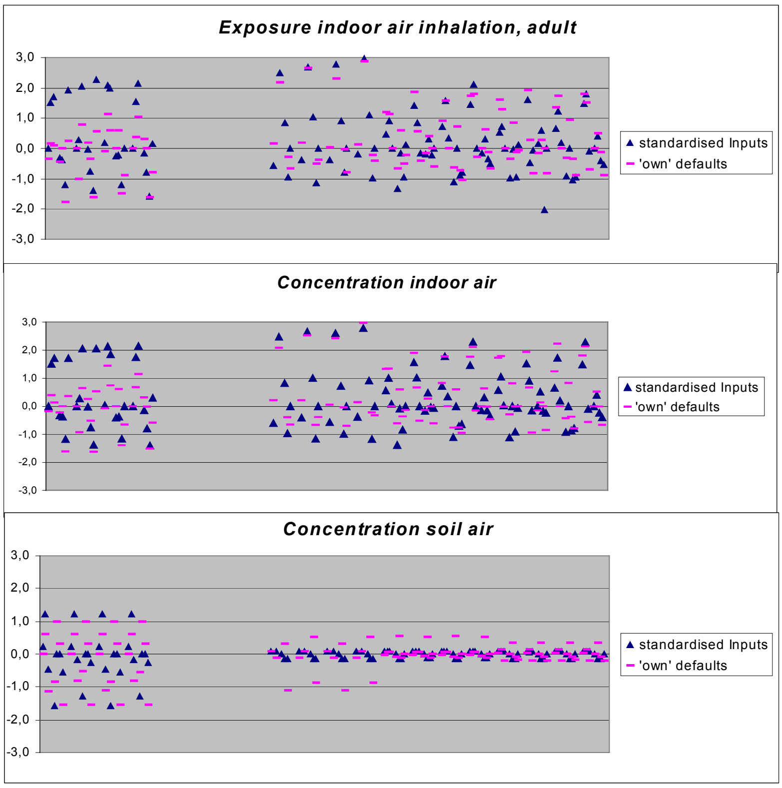

Figure 5.17: RDs (relative deviation from the scenario-medians) for Exposure via indoor air inhalation, adult, Concentration in indoor air and for Concentration in soil air as a function of type of input parameters.
RDs at log scale. Each symbol represents an individual model calculation.

From the graphs in Figure 4.1, 5.9 and 5.17 the following can be concluded:

- The variation in *Exposure via indoor air inhalation, adult* is similar to the variation in *Concentration in indoor air*, for both types of input parameters. This is more clearly illustrated in Figure 5.18, in which the quotients between the RDs for *Exposure via indoor air inhalation, adult* versus *Concentration in the indoor air* are presented. In case there is a strong relation between these two outputs, the quotients will be close to 1. Figure 5.18 shows that deviations from the scenario medians for *Exposure via indoor air inhalation, adult* indeed follow a similar pattern as deviations from the scenario medians for *Concentration in indoor air*, for both type of input parameters. This suggests that the factors that control the variation in *Concentration in the indoor air* also control the variation in *Exposure via indoor air inhalation, adult.*
  In general, variation in *Concentration in indoor air* is huge: the majority of the individual calculations of *Concentration in indoor air water* is within the range from a factor of 10 lower up to a factor of 10 higher than the scenario medians. The 90%-confidence interval for *Concentration in indoor air* ranges from a factor of 25 lower up to a factor of 80

higher than the scenario medians. (The 90%-confidence interval for *Exposure via indoor air inhalation, adult* ranges from a factor of 27 lower up to a factor of 71 higher than the scenario medians).

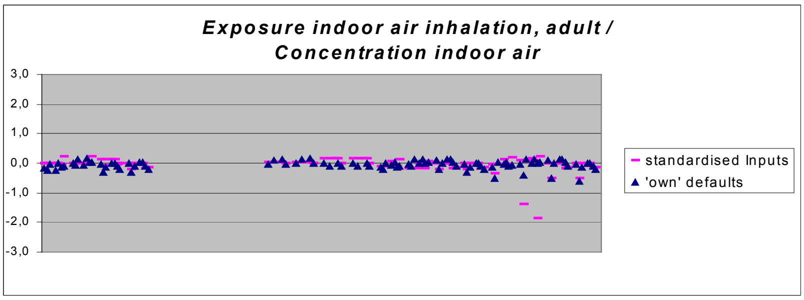

Figure 5.18: Quotients between the RDs (relative deviation from scenario medians) for Exposure via indoor air inhalation, adult and the RDs for Concentration in indoor air
Quotients between RDs at log scale. Each symbol represents an individual model calculation.

- The variation in *Exposure via indoor air inhalation, adult* is different than the variation in *Concentration in soil air*, for both types of input parameters. This is more clearly illustrated in Figure 5.19, in which the quotients between the RDs for *Exposure via indoor air inhalation, adult* versus *Concentration in the soil air* are presented. In case there is a strong relation between these two outputs, the quotients will be close to 1. Figure 5.19 shows that deviations from the scenario medians for *Exposure via indoor air inhalation, adult* indeed follow a different pattern than deviations from the scenario medians for *Concentration in soil air*, for both type of input parameters.
  Variation in *Concentration in soil air* shows two different clusters: one cluster concerns the variation in *Concentration in soil air* for benzo(a)pyrene and is huge: the variation in *Concentration in soil air* for benzo(a)pyrene is within the range from a factor of 100 lower up to a factor of 100 higher than the scenario medians. The other cluster concerns the variation in *Concentration in soil air* for atrazine, benzene and trichloroethene and is limited: the majority of the individual calculations of *Concentration in indoor air* is within the range from a factor of 1.5 lower up to a factor of 4 higher than the scenario medians. The 90%-confidence interval for *Concentration in soil air* ranges from a factor of 6 lower up to a factor of 5 higher than the scenario medians. (The 90%-confidence interval for *Exposure via indoor air inhalation, adult* ranges from a factor of 27 lower up to a factor of 71 higher than the scenario medians).

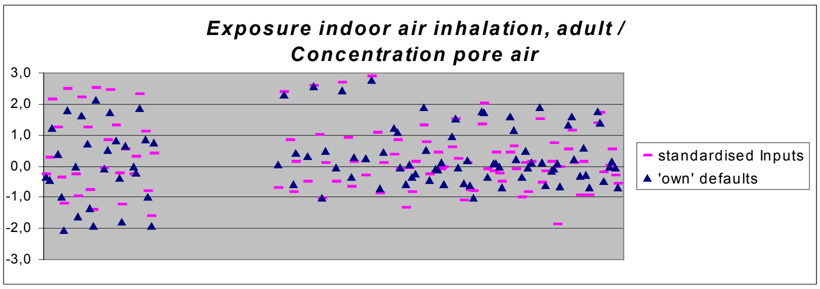

Figure 5.19: Quotients between the RDs (relative deviation from scenario medians) for *Exposure via indoor air inhalation, adult* and the RDs for *Concentration in soil air*
Quotients between RDs at log scale. Each symbol represents an individual model calculation.

- *Breathing volume, adult* (from 20 up to 22 m^3/d) is almost similar for all models, so that the influence of variation in this input parameter on *Exposure via indoor air inhalation, adult* (and on *Concentration in indoor air)* is negligible.
- The *residence time in the house, adult* (from 14 up to 24 h/d)*; ventilation frequency house* (from 0.3 up to 1.25 1/h), *residence time in the building at an industrial site, adult* (from 5 up to 10 h/d) and *ventilation frequency in the building at an industrial site* (from 0.5 up to 1.25 1/h) vary substantially. There is a relation between these variations and the *Exposure via indoor air inhalation, adult.* For the Vlier-humaan model, for which residence times are relatively low, ventilation frequencies relative high and a concrete basement floor has been assumed for the industrial building, *Exposure via indoor air inhalation, adult* is lower when country-specific default parameters are used. For the NoNameSweden model, for which residence times are relatively high and ventilation frequencies are relative low, *Exposure via indoor air inhalation, adult* is higher when country-specific default parameters are used. Because the variation in *Exposure via indoor air inhalation, adult* is similar to the variation in *Concentration in indoor air* the same conclusions can be drawn for the relation between these input parameters and the *Concentration in soil air*.
- There is a large variation in *surface of the house* (from 50 up to 225 m^2), *surface of the building at an industrial site* (from 50 up to 2500 m^2), *volume of the house* (from 25 up to 450 m^3) and *volume of the building at an industrial site* (240 up to 10000 m^3). This might have to do with differences in building construction types in different countries. In some approaches transport of volatile contaminants from the soil to a crawl space, having a different surface and volume, is considered.
- There is no clear relation between the variation in *Concentration in indoor air* and the variation in *Concentration in soil air.* This is more clearly illustrated in Figure 5.20, in which the quotients between the RDs for *Concentration in indoor air* versus the RDs for *Concentration in soil air* are presented. Figure 5.20 show that deviations from the scenario medians for *Concentration in indoor air* indeed follow a quite different pattern than deviations from the scenario medians for *Concentration in soil air*, for both type of input parameters.
  (The 90%-confidence interval for *Concentration in soil air* ranges from a factor of 6 lower up to a factor of 5 higher than the scenario medians. The 90%-confidence interval for *Concentration in indoor air* ranges from a factor of 25 lower up to a factor of 80 higher than the scenario medians).

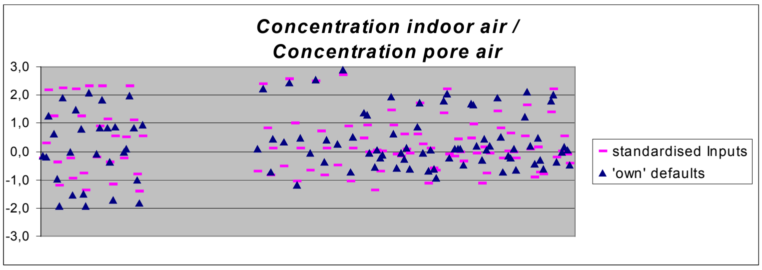

Figure 5.20: Quotients between the RDs (relative deviation from scenario medians) for calculated Concentration in indoor air and the RDs for Concentration in soil air.
Quotients between RDs at log scale. Each symbol represents an individual model calculation.

5.7 Discussion

In Section 5.6 the results of this human exposure comparison study were presented. In the present section discussion is focused on the following questions:

- Is the variation in calculated human exposure acceptable?
- What is the role of communication in regard to variation in calculated human exposure?
- Should human exposure calculations be harmonised and how should this be done?

5.7.1 Acceptance of the variation in calculated exposure

Whether the variation in exposures as has been described in Section 5.6 is acceptable or not depends on:

- “natural” variation in exposure between countries due to geographical/ ethnological factors;
- purpose of the calculated human exposure;
- policy decisions on choice of parameter values;
- other standards that are used in (human toxicological) risk assessment.

Variation in exposure due to geographical/ ethnological factors

As was mentioned in the introduction of Chapter 5 calculated human exposure from the same source is not necessarily equal within Europe, because of geographical and ethnological differences. It is difficult to quantify the influence of geographical or ethnological factors on (variation in) exposure. However, it can be assumed that differences might increase in the order of exposure via soil ingestion, exposure via crop consumption and exposure via indoor air inhalation. The reason for this is that in this order the role of fate and transport processes, which are influenced mainly by geographical factors like soil and climate, increase. Ethnological factors mainly influence residence times (exposure via soil ingestion), fraction of vegetables that is homegrown and type of vegetables (exposure via crop consumption), handmouth behaviour and time spent outside (exposure via soil ingestion), construction of buildings (exposure via indoor air inhalation). In table 5.2 examples of geographical and ethnological factors influencing the separate exposure pathways have been listed.

Table 5.2: geographical and ethnological factors influencing exposure via the separate exposure pathways.

	Geographical	Ethnological
Exposure via soil ingestion	• snow and ground frost	• residence time in the garden
Exposure via crop consumption	• type of crops • bio-availability of contaminants	• fraction of total root and leafy vegetable consumption that is homegrown
Exposure via indoor air inhalation	• groundwater table • affinity for diffusion • soil temperature	• type of construction of buildings • ventilation behaviour of building • residence time indoors/ outdoors

Although most factors are fixed in this human exposure comparison study several concepts of the models involved include empirical elements that are valid for regional conditions only. Exposure via indoor air inhalation, for example, can vary substantially between different countries due to different groundwater levels and differences in construction types. In the present study the groundwater level was fixed. However, several models use concepts for the calculation of exposure via indoor air inhalation is calculated that include empirical elements that are valid for regional conditions only, e.g. a diffusion flux in soil.

For a detailed analysis of the influence of geographical/ ethnological factors on (variation in) calculated exposure, boundary conditions, model concepts, and input parameters should be compared. This would only be possible with direct involvement of the human exposure model experts, i.e. in an international project. In the present study it is assumed that the variation in calculated exposures due to geographical and ethnological factors will affect the ratio between the extreme values in the majority of the calculated outputs no more than one order of magnitude.

Purpose of calculating human exposure

It is relevant to realise that human exposure models are used for different purposes. In many cases calculated human exposure, usually based on a conservative estimate, is used in a first tier of a more sophisticated human risk assessment ("trigger function"). The purpose of this first step in human risk assessment is often to exclude these contaminated sites for which it is evident that, even under worst case conditions, there is no risk for human beings. In all other cases the human risk should be assessed in more detail, usually with the aid of measured

concentrations in the contactmedia (crops, indoor air). As a first tier of a more sophisticated human risk assessment most (conservative) human exposure calculations will be acceptable, although in some cases there will be over-conservatism.
But also when site-specific human exposure is calculated it is generally recognised that often the result is conservative. The reason for this is that input parameter selection is usually based on Reasonable Maximal Exposure: in case that an input parameter is well known (e.g. body weight) the average value is chosen; when on the contrary the input parameter is difficult to quantify (e.g. amount of soil ingestion of adults) usually a conservative estimate is chosen. Besides there is a general tendency, for the sake of public safety, to intentionally use high-point estimates (Paustenbach, 1995). As a result the overall effect is a conservative calculated human exposure.
A source of variation in calculated exposures with the seven European models is that the models have been developed and used for different purposes and (hence) input parameters are based, intentional or unintentional, on a different choice in the range best case – worst case. Again it is difficult to quantify the influence of this phenomenon on variation in calculated human exposure. In the present study it is assumed that the variation in calculated exposures due to the different purposes for which these models have been developed will affect the ratio between the extreme values in the majority of the calculated outputs with a factor between one and two order of magnitude.

<u>Other standards that are used in risk assessment</u>

Absolute values of calculated human exposure are only useful when these values can be compared to a reference like *(maximal) permissible* exposure. Although geographical/ ethnological factors scarcely will influence effects on human beings, permissible exposures show huge differences between different countries. This is due to political decisions (for example different protection levels for carcinogenic contaminants in different countries), different experimental results, and different procedures (for example in regard to the use of extrapolation and uncertainty factors).
In many cases risk assessment is also focused on other targets than human beings alone, e.g. ecosystems, groundwater. In general all elements of risk assessment are characterised by large uncertainties. It would not make sense to reject risk assessments based on calculated exposures because these calculations are unreliable, unless uncertainties are larger than for other targets or for permissible exposure.

<u>Résumé</u>

It is not possible to give a quantitative criterion for acceptance of variation in calculated exposure. However the bottom line is that exposure from the same source is not necessarily equal within Europe, because of differences in geographical and ethnological conditions and differences in the choice of input parameters/ model concepts in the range best case – worst case. In the present study it is assumed that the variation in calculated exposures due to the country-specific differences combined will scarcely affect the ratio between the extreme values in the majority of the calculated outputs with a factor of one order of magnitude. Besides, variation in other standards used in risk assessment is (also) characterised by large uncertainties.

In Table 5.3 an overview is given of the 90%-confidence intervals (the 5-percentiles and the 95-percentiles) of the relevant outputs. Besides, the number of calculated outputs, minimum values, maximum values, standard deviations and coefficient of variation of the relevant outputs are given in this table.

Table 5.3: Characteristics of the relevant outputs, including the 90%-confidence intervals (the 5-percentiles and the 95-percentiles)

	Total exposure	Exp.via soil ing.	Exp.via crop cons.	Exp.via ind.air inh.	Conc.root veg.	Conc. Leafy Veg.	Conc. ind.air	Conc. pore water	Conc. soil air
Number of data	**260**	**260**	**110**	**204**	**110**	**110**	**204**	**232**	**204**
Minimum	1.63E-03	3.48E-02	5.25E-03	9.88E-03	4.20E-03	6.33E-03	2.35E-02	1.66E-06	2.66E-02
Maximum	8.07E+01	2.29E+00	4.83E+01	9.40E+02	1.20E+01	2.05E+03	9.45E+02	1.43E+03	1.67E+01
Average	4.85E+00	1.01E+00	2.71E+00	2.92E+01	1.43E+00	1.86E+02	2.99E+01	1.35E+01	1.56E+00
Standard dev.	11.20	0.52	5.97	108.34	2.07	463.01	99.56	132.02	2.57
Coeff.of var.	2.31	0.52	2.20	3.70	1.45	2.49	3.33	9.82	1.64
95-perc.	**21**	**3**	**11**	**71**	**8**	**1750**	**80**	**9**	**5**
5-perc.	**20**	**5**	**13**	**27**	**21**	**34**	**25**	**12**	**6**

From Table 5.3 and the qualitative analysis given in section 5.6 it can be concluded that the variation in the several calculated outputs is substantially higher than could be explained on the basis of the above mentioned “country-specific” factors. This suggests that for most of the outputs additional variation can be explained by differences in model concepts and in input parameters.

5.7.2 Communication

The success of a comparison study is dependent on the quality of communication, i.e. the way that definitions, methodologies and boundary conditions are formulated clearly and unambiguous, the way participants interpret this information and the carefulness how participants carry out the calculations. Well-known pitfalls are:

- using deviant (own, familiar) starting-points or boundary conditions;
- basing input parameter selection on a deviant choice in the range best case – worst case;
- using deviant dimensions (a notorious example concerns BioConcentration Factors expressed on dry weight instead of wet weight, or vice versa).

Starting-points, boundary conditions and input parameters

In many cases starting-points or boundary conditions and, particularly, the choice in the range best case – worst case input parameters have not been based on intentional positions. This phenomenon usually has its origin in the character of the available data. The available input parameters relating to human behaviour, for example, determine the boundary condition which group of human beings is considered ("average" human being, vulnerable human being, et cetera). In case BioConcentrationFactors crop–soil for metals, for example, are generally based on experiments in which the metals are relatively bio-available, this average BioConcentrationFactor is a conservative estimate, although no intentional position was made for the choice in the range best case – worst case. Moreover, the exact degree of conservatism of input parameters, and particularly the influence of this conservative estimate on calculated exposure, is often unknown. In some studies, however, this problem has been solved by using Monte Carlo techniques. Using this probability density functions of the input parameters (if available) are used, while the choice of a point estimate of the input parameters can be avoided. A disadvantage of this technology is that the calculated exposure, also given as a probability function, is more difficult to understand. Another advantage is that is gives politicians more insight in variation in exposure and the possibility to select different degrees of conservatism (e.g. mean exposure, 90-percentile of exposure) for different purposes.

Only is one case a participant tended to use a clearly defined worst case calculation, although an average exposure was asked for. Because best case to worst case human exposure calculations concern a sliding scale, it is hard to tell in how far every exposure model calculated the same, i.e. average exposure. Most models tend to calculate the Reasonable Maximal Exposure, based on average input parameters in case the distribution of the input parameter is well known (like body weight) and on a conservative estimate in case of not much information of the input parameter is available (for example the amount of soil ingestion of adults). It must be concluded that in case country-specific default input parameters are used the type of calculated exposure is somewhere else in the range from best to worst case for every approach, but most models probably have calculated "slightly worst case" exposure. This kind of bias can hardly be avoided, because the type of calculated exposure on the scale of worst case to best case is dependant on the concepts of the model (these were only adapted in this human exposure comparison study when certain exposures or concentrations in contactmedia could not be calculated with the existing model) and on many input parameters. In case model users use a clearly defined type of exposure (e.g. a 90 percentile) this can only be avoided in bilateral communication when this participant reveal this clearly.

Deviate dimensions

The consequence of using deviant dimensions can range from absent to severe. When exposure is expressed in μg/kg$_{\text{body weight}}$/day (*micro*gram) instead of mg/kg$_{\text{body weight}}$/day (*milli*gram), for example, this unwanted deviation could be easily detected and corrected in a comparison study like the present one. In case that site-specific human exposure is calculated, deviation in dimensions would only result in an incorrect risk assessment when calculated exposure is compared to a reference like tolerable exposure based on deviant dimensions, which is not likely to happen. However, when deviant dimensions are used in input

parameters or intermediate calculations, it is questionable if this is detected in both this comparison study and site-specific risk assessment.
In a few cases participants tended to use deviant (own, familiar) starting-points or boundary conditions, like default age ranges. This proves that definitions, methodologies and boundary conditions were not formulated clearly and unambiguous and/or participants did not interpret this information carefully.
During the performance of the project several cases of miscommunication were simply cleared up in bilateral communication. However, it can never be guaranteed that every use of deviant dimensions is identified and, hence, avoided.

Résumé

As a résumé it can be stated that sound communication, in case of this comparison study, but certainly also in real practice, is essential in every case in which exposure models are used. Probably in many cases the client will ask for calculated human exposure without realising exactly what the model expert returns: internal or external exposure, best case or worst case exposure, for average or vulnerable human beings, et cetera.
In this human exposure comparison study deviant starting-points or boundary conditions and the use of input parameter that are based on a deviant choice in the range best case – worst case are a source for improper variation in calculated exposure for the calculations in which "own" default parameters have been used. In the present study it is assumed these differences will not affect the variation in calculated exposures in such a way that the ratio between the extreme values in the majority of the calculated outputs exceeds one order of magnitude. Furthermore, it has been assumed that most use of deviant dimensions was cleared up in bilateral communication. However, it can never be guaranteed that every use of deviant dimensions is identified and, hence, avoided.

5.7.3 Harmonisation of human exposure calculations

From an European political point of view it would be favourable to have one ideal human exposure model, including one ideal input parameter set, that can be used along the lines of one ideal general procedure throughout, lets say, all countries of the European Union. However, from a technical point view this is an utopia for the following reasons:
- exposure differs throughout Europe due to geographical/ ethnological factors (see Section 5.7.1);
- several political elements are involved in the concepts and input parameters of human exposure models.

At the other side many aspects in the calculation of human exposure are not, or scarcely, affected by geographical/ ethnological factors or political choices and are suited for harmonisation and standardisation. Some examples of model concepts that can be standardised are:
- the calculation of the distribution of the contaminants over the soil compartments (solid phase, pore water, soil air);
- the model concepts for exposure via soil ingestion and via crop consumption.

Some examples of input parameters that can be standardised are:
- contaminant-specific input parameters;
- correction factor for the limited bioavailability in the human body.

Some examples of methodical guidance that can be harmonised are:
- a guideline on when and how to measure concentrations in contactmedia;
- the way how to deal which exposures that follow different exposures patterns, i.e. via oral, inhalative or dermal exposure pathways: adding up or considering separately.

Several other aspects in the calculation of human exposure can be subdivided in a technical, unambiguous aspect and elements in which geographical/ ethnological factors and/or political choices are involved. For example in the case of input parameter identification for oral exposure via soil ingestion the following aspects are unambiguous: the determination of the total concentration in soil, for which international (ISO) protocols exists, correcting for the limited bioavailability in the human body, which is assumed to be more or less similar for all human beings throughout Europe. Methodologies to determine these relative absorption factors should be harmonised and possible (minor) differences between European countries, e.g. bioavailability in the human body is affected by the diet, should be quantified. Many of these aspects are given attention in the international initiative BARGE (Oomen et al., 2002). However, when human-toxicologically based guidelines have to be derived in a specific country or region in Europe there should be space for incorporating region- or country specific amounts of soil ingestion for adults and children. This value can be determined on the basis of geographical/ ethnological factors and/or political choices: a region- or country-specific amount of soil ingestion could be selected (geographical/ ethnological factor) for a specified group of human beings, e.g. average, sensitive, vulnerable human beings (political factor).

A major recommendation from this project is that an international project or co-operation should be initiated, with the purpose to develop a common *toolbox* to assess human exposure. This toolbox should at least include the following elements:
- Identification of which elements of the human exposure calculation, i.e. boundary conditions, (part of) model concepts, input parameters should be standardised throughout Europe.
- Fixed model concepts, for these model concepts that are suitable for standardisation and harmonisation (“fixed model tools”).
- Fixed input parameters for these input parameters that are suitable for standardisation and harmonisation (“fixed input parameter tools”).
- Flexible model concepts that are suitable for standardisation and harmonisation, but for which place for political choices is desired (“flexible model tools”).
- Options for input parameters for these input parameters that are suitable for standardisation and harmonisation, but for which place for political choices is desired (“optional parameter tools”).
- A procedure on assessing human exposure, including documentation on the sensitivity of calculated human exposure to the input parameters and a guideline on when and how to measure concentrations in contactmedia.
- Information on the uncertainty/ reliability of the calculated human exposure.

6. Conclusions and recommendations

6.1 Conclusions

6.1.1 Exposure models

On the basis of the general model information (Chapter 3) the following conclusions can be drawn:
- The model concepts and the input parameters of the exposure models CETOX-human, NoNameFrance 2000, Vlier-humaan and CSOIL 8.0 are related to each other. Besides, the model concepts of the exposure model NoNameSweden are related to the four models mentioned and vice versa.

Layout of the European exposure models:
- The soil compartment and the unsaturated groundwater zone are included in most of the models; besides most models include several other compartments (air, surface water, saturated groundwater zone).
- The following exposure pathways are incorporated in all models: Soil ingestion, Crop consumption (except for ROME 01), Indoor air inhalation (inhalation of vapours only, excluding suspended particles in the air), Dermal uptake, Inhalation of dust/ soil particles; besides most models include several other exposure pathways.
- All model concepts and default input parameters are based on Maximal Reasonable Exposure or (realistic) worst case. As a consequence, all models rather calculate at least "slightly worst case" exposure.
- All models use the total soil content as starting point.
- The distribution of the contaminants over the soil compartments is mainly calculated on the basis of partition coefficients.

Possibilities of the European exposure models:
- Only part of the models includes the possibility for probabilistic application, background exposure, kinetic processes, or standards that limit the concentration in contactmedia.
- Most models do not offer the possibility for acute exposure, degradation and exposure to a mixture of contaminants.

Use of the European models:
- All models are used for the derivation of soil quality standards, although not all standards have been (legally) formalised . Besides all models are used for at least one additional purpose.
- The soil uses Residential site and Industrial site are incorporated in all models; besides all models includes several other soil uses.
- No model includes phytotoxicity (a maximal permissible concentration in the crop).
- Most models do not include guidelines for selection of input parameters or recommendations or guidelines for measurements in contactmedia.

- All models offer the possibility for the site-specific calculation of the concentration in the indoor air, but only two models offer the possibility for the site-specific calculation of the concentration in crops.

6.1.2 Input parameters

On the basis of the overview of the input parameters (Chapter 4) the following conclusions can be drawn[4]:

Human characteristics (for details see Section 4.2.1):
- The *Body weight* and *Breathing volume* are similar for all approaches.
- The variation in most *Residence times,* the *Amount of total consumption of root vegetables* for children and the *Average daily soil intake at a residential site for adults* are substantial
- The variation in the *Average daily soil intake at a residential site for children* and the *Average daily soil intake at an industrial site for children* and *adults* is large.

In relation to exposure via crop consumption (for details see Section 4.2.2):
- The *Moisture content of root* and *leafy vegetables* is similar for all approaches.
- The variation in the *Fraction of total root and leafy vegetable consumption that is homegrown for root* and *leafy vegetables* is substantial.

In relation to exposure via indoor air inhalation (for details see Section 4.2.3):
- The variation in the *Ventilation frequency of a house* and the *Ventilation frequency of a building at an industrial site* is substantial.

The *Surface of a house*, the *Surface of a building at an industrial site,* the *Volume of a house* and the *Volume of a building at an industrial site* has not been compared, because of differences in building construction types in different countries.

In relation to exposure via other exposure pathways (for details see Section 4.2.4):
- The *Fraction soil particles in suspended air, indoors* and the *Fraction soil particles in suspended air, outdoors* is similar.
- The variation in the *Concentration in suspended particles in the air at a residential site, indoors* is substantial.
- The variation in the *Concentration in suspended particles in the air at an industrial site, indoors* is large).

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[4] The following (abitrary) categorisation has been used:
- The difference between the extreme values is within a factor of 2: default input parameters are "similar".
- The difference between the extreme values is in between a factor of 2 and 10: there is a "substantial variation" in the default input parameters.
- The difference between the extreme values is in between a factor of 10 and 100: there is a "large variation" in the default input parameters.
- The difference between the extreme values is more than a factor of 100: there is a "huge variation" in the default input parameters.

Contaminant-specific input parameters (only for benzo(a)pyrene, cadmium, benzene and trichloroethene, not for atrazine; for details see Section 4.2.5):

- The *Molecular weight* is similar for all contaminants.
- The *Solubility* is similar for benzene; however, the variation in the *Solubility* for benzo(a)pyrene and trichloroethene is large.
- The *Vapour pressure* is similar for benzene and trichloroethene; however, the variation in the *Vapour pressure* for benzo(a)pyrene is large.
- The *Henry coefficient* is similar for benzene and trichloroethene; however, the variation in the *Henry coefficient for* benzo(a)pyrene is large.
- The *Octanol-water partition coefficient Kow* is similar for benzene; however, the variation in the *Octanol-water partition coefficient Kow* for benzo(a)pyrene and trichloroethene is substantial.
- The *Diffusion coefficient in water* and the *Diffusion coefficient in air* are similar for benzene, trichloroethene and for benzo(a)pyrene.
- The *Octanol-carbon partition coefficient Koc* is similar for benzo(a)pyrene and for benzene; however the variation in the *Octanol-carbon partition coefficient Koc* for trichloroethene is substantial. The variation in the *Partition coefficient solid phase/ pore water* for cadmium is huge.
- The variation in the *BioConcentrationFactor for root* and *leafy vegetables* for benzo(a)pyrene and for cadmium are huge.
- Half of the models use a *Relative retention factor for soil particles in lungs* of 0,75, while the other half of the models use a *Relative retention factor for soil particles in lungs* of 1.0.

Note that for the CLEA C.C. model several input parameters have been given in a probabilistic format. Therefore, it was not possible to compare one specific value from this models with the other input parameters.

6.1.3 Variation in exposure

In Table 6.1 the variation in the outputs, based on the calculation of exposures to adults according to the same 40 exposure scenarios, using seven different European models, is listed in a qualitative way. This table gives insight in the variation in the majority of the data (excluding extreme values). Besides in Figure 6.1 the 90%-confidence intervals of the outputs have been presented. These figure gives insight in the variation in the complete calculated data sets.

Table 6.1: Variation in the outputs

	Total exposure	Exp.via soil ing.	Exp.via crop cons.	Exp.via indoor air inh.	Conc.root veg.	Conc. Leafy Veg.	Conc. indoor air	Conc. Pore water	Conc. soil air
Limited		x							x
Substantial			x		x			x	
Large	x			x		x	x		

The following (arbitrary) categorisation has been used:

- *Limited* variation: The majority of the outputs is within a factor of 5 higher and a factor of 5 lower than the scenario medians.
- *Substantial* variation: The majority of the outputs is in between a factor of 10 higher and a factor of 10 lower than the scenario medians: there is a "substantial variation" in the calculated human exposures.
- *Large* variation: The majority of the outputs is in between a factor of 100 higher and a factor of 100 lower than the scenario medians.
- *Huge* variation: The majority of the outputs is *not* in between a factor of 100 higher and a factor of 100 lower than the scenario medians.

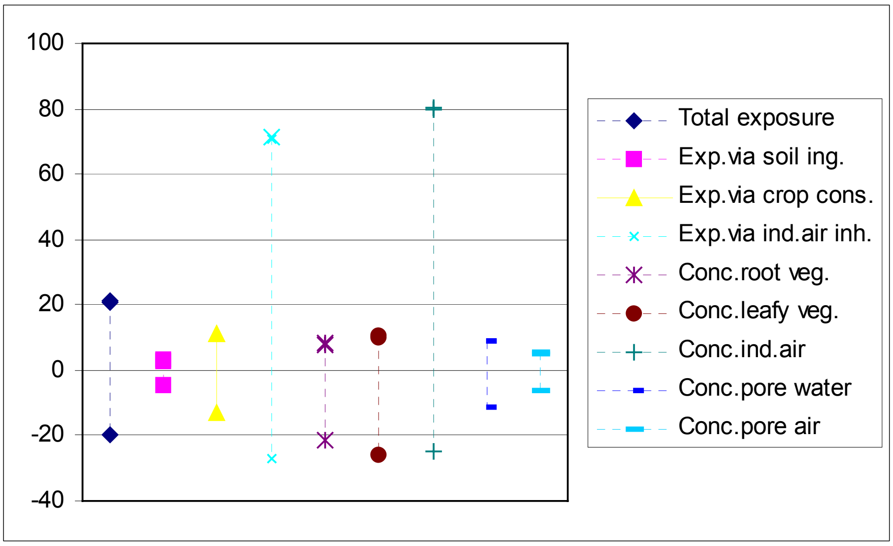

Figure 6.1: 90%-Confidence intervals (5%-confidence limit and 95%-confidence limit), expressed as "factor x higher" (positive values), or "a factor y lower" than the median value (negative value).

It is assumed that the country-specific differences combined will scarcely affect the overall variation in calculated exposures in such a way that the ratio between the extreme values in the majority of the calculated outputs exceeds one order of magnitude. Because in general variation in calculated output is substantial higher, this suggests that for most of the outputs additional variation can be explained by differences in model concepts and in input parameters.

Furthermore, the following conclusions can be drawn:

<u>Insight in variation in exposures:</u>

- The variation in *Total exposure* does not clearly increase when country-specific default parameters are used instead of standardised input parameters. This suggests that the variation from different model concepts dominates over the variation from using different input parameters. The same conclusions can be drawn for *Exposure via crop consumption, Exposure via indoor air inhalation.* Only for *Exposure via soil ingestion* variation clearly increase when country-specific default parameters are used instead of standardised input parameters. For this exposure pathway it seems that the variation from using different input parameters dominates over the variation from different model concepts.
- For each type of exposure a few extreme values have been calculated, i.e. values that are "very different" from the median value. Most extreme values are calculated in the following order: *Exposure via indoor air inhalation* (high extremes) > *Total exposure* (low extremes) > *Exposure via crop consumption* (low and high extremes) > *Exposure via soil ingestion* (low extremes).

<u>Influence of contaminant on variation in exposures:</u>

- The variation in *Total exposure* is dependent on contaminant (most variation for exposure to atrazine). The variation in *Exposure via soil ingestion* is scarcely dependent on contaminant. The variation in *Exposure via crop consumption* is strongly dependent on contaminant (most variation for exposure to cadmium and to a lesser extent to benzo(a)pyrene and trichloroethene). The variation in *Exposure via indoor air inhalation* is also dependent on contaminant (most variation for exposure to atrazine and to benzo(a)pyrene), although the variation is high for all contaminants.

<u>Influence of exposure model on variation in exposure:</u>

- The variation in *Total exposure* is strongly dependent on exposure model, although the majority of the models contribute to large variation. The variation in *Exposure via soil ingestion* is scarcely dependent on exposure model. The variation in *Exposure via crop consumption* is strongly dependent on exposure model (most variation for calculations with CLEA D.D.) The variation in *Exposure via indoor air inhalation* also is strongly dependent on exposure model (most variation for calculations with CSOIL 8.0, CETOX and ROME 01). Again, the majority of the models contribute to large variation in *Exposure via indoor air inhalation*.

<u>Influence of soil use and soil type on variation in exposure:</u>

- The variation in *Total exposure, Exposure via soil ingestion, Exposure via crop consumption* and *Exposure via indoor air inhalation* is scarcely dependent on soil use and even less dependent on soil type.

<u>Understanding variation in exposure:</u>

- There is a strong relation between variation in *Exposure via indoor air inhalation* and variation in *Concentration in indoor air*. This suggests that the factors that control the variation in *Concentration in the indoor air*, i.e. *Concentration in soil air*, *Surface and*

Volume of the house or building, *Ventilation frequency*, also control the variation in *Exposure via indoor air inhalation.*
- On the contrary there is no clear relation between the variation in *Exposure via crop consumption* and the variation in *Concentration in crop* (root or leafy vegetables). This suggests that the input parameters *Total (root and leafy) vegetable consumption* and *Fraction of root and leafy vegetables that is homegrown* (also) control the variation in *Exposure via crop consumption*.
- The variation in *Concentration in pore water* is not clearly related to the variation in *Exposure via crop consumption* or to the variation in *Concentration in leafy root or leafy vegetables.*
- The variation in *Concentration in soil air* is not clearly related to the variation in *Exposure via indoor air inhalation* or to the variation in *Concentration in indoor air.*

6.1.4 Procedure on calculating human exposure

- Intensive communication between model client and model user is essential to tune calculated human exposure to the client's expectations and is sometimes even necessary to avoid serious miscalculations.
- Because of geographical/ ethnological and political differences throughout Europe it is an utopia to have one ideal human exposure model, including one ideal input parameter set, that can be used along the lines of one ideal general procedure.

6.2 Recommendations

The following recommendations can be given:
- The variation in calculated human exposure should be investigated in more detail. As part of this further research the differences in the model concepts on variation in exposure should be evaluated in more detail, taking into account the mathematical description of the model concepts. To this purpose international human exposure model experts should participate actively in this further research.
- On the long term a tool box should be constructed for use in (a part of) Europe, including:
    - Identification of which elements of the human exposure calculation, i.e. boundary conditions, (part of) model concepts, input parameters should be standardised throughout Europe.
    - Fixed model concepts, for these model concepts that are suitable for standardisation and harmonisation ("fixed model tools").
    - Fixed input parameters for these input parameters that are suitable for standardisation and harmonisation ("fixed input parameter tools").
    - Flexible model concepts that are suitable for standardisation and harmonisation, but for which place for political choices is desired ("flexible model tools").
    - Options for input parameters for these input parameters that are suitable for standardisation and harmonisation, but for which place for political choices is desired ("optional parameter tools").

- A procedure on assessing human exposure, including documentation on the sensitivity of calculated human exposure to the input parameters and a guideline on when and how to measure concentrations in contactmedia.
- Information on the uncertainty/ reliability of the calculated human exposure.

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77 Ir. A.H.M. Bresser (hLWD)
78 Dr. A. Opperhuizen (hLEO)
79 Ing. P.F. Otte (LER)
80 Ir. J.P.A, Lijzen (LER)
81 Drs. D. de Zwart (LER)
82 Drs. T.G. Vermeire (CSR)
83 Drs. M.G.J. Rikken (CSR)
84 Drs. T. Traas (CSR)
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86 Ms.dr. A.G. Oomen (SIR)
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91 Author
92 SBC/Communicatie
93 Bureau Rapportenregistratie
94 Bibliotheek RIVM
95 Bibliotheek CSR
98-107 Bureau Rapportenbeheer
108-200 Reserve-exemplaren

Appendix 2: Detailed information on the European human exposure models

CETOX-human (Denmark)

1. AFFILIATION CONTACT PERSON

1.1 Dorte Rasmussen, DHI Water and Environment, Agern Allé 11, DK-2970 Horsholm, DOR@dhi.dk

2. MODEL CHARACTERISTICS

2.1 Name: CETOX-human
Report in Danish: Humantoksikologiske vurderinger i forbindelse med depotindsatsen. Arbejdsrapport nr. 16 1996.
Report in Danish: Forholdsregler mod forurenet jord. Arbejdsrapport nr. 15 1996.

Is the model based on existing exposure models?
2.2a In regard to model concept
- Yes. Several of the sub-models are based on existing exposure models, e.g. the volatilisation is based on the model of Jury et al. (Thomas, 1982), the dilution in the air is taken from Veerkamp & ten Berge, 1992).

2.2b In regard to input parameters
- Yes. Some of the input parameters have been defined specifically for the CETOX-human model, others are literature values; e.g. N&R Consult (1990), Dansk Standard (1995), van den Berg & J.M. Roels (1991), IPCS (1994), Veerkamp & ten Berge (1992), AIHC (1994), de Silva 1994). The compound data are derived on the basis of a review and evaluation of literature data.

2.3 What compartments are considered in the model
- soil

2.4 What exposure pathways are incorporated? Exposure via
- soil ingestion
- crop consumption
- inhalation of indoor air.
- inhalation of outdoor air
- inhalation of dust/ soil particles
- dermal uptake through soil, inside
- dermal uptake through soil, outside

Remarks: The first model did not consider inhalation of indoor air. An extension, where this exposure pathway has been included, has been added.

2.5 CETOX-human can be used for:
- calculation of site-specific human exposure
- characterisation of the polluted site with respect to "free use", "advisory action" (the users will be advised about the appropriate use of the soil), and "exposure cut-off" (denotes the uses of the soil, which cannot be recommended)
- ad hoc risk assessment

2.6 Does the model offer possibilities for probabilistic analysis:
- no, not at present.

2.7 Is the model available for third parties?
- no, not at present

2.8 Is the model in “general” use?
- no

2.9 Is background exposure taken into account?
- yes

3. DEFAULT SCENARIOS AND INPUT PARAMETERS

3.1 What standard exposure scenario's do you use:
- residential: included in these calculations, were not included originally
- industrial: included in these calculations, were not included originally.
- vegetable garden
- kindergarten
- parks
- ornamental gardens (crops like flowers, no consumption), incl. common grounds around apartment housing
- sports grounds
- consolidated grounds (partly un-permeable coating, e.g. asphalt, concrete, flagstones)

3.2 The following standard age ranges are defined:
- children is around 1-3 years
- adults is around 20 – 60 years

3.3 Are differences in exposure for men and women taken into consideration?
- no

3.4 How is dealt with exposure to children and adults?
- calculated separately

3.5 Do you (also) consider acute (short-term) exposure (i.e. exposure that takes place during several hours)?
- no

3.6 Are any kinetic (time dependent) processes included in the model?
- no

3.7 Is the possibility for degradation included in the model?
- no

3.8 Are any standards incorporated in the model that limit the maximal concentration in contactmedia (e.g. crop concentration does not exceed x mg/kg, or indoor air concentration does not exceed y mg/m^3)?
- no

3.9 Is exposure to mixtures of contaminants included in the model?
- no

What principal basis do you use in the range of worst case - best case?

3.10a For model concepts:
- realistic worst case

3.10b For input parameters:
- different, namely a min, max and average

Remarks: The CETOX-human model operates with a minimum, average and maximum exposure via the different exposure pathways. This means that three estimated total exposures could be obtained from the model: a minimum, an average and a maximum exposure.

3.11 Are there any guidelines for selection of input parameters?
- no

Remarks: The references to the model describe how parameters for 5 compounds have been derived. It also can be used as a guideline on how to derive parameters for other compounds.

3.12 Are there any recommendations and/or guidelines for measuring concentrations in contactmedia (crops, indoor air)?
- no

3.13 What is the “starting point” of the human exposure calculation?
- total soil content

3.14 How is the distribution of contaminants into the soil phases incorporated in the model?
- using partition coefficients (Kd, Koc, Khenry)

In case that the exposure pathway “exposure via crop consumption” is included:

3.15a Is it possible to calculate the *site-specific* uptake/accumulation in crops (as function of soil characteristics)?
- yes

3.15b What crops do you consider?

- consumption crops only. A dietary model composed of different vegetables and fruits is included.

Remark: An adult and a child is assumed to eat a certain amount of potatoes, tomatoes, fruits etc per day. A BCF for each crop and chemical is determined. Average BCFs are then determined where the BCF of each crop is weighed with respect to the relative amount of the crop eaten per day.

3.15c Is phytotoxicity included (a maximal permissible concentration in the crop)?

- no

In case that the exposure pathway “exposure via inhalation of indoor air” is included:

3.16 Is it possible to calculate the *site-specific* indoor air concentration (as function of soil characteristics, groundwater table, building characteristics, etc.)?

- yes, but a number of parameters have to be determined.

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CLEA D.D. (United Kingdom)

1. AFFILIATION CONTACT PERSON

1.1 Paul Nathanail, Land Quality Management Ltd, School of Chemical Environmental and Mining Engineering, University of Nottingham, University Park, Nottingham NG7 2RD, naomi.earl@nottingham.ac.uk

2. MODEL CHARACTERISTICS

2.1 Name: Contaminated Land Exposure Assessment Model, CLEA97, references
Remarks: Developed by Professor Colin Ferguson for Department of the Environment, now Department of the Environment, Food and Rural Affairs (DEFRA), in Visual Basic. The non-compiled version has been held by Land Quality Management Ltd until recently and all variables can be changed and manipulated. Since this model comparison was performed, CLEA 2002 has been published.

A compiled version of CLEA in C++ has been commissioned by DEFRA, the Environment Agency of England and Wales and the Scottish Environment Protection Authority. Some input parameters can be changed but others (e.g. soil properties, depth of contamination) and the source code cannot be manipulated without access to the software company.

Is the model based on existing exposure models?
2.2a In regard to model concept
- no (in the main)

Remarks: The model was designed for UK conditions, soil types, land-use scenarios and applicable pathways. However some of the algorithms are based on the algorithms in other models.
2.2b In regard to input parameters
- no

Remarks: The input parameters have been chosen on a case-by-case basis from extensive literature review. Receptor characteristics and behaviour and time spent in various activities are based on UK data.

2.3 What compartments are considered in the model
- soil
- groundwater- only in unsaturated zone, when in equilibrium with soil

2.4 What exposure pathways are incorporated? Exposure via
- soil ingestion
- crop intake-garden vegetables only
- inhalation of indoor air
- inhalation of outdoor air
- inhalation dust/ soil particles-separated into inside and outside
- inhalation of bathroom air-not usually considered but present in one of background routines
- dermal uptake through soil, inside
- dermal uptake through soil, outside
- dermal uptake during bathing/showering- not usually considered but present in one of background routines
- soil attached to garden vegetables

2.5 CLEA can be used for
- calculation of site-specific assessment criteria.
- deriving soil quality standards (UK Soil Guideline Values for contaminants in soils) in the framework of UK regulation, (planning regime and Part IIA of 1990 Environmental Protection Act).
- ad hoc risk assessment (only with manipulation of source code at present. This will change if an external version of the model is released).

2.6 Does the model offer possibilities for probabilistic analysis:
- yes

Remarks: CLEA has been developed solely as a probabilistic model (with manipulation of the source code this can be used for sensitivity and uncertainty analysis but neither is the primary purpose.) Many of the input parameters for calculating exposure have an input range of values with a probability density function appropriate for each variable. In order to input the standard defaults required for this exercise the source code within the model must be overwritten, in order the eliminate the probabilistic nature of the model and input single values.

2.7 Is the model available for third parties?
- yes

Remarks: the model is available from available from www.environment-agency.gov.uk or www.defra.gov.uk.

2.8 Is the model in "general" use?
- yes

Remarks: CLEA2002 has been in general use since March 2002.

2.9 Is background exposure taken into account?
- optional

Remarks: UK policy is that background exposure to air, water and food and also exposure to contaminated soil on other sites should be taken into account for threshold substances. They are not, however, included for non-threshold substances.

3. DEFAULT SCENARIOS AND INPUT PARAMETERS

3.1 What standard exposure scenario's do you use:
- residential-with-plant uptake
- residential-without-plant uptake
- industrial
- vegetable garden (called allotments)

Remarks: Exposure to parks, playing fields and open spaces was included is CLEA97, were it was treated as the same as the residential-without-gardens scenario, with the exception that the vapour intrusion pathway is not included. This conservative assumption is to take account of the fact that some inner city parks will be used by children as if they were back gardens. If site-specific information was available, this assumption would not need to be made. In CLEA2002 it is not included.

3.2 The following standard age ranges are defined:
- The first 16 years of life are treated as individual age classes. The working life (between 16 and 59, i.e. 43 years of exposure) is treated as another age class. Retirement (between 59 and 70, i.e. 11 years of exposure is treated as another standard age class.

Remarks: For the purpose of deriving Soil Guideline Values, different combinations of age classes are used by CLEA2002 for exposure and averaging periods, depending on the land use and whether the contaminant considered is a non-threshold or a threshold substance. These are shown in the table below.
For threshold substances

Land use	Exposure Period	Averaging Period
Residential-with-plant uptake	0-6 years	6 years
Residential-without-plant uptake	0-6 years	6 years
Allotments	0-70 years	70 years
Commercial/industrial	16-59 years	43 years

For threshold substances

Land use	Exposure Period	Averaging Period
Residential-with-plant uptake	0-30 years	70 years
Residential-without-plant uptake	0-30 years	70 years
Allotments	0-70 years	70 years
Commercial/industrial	16-59 years	70 years

3.3 Are differences in exposure for men and women taken into consideration?
- yes

Remarks:
Men and women are assumed to have different physiological characteristics (e.g. body weights and inhalation rates) and also slightly different activity patterns in some instances. The female receptor is used as the default for the derivation of Soil Guideline Values.

3.4 How is dealt with exposure to children and adults?
- Calculated separately or summed up

Remarks: This depends on the land use and nature of contaminant as shown in the table above. An important feature is that childhood is assumed to last until the 16th birthday, not just the sixth birthday. Each year of the 16 years is modelled differently in terms of bodyweights, inhalation rates and exposure patterns.

3.5 Do you (also) consider acute (short-term) exposure (i.e. exposure that takes place during several hours)?
- no

Remarks: Short-term risk is not taken into account in the model. However the as yet unpublished Soil Guideline Value for cyanide is based on acute exposure- this is calculated separately, not using the CLEA model itself.

3.6 Are any kinetic (time dependent) processes included in the model?

- yes, namely “degradation” in terms of half life, and penetration through the skin in one of the dermal algorithms.

Remarks: The term “degradation” includes all the processes in soil which may contribute to the half-life e.g. biodegradation, leaching and volatilisation. Although the model is able to take degradation into account, it is not included when deriving Soil Guideline Values in order to be protective of human health. A fixed contact period is used to calculate penetration into the skin.

3.7 Is the possibility for degradation included in the model?
- yes, namely use of half life-see above.

3.8 Are any standards incorporated in the model that limit the maximal concentration in contactmedia (e.g. crop concentration does not exceed x mg/kg, or indoor air concentration does not exceed y mg/m^3)?
- no

Remarks: CLEA97 is able to incorporate limits to vegetable concentration due to phytotoxicity. However insufficient data was found in the literature about a) what constituted phytotoxicity (varies between minor decrease in plant yield and death of plant) and b) phytotoxic limits for different contaminants and plants for this facility to be used when generating Guideline Values.

3.9 Is exposure to mixtures of contaminants included in the model?
- no

What principal basis do you use in the range of worst case - best case?

3.10a For model concepts:
- probabilistic modelling is used in many cases (e.g. amount of contaminant taken up by plants, in other cases reasonable maximal exposure (best estimates in case there is enough knowledge; upper bound estimate in case of doubt)

Remarks: Each model concept was examined on an individual basis, in order to make these decisions.

3.10b For input parameters:
- many of the variables e.g. body weight, vegetable consumption rate, proportion of vegetables that are site-grown, childhood soil ingestion rate are calculated probabilistically from Probability Density Functions using Monte Carlo simulation. In other cases e.g. time on site CLEA 97 uses a best reasonable guess (realistic in case there is enough knowledge; worst case in case of doubt)

3.11 Are there any guidelines for selection of input parameters?
- yes

Remarks: Guidance is provided in the CLR9 and CLR10 and individual substance reports.

3.12 Are there any recommendations and/or guidelines for measuring concentrations in contactmedia (crops, indoor air)?
- no

3.13 What is the “starting point” of the human exposure calculation?
- total soil content

Remarks: The hard code of the model may be fixed to start with e.g. a groundwater concentration but this is not usually done.

3.14 How is the distribution of contaminants into the soil phases incorporated in the model?
- different, namely mainly using partition coefficients (Kd, Koc, Khenry) but some of the algorithms (e.g. dermal, plant uptake) may use fugacity theory.

In case that the exposure pathway “exposure via crop intake” is included:

3.15 Is it possible to calculate the *site-specific* uptake/accumulation in crops (as function of soil characteristics)?
- yes

Remarks: As a function of pH (cadmium) and % soil organic matter (mercury, organic contaminants).

3.15b What crops do you consider?
- different crops, namely potatoes; carrots; onions and leeks (treated as one category); brussels sprouts, cabbage, lettuce.

Remarks: These vegetables have been selected because they are the most commonly home-grown vegetables in the UK.

3.15c Is phytotoxicity included (a maximal permissible concentration in the crop)?
- no

Remarks: CLEA97 is able to incorporate limits to vegetable concentration due to phytotoxicity. However insufficient data was found in the literature about a) what constituted phytotoxicity (varies between minor decrease in plant yield and death of plant) and b) phytotoxic limits for different contaminants and plants for this facility to be used when generating Guideline Values.

3.16 Is it possible to calculate the *site-specific* indoor air concentration (as function of soil characteristics, groundwater table, building characteristics, etc.)?

- yes

Remarks: The indoor air concentration depends on %Soil Organic Matter and soil type (sand, loam or clay) and building type (ground-bearing slab or suspended floor) which can all be altered easily on the screen. Separate Soil Guideline Values may be published for 1, 2.5, 5, and 10% SOM and also for building type. All published Guidelines will be for sandy soil because this is a worst case scenario. The building characteristics (ventilation rate, volumes, thickness of layers etc) are in data files and the pathlength is in the hard code. It is anticipated that all of these variables will be easily changeable when the model is available commercially. At the time of writing no CLR10 report for volatile substances has been published.

4. REFERENCES

List: References that were given in the questionnaire.

CSOIL 8.0 (The Netherlands)

1. AFFILIATION CONTACT PERSON

1.1 Piet Otte, National Institute of Public Health and the Environment (*RIVM*), P.O. Box 1, 3720 BA Bilthoven, The Netherlands, pf.otte@rivm.nl

2. MODEL CHARACTERISTICS

2.1 name: CSOIL 8.0
Remarks: CSOIL calculates exposure to contaminated terrestrial soils. Other relevant models are VOLASOIL for the site-specific calculation of the indoor air and SEDISOIL for the calculation of exposure to contaminated sediments. The information in this questionnaire refers to CSOIL, unless it is said otherwise.

Is the model based on existing exposure models?
2.2a In regard to model concept
- no

Remarks: CSOIL was partly developed in co-operation with the developers of HESP (ECOTOC/Veerkamp, 1990).
2.2b In regard to input parameters
- no

2.3 What compartments are considered in the model
- soil
- groundwater (unsaturated zone)

2.4 What exposure pathways are incorporated? Exposure via
- soil ingestion
- crop consumption
- intake of municipal drinking water, which is contaminated due to permeation of contaminants through groundwater tubes.
- inhalation of indoor air
- inhalation of outdoor air
- inhalation of dust/ soil particles
- inhalation of bathroom air
- dermal uptake through soil, inside
- dermal uptake through soil, outside
- dermal uptake during bathing/showering

Remarks: as part of the procedure of the calculation of the Intervention Values exposure via direct intake of groundwater as drinking water is considered.

2.5 CSOIL can be used for
- derivation of soil quality standards (Intervention Values) in the framework of the Dutch Soil Protection Act
- derivation of remediation objectives
- determination of the urgency of remediation
- calculation of site-specific exposure

2.6 Does the model offer possibilities for probabilistic analysis:
- no

2.7 Is the model available for third parties?
- no

Remarks: The CSOIL formulae have been incorporated in the model Risk human (Van Hall Institute) and in the (human exposure part of the) SUS model (also Van Hall Institute) which is formally used for the determination of the urgency of remediation in the case of serious soil contamination in the framework of the Dutch Soil Protection Act. These models are available.
In 2003 it is planned to give a overview of the model on the RIVM website (www.RIVM.nl).

2.8 Is the model in “general” use?
- yes

Remarks: Although CSOIL was never made available many consultants perform site-specific risk assessment on the basis of the CSOIL formulae. Besides, CSOIL is incorporated in the SUS computer package, which is formally used to assess the determination of the urgency of remediation in the case of serious soil contamination in the framework of the Dutch Soil Protection Act.

2.9 Is background exposure taken into account?
- no

3. DEFAULT SCENARIOS AND INPUT PARAMETERS

3.1 What standard exposure scenario's do you use:
- residential with vegetable garden
- residential with normal garden (standard scenario)
- residential without garden
- industrial
- infrastructure
- recreational areas
- parks
- social-cultural areas

Remark: The Intervention Values for soil were derived on the basis of the scenario residential with normal garden (the so called standard scenario).

3.2 The following standard age ranges are defined:
- 0 – 6 years (children) and 6 - 70 years (adults)

3.3 Are differences in exposure for men and women taken into consideration
- yes

3.4 How is dealt with exposure to children and adults?
- calculated separately or summed up

3.5 Do you (also) consider acute (short-term) exposure (i.e. exposure that takes place during several hours)?
- no

3.6 Are any kinetic (time dependent) processes included in the model?
- no

3.7 Is the possibility for degradation included in the model?
- no

3.8 Are any standards incorporated in the model that limit the maximal concentration in contactmedia (e.g. crop concentration does not exceed x mg/kg, or indoor air concentration does not exceed y mg/m^3)?
- yes, namely solubility should not exceed the maximal solubility.

Remarks: for the derivation of soil quality standards (Intervention Values) also the Tolerable Concentration in Air (TCA) limits the calculated indoor air concentration and drinking water quality standards limit the calculated concentration in groundwater.

3.9 Is exposure to mixtures of contaminants included in the model?
- no

What principal basis do you use in the range of worst case - best case?

3.10a For model concepts:
- reasonable maximal exposure (best estimates in case there is enough knowledge; upper bound estimate in case of doubt)

3.10b For input parameters:
- best reasonable guess (realistic in case there is enough knowledge; worst case in case of doubt)

3.11 Are there any guidelines for selection of input parameters?
- not officially

Remarks: However, for the derivation of the Intervention values the major input parameters have been identified on the basis of a sensitivity analysis. Besides the input parameters of the VOLASOIL model has been categorised as sensitive/ average sensitive and not sensitive.

3.12 Are there any recommendations and/or guidelines for measuring concentrations in contactmedia (crops, indoor air)?

- it is recommended in the Manual on the determination of urgency of remediation, besides the assessment of the calculation of exposure to the indoor air, to measure the concentration in indoor air and compare this to the TCA. Besides it is recommended to measure the concentration in crops.

3.13 What is the “starting point” of the human exposure calculation?
- total soil content

3.14 How is the distribution of contaminants into the soil phases incorporated in the model?
- using the fugacity theory
- using partition coefficients (Kd, Koc, Khenry)

In case that the exposure pathway “exposure via crop consumption” is included:
3.15a Is it possible to calculate the *site-specific* uptake/accumulation in crops (as function of soil characteristics)?
- no, only generic

3.15b What crops do you consider?
- consumption crops only

3.15c Is phytotoxicity included (a maximal permissible concentration in the crop)?
- no

Remarks: a model for site-specific calculation of the uptake/accumulation in crops (as function of soil characteristics) is in progress.

In case that the exposure pathway “exposure via inhalation of indoor air” is included:
3.16 Is it possible to calculate the *site-specific* indoor air concentration (as function of soil characteristics, groundwater table, building characteristics, etc.)?
- no, only generic

Remarks: for calculation of the site-specific indoor air concentration the VOLASOIL model is available.

4. REFERENCES

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LUR (Basque Country, Spain)

1. AFFILIATION CONTACT PERSON

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2. MODEL CHARACTERISTICS

2.1 Full-name: LUR

References:

- T. Martínez, K. Cambra, Y. Cuetos, A. Urzelai. 1998. Valores máximos admisibles en suelo (VIE-B) para la protección de la salud. En: *Calidad del Suelo. Valores Indicativos de Evaluación.* Gobierno Vasco - Departamento de Ordenación del Territorio, Vivienda y Medio Ambiente. IHOBE S.A., Bilbao.
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Is the model based on existing exposure models?

2.2a In regard to model concept

- yes

Remarks: It is based in a review of bibliography and models existing at that time

2.2b In regard to input parameters

Remarks: It is based in a review of bibliography and models existing at that time

2.3 What compartments are considered in the model

- soil

2.4 What exposure pathways are incorporated? Exposure from

- soil ingestion
- crop intake
- inhalation of indoor air
- inhalation of outdoor air
- inhalation dust/ soil particles
- dermal uptake through soil, outside

2.5 LUR can be used for

- deriving soil quality standards in the framework of Contaminated Soil Policy in the Basque Country

Remarks: In parallel to the development of LUR, a methodological guide for site–specific risk assessment was published, which incorporates the criteria, assumptions, guidelines, default values, etc. adopted by LUR.

2.6 Does the model offer possibilities for probabilistic analysis:

- no

2.7 Is the model available for third parties?

- no

Remarks: No, in the form of software, but it is published (see references).

2.8 Is the model in "general" use?

- yes

Remarks: The soil values derived using the model are of general use in the Basque Country, but only in few cases it is used for site-specific assessment (only by Government and very specialised consultancies)

2.9 Is background exposure taken into account?

- yes

Remarks: If data are available.

3. DEFAULT SCENARIOS AND INPUT PARAMETERS

3.1 What standard exposure scenario's do you use:

- residential
- industrial

- children play ground
- parks
- others, namely: residential with vegetable garden...........

3.2 The following standard age ranges are defined: Child (0-6 years); Adult (7-70 years).

3.3 Are differences in exposure for men and women taken into consideration?
- no

3.4 How is dealt with exposure to children and adults?
- calculated separately

Remarks: For carcinogenic substances the long-life exposure is calculated.

3.5 Do you (also) consider acute (short-term) exposure (i.e. exposure that takes place during several hours)?
- no

3.6 Are any kinetic (time dependent) processes included in the model?
- no

3.7 Is the possibility for degradation included in the model?
- no

3.8 Are any standards incorporated in the model that limit the maximal concentration in contactmedia (e.g. crop concentration does not exceed x mg/kg, or indoor air concentration does not exceed y mg/m^3)?
- no

3.9 Is exposure to mixtures of contaminants included in the model?
- no

What principal basis do you use in the range of worst case - best case?
3.10a For model concepts:
- worst case
- reasonable maximal exposure (best estimates in case there is enough knowledge; upper bound estimate in case of doubt)

Remarks: Somewhere between these two options.

3.10b For input parameters:
- best reasonable guess (realistic in case there is enough knowledge; worst case in case of doubt)

3.11 Are there any guidelines for selection of input parameters?
- yes

3.12 Are there any recommendations and/or guidelines for measuring concentrations in contactmedia (crops, indoor air)?
- recommendations yes, guidelines no

3.13 What is the “starting point” of the human exposure calculation?
- total soil content

3.14 How is the distribution of contaminants into the soil phases incorporated in the model?
- using partition coefficients (Kd, Koc, Khenry)

In case that the exposure pathway “exposure via crop intake” is included:
3.15 Is it possible to calculate the *site-specific* uptake/accumulation in crops (as function of soil characteristics)?
- no, only generic

3.15b What crops do you consider?
- consumption crops only

3.15c Is phytotoxicity included (a maximal permissible concentration in the crop)?
- no

In case that the exposure pathway “exposure via crop intake” is included:
3.16 Is it possible to calculate the *site-specific* indoor air concentration (as function of soil characteristics, groundwater table, building characteristics, etc.)?

- no, only generic

NoNameGiven (France)

1. AFFILIATION CONTACT PERSON

1.1 Roseline Bonnard, National Institute for Industrial Environment and Risks (*INERIS*), Parc technologique Alata, BP n°2, 60550 Verneuil-en-Halatte, roseline.bonnard@ineris.fr

2. MODEL CHARACTERISTICS

2.1 Model name: there is no official name. This model has been constructed by INERIS and it is used to make site-specific risk assessment and the appraisal of the third party's studies. Some parts are used to define generic warning values (VCI : valeurs de constat d'impact). It is a tool with a modular structure to adapt it to the specific pathways and pathways of exposure of a specific site.

Is the model based on existing exposure models?
2.2a In regard to model concept
- yes, HESP 2.1, Johnson and Ettingher's model, Thibodeaux's model, USEPA's models for dermal exposure (92), Volasoil

2.2b In regard to input parameters
- yes, HESP 2.1 but also other sources from France, USEPA and more generally from the international scientific literature

2.3 What compartments are considered in the model
- soil
- water
- air

2.4 What exposure pathways are incorporated? Exposure via
- soil ingestion
- crop consumption
- intake of water, which is contaminated due to permeation of contaminants through tubes.
- inhalation of indoor air
- inhalation of outdoor air
- inhalation of dust/ soil particles
- inhalation of bathroom air
- dermal uptake through soil, inside
- dermal uptake through soil, outside
- dermal uptake during bathing/showering

Remarks: For site-specific modelling, we try to incorporate all the pathways which are relevant: exposure via meat and milk consumption could be calculated if these pathways were relevant for the use of the site.

2.5
The INERIS model can be used for and has been used for:
- assessing the level of risk linked to specific sites for human health
- support to identifying remediation solutions

2.6 Does the model offer possibilities for probabilistic analysis:
- yes, to the following purpose:
  - sensitivity analysis (evaluating the contribution of input-parameters)
  - uncertainty analysis (evaluating the uncertainty in the calculated exposure) owing to an add-in software

Remarks: But for uncertainty analysis, we do not have an identified method to define distributions for input parameters

2.7 Is the model available for third parties?
- no

Remarks: But, we always present the origin of all the equations and values of the input parameters

2.8 Is the model in "general" use?
- no

Remarks: Consultants are free to use the model they want, but INERIS can be asked by the French administration to check the risk assessment studies for health, including the exposure modelling

2.9 Is background exposure taken into account?
- no

3. DEFAULT SCENARIOS AND INPUT PARAMETERS

3.1 What standard exposure scenario's do you use:
The most common scenarios are
- residential with or without a vegetable garden
- industrial
- recreational

Remarks: For specific risk assessment, we try to define all the pathways and pathways which are relevant according to the specific use of the site. So there is no real predefined scenario.

3.2 The following standard age ranges are defined:
- child (0-6 year), adult (6-70 years)

3.3 Are differences in exposure for men and women taken into consideration?
- no

3.4 How is dealt with exposure to children and adults?
- calculated separately for non-carcinogens
- summed up for carcinogens

3.5 Do you (also) consider acute (short-term) exposure (i.e. exposure that takes place during several hours)?
- no

3.6 Are any kinetic (time dependent) processes included in the model?
- Yes, the gas emission is time dependent

3.7 Is the possibility for degradation included in the model?
- no

Remarks: It is used at the moment but a first order degradation function could be easily included

3.8 Are any standards incorporated in the model that limit the maximal concentration in contactmedia (e.g. crop concentration does not exceed x mg/kg, or indoor air concentration does not exceed y mg/m^3)?
- no

3.9 Is exposure to mixtures of contaminants included in the model?
- no

Remarks: We can manage several substances at the same time. But we cannot take into account the chemistry and the interactions of the mixtures of contaminants. Petroleum products can be treated by fractions like in the TPH approach.

What principal basis do you use in the range of worst case - best case?
3.10a For model concepts:
- reasonable maximal exposure (best estimates in case there is enough knowledge; upper bound estimate in case of doubt)

3.10b For input parameters:
- best reasonable guess (realistic in case there is enough knowledge; worst case in case of doubt)

3.11 Are there any guidelines for selection of input parameters?
- yes

Remarks: There are some rules to choose values of input parameters. Values are chosen with regard to representatively and experimental conditions. Values from experiments are preferred compared to calculated values. In a specific site assessment the references must be given and the assessor has to motivate parameter identification. For substances, there are some reports with the chemical parameters.

3.12 Are there any recommendations and/or guidelines for measuring concentrations in contactmedia (crops, indoor air)?
- no

3.13 What is the “starting point” of the human exposure calculation?
- total soil content but the results of measures made in the different compartments can be used as inputs

3.14 How is the distribution of contaminants into the soil phases incorporated in the model?

- using partition coefficients (Kd, Koc, Khenry)

In case that the exposure pathway “exposure via crop consumption” is included:
3.15a Is it possible to calculate the *site-specific* uptake/accumulation in crops (as function of soil characteristics)?
- no, only generic

Remarks: We try to choose parameters, including BCFs, for which the experimental conditions are representative for the relevant site. But for BCF, it is often difficult to find well-adapted values
3.15b What crops do you consider?
- all crops for which relevant data (i.e. BCFs) are available

3.15c Is phytotoxicity included (a maximal permissible concentration in the crop)?
- no

In case that the exposure pathway “exposure via inhalation of indoor air” is included:
3.16 Is it possible to calculate the *site-specific* indoor air concentration (as function of soil characteristics, groundwater table, building characteristics, etc.)?
- yes

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NoNameGiven (Sweden)

1. AFFILIATION CONTACT PERSON

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Mark Elert, B Sc, Kemakta Konsult AB, Box 12655, S-112 93 Stockholm, mark@kemakta.se

2. MODEL CHARACTERISTICS

2.1 Name:
- No name given, published in Swedish EPA Reports 4639 and 4889. Report 4639 reports the version of the model used for development of generic guidelines for contaminated soils. This model has later been extended for the development of guidelines at petrol stations (report 4889). The extensions comprise the use of different soil types, different depths of the pollutant, new models for indoor air concentration and dilution in groundwater wells.

Is the model based on existing exposure models?
2.2a In regard to model concept
- yes: CSOIL, HESP, Massachusetts Department of Environmental Protection, US EPA Soil Screening Levels, Ontario MOEE

2.2b In regard to input parameters
- yes, same as above for exposure data. Chemical-physical data primarily from US EPA SSL and toxicological data from WHO, except for petroleum hydrocarbons where data are taken from Total Petroleum Hydrocarbon Working Group.

2.3 What compartments are considered in the model
- soil
- groundwater
- surface water

2.4 What exposure pathways are incorporated? Exposure via
- soil ingestion
- crop consumption
- direct groundwater intake
- inhalation of indoor air
- inhalation of outdoor air (see remarks)
- inhalation of dust/ soil particles
- dermal uptake through soil, inside (not distinguished from outside)
- dermal uptake through soil, outside (not distinguished from inside)
- fish intake

Remarks: Inhalation of outdoor air included for land-uses: Park and Land with limited use (see 3.1).

2.5 The model can be used for
- calculation of site-specific human exposure
- deriving soil quality standards
- ad hoc risk assessment

2.6 Does the model offer possibilities for probabilistic analysis?
- no

Remarks: Simple sensitivity analyses can be performed.

2.7 Is the model available for third parties?
- no

Remarks: Software form is Excel spreadsheets.

2.8 Is the model in "general" use?
- no

Remarks: The calculation methodology and formulas are in general use by consultants and public servants.

2.9 Is background exposure taken into account?
- yes

For some metals where background exposure through diet is high in relation to TDI

3. DEFAULT SCENARIOS AND INPUT PARAMETERS

3.1 What standard exposure scenario's do you use:
- residential
- industrial
- vegetable garden
- children play ground
- kindergarten
- infrastructure
- agriculture
- nature reserves
- recreational areas
- parks
- less sensitive land use but with groundwater extraction

Remarks:
Three categories of land use are defined in Report 4639:
- Sensitive land use (basically multifunctionality) i.e. residential areas, kindergartens, play grounds, vegetable garden, agricultural use
- Less sensitive use *without* groundwater extraction (i.e. commercial use, offices, industry, roads etc)
- Less sensitive land use *with* groundwater extraction within 500 m of the site (exposure through drinking water included)

In report 4889 two additional categories are included:
- Park, i.e. land without buildings but occasionally frequented by humans. High environmental value. Groundwater protection. (parks, recreational areas, nature reserves.)
- Land with limited use, land without buildings but occasionally frequented by humans. Moderate environmental value. Groundwater protection.

3.2 The following standard age ranges are defined:
- 0 – 6 years and 6 - 64 years

3.3 Are differences in exposure for men and women taken into consideration?
- no

3.4 How is dealt with exposure to children and adults?
- calculated separately or summed up

Remarks: Exposure for both children and adults are evaluated. For non-genotoxic contaminants group with highest long-term exposure considered (i.e. children). For genotoxic contaminants lifetime average exposure used.

3.5 Do you (also) consider acute (short-term) exposure (i.e. exposure that takes place during several hours)?
- yes

Remarks: For some chemicals with high acute toxicity, such as cyanide and As (pica-children at high risk)

3.6 Are any kinetic (time dependent) processes included in the model?
- yes, evaporation of volatile organic compounds.

Remarks: Release rate from soil will decrease with time due to depletion of soil layers near surface. An average rate over a period of 5 years used.

3.7 Is the possibility for degradation included in the model?
- no

3.8 Are any standards incorporated in the model that limit the maximal concentration in contactmedia (e.g. crop concentration does not exceed x mg/kg, or indoor air concentration does not exceed y mg/m^3)?
- yes: groundwater concentrations should be below drinking water standards and indoor air concentrations should be below reference concentrations for air

3.9 Is exposure to mixtures of contaminants included in the model?
- yes, for petroleum hydrocarbons

What principal basis do you use in the range of worst case - best case?

3.10a For model concepts:
- reasonable maximal exposure (best estimates in case there is enough knowledge; upper bound estimate in case of doubt)

3.10b For input parameters:

- best reasonable guess (realistic in case there is enough knowledge; worst case in case of doubt)

3.11 Are there any guidelines for selection of input parameters?

- no

3.12 Are there any recommendations and/or guidelines for measuring concentrations in contactmedia (crops, indoor air)?

- recommendations and guidelines

Remarks: As detailed in Swedish EPA Reports 4310-0, 4310-2

3.13 What is the “starting point” of the human exposure calculation?

- total soil content

Remarks: Total (integrated) exposure should be below TDI

3.14 How is the distribution of contaminants into the soil phases incorporated in the model?

- using partition coefficients (Kd, Koc, Khenry)

In case that the exposure pathway “exposure via crop consumption” is included:

3.15a Is it possible to calculate the *site-specific* uptake/accumulation in crops (as function of soil characteristics)?

- no, only generic

3.15b What crops do you consider?

- no specific crops

3.15c Is phytotoxicity included (a maximal permissible concentration in the crop)?

- no

Remark: Only for ecotoxicology

3.16 In case that the exposure pathway “exposure via inhalation of indoor air” is included:
Is it possible to calculate the *site-specific* indoor air concentration (as function of soil characteristics, groundwater table, building characteristics, etc.)?

- yes

In Swedish EPA Report 4889

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ROME 01 (Italy)

1. AFFILIATION CONTACT PERSON

1.1 Francesca Quercia, National Environmental Protection Agency (*ANPA*), Via V. Brancati 48 – 00144, Roma – Italy, quercia@anpa.it
Remarks: additional contact person: Ivano Aglietto, Politecnico di Torino (DIGET), C.so Duca degli Abruzzi 24 – 10129 Torino – Italy, aglietto@polito.it

2. MODEL CHARACTERISTICS

2.1 Name: ReasOnable Maximum Exposure, ROME 01,
Remarks: ROME 01 is an "experimental" or "provisional model", i.e. it is being tested and improved, but at the same time Version 01 is widely used in the country.

Is the model based on existing exposure models?
2.2a In regard to model concept
- yes, namely ASTM RBCA *and CONCAWE*

2.2b In regard to input parameters
- yes, namely U.S. EPA Databases *mostly*

2.3 What compartments are considered in the model
- soil
- groundwater
- air

2.4 What exposure pathways are incorporated? Exposure from
- soil ingestion
- direct groundwater intake
- inhalation of indoor air
- inhalation of outdoor air
- inhalation of dust/ soil particles
- dermal uptake of soil
- inhalation of vapours from groundwater and from free product

Remarks: crop consumption might be added in the future.

2.5 ROME 01 has been used for
- Calculation of site-specific human exposure
- Determination of site-specific clean up objectives
- Real cases of risk assessment (by consultants and local authorities)
- Proposal for National Generic Limit Values (not implemented so far)
- Elaboration for Screening Values (Region Lombardia) for chemicals not included in the present national norm

2.6 Does the model offer possibilities for probabilistic analysis:
- no

2.7 Is the model available for third parties?
- yes (user friendly and windows compatible, free of charge)

2.8 Is the model in “general” use?
- yes

2.9 Is background exposure taken into account?
- no

3. DEFAULT SCENARIOS AND INPUT PARAMETERS

3.1 What standard exposure scenario's do you use:
- residential
- industrial

Remarks: recreational areas are assimilated to residential, children playground is assimilated to residential for limited age range. Vegetable gardens might be added by including crop consumption in the residential scenario, but this should fit with criteria for agricultural soils, that are presently missing.

3.2 The following standard age ranges are defined:
- 0 – 6 years and 6 - 70 years

3.3 Are differences in exposure for men and women taken into consideration
- no

3.4 How is dealt with exposure to children and adults?
- calculated separately

Remarks: for carcinogenic substances children and adult exposure are summed up and averaged over lifetime.

3.5 Do you (also) consider acute (short-term) exposure (i.e. exposure that takes place during several hours)?
- no

3.6 Are any kinetic (time dependent) processes included in the model?
- no

3.7 Is the possibility for degradation included in the model?
- yes, namely first order

3.8 Are any standards incorporated in the model that limit the maximal concentration in contactmedia (e.g. crop concentration does not exceed x mg/kg, or indoor air concentration does not exceed y mg/m^3)?
- yes, namely maximum concentration for groundwater.

3.9 Is exposure to mixtures of contaminants included in the model?
- yes

Remarks: TPH diesel and gasoline ranges

What principal basis do you use in the range of worst case - best case?

3.10a For model concepts:
- reasonable maximal exposure (best estimates in case there is enough knowledge; upper bound estimate in case of doubt)

3.10b For input parameters:
- reasonable worst case
- reasonable case

3.11 Are there any guidelines for selection of input parameters?
- yes

Remark: defaults mostly from U.S. EPA, ASTM Guidelines, ranges given in ROME 01 manual.

3.12 Are there any recommendations and/or guidelines for measuring concentrations in contactmedia (crops, indoor air)?
- recommendations and guidelines

Remarks: National Technical Regulation and International recommendations and guidelines for soil, water, vapours, sludge, wastes and crops

3.13 What is the “starting point” of the human exposure calculation?
- total soil content AND / OR groundwater concentration
- leachate concentration from tests

3.14 How is the distribution of contaminants into the soil phases incorporated in the model?
- using partition coefficients (Kd, Koc, Khenry)

In case that the exposure pathway “exposure via crop consumption” is included:

3.15a Is it possible to calculate the *site-specific* uptake/accumulation in crops (as function of soil characteristics)?
- no, only generic

Remark: The Model, for the time being, does not include crop intake (generic and site-specific) since the national law for site remediation does not include agricultural use of land. In the residential land-use, home-grown crops consumption is not considered relevant so far, but could be considered in the future.

3.15b What crops do you consider?
- no specific crops (see 15a)

3.15c Is phytotoxicity included (a maximal permissible concentration in the crop)?

- no

In case that the exposure pathway “exposure via inhalation of indoor air” is included:

3.16 Is it possible to calculate the *site-specific* indoor air concentration (as function of soil characteristics, groundwater table, building characteristics, etc.)?

- yes

4. REFERENCES

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Vlier-humaan (Flanders, Belgium)

1. AFFILIATION CONTACT PERSON

1.1 Christa Cornelis, Flemish Institute of Technology and Development (*VITO*), Boeretang 200, B-2400 MOL, Belgium, cornelic@vito.be

2. MODEL CHARACTERISTICS

2.1 Name: Vlaams Instrument voor de evaluatie van risico's - humaan, Vlier-humaan version 1.0, Van Hall Institute

Is the model based on existing exposure models?

2.2a In regard to model concept

- yes, namely HESP. Formulas are based on HESP and are almost not modified. Scenarios were modified.

2.2b In regard to input parameters

- yes, namely input parameters are chosen from the HESP model and from other available models (as CSOIL)

2.3 What compartments are considered in the model

- soil
- groundwater
- air

2.4 What exposure pathways are incorporated? Exposure via

- soil ingestion
- crop consumption
- direct groundwater intake
- intake of groundwater as drinking water, which is contaminated due to permeation of contaminants through drinking water tubes.
- meet/milk consumption
- inhalation of indoor air
- inhalation of outdoor air
- inhalation of dust/ soil particles
- inhalation of bathroom air
- dermal uptake through soil, inside
- dermal uptake through soil, outside
- dermal uptake during bathing/showering

2.5 Vlier-humaan can be used for

- derivation of clean-up values within the Flemish legislation on soil remediation. These clean-up values are meant to decide whether a site has to be remediated in the case of recent soil pollution (originated after 28 October 1995). The clean-up values are also used to give a first indication of the presence of a "serious threat" in the case of historical soil pollution.
- to calculate the minimal required clean-up goals. However, this must fit in the whole legal framework (reaching background values in principle, but BATNEEC can lead to higher values not giving rise to unacceptable risks).

2.6 Does the model offer possibilities for probabilistic analysis:

- yes, to the following purpose: sensitivity analysis (evaluating the contribution of input-parameters)

Remarks: No, in the sense that there is no module provided to do this. Manual performance of sensitivity analysis is possible

2.7 Is the model available for third parties?

- yes (diskette, Van Hall Institute, circa 900 Euro)

2.8 Is the model in "general" use?

- The OVAM (in Flanders responsible for soil pollution problems) has formalised this model for use in risk assessments. It is for the moment the only model that is formally recognised. In principle, consultants need to use this model, so it is in general use. However, other models are also used.

2.9 Is background exposure taken into account?

- yes

3. DEFAULT SCENARIOS AND INPUT PARAMETERS

3.1 What standard exposure scenario's do you use:
- residential
- industrial
- agriculture
- recreational areas
- parks (same as recreational)

Remarks: Recreational and industrial land use each have two different exposure scenarios

3.2 The following standard age ranges are defined:
- 0 – 6 years and 6 - 70 years

3.3 Are differences in exposure for men and women taken into consideration
- no

3.4 How is dealt with exposure to children and adults?
- calculated separately or summed up

Remarks: Both options are possible, depending on the type of contaminant, i.e. carcinogen (lifetime average) or non-carcinogen (separately). In each case results can be seen separately.

3.5 Do you (also) consider acute (short-term) exposure (i.e. exposure that takes place during several hours)?
- no

3.6 Are any kinetic (time dependent) processes included in the model?
- no

3.7 Is the possibility for degradation included in the model?
- no

3.8 Are any standards incorporated in the model that limit the maximal concentration in contactmedia (e.g. crop concentration does not exceed x mg/kg, or indoor air concentration does not exceed y mg/m^3)?
- yes, namely drinking water concentration, crop concentration, air concentration (indoor and outdoor), meat concentration

3.9 Is exposure to mixtures of contaminants included in the model?
- no

What principal basis do you use in the range of worst case - best case?

3.10a For model concepts:
- probably worst case.

3.10b For input parameters:
- best reasonable guess (realistic in case there is enough knowledge; worst case in case of doubt)

3.11 Are there any guidelines for selection of input parameters?
- we make a difference between type of parameters. Fixed parameters can not be modified. Values are reasonable worst case. Secondly, there are default parameters. Values are reasonable worst case. The default parameters can be modified in case of clear site-specific deviations from the default scenario. Thirdly there are variable parameters. These should be identified depending on the local situation. No specific guidelines exist, although the impression is that OVAM prefers worst case, while consultants not always use it (which is of course sometimes reasonable).

3.12 Are there any recommendations and/or guidelines for measuring concentrations in contactmedia (crops, indoor air)?
- no

3.13 What is the “starting point” of the human exposure calculation?
- total soil content

Remarks: It is to a certain extent possible to use measured data in the model.

3.14 How is the distribution of contaminants into the soil phases incorporated in the model?
- using the fugacity theory
- using partition coefficients (Kd, Koc, Khenry)

In case that the exposure pathway “exposure via crop consumption” is included:

3.15a Is it possible to calculate the *site-specific* uptake/accumulation in crops (as function of soil characteristics)?

- no; however, it is possible to use measured crop concentrations or measured BCF-factors. But there are no BCF-factors available that are dependent on soil characteristics.

3.15b What crops do you consider?

- as default we use consumption crops. It is however possible to change values in order to calculate uptake in other crops.

3.15c Is phytotoxicity included (a maximal permissible concentration in the crop)?

- no

In case that the exposure pathway "exposure via inhalation of indoor air" is included:
3.16 Is it possible to calculate the *site-specific* indoor air concentration (as function of soil characteristics, groundwater table, building characteristics, etc.)?

- yes (partly)

Remarks: but not as a function of groundwater table.

4. REFERENCES

List: References that were given in the questionnaire.