Human Exposure Model Comparison Study: State of Play

Frank A. Swartjes

Abstract
The use of human exposure models for the determination of the levels of human exposure to contaminants in soils can lead to a wide range of results, depending upon the model and parameters selected. The consequences can be far-reaching. Therefore a better insight into the accuracy of exposure models is required. For this reason model calculations using different models from seven European countries are compared on the basis of questionnaires. The calculations are based on the same scenarios – with differences in soil use, soil type and contaminant used in the comparisons. In addition, an overview is given of default values for the input parameters used in different exposure models as well as the proposed exposure input parameters of NICOLE. The study will be finished in 2001.

Key words: human exposure model, human exposure parameters

INTRODUCTION

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 a 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*. 1996).
- 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 intake (Stanek and Calabrese 1995). In addition, there may be regional variations in input parameters, for example, in the organic matter content of the soil.

Statistical procedures (like Monte Carlo techniques) can be used to eliminate the influence of uncertain parameters, or uncertain model concepts. However, these procedures are relatively time-consuming.

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 misuse of human exposure models. For example, if an exposure model in which the transport of volatile contaminants derived for homogeneous soils with an average soil temperature of around 10°C, 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 misuse are hard to assess, but they might become more widespread as a variety of commercial user-friendly software packages become available.

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 based on 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’, or for the social and financial situation of organisations and individuals, if a site is incorrectly diagnosed as ‘dangerous’.

The combination of ‘limited accuracy’ and ‘major consequences’ is a serious problem which requires a better insight into the accuracy of exposure models.

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This requirement can be most directly addressed by performing a validation study, i.e. comparing calculated exposure with measured exposure. However, measuring exposure in the human body is difficult, both for ethical and technical reasons. Another way to gain insight in model performance 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 possible variation in calculated human exposures.

PURPOSE

This comparative study, which is sponsored by the Dutch Ministry of Housing, Spatial Planning and the Environment (*VROM*) has the following aims:

- Gaining insight into the possible variation in calculated human exposure.
- Gaining insight into (differences in) default values for the input parameters used in different countries.
- Evaluating the differences in calculated exposure via different major exposure routes on the basis of differences in model concepts and input parameters.

Its results 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 will have a seminal influence on future research and development in this area, and the study itself may be a precursor to a larger R&D proposal.

PROCEDURE

Recognising the value of a comparative study of human exposure models, a number of organisations involved with CLARINET and/or NICOLE 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 of Technology and Development (VITO), Flanders, Belgium;
- The National Institute of Public Health and the Environment (RIVM), The Netherlands;
- Kemakta Konsult AB, Sweden;
- DHI Water and Environment, Denmark; and possibly
- The University of Nottingham, UK.

The models used are described in Table 1.

The following procedure has been used to conduct the ‘Human exposure model comparison study’:

- Comparison of calculated exposure via different major exposure routes (oral soil ingestion, crop consumption, inhalation indoor air) using the different human exposure models listed in Table 1: (a) by using the same prescribed input parameters; and (b) by using the input parameters that are used in different countries (‘own’ default input parameters).
- Overviewing default values used for the main input parameters in the different approaches in the different countries ascertained from questionnaires.
- Evaluating the differences in calculated exposure on the basis of model concepts and input parameters. However, this evaluation might be difficult without direct participation of the human exposure model experts (workshop).
- Informing ‘a broad audience’ on the model comparison study, possibly at the final CLARINET meeting in Vienna in June 2001, or at a workshop on human exposure models.

VARIATIONS IN CALCULATIONS

Twenty hypothetical scenarios have been defined. These scenarios differ in respect to two land uses (residential and industrial), two soil types, and five different contaminants.

The soil types are described as follows:

- Sandy soil, 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, 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 route: oral soil ingestion.
- Cd (metals); major exposure route: crop consump-

tion;
- Atrazine (pesticides); major exposure route: crop consumption;
- Benzene (aromatic compounds); major exposure route: inhalation indoor air;
- Trichloroethene (volatile aliphatic compounds); major exposure route: inhalation 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 $mg.kg_{dw}^{-1}$;
  - Cd: 12 $mg.kg_{dw}^{-1}$;
  - atrazine: 6 $mg.kg_{dw}^{-1}$;
  - benzene: 1 $mg.kg_{dw}^{-1}$;
  - trichloroethene: 60 $mg.kg_{dw}^{-1}$.

- 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).

- Exposure from the following exposure routes:
  - oral soil ingestion;
  - crop consumption;
  - inhalation indoor air.

Total exposure via all exposure routes combined will also be calculated.

All exposure calculations have to be performed twice for all twenty scenarios:

- Once with 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.
- And once with the data that is used in different countries, i.e. each model's 'own' default parameters.

Seventeen different outputs have been defined for each calculation (see Figure 1):

- lifelong exposure and exposure to children and adults via the major exposure routes (oral soil ingestion, crop consumption, inhalation indoor air);
- lifelong exposure and exposure to children and adults via all exposure routes combined; and
- concentrations in contact media (pore water, soil air, root vegetables, 'green' vegetables, indoor air).

There is an interaction between several outputs. Please note 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 groundwater is not considered in this study.
- Background exposure, i.e. exposure from sources other than contaminated soil, is not taken into consideration in this study.

DEFINITIONS

The comparative study also employs standard definitions for use in all of the human exposure models being used. These are as follows:

General
- One's 'own' input parameters: input parameters used for the derivation of soil quality standards, in risk assessment procedures and/or described or listed in manuals.

Exposure
- Exposure: amount of a contaminant expressed in [$mg.kg_{body\ weight}^{-1}.day^{-1}$] 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 from oral soil ingestion: potential exposure due to unconscious oral intake of soil particles (i.e. not including inhalative intake of suspended soil particles or dust).
- Exposure from crop consumption: potential exposure due to oral intake of contaminated home-grown 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

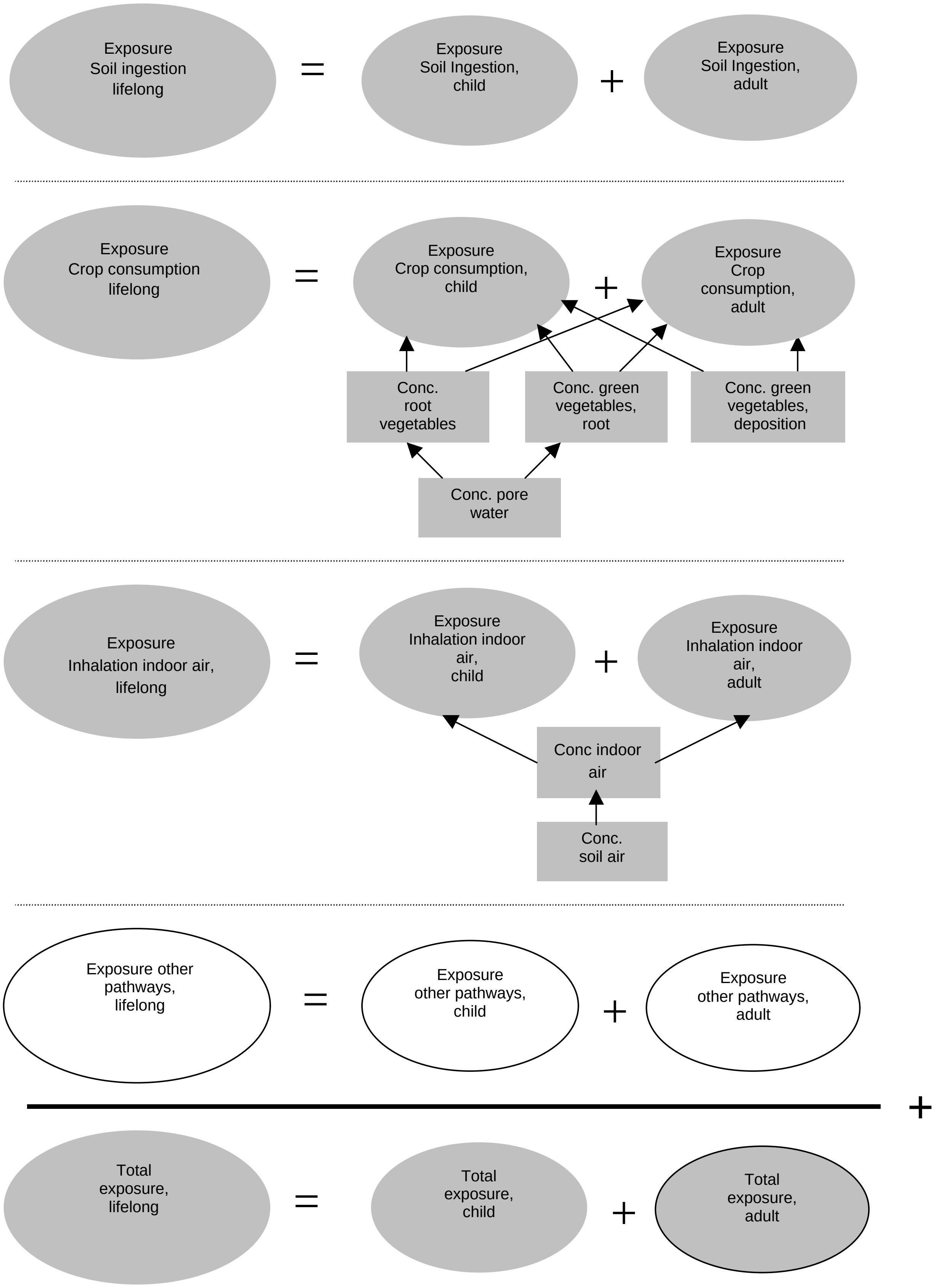

Figure 1: Outputs calculated in the 'Human exposure model comparison study' (shaded) and their interactions; ovals represent exposure, boxes represent concentrations in contact media.

crops originating from the site); no crop uptake from vapours is considered.
  - Root vegetables: the part of the crop growing under the soil surface, including potatoes.
  - 'Green' vegetables: the part of the crop growing above the soil surface.
- Exposure from inhalation of indoor air: potential exposure due to unconscious inhalative intake of contaminated indoor air, 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 production is not the main function of the garden.
- Industrial site: site where industrial activity is the main function; crop cultivation is excluded.

MODELS PARTICIPATING

The models used in this human exposure model comparison study are summarised in Table 1, which also

Table 1. The models used in the human exposure model comparison study, including developers, contact persons and model application

	DEVELOPER	CONTACT	MODEL APPLICATIONS
CETOX-human	DHI Water and Environment (former VKI) and Danish Toxicological Center	DHI Water and Environment, D. Rasmussen, Agern Allé 11, DK-2970 Hørsholm, Denmark	Management of risks arising from polluted soil. The model is tied to the specific polluting substance, land use and outlines how to minimize exposure to soil, which crops not to grow on the land and the like.
CLEA*	University of Nottingham	University of Nottingham, Land Quality Management Ltd., N. Earl, Nottingham NG7 2RD, UK	
CSOIL	National Institute of Public Health and the Environment (RIVM)	RIVM, P. Otte, PO 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)
No name given	National Institute for Industrial Environment and Risks (INERIS)	INERIS, R. Bonnart, Parc Technologique Alata, BP no. 2, 60550 Verneuil-en-Halatte, France	Derivation of generic warning quality standards. Site-specific risk assessment
No name given	Kemakta Konsult AB	Kemakta Konsult AB, M. Elert, PO 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	National Environmental Protection Agency (ANPA)	ANPA, F. Quercia, Via V. Brancati 48, 00144 Rome, Italy	Derivation of generic screening values and 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)

*Possible participating model

provides an overview of each model developer, contact person and model applications. For these models the calculations are performed for the twenty scenarios mentioned above, using prescribed and one's 'own' default input parameters.

The NICOLE (1999) data set is included in the overview of input parameters, together with input parameters used in the different models mentioned in Table 1. This overview illustrates the range of values of input parameters used in different countries. This information could be of use to both those who develop models and those who use or apply models, as well as to policy makers. The complete overview of input parameters will be presented in the final report.

CURRENT STATUS

Most of the participants mentioned in Table 1 conducted the calculations, which yielded a series of values for the seventeen outputs, for all twenty scenarios, once with the prescribed set of parameters, and once with their 'own' default parameters. At the moment statistical data analysis is being performed at the National Institute of Public Health and the Environment (RIVM). The study will be finished in 2001. All participants will be asked to respond to the intermediate results – a small-scale workshop will maybe be organised for this purpose. (Intermediate) results will be presented at the CLARINET final workshop in Venice, June 2001. The final results will be published in a RIVM-report in the second half of 2001.

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