

project description

Validation of Exposure Models and Parameters

enterprise

In order to realise EU legislation, the environmental risk of new and existing chemical substances has to be assessed. The methods for risk assessment are laid down in the **Technical Guidance Documents - TGD** (EC 1996A).

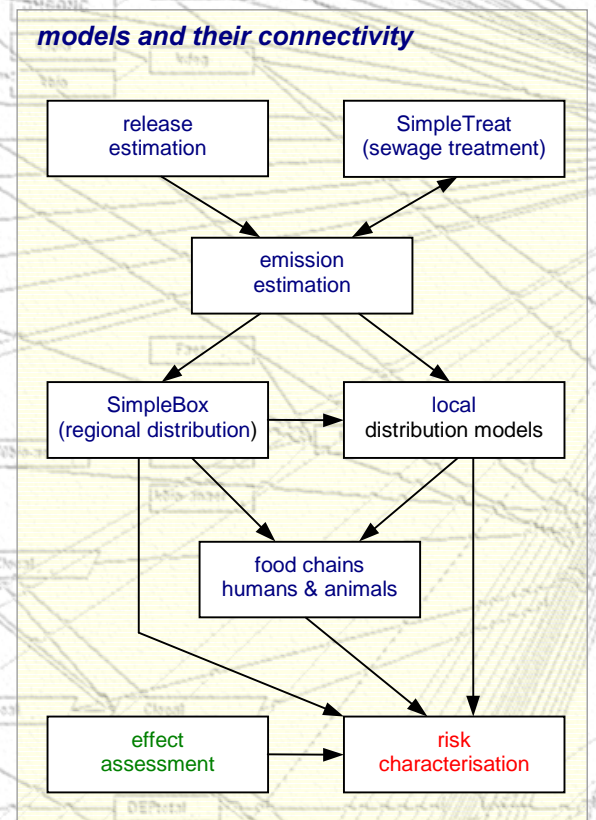
Basically, risk assessment consists of a comparison of predicted environmental concentrations (exposure assessment) and concentrations which may cause adverse effects (effect assessment). For exposure assessment various exposure models (regression equations, simple generic models, multimedia compartment models) are used.

Despite their wide economic and ecological impact, the applicability and usefulness of the models and software were not clarified.

It is determined for which substances and for which environmental segments the models deliver realistic values. One of the aims is to point out and evaluate uncertainty in models and data arising in model application. Scientific justification of underlying equations, limitations, and respective software are tested and checked for possible errors.

models

There are numerous different exposure modelling approaches (a survey can be found in, e.g. TRAPP & MATTHIES 1998 or LEEUWEN & VAN HERMENS 1995). Those models designed for official risk assessment cover all relevant exposure pathways.



The concatenation of diverse submodels enables a more comprehensive and more realistic assessment. Simultaneously the whole system becomes more complex. This reveals the necessity to analyse the models and their connectivity.

EUSES

With the **European Union System for the Evaluation of Substances - EUSES** (EC 1996B) a decision support system is available which integrates the models presented in the TGD into a Windows 95/NT-based software product. Meanwhile, EUSES has attained a far reaching and extensive use in governments, industry, and research institutes.

Besides the actual validation of the models and parameters used, an evaluation of available software and especially of EUSES with respect to quality assurance measures is realised.

methods

In the scientific community the concept of **validation** is debatable and not defined consistently (BECK ET AL. 1997). However, in a pragmatic manner validation can be realised as a method of model analysis, comprising various facets.

- working packages of the project**
- comprehensive data recherche
 - data evaluation
 - conceptual validation
 - model simulations
 - sensitivity and uncertainty analyses
 - comparison of model results with measured values (numerical validation)
 - appropriateness of models (operational validation)
 - comparison with alternative models
 - software evaluation

Together with data recherche and software evaluation these facets form the working packages of the project.

substances

Within this project exposure assessments are carried out for different substances. Substances of interest are those which are used in numerous products or chemical processes and which are frequently found in the environment. Due to their relatively good database, typical and well-known pollutants, such as dioxins and PCBs, are also investigated.

Furthermore, this selection considers the different environmental compartments.

Selected substances and mixtures

- Polychlorinated dibenzo-*p*-dioxines (PCDD)
- Polychlorinated biphenyls (PCB)
- Di-(2-ethylhexyl)phthalate (DEHP)
- Linear alkylbenzene sulphonate (LAS)
- Ethylenediaminetetra acetic acid (EDTA)
- 1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethyl-cyclopenta- γ -2-benzopyrane (HHCb)
- 1,2-Dichloroethane (EDC)
- Benzene

scenario

For validation studies, in particular to compare measured concentrations with predicted ones, spatially and temporally coherent data sets must be available.

Thus, before starting the project an environmental segment of regional scale had to be chosen. The German state of **North-Rhine Westphalia** (approximately 34 000 km²) was selected.

by order of

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time schedule

There are plans to complete the work within three years. The project began in March 1997.

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