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Feasibility of validating the Uniform System for the Evaluation of Substances (USES)

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ABSTRACT

USES, the Uniform System for Evaluation of Substances, is a decision-supporting tool, that can be used for rapid, quantitative assessment of the hazards and risks of chemical substances. Since risk assessment is an inherently uncertain process, a thorough model analysis is advisable. A previous version of USES was only partially validated, which was not sufficient sofar. Risks cannot be measured in the field, therefore, the effort will be aimed at validating the separate (sub-) modules of USES. This report describes the procedure that can be followed to show the user of the system the degree of accuracy that USES is able to give. This gives decision makers the opportunity to take the accuracy of USES into account in risk assessment. In this report, the validation status of the present modules of USES is discussed. A framework and recommendations for future validation are given. Furthermore, the assumptions and choices for the exposure scenario (often made implicitly) are listed.

It was concluded that for many modules, numerical validation has been performed or initiated. Operational validation of the appropriateness of the model chosen, and conceptual validation of the exposure scenario are however, still lacking. Furthermore, since many of the validation activities are performed outside the framework of the USES project, inventarisation of all the results is needed.

This report also describes an experiment to 'validate' the risk estimates of USES. This was done by comparing priorities of substances by experts to the ranking of USES. Despite many limitations, this approach gives more insight in the relation between the 'objective' risk estimate of USES and experts 'risk perception'.

In 1995 and 1996, a European risk assessment system will be developed, based on the present version of USES. The inventarisation and discussion in this report of the present modules and scenarios can be used in this development. Validation of the present version of USES is not planned. When the European risk assessment system is finalised, this system can be thoroughly analyzed, using this report as a basis.

SAMENVATTING

UBS, het Uniforme Beoordelingssysteem Stoffen, is een beslissings-ondersteunend gereedschap voor een snelle, kwantitatieve analyse van de risico's verbonden aan de levenscyclus van een chemische stof. Omdat risico-analyse een inherent onzeker proces is, is een grondige modelanalyse aan te bevelen. Een vorige versie van UBS was slechts gedeeltelijk gevalideerd, wat onvoldoende was voor een volledige validatie. Risico's kunnen niet in het veld gemeten worden, daarom zal de aandacht voornamelijk gericht zijn op validatie van de afzonderlijke modellen en modulen van UBS. Dit rapport beschrijft de procedure die gevolgd kan worden om de gebruiker te tonen wat de nauwkeurigheidsgraad is die UBS kan geven. Dit geeft de beleidsmaker de mogelijkheid om de nauwkeurigheid van UBS bij risico-analyse in overweging te nemen. In dit rapport wordt de validatie-status van de huidige modulen van UBS bediscussieerd. Een kader en aanbevelingen voor toekomstige validatie wordt gegeven. De aannamen en keuzen (vaak impliciet gemaakt) zijn nu geëxpliciteerd.

Geconcludeerd kan worden dat voor vele modulen numerieke validatie reeds is uitgevoerd of geïnitieerd. Operationele validatie van de toepasbaarheid van het gehanteerde model en conceptuele validatie van het blootstellingsscenario ontbreekt echter. Omdat veel van de validatieactiviteiten buiten het kader van het UBS-project plaatsvinden, is inventarisatie van al de resultaten noodzakelijk.

Dit rapport beschrijft tevens een experiment om de risicoschattingen van UBS te 'valideren'. Dit gebeurde door prioritering van stoffen door experts te vergelijken met prioritering door UBS. Ondanks vele onzekerheden geeft deze aanpak meer inzicht in de relatie tussen 'objectieve' risico-schatting van UBS en de 'risico-perceptie' van experts.

In 1995 en 1996 zal een Europees systeem voor risico-analyse ontwikkeld worden, gebaseerd op de huidige versie van UBS. De inventarisatie en discussie in dit rapport van de huidige modulen en scenario's kan gebruikt worden bij deze ontwikkeling. Een validatie van het huidige UBS is niet gepland. Als het Europese systeem afgerond is kan dit systeem grondig geanalyseerd worden waarbij dit rapport de basis kan vormen.

1. INTRODUCTION

This report examines the feasibility of validating USES, the Uniform System for the Evaluation of Substances. Firstly, this means defining a framework, objectives, and approach for a validation. The main part of this report is an inventarisation of the validation status of the separate models of the system. This includes the activities that were already performed, the activities already initiated, and the activities that are required. It should be noted that the literature references for the first two chapters are displayed at the end of each chapter. For the third chapter (inventarisation per separate sub-module) the references are given in each section.

1.1. Introduction to USES

The Uniform System for the Evaluation of Substances (USES, RIVM *et al.*, 1994) is a decision-supporting tool, that can be used for rapid, quantitative assessment of the hazards and risks of chemical substances. USES was described in a series of articles (Vermeire *et al.*, 1994; Jager *et al.*, 1994a/b; Van der Poel, 1994; Linders & Luttik, in prep.). Risks are expressed as the ratio of the PEC (Predicted Environmental Concentration) to the NEC (No-Effect Concentration). Estimation of PECs starts with an estimation of the emission of a substance followed by its subsequent distribution through the environment, and completed with an estimate of exposure or intake. NECs are derived from single-species toxicity data using extrapolation procedures.

In 1995/1996 USES will be developed towards a European risk assessment system for new and existing chemicals. Future validation will therefore be aimed at this European risk assessment system. This report does not describe USES in detail. For more background information and the actual mathematical process descriptions, the reader is referred to the USES documentation (RIVM *et al.*, 1994).

USES aims at the protection of the following:

1. aquatic ecosystems;
2. terrestrial ecosystems;
3. predators indirectly exposed through the environment; represented by birds/mammals that feed on fish or earthworms;
4. humans, exposed via:
   - the environment (indirect exposure),
   - consumer products (direct exposure);
5. micro-organisms residing in a sewage treatment plant;
6. specific terrestrial organisms residing in/on an agricultural area, treated with pesticides;
7. specific aquatic organisms residing in a ditch, surrounding an agricultural area, treated with pesticides.

The estimation of exposure levels requires the use of exposure scenarios for the specific groups to be protected. Estimation of exposure concentrations takes place at three spatial scales:

- Local scale: emissions from a point source are considered, targets are exposed near this source. In USES, the concept of a realistic worst case scenario is applied for the individual protection targets. This creates a hypothetical site, the standard environment. Although this standard environment, in which all routes and protection targets are combined, represents an unfavourable situation, it provides insight in all processes encountered in the real world. In some cases, worst case scenario assumptions are necessary due to lack of knowledge.
- Regional scale: emissions are considered as diffuse; the default compartment definition is an approximation of the Dutch situation.
- Continental scale: emissions are regarded as diffuse; this spatial scale is defined as 'Western Europe'. No targets are considered, the only purpose is to compute continental concentrations as a boundary condition for the regional computations.

In the present version of USES, regional and local exposure estimations are made separately. A specification of the targets and their exposure, as well as the way in which this exposure is estimated, is given in Table 1. It includes aspects of the spatial and temporal scales. Continental and regional computations are done sequentially, using the model SimpleBox (Van de Meent, 1993), which is a model of the so-called 'Mackay-type'. The continental concentrations form the background conditions of the regional system.

Table 1 *Exposure scenarios.*

target	medium of exposure	exposure scenario	
		regional	local
aquatic ecosystems	surface water	steady state surface water concentration	average concentration during an emission episode
terrestrial ecosystems	agricultural soil	steady state concentration in agricultural soil	concentration in agricultural soil*
fish eating predators	fish	equilibrium concentration in fish caught in surface water	equilibrium concentration in fish caught in surface water (annual average water concentration used)
worm eating predators	worms	equilibrium concentration in worms from agricultural soil	equilibrium concentration in worms from agricultural soil*
micro-organisms	water in the STP** aeration tank	not relevant (always lower than local)	concentration during emission episode
specific non-target organisms (in the case of pesticide application)	exposure through several pathways possible	-	exposure concentrations are defined through specific application scenarios (short term as well as long term)
man (exposed via the environment)	air	steady state concentration in air	annual average concentration in air, at 100 m from point source or STP**
	drinking water	steady state concentration in groundwater or purified surface water, supplied by sources in *agricultural areas*	annual average concentration in purified surface water or maximal concentration in ground water below agricultural soil*
	fish	equilibrium concentration in fish, from surface water (steady state concentration used)	equilibrium concentration in fish, from surface water (annual average water concentration used)
	crops	equilibrium concentration in crops grown on agricultural soil	equilibrium concentration in crops grown on agricultural soil*
	meat, milk	equilibrium concentration in meat/milk of cattle grazing on agricultural soil	equilibrium concentration in meat/milk of cattle grazing on agricultural soil*
man (exposed as consumer)	consumer products	not applicable	exposed on the personal scale through concentrations in air, in food or in contact media, defined by specific scenarios

* On the local scale, concentrations in agricultural soil and ground water are principally estimated as long term steady state concentrations due to atmospheric deposition and/or application of sludge from a sewage treatment plant. The concentration in sludge is taken from an annual average emission.
** STP: Sewage Treatment Plant.

In USES, several modules can be distinguished. Figure 1 shows the main modules, and the flow of data between these modules.

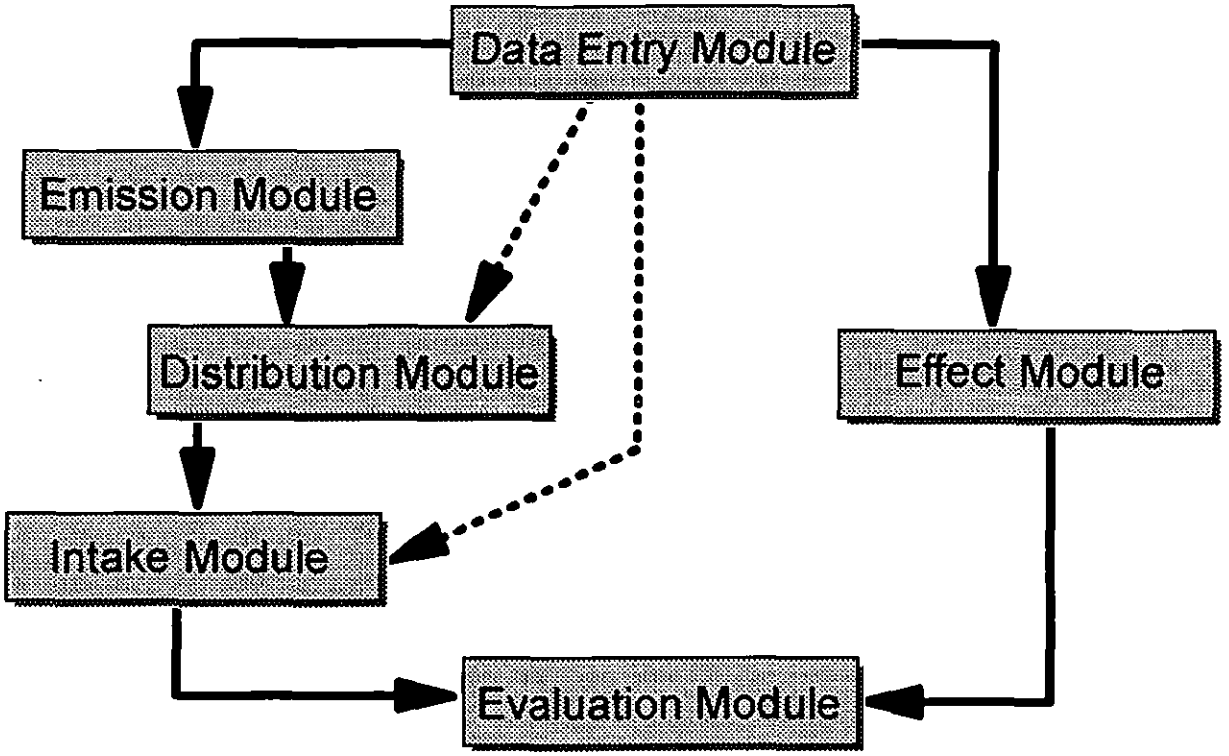

Figure 1 *The main modules of USES 1.0. and the flow of data between them.*

1.2. Earlier validation attempts

A previous version of USES was subject to validation, a comparison was made between environmental concentrations and human intakes for 25 existing chemicals and concentrations and intakes calculated with DRANC 1.0. (Toet *et al.*, 1991; De Nijs *et al.*, 1988; De Nijs *et al.*, 1993; RIVM *et al.*, 1994). The conclusions that could be drawn from these studies were:

- The Sewage Treatment Plant (STP) model SimpleTreat performed satisfactorily to predict concentrations in effluent and sludge from influent concentrations.
- The drinking water module performed quite well, even though a conservative approach was followed in the modelling process.
- The estimation of bioconcentration factors for fish, crops and cattle seems quite inaccurate.
- The concentrations calculated in fish, plants and cattle deviated even more from measured values. It has to be noted that in this version of the system, the air route to plants and cattle was not implemented yet.

Several major problems concerning validation of USES and its predecessors were identified by Toet *et al.* (1991) and have been reiterated in USES (RIVM *et al.*, 1994):

- The hazard ratios cannot be measured directly. Only intermediate results of the exposure assessment can be measured, like emission fluxes, concentrations in the environment, bioconcentration factors, and daily doses.
- One of the purposes of the model is to predict the risk of new chemicals, notified within the scope of EC Directive 67/548/EEC, before they enter the market. Measured data for comparison with intermediate model results are not available. A validation of the risk

assessment system must therefore be carried out with existing chemicals, which are already *in production*.

- It is extremely difficult to find a consistent data set of measurements over the same distribution pathways as described in USES. For example, measured concentrations in the environment generally cannot be related to a specific emission point. Moreover, substances may very well be released by other sources and distribution pathways than assumed in USES.
- The system makes use of a 'standard environment'. Reported data will invariably not only be non-representative for the standard environment, but also be incomplete and often ill-defined with respect to time and spatial scales of the measurements. Measurements will often originate from many different locations.

Toet *et al.* (1991) selected 25 chemicals to perform validation with. In my opinion, it is not necessary to validate each sub-module with the same set of chemicals. As Toet and coworkers pointed out: *even after extensive literature search, many values were still missing. Without* the restricting set of 25 chemicals, it is probably easier to collect a larger amount of data for several modules.

1.3. References

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2. APPROACH FOR VALIDATING USES

2.1. Framework and definitions

A model is a simplified representation of a part of reality. USES can be seen as a 'policy oriented model', the system aims at predicting the 'risk' of a substance in causing some kind of adverse effects. The process of modelling may proceed through a number of predefined steps; an example is given in Figure 2 (adapted from Anderson & Woessner, 1992).

The top two blocks have already been performed for USES, but the last block, the model analysis has not been satisfactorily fulfilled yet. The development of an uncertainty analysis, as a part of the USES system, is handled in a separate report (Jager & Slob, 1995).

Model analysis should be a part of the development of a model. Validation is a crucial step in model analysis. In fact, it is the final check if the model produces results that are acceptable for its purpose. The following definition of validation can be used (taken from Boekhold *et al.*, 1993):

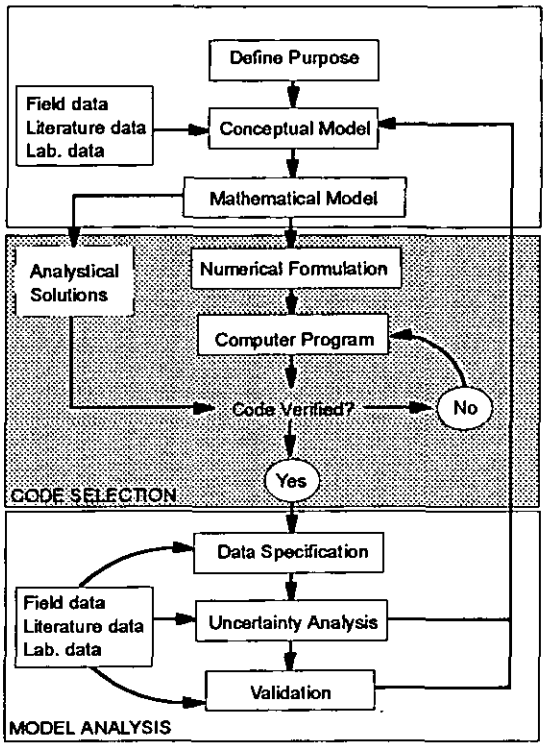

Figure 2 *The modelling process relevant to USES (adapted from Anderson & Woessner, 1992)*

Model validation: The process of proving (with a predefined degree of accuracy) that the model is an adequate representation of (a part of) the reality.

Validation may consist of several parts:
1) Are assumptions and theories correct (conceptual validation)?
2) Is the model appropriate for the intended use (operational validation)?
3) Do model results sufficiently correspond with independent measurements (numerical validation)?

Numerical validation of risk assessment systems is, in the strictest sense, impossible since risks cannot be measured. Nevertheless, the accuracy with which the system predicts concentrations and effects can be expressed (semi-)quantitatively. Validation of a general system like USES is troublesome; the system should perform adequately for *all* organic substances, in all situations. In fact, it is clear beforehand that no model whatsoever is able

to give *accurate* predictions for *all* chemicals. Therefore, the word *adequate*, in the definition of validation, needs more elaboration. It is difficult to say what degree of certainty the decision maker requires when assessing hazards of chemicals. Nevertheless, the user of a system should be aware of the (in)accuracy of the model. It is important for a validation that the results are transparently, and quantitatively, presented. In this case, each user can conclude if this is an adequate model for his intended use. This means that 'validation', in this context, must be seen as the process of indicating *what* the degree of accuracy of the model *is*, rather than proving that the degree of accuracy is *adequate*. Therefore, the definition of validation that I will use, with respect to validating USES, can be written as:

Model validation: The process of *transparently showing* the degree of accuracy of (parts of) the model in giving a representation of (a part of) the reality. The user of the model has the possibility of judging this degree of accuracy to be sufficient or not for the intended use of the model.

When USES is judged insufficiently valid, the validation results can be used to steer future research. The required data for validation may be obtained from:

- Measured (laboratory or field) data, obtained from:
  - published literature
  - unpublished data from industry and others (e.g., emission data, effluent concentrations, environmental concentrations)
  - factual data banks (e.g., physico-chemical properties, bioconcentration factors)*
- Other (more elaborate) models (e.g., environmental distribution models)

* E.g., the Chemical Evaluation Search and Retrieval System (CESARS) by the Michigan Department of Natural Resources and the Ontario Ministry of the Environment.

The major problem in using field data to validate environmental computer models is the large spatial and temporal variability of experimental data measured in the field. For instance, it is not abnormal for the concentration of a chemical in sediment samples, taken from within the same square meter, to vary by more than a factor of 10 or even 100 (ECETOC, 1992). Therefore, care has to be taken in interpreting field data and validation results. Obviously, the optimal situation would be to have an extensive set of field observations to allow a full statistical evaluation (ECETOC, 1992). As extensive field data sets are bound to be scarce, we must ensure a careful interpretation of validation results.

Even in the case that all submodules are satisfactorily validated, the combination of all submodules into a chain of models may not be valid if models are inappropriately linked. Here we will probably have to rely on 'common sense' or expert judgement to validate this step as coherent data sets, covering all submodules, will be scarce or non-existent. Nevertheless, we may be able to find data sets covering several modules which may provide additional validation to the model.

Another important part of model analysis is uncertainty analysis; showing the influence of

uncertainty and natural variance of parameters on the model's results. Validation and uncertainty analysis are linked. Uncertainty analysis can indicate where the main uncertainties in the system are, and therefore, steer validation activities. The other way around, validation activities can be used to quantify the uncertainty in parameters. Uncertainty analysis of USES is discussed by Jager & Slob (1995).

2.2. Procedure for validation

In USES, the scenario concept holds a key position in the system. The environmental distribution of a substance is followed in a 'standard' environmental scenario. This scenario also includes assumptions, as for example, the assumption of steady state between fish and surface water. In principle, the assessments performed with USES are only valid under the defined assumptions of the standard scenario. However, calculating actual environmental exposure is not the main purpose of USES. USES should be able to put substances on an ordinal risk scale (this means that the system should be able to tell if substance A is more hazardous than substance B). It is assumed that when the environmental distribution and the effects assessment are calculated realistically, the subsequent risk estimate will be (at least in a relative manner) appropriate to support risk management.

A complete validation of USES requires several steps:
- Conceptual and operational validation of the separate models.
- Conceptual validation of the standard scenario (per sub-module or model).
- Numerical validation of each separate model with measured values.
- Conceptual and operational validation of the links between each (sub-)module or model.
- Numerical validation of a chain of models (if possible) with measured values.
- Validation of the (relative) risk level, as estimated with USES.

It is clear that numerical validation only, is not sufficient to validate a risk assessment system like USES. Individual models can be validated with measured values, but first, one has to check whether this particular model is appropriate (operational validation) and whether the assumptions are acceptable (conceptual validation). As an example, the calculation of concentrations in fish involves the use of a bioconcentration factor (BCF). The use of a BCF implies the assumption that an equilibrium between fish and the water occurs. Even though the bioconcentration model may perform very well to predict concentrations in fish due to long term exposure (and thus be numerically valid), the assumption of equilibrium may be incorrect if emission only takes place a few days a year.

Conceptual validation of the standard exposure scenario requires expert judgment. The question in this step is the following: is the scenario relevant in view of the purpose of the assessment, and does 'realistic worst case' apply? The relevance of the scenario is something that need to be thoroughly discussed. A 'validated' scenario in this context, is a scenario that is agreed upon by all parties involved in the risk assessment process.

Conceptual and operational validation of the links between the models means that for each link it must be discussed whether it is logical or not. For example, a substance emitted during a batch process, only a few days a year, linked to an annual average dispersion model is

questionable. A thorough analysis of the exposure models is required. For some substances, measured data covering several dispersion steps is present. For example, for dioxines, much information has been gathered concerning emissions, levels in water and soil, levels in food products, and exposure of humans. This might give a possibility to numerically validate a chain of models applied in USES.

Risk or hazard quotients cannot be measured in the field. As pointed out in the previous section, consistent data sets over the same distribution routes as described in USES are scarce. Therefore, one of the main objectives of validation will be the validation of separate modules, using measured input values and comparing the outcomes to measured output values. This procedure is schematically drawn in Figure 3.

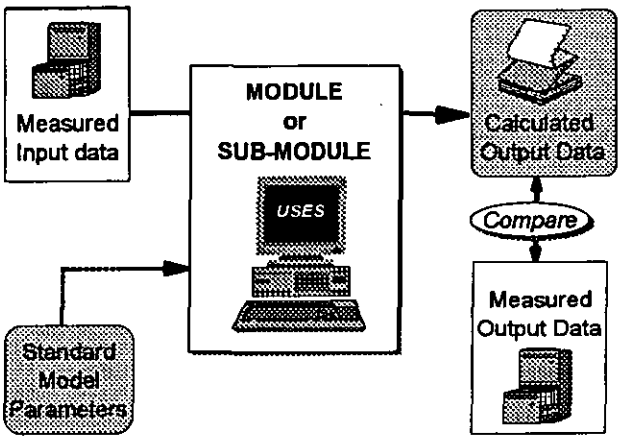

Figure 3 *Schematic procedure for numerical validation.*

To illustrate this procedure, lets look at the submodule 'Sewage Treatment Plant'. The measured input data that we need are emission fluxes, discharged to wastewater. Standard model parameters are for instance the characteristics of the average sewage treatment plant (a fixed scenario in USES 1.0.). The outputs of the STP module, concentrations in effluent, sludge, air near the STP and biodegradation, can be compared to measured values. In fact, with this procedure we are not just validating the STP model, but we may also be able to check the applicability of several scenario choices.

2.3. Validating 'risks'

Validation of the relative risk levels, as estimated with USES, is a more complex problem. Unfortunately, it is impossible to measure hazards or risks (or even PEC/NEC ratios) in the field. Nevertheless, it may be possible to *indicate* if the hazard evaluation by USES is valid. USES assumes that, the better the estimation of exposure levels and no-effect levels, the better the risk estimate will be. Therefore, numerical validation of the separate models is an appropriate attempt to validating USES. No matter how good the models of USES are, the real world is very heterogeneous, USES will never be able to predict accurately all concentrations occurring in the real environment.

The main purpose of USES is not to predict environmental concentrations, but to screen chemicals for potentially hazardous ones. The most important question in a validation of USES is: are substances with a higher PEC/NEC ratio than others really more risky in the real environment? Since PEC/NEC ratios do not exist in the real environment, the question is more about the validity of the relative risk levels as estimated by the system.

In the above paragraphs we have used the terms 'hazard' and 'risk' interchangeable. In USES

Hazard: The inherent potential of a substance to cause adverse effects
Risk: The probability of a substance to cause adverse effects

1.0 the definitions as given by the EU and the OECD are used. Usually the term 'risk' is an impact multiplied with a probability that this impact occurs. In USES, the PEC/NEC ratio is taken as a measure of risk. This is not entirely appropriate given the definitions, but this discussion will not be pursued in this report. This problem is handled in the definitions of risk characterisation and risk estimation as defined in USES.

Risk characterisation: The process designed to estimate the incidence and severity of the adverse effects likely to occur
Risk estimation: The quantitative estimation of the probabilities of clearly described effects by including uncertainty analysis; the risk assessment is complete when the risk characterization includes 'risk estimation'

With these definitions, the risk characterisation implies the derivation of a PEC/NEC ratio. Uncertainty analysis completes the risk estimation by quantifying the probability of the PEC exceeding the NEC.

Validation of risk levels may be performed with existing chemicals where we have experience. Properties of substances with *known adverse effects* for a group to be protected in the field can be entered in USES. USES should predict a PEC/NEC ratio > 1 for this substance and this group to be protected. The other way around is also possible: substances which are known to cause *no adverse effects whatsoever* can be entered in USES. USES should then predict a PEC/NEC < 1. This procedure requires further elaboration, but may provide a means for validating the ultimate ability of USES to predict risks. Furthermore, if this kind of validation is performed accurately, it may help interpreting hazard and risk levels given by USES.

Another possibility of validating risk levels, is to consult experts in the field of risk assessment and risk management. The ranking given by experts to a number of known chemicals can be compared to the ranking made by USES. This should give information on the applicability of USES in predicting (relative) risks. One should keep in mind, however, that risk perception in the experts view differs from the risk estimates of USES. This option is worked out in a small experiment with members of the Dutch Society of Toxicology during a meeting at the RIVM. The results of this experiment are discussed in chapter 4.

2.4. Presentation of validation results

The 'comparison' of model results with measured data can be presented graphically, as shown in Figure 4. The measured values are plotted on the x-axis, the calculated values on the y-axis. The (vertical or diagonal) distance of each point to the y=x line is a measure of the validity of the model.

The procedure of constructing 'correlation areas', as done by Toet *et al.* (1991), is not

advisable. Calculated output data are dependent on measured input data, when there is a range of input data, a range of output data is constructed. A 'correlation area' is constructed by drawing a rectangle through the minimum and maximum point (see Figure 5). The validation can, according to Toet and coworkers be called satisfactory if this area crosses the y=x line. Individual results are not shown and the rectangle is not a property of the individual data points. This problem is exemplified in Figure 6. Suppose only two data points are available, one of which will be marked *min* and the other *max* as in Figure 5. Suppose that another data point can be found instead of *max*, with a value closer to the y=x line. This point is called *max 2* in Figure 6. The points are now, closer to the y=x line, the average distance of calculated to measured values has decreased. Nevertheless, the correlation area does *not* cross the line anymore, and the model has to be judged *less* valid. The validity of the model seems to increase with increasing input and output *ranges*. This is, in my opinion, not a proper way to represent validation results. It is more appropriate to plot each individual data point (as done in Figure 4).

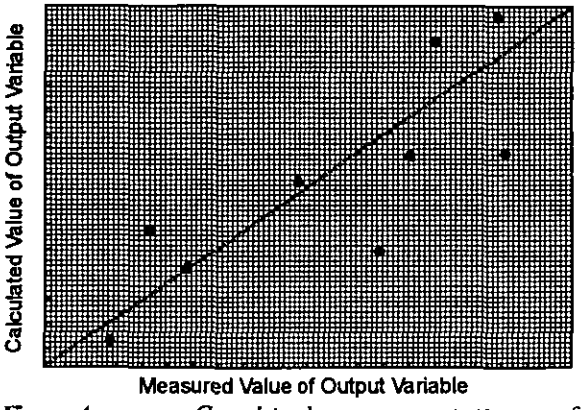

Figure 4 *Graphical representation of validation results.*

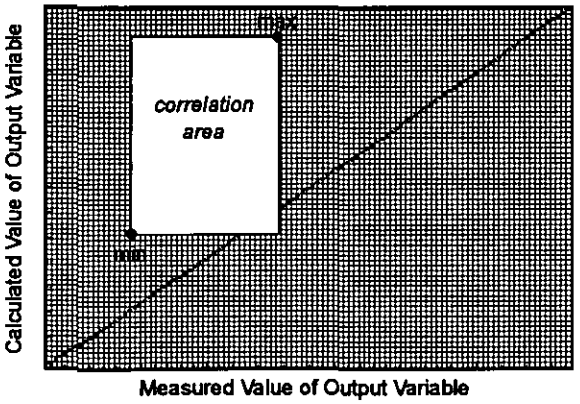

Figure 5 *Example of a "correlation area".*

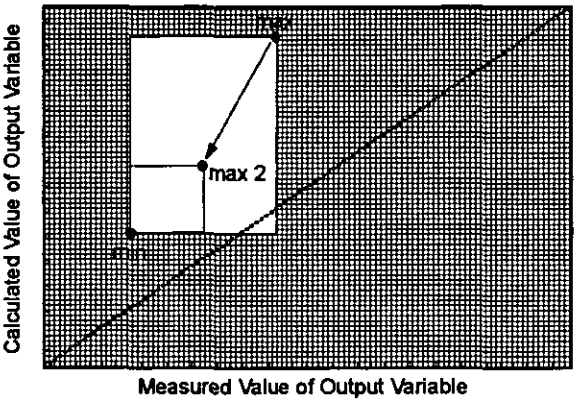

Figure 6 *Example of the problem with alternative value* max 2 *instead of* max.

There are several methods of presenting the results of a validation study with statistical methods. Because the validation results must be readily interpretable by users of the system, the choice for a graphical representation seems the most appropriate.

2.5. References

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3. VALIDATION ACTIVITIES PER (SUB-)MODULE

In this chapter *all* sub-modules are investigated concerning their validation status or requirements.

Each section will be structured as follows:
- First, a short description of the module.
- A discussion of the validation status of this module or the activities needed for validation.
- A table with the assumptions made for this module, and the scenario choices made. These assumptions and choices can be subjected to conceptual validation .
- A table to indicate which measured input parameters should be used for validation of the sub-module, and which output parameters can be compared to measured data (a procedure as shown in Figure 3).
- A list with the literature references, references are given per sub-module to facilitate research..

3.1. Data entry module

In the data entry module, the input parameters are entered by the user. Missing data will be filled with defaults or estimates, and secondary parameters are derived from primary data. The estimation routines, or QSARs (Quantitative Structure-Activity Relationships), and the derivation of secondary data can be subject to validation. The numerical validity of QSARs is often quite trivial. Since QSARs are usually regressions based on measured data (the training set), the validity is directly shown in the goodness of fit of the regression. Therefore, the validity can be immediately derived from the original publication of the QSAR. However, the way in which the QSAR is applied in USES may be subject to operational validation. When a QSAR is applied, it should be clear what the boundary conditions are. Furthermore, it *is* possible to numerically validate a QSAR, to check its validity *outside* the ranges of the training set. As an example, the relations between soil and plant where derived for one plant species only, but are applied for all crops. This indicates a clear need for validation (which was performed already).

3.1.1. Physico-chemical properties

The sub-module 'Physico-chemical properties' contains two QSARs, one to estimate the octanol-water partitioning coefficient (*Kow*) from the water solubility, and the other for the reciprocal estimation. The relations were derived by Isnard & Lambert (1989), but for the derivation of solubility from *Kow* the relation of Veith (unpublished) (taken from Hunter *et al.*, 1986) is used when no melting point is given. It should be noted that the implementation of the relations by Isnard & Lambert in USES, is not entirely correct. The correct formulation is given in Jager & Slob (1995). This makes use of the unpublished data of Veith unnecessary.

The validity of this QSAR can be directly taken from the article of Isnard & Lambert (1989).

The applicability of the QSARs may be tested by using (groups of) substances not used in the training set. The required data (solubility, *Kow*, and melting point) are readily available from on-line data bases such as the Chemical Evaluation Search and Retrieval System (CESARS).

Validation of this module is not urgently required as *Kow* and solubility are both part of the required base set for new and existing substances, and pesticides. Therefore, this estimation will only be used in the rare occasion that one of these values is not given. In that case, the extra uncertainty will be accounted for in the uncertainty analysis (Jager & Slob, 1995). Furthermore, the correlations between *Kow* and solubility are relatively reliable and commonly applicable (Verhaar & Hermens, 1990).

Input	Symbol	Output	Symbol
water solubility	*SOL*	Kow	*Kow*
melting point	*TEMPmelt*		
Kow	*Kow*	water solubility	*SOL*
melting point	*TEMPmelt*		

References

Hunter, R.S., F.D. Culver, J.R. Hill and A. Fitzgerald (1986). QSAR System user manual. EPA-ERL, Duluth, Minnesota & Montana State University, Bozeman, Montana.

Isnard, P. and S. Lambert (1989). Aqueous solubility and n-octanol/water partition coefficient correlations. Chemosphere 18, 1837-1853.

Jager, D.T. and W. Slob (1995). Uncertainty analysis of the Uniform System for the Evaluation of Substances (USES). Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102027.

Verhaar, H.J.M. and J.L.M. Hermens. (1990). QSAR System, een evaluatie. Utrecht, Research Institute Toxicology (RITOX), Report for RIZA and VROM (in dutch). *(QSAR System, an evaluation)*

3.1.2. Characterisation of the environment

This sub-module calculates values for the bulk density of soil, sediment, suspended matter, and biota from default values. Each compartment is assumed to consist of solids, water, and air. The volume fractions of each phase define the bulk density of the compartment. (Bulk density of sediments is only used in the regional calculations with SimpleBox). This sub-module also calculates the volumes of the regional and continental compartments.

Of course, a range of bulk densities will inevitably be found when looking at all possible soils/sediments/suspended matter/biota in a certain environment. The choice for a specific bulk density can be subjected to conceptual validation (are these typical values agreed upon?). This question may also be raised for other defaults concerning the characterisation of the environment in USES, e.g., the fraction organic carbon in soil etc. These bulk densities, and the other defaults characterising the environment, were already extensively discussed in the framework of harmonisation of several risk assessment systems (Heijna-Merkus & Hof, 1993). For the EU-project in 1995/1996, these values will have to be reexamined for the European situation. Therefore, validation is not required at this moment.

Assumptions in the standard scenario:

- Typical characteristics of the Dutch environment are used by default. These characteristics are harmonised between several risk assessment systems and therefore, have a broader consensus.

Input	Symbol	Output	Symbol
		density soil	RHO_{soil}
		density susp. matt.	RHO_{susp}
		density biota	RHO_{bio}
		density sediment	$RHO_{sediment}$

References

Heijna-Merkus, E. and M. Hof (1993). Harmonization of model parameters. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102022.

3.1.3. Intermedia partitioning

In this sub-module, parameters are derived to calculate the partitioning between environmental media (biota excluded). Partitioning between water and solids is described with a *Kp* (partitioning coefficient) in each compartment. If *Kp* values are not entered by the user, they are estimated using the approach of Karickhoff (1981). (*Kp* of sediment and scavenging ratio are only used in the SimpleBox regional calculations).

Partitioning between air and water is described with the Henry's law constant and/or the air-water partitioning coefficient.

The validity of the QSAR linking *Koc* to *Kow* can immediately be derived from Karickhoff (1981). The applicability of this QSAR can be subject of conceptual validation. It should be noted that the derivation of *Kp* values from *Kow* is only valid for non-ionic organic chemicals. For all other chemicals (e.g., ionic substances, surfactants, metals) measured data or specific models should be used. USES also allows the input of measured data. Therefore, as long as the uncertainty in the estimate is adequately quantified, validation is not urgently needed.

Input	Symbol	Output	Symbol
vapour pressure	*VP*	frac. ass. aerosol	$Fass_{aer}$
Kow	*Kow*	solids-water part.	Kp_{soil}
Frac. organic carbon	$Foc_{compartment}$		Kp_{susp}
			Kp_{suspPS}
			$Kp_{suspATSLS}$
vapour pressure	*VP*	Henry's law const.	*HENRY*
water solubility	*SOL*	air-water part.	$K_{air\text{-}water}$
molecul. weight	*MOLW*		

References

Karickhoff, S.W. (1981). Semi-empirical estimation of sorption of hydrophobic pollutants on natural sediments and soils. Chemosphere **10**, 833-846.

3.1.4. Biodegradation

Usually, at base set level, all the information given on the biodegradability of a substance is the result of a standard biodegradability test in water. The result is given as 'readily biodegradable' or 'not readily biodegradable'. From this classification, degradation rates in water, soil, sediment, and sewage treatment are derived. These estimation routines are all based on default degradation rates. It may not be very opportune to validate these defaults as they are conservatively chosen. It may, however, be possible to validate the assumptions made in the derivation of biodegradation rates in soil and sediment. The degradation rate in water (a measured rate, or a default based on the 'readily' test) is rescaled to the number of bacteria present in soil or sediment. The degradation is assumed only to occur in the porewater phase.

Degradation in sediment is only modelled in the regional and continental calculations of SimpleBox. This procedure to derive a degradation rate constant from a readily biodegradability test applies only to aerobic sediments. Generally, only the top few millimetres of the sediment are aerobic. A standardised anaerobic test is under development.

Validation of this sub-module is not advisable at this moment. In the framework of the EU-project, the extrapolation of environmental degradation rates from standard tests will be discussed.

Assumptions in the standard scenario:

- Biodegradation rates in porewater of soil and sediment are equal to those in the degradation test, when scaled to the number of bacteria.
- Biodegradation in soil and sediment only occurs in the water-phase, chemicals associated with particles are not available for biodegradation.
- Partitioning of a compound between the particle and the aqueous phase is governed by a thermodynamic equilibrium occurring at a rate which is fast with respect to degradation processes.
- Biodegradation can be described with a first order process.
- The soil or sediment system under consideration is an aerobic system.

Input	Symbol	Output	Symbol
degr. rate test	$kdeg_{test}$	degr. rate soil	$kdeg_{soil}$
soil-water part.	Kp_{soil}		
bacteria in soil	$BACT_{soil}$		
soil characteristics	RHO_{soil}, $RHOsolid$, $Fwater_{soil}$, $Fsolid_{soil}$		
degr. rate test	$kdeg_{test}$	degr. rate sediment	$kdeg_{sed}$
sed.-water part.	Kp_{sed}		
bacteria in sediment	$BACT_{sed}$		
sed. characteristics	RHO_{sed}, $RHOsolid$, $Fwater_{sed}$, $Fsolid_{sed}$		

3.1.5. Bioaccumulation

In this sub-module, bioconcentration or biotransfer factors are estimated from physico-chemical properties. This estimation is usually a regression on measured data. The use of fixed bioconcentration factors implies the assumption that a steady-state situation occurs in which the ratio between concentration in organism and its exposure medium remains constant. It should be noted that in 1995 the bioconcentration process will be subject of a more in depth investigation as part of the USES project. This project will specifically examine the

appropriateness of the assumption of equilibrium between organisms and exposure medium.

3.1.5.1. Fish

As discussed in the report concerning uncertainty analysis (Jager & Slob, 1995), we propose to change the present approach of USES 1.0 to a more median one. The proposed approach is to use the log-linear regression on the extensive data set of Veith & Kosian (1983). This data set includes substances that are metabolised, and substances that are not. This regression leads to a more median case estimation, with the additional benefit that uncertainties are easily quantified. This data set consists of 122 data points from several classes of organic chemicals (log *Kow* from 1 to 6) with different fish species. This QSAR should not be used for substances with a molecular weight of more than 700.

Numerical validation of this approach is not urgently needed. If additional data are gathered these can be easily included in the data set, leading to a new regression. Of course, the applicability of the derived regression can be tested with (classes of) chemicals not present in the training set. Furthermore, measured values can be used to overwrite the estimates made by USES. The validation activities of Toet *et al.* (1991) suggest that the formula applied in USES is not very valid as discrepancies of more than a factor of 100 occur. It should however be noted that measured data showed large amounts of variation for the same substance.

Bioconcentration factors for fish are relatively easily available. This process is also relatively easy to examine experimentally, compared to the bioaccumulation process in worms, plants, or cattle. Experimental BCFs are, for example, reported by De Wolf *et al.* (1994), Fox *et al.* (1994), Kalsch *et al.* (1991), Mackay *et al.* (1982), Porte & Albaiges (1994), Saito *et al.* (1991, 1994). Experimental BCFs can also be obtained from on-line research (e.g., CESARS).

Assumptions in the standard scenario:

- The bioconcentration process can be seen as a hydrophobic partitioning between the lipid content of the fish and the surface water, therefore, dietary uptake can be ignored.

Input	Symbol	Output	Symbol
Kow	*Kow*	BCF for fish	BCF_{fish}

References

De Wolf, W., E.S.E. Yedema, W. Seinen and J.L.M. Hermens (1994). Bioconcentration kinetics of chlorinated anilines in guppy, *Poecilia reticulata*. Chemosphere **28**, 159-167.

Fox, K., G.P. Zauke and W. Butte (1994). Kinetics of Bioconcentration and Clearance of 28 Polychlorinated Biphenyl Congeners in Zebrafish (*Brachydanio rerio*). Ecotoxicol. Environ. Saf. **28**, 99-109.

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Kalsch, W., R. Nagel and K. Urich (1991). Uptake, elimination, and bioconcentration of ten anilines in zebrafish (*Brachydanio rerio*). Chemosphere **22**, 351-363.

Mackay, D. (1982). Correlation of bioconcentration factors. Environ. Sci. Technol. **16**, 274-278.

Porte, C. and J. Albaiges (1994). Bioaccumulation patterns of hydrocarbons and polychlorinated biphenyls in bivalves, crustaceans, and fishes. Arch. Environ. Contam. Toxicol. **26**, 273-281.

Saito, H., M. Hirano and T. Shigeoka (1994). Uptake, distribution, metabolism and excretion of tebufenpyrad by carp, *Cyprinus carpio*. J. Pestic. Sci. **19**, 93-101.

Saito, S., A. Tanoue and M. Matsuo (1991). The i/o-characters to describe bioconcentration of organic chemicals in fish. Chemosphere **23**, 789-799.

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Veith G.D., and P. Kosian (1983). Estimating bioconcentration potential from octanol/water partition coefficients. In: Physical behaviour of PCBs in the Great Lakes. D. Mackay et al (eds.), 269-282. Ann Arbor, Mich. USA.

3.1.5.2. Worm

The concentration in earthworms is only relevant for exposure of predating birds or mammals. Connell & Markwell (1990) collected available data to construct the regression as applied in USES. Again, the validity of the regression can be taken from their article. The regression is based on 100 data points of 32 substances, all pesticides (log *Kow* of 1-6.5). The inaccuracy of this QSAR is reflected in the high level of uncertainty (see Jager & Slob, 1995); an uncertainty factor of 17 was derived. Furthermore, the range of substances tested is small. Information on the bioconcentration process from soil to earthworms will be scarce. Therefore, this BCF is not easily validated. An example of experimental work is given by Hans *et al.* (1994).

Belfroid (1994) has done research on the applicability of the equilibrium partitioning assumption. Furthermore, Belfroid has examined BCF values of earthworms for several substances in the lab and in the field. Under most circumstances, the contribution of dietary intake is small, except for hydrophobic chemicals (log *Kow* > 5) in soils with a very high organic matter content (approx. 20%). Model calculations of Belfroid (1994) showed that in a soil with a fraction organic matter of 3%, even for a very lipophilic compound (log *Kow* of 7) dietary uptake was small (11%). In USES a fraction organic matter of 5% is applied (frac. organic carbon of 2.9%). This indicates the validity of equilibrium partitioning assumption for application in USES.

Assumptions in the standard scenario:

- The bioconcentration process can be seen as a hydrophobic partitioning between the lipid content of the worm and the porewater, therefore, dietary uptake may be ignored. Validity indicated by results of Belfroid (1994).

Input	Symbol	Output	Symbol
Kow	*Kow*	BCF for worms	BCF_{worm}
soil-water part.	Kp_{soil}		

References

Belfroid, A.C. (1994). Toxicokinetics of hydrophobic chemicals in earthworms. Validation of the equilibrium partitioning theory. Phd. Thesis. Utrecht University, The Netherlands.
Connell, D.W. and R.D. Markwell (1990). Bioaccumulation in the soil to earthworm system. Chemosphere **20**, 91-100.
Hans, R.K., M. Farooq, R.C. Gupta and M.U. Beg (1994). Dissipation and accumulation kinetics of endosulfan in soil and earthworm - *Pheretima posthuma*. J. Environ. Biol. **15**, 127-133.
Jager, D.T. and W. Slob (1995). Uncertainty analysis of the Uniform System for the Evaluation of Substances (USES). Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102027.

3.1.5.3. Plant

Validation of the plant-module has already been started. The uptake and translocation of chemicals from soil to plants ($BCFstem_{plant}$ and $BCFroot_{plant}$) as described by Briggs *et al.* (1982, 1983) was validated by Polder *et al.* (1994). The estimated concentration factor between root and soil ($BCFroot_{plant}$) showed a good correlation with measured data.

Furthermore, there was no marked difference between nutrient medium experiments and laboratory soil and field soil data. This suggests the validity of the assumptions that uptake is a passive sorption process and only the dissolved concentration is bioavailable.

For the concentration factor between soil and above-ground plant parts, the correlation was less satisfactory. Deviations were higher and lower than the estimated values (up to a factor 100) without showing distinct patterns. Partly, the deviations could be ascribed to the experimental design, but the validation clearly indicated that the model formulation is not valid for the intended use.

It should be stressed that the relations reported by Briggs and coworkers were derived for a small group of compounds (O-methylcarbamoyloximes and substituted phenylureas) in one plant species only (barley). The substances had a log *Kow* from -0.57 to 4.6. It is clear that for this QSAR it is necessary to know if it can be successfully applied outside its narrow boundaries.

The route from air to plant is divided into two main routes: deposition on leafs and gasuptake. Relations for both were derived on theoretical grounds by McKone & Ryan (1989) and Riederer (1990) respectively. The work of Bacci *et al.* (1990) seems to indicate the validity of the relations for gasuptake, but uncertainties remain large. An extensive numerical validation of the route air to plant (gasuptake and deposition) is already planned as part of the USES project for 1995. In 1995, alternatives for this sub-module will be investigated within the framework of the USES project. The model of Trapp *et al.* (1994) may provide an interesting alternative. In this model, uptake from soil and air is handled simultaneously. The data set collected by Polder *et al.* (1994) will be used to test these alternatives.

Assumptions in the standard scenario:

- The BCFs derived for barley by Briggs *et al.* are valid for all crops and grass. This assumption has been partially validated by the work of Polder *et al.* (1993) for *BCFroot*.
- Plants are only taking up substances from the water phase of the soil (the concentration in the water phase is assumed constant over the time period considered).
- Uptake of substances by roots of plants can be viewed as a passive sorption process.
- Transformation and degradation in plants can be ignored.
- Uptake of substances from the air (as gas and deposition) can be described as a partitioning between plant and air. *This will be examined in 1995 as part of the USES project.*

Input	Symbol	Output	Symbol
Kow	Kow	BCF for roots	$BCFroot_{plant}$
soil-water part.	Kp_{soil}	BCF for stems	$BCFstem_{plant}$
Kow	Kow	gas-plant. part.	$K_{gas\text{-}plant}$
air-water part. coeff.	$K_{air\text{-}water}$		
		aerosol-plant part.	$K_{aerosol\text{-}plant}$

References

Bacci, E., D. Calamari, C. Gaggi and M. Vighi (1990). Bioconcentration of organic chemical vapors in plant leaves: Experimental measurements and correlation. Environ. Sci. Technol. **24**, 885-889.

Briggs, G.G., R.H. Bromilow and A.A. Evans (1982). Relationships between lipophility and root uptake and translocation of non-ionised chemicals by Barley. Pestic. Sci. **13**, 495-504.

Briggs, G.G., R.H. Bromilow, A.A. Evans and M. Williams (1983). Relationships between lipophility and the distribution of non-ionised chemicals in barley shoots following uptake by the roots. Pestic. Sci. **14**, 492-500.

McKone, T.E. and B. Ryan (1989). Human exposure to chemicals through food chains: an uncertainty analysis. Environ. Sci. Technol. **23**, 1154-1163.

Polder, M.D., E.M. Hulzebos and D.T. Jager (1994). Validation of models on uptake of organic chemicals by plant roots. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102024.

Riederer, M., (1990). Estimating partitioning and transport of organic chemicals in the foliage/atmosphere system: Discussion of a fugacity-based model. Environ. Sci. Technol. **24**, 829-837.

Trapp, S., C. Mc Farlane and M. Matthies (1994). Model for uptake of xenobiotics into plants: validation with bromacil experiments. Environ. Toxicol. Chem. **13**, 413-422.

3.1.5.4. Meat and Milk

The relation between daily intake of the chemical by the cow and the concentrations in meat and milk are described with biotransfer factors. The relationship applied in USES is taken from Travis & Arms (1988). The relation is a log-linear regression on a collected set of measured biotransfer data. For the transfer to meat, 36 data points were used of different organic substances (log *Kow* from 1.3-6.9). For the transfer to milk, 28 data points were used of different organic substances (log *Kow* from 2.8-6.9). The accuracy of these QSARs is low, as reflected in the large uncertainty factors of 64 for meat and 36 for milk (see Jager & Slob, 1995). Due to these large uncertainties (even for estimating data from the training set) more accurate approaches need to be developed, and validation can be postponed.

Further research on biotransfer factors can for example be found in Fries (1982) and Kenaga (1980).

Assumptions in the standard scenario:

- Kow is the only indicator for bioaccumulation. This is questionable, given the low prediction ability of the QSAR.

Input	Symbol	Output	Symbol
Kow	*Kow*	BCF for meat	BCF_{meat}
		BCF for milk	BCF_{milk}

References

Fries, G.F. (1982). Potential polychlorinated biphenyl residues in animal products from application of contaminated sewage sludge to land. J. Environ. Qual. **11**,14-20.

Jager, D.T. and W. Slob (1995). Uncertainty analysis of the Uniform System for the Evaluation of Substances (USES). Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102027.

Kenaga, E.E. (1980). Correlation of bioconcentration factors of chemicals in aquatic and terrestrial organisms with their physical and chemical properties. Environ. Sci. Technol. **14**,553-556.

Travis, C.C. and A.D. Arms (1988). Bioconcentration of organics in beef, milk and vegetation. Environ. Sci. Technol. **22(3)**,271-274.

3.2. Emission module

The emission module consists of a large number of tables. Depending on the intended or actual use pattern of the substance (and physico-chemical properties of the chemical), emission releases to air, waste water, and industrial soil are estimated. For local emission estimates, the fraction of a main source and the number of emission days are estimated from the use pattern and the production volume of the substance. Estimations are made on the basis of experience in emission estimations at the RIVM. For some characteristic groups, results of specific studies have been used.

It is impossible to validate the entire emission module extensively because of lack of data. If data where available, this would automatically lead to other, more accurate, emission estimates. If this module would be subject of validation activities, we must be satisfied with some sample categories of substances. This could give some insight in the validity of this module. This is extremely important, as the risk estimate is related linearly to emission rates (a doubled emission leads to doubled risks). It can be concluded that numerical validation of this module is not advisable, but further research is very much needed. It is also necessary to critically evaluate the assumptions made in the scenario.

In 1995 the emission estimates of USES 1.0 will be discussed in the framework of the EU-guidance document on environmental risk assessment of substances. New studies will be performed on emissions of industrial category 9 (mineral oil and fuel) and 14 (paints, lacquers, and varnishes). Existing documents will be used to amend the emission database of USES for the following categories: paint industry, oil industry, production of plastics, intermediates and other available documents.

Assumptions in the standard scenario:

- Emission releases are dependent on use pattern of the substance, tonnage, and also on water solubility and vapour pressure.
- The entire production volume is placed on one use pattern of the substance. This is not relevant for many chemicals. A mixed use pattern should be considered.
- For local estimates, a main point source is considered.
- For local estimates, only the process with the highest emission to water is considered.
- For local estimates, only the emission to air belonging to the above-mentioned process is considered.
- For calculating exposure levels for humans, soil organisms, and predators, emissions are averaged over a year.

Input	Symbol	Output	Symbol
main Cat.		frac. to air	
industr. Cat.		frac. to wastew.	
use Cat.		(frac. to soil)	
tonnage	*TONNAGE*	frac. main source	
(specific. questions)		no. of emiss. days	$T_{emission}$
vapour pressure	*VP*		
water solubility	*SOL*		

3.3. Distribution module (local)

The local distribution module estimates the concentrations in air, surface water, groundwater, and agricultural soil in the surroundings of an emission source of the substance. Four sub-modules are distinguished: the Sewage Treatment Plant (STP), the air module, the surface water module, and the soil-groundwater module. Assumptions are made on the exposure location, relative to the source, and on the characteristics of the environment. It should be noted that the latter are extensively discussed in a project on harmonisation of several risk assessment systems in The Netherlands (Heijna-Merkus and Hof, 1993). Although this does not imply that these values are validated, it means that a broader consensus was reached.

At this moment, the Danish National Environmental Research Institute is also examining the exposure models of USES in detail to examine its applicability for the Danish conditions. The work includes testing of the models, and comparison with other models. The results of this project can be taken into account in a validation of USES.

References

Heijna-Merkus, E. and M. Hof (1993). Harmonization of model parameters. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102022.

3.3.1. Sewage treatment plant

In USES, all emissions to water are treated in a sewage treatment plant (STP). The process of sewage treatment, as modelled with SimpleTreat (Struijs *et al.*, 1991a,b), can be described as a redistribution of the emission via waste water to effluent, sludge, and air. The remainder is degraded. Struijs *et al.* (1991b) compared some results to field data, concluding that estimated emissions to air for five persistent volatile compounds were in good agreement with measured data (within a factor of 1.5). Estimated concentrations in sludge were compared to field data only for LAS (linear alkylbenzenes sulphonates) for which the authors concluded that agreement was good. The results of Toet *et al.* (1991) also indicate the validity of this model with respect to concentrations in effluent and sludge (usually within a factor of 10 with a broad range of substances and plants, with the default STP definition).

Half-lifetime for biodegradation is shown as input parameter. It is possible to run USES without input of this parameter, but the defaults have been chosen conservatively.

Validation activities have already been initiated, as described by Temmink *et al.* (subm.). The Department of Environmental Technology of the Wageningen Agricultural University will conduct an experimental validation of a number of available models, including SimpleTreat as applied in USES 1.0. The experiments will be conducted in a pilot-scale activated sludge plant which is operated at two extremely different sludge loading rates and with test compounds which vary in their physico-chemical properties and biodegradation rates. Experiments are set up to verify the individual processes which determine the distribution of chemicals (sorption, stripping and biodegradation) and validation focused on the reliability of the models as a whole.

Assumptions in the standard scenario:

- All of the emission to water is treated in a sewage treatment plant. This assumption is valid for the situation in The Netherlands.
- Average characteristics of a Dutch municipal plant are assumed as default.
- Only removal by volatilisation, biodegradation (which may include hydrolysis), sorption to solids is taken into account.
- The steady state situation in the STP is relevant with respect to exposure concentrations in air, effluent, and sludge.

Input	Symbol	Output	Symbol
emission to w.w.	$Edirect_{water}$	frac. to effluent	
half-life STP	$kdeg_{stp}$	frac. to sludge	
Kow	Kow	frac. to air	
Henry coeff.	$HENRY$	frac. degraded	
solids-water part.	$Kp_{susp/S}$		
	$Kp_{susp/TSLS}$		
molec. weight	$MOLW$		

References

Struijs, J., D. van de Meent and J. Stoltenkamp (1991a). SimpleTreat: a spreadsheet-based box model to predict the fate of xenobiotics in a municipal waste water treatment plant. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 670208002.

Struijs, J., J. Stoltenkamp and D. van de Meent (1991b). A spreadsheet-based model to predict the fate of xenobiotics in a municipal wastewater treatment plant. Wat. Res. **7(25)**, 891-900.

Temmink, H., P. Kuiper and A. Klapwijk (submitted for publication). Validatie van modellen die het gedrag van milieuvreemde stoffen in rwzi's voorspellen. (in Dutch). *(Validation of models that predict the fate of xenobiotics in sewage treatment plants)*

Toet, C., A.C.M. de Nijs, T.G. Vermeire, P. van der Poel and J. Tuinstra. Risk Assessment of New Chemical Substances; System Realisation and Validation II. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102004.

3.3.2. The air module

Emissions to air are linked to (long term average) concentrations and deposition fluxes with results obtained from the OPS model (Van Jaarsveld, 1990). For validation, concentrations in air have to be found related to a point source with known emission flux. These conditions are not easily met, and concentrations in air are likely to vary appreciably in time and space. Another possibility is to validate the approach in USES with other, more specific, models.

The air module of USES is currently being analyzed. This includes the numerical models, as well as relevance of the exposure scenario. This could well lead to a different air module. Especially the assumption of averaging emissions over a year is questionable when looking at batch processes or spraying of pesticides. It is, however, yet unclear how concentrations varying in time can be linked to, for example, chronic human exposure.

Assumptions in the standard scenario:

- Only annual average concentrations are generated by averaging emissions over the year.
- Concentrations are calculated at 100 m from the source.
- Deposition will be calculated as averaged over a circular area with a range of 1 km around the source.
- Standard source characteristics and environmental and meteorological data are used.
- A typical value is taken for the area of aerosol particles. This value is harmonised between several risk assessment systems (Heijna-Merkus & Hof, 1993).

Input	Symbol	Output	Symbol
emiss. to air	$Edirect_{air}$	conc. in air	$Cdirect_{air}$
(no. emiss. days)	$T_{emission}$	deposition flux	$Dtot$
frac. ass. aerosol	$Fass_{air}$		

References

Van Jaarsveld, J.A. (1990) An operational atmospheric transport model for Priority Substances; specification and instructions for use. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 222501002.

Heijna-Merkus, E. and M. Hof (1993). Harmonization of model parameters. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102022.

3.3.3. The surface water module

This sub-module describes the dilution process occurring in surface water and includes partitioning with suspended solids. The concentration in surface water shows a large amount of variation due to the variability in flowrate of the receiving surface water. In USES this is reflected in the high uncertainty factor of 148. This large range of dilution factors is calculated using a model on the characteristics of the receiving surface water of each STP in the Netherlands (De Greef & De Nijs, 1990).

The research behind the dilution factor is quite extensive. Therefore, numerical validation of this module is not necessary for the situation in The Netherlands. In the process of developing a European risk assessment system, this module needs further investigation. The assumptions and scenario choices may however, be examined more closely.

Assumptions in the standard scenario:

- Concentration at 1000 m from the STP is used as relevant exposure concentration. This a more or less arbitrary location.
- Dilution and partitioning to suspended solids are the main removal processes. Other processes as, e.g., sedimentation, degradation, hydrolysis, and volatilization are neglected. This assumption needs further investigation. This may be valid in view of the short residence time between the STP and the exposure location.
- Typical characteristics of suspended solids are assumed. These default parameters were harmonised between several risk assessment systems (Heijna-Merkus & Hof, 1993).

Input	Symbol	Output	Symbol
conc. effluent	$Ctot_{effl}$	conc. surf. water	$Cdiss_{surf,epi}$
solid-water part.	Kp_{susp}		

References

De Greef, J. and A.C.M. De Nijs (1990). Risk Assessment of New Chemical Substances; Dilution of effluents in The Netherlands. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 670208001.

Heijna-Merkus, E. and M. Hof (1993). Harmonization of model parameters. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102022.

3.3.4. The *soil and groundwater module*

The soil-groundwater module calculates long-term concentrations in soil and groundwater at given input rate from sludge application and aerial deposition. Results from the model PESTLA, run with a standard environmental scenario are used. Two input parameters are used to characterise the behaviour in soil: a sorption coefficient (*Kom*, estimated from *Kow*) and a degradation rate (*DT50soil*).

Validation of the original PESTLA model was performed in detail in 1994 with respect to pesticide application. The procedure for validating PESTLA has been outlined by Boekhold *et al.* (1993a). A field test with PESTLA is described by Boekhold *et al.* (1993b). It was concluded that PESTLA simulated the behaviour in soil of bentazon well. Several other reports are in preparation and, at this moment, a summary report with conclusions is being finalised. A large problem in validating PESTLA was the lack of data, especially for levels in groundwater. Therefore, the validation was mainly performed by comparison of measured and calculated soil concentration-depth profiles and to a lesser extent by comparing measured and calculated concentration in groundwater.

Validation of the way in which PESTLA is implemented in USES (as reflected in the assumptions of the scenario) is required. Especially the summation of sludge and continuous deposition, and the derivation of concentrations in soil from the fraction accumulation needs further investigation. Furthermore, the choices for a characteristic soil type, meteorological data, type of crops grown, etc. need to be reconsidered for the EU-project.

Assumptions in the standard scenario:

- Only one type of soil considered. Sludge is applied once each year (the maximum amount of 2000 $kg.ha^{-1}.yr^{-1}$).
- The concentration in sludge, that is used on agricultural land, is calculated with annual average emissions.
- The soil receives deposition as averaged over a circular area with a range of 1 km.
- The soil type is more or less best case with respect to accumulation, but worst case with respect to leaching to groundwater. Furthermore, no dilution of the groundwater is assumed before water is taken in for drinking water production.
- For other soil characteristics (density, fraction organic matter, etc.), average Dutch values are applied. These values are harmonised between several risk assessment systems (Heijna-Merkus & Hof, 1993).
- A top-soil layer of 20 cm is assumed. This default parameter is also harmonised (Heijna-Merkus & Hof, 1993).
- The concentration in the soil is calculated as average over 180 days. This value is used for exposure of soil organisms and indirect human exposure. This assumption is not consistent with the EC directive on the use of sewage sludge in agriculture (EC, 1986), and therefore, further investigation is required.
- The fraction accumulation, given by PESTLA, can be translated to a first-order removal rate from the top-soil layer. This assumption needs further investigation, but some test runs with the original PESTLA show that the error due to this assumption is small (less than a factor 2).
- For calculating the concentration in groundwater, the total annual deposition and sludge application are summed into one single application. Again, this assumption was tested with a original PESTLA model, the error made was small (also within a factor 2).

Input	Symbol	Output	Symbol
conc. in sludge	C_{sludge}	conc. in soil	$Ctot_{agr}$
degr. rate in soil	$kdeg_{soil}$	conc. in groundw.	C_{grw}
deposition	$Dtot$		
Kow	Kow		

References

Boekhold, A.E., H. van den Bosch, J.J.T.I. Boesten, M. Leistra, F.A. Swartjes and A.M.A. van der Linden (1993a). Validation of the PESTLA model: Definitions, objectives and procedure. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 715802001.

Boekhold, A.E., F.A. Swartjes, F.G.G. Hoogenboom and A.M.A. van der Linden (1993b). Validation of the PESTLA model: Field test using data from a sandy soil in Schaijk (the Netherlands). Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 715802002.

EC (1986). Council directive of 12 June 1986 Regarding the protection of the environment, especially soil, when using sewage sludge in agriculture (86/278/EEC). Official Journal of the European Communities, L181.

Heijna-Merkus, E. and M. Hof (1993). Harmonization of model parameters. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102022.

3.4. Distribution module (regional)

For environmental distribution on a regional scale, the model SimpleBox is applied in USES (Van de Meent, 1992). This model calculates steady-state concentrations in several environmental compartments, assuming a constant, diffuse, emission pattern. Validation of SimpleBox can be viewed in three ways:

- Validation of the ability of SimpleBox to predict *actual occurring* environmental concentrations from physico-chemical properties of the substance and its emission pattern.
- Validation of the ability of SimpleBox to predict the distribution of a substance between environmental compartments
- Validation of the *relative* environmental exposure levels (PECs).

Validation in the first context requires environmental concentrations of chemicals with a (more or less) diffuse emission pattern. The substance must have been used over a longer period of time to accommodate the steady-state assumption. However, the problem arises that environmental concentrations are highly variable in time and in space. By stating this, one of the assumptions is immediately invalidated: the region under consideration in *not* made up of homogeneous compartments, therefore, SimpleBox will *not* be able to predict regional concentrations occurring at a specific place or time. Of course, the criterium can be put less stringent: is SimpleBox able to predict spatially and temporally averaged concentrations? The problem remains that substances which will fit the assumptions and are measured extensively (also in unpolluted areas) are scarce.

A case study on environmental distribution of 7 substances was performed by ECETOC (1994a). For the calculations, the regional model of HAZCHEM (ECETOC, 1994b) was used. This model is also a Mackay level 3 multimedia model, and the differences with SimpleBox are small.

in Figure 7, the results of the case study are summarised. The values in this figure are environmental concentrations in air (mg/m^3), surface water (mg/l), groundwater (mg/l), sediment (mg/kg), and soil (mg/kg). Minimum-maximum ranges are shown. The measured concentrations are, whenever possible, background concentrations, to allow for a realistic comparison with HAZCHEM. It should be noted however, that measurements are often made on contaminated sites. Despite many uncertainties, several conclusions can be made. There is a correlation between the estimated concentrations and the measured concentrations. Secondly, large deviations between measured and estimated concentrations occur, more specifically, HAZCHEM tends to underestimate environmental concentrations (up to 5 orders of

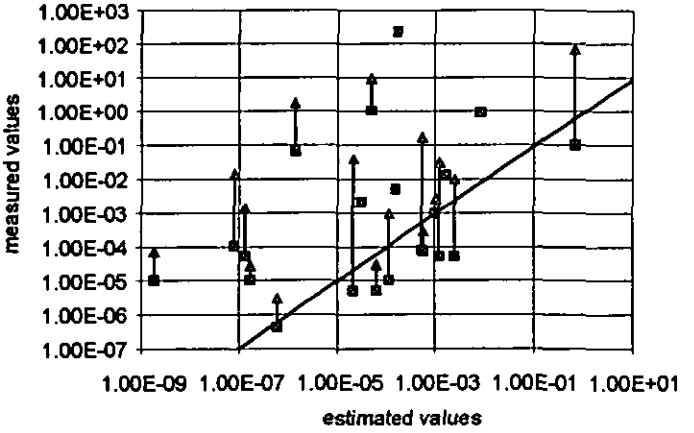

Figure 7 *Summarized results of the case study with a regional model (HAZCHEM). Environmental concentrations are compared.*

magnitude). It should be noted that the measured data showed an enormous amount of variability. The results of this case study must be interpreted carefully, but it indicates that use of the regional model can lead to serious underestimation of the environmental concentrations, and therefore, underestimation of the absolute risk of substances.

Even if SimpleBox would not be valid in predicting averaged environmental concentrations, this would not mean that the model is not appropriate for the purpose of USES. A more promising way to validate this model is to validate the *relative* environmental concentrations. Again, selection and gathering of the required data will be the main problem. No activities to validate SimpleBox are planned for the near future. A more in depth validation analysis of SimpleBox is advisable.

Assumptions in the standard scenario:

- The region under considerations is made up of a few, well-mixed, compartments (3 soil types, sediment, surface water, suspended matter, air, biota).
- Emissions are regarded as diffuse and continuous.
- Default definition is that of the Netherlands, separate calculations on the scale of Western Europe calculate the background conditions for the regional calculation.
- A steady-state situation occurs, and is the relevant situation with respect to exposure of the groups to be protected.

Input	Symbol	Output	Symbol
physico-chem. prop.		conc. in soil	$Ctot_{agr,reg}$
emission pattern		conc. in surf. water	$Cdiss_{surf,reg}$
		conc. in air	$C_{air,reg}$
		conc. in sediment	$Ctot_{sed,reg}$
		conc. in groundw.	$C_{grw,reg}$

References

ECETOC (1994a). Assessment of non-occupational exposure to chemicals. Technical Report no. 58, ECETOC, Brussels.

ECETOC (1994b). HAZCHEM, a mathematical model for use in risk assessment of substances. Special report no. 8, ECETOC, Brussels.

Van de Meent, D. (1993). SIMPLEBOX: a generic multimedia fate evaluation model. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 672720001.

3.5. Intake module

In this module, concentrations in consumption media for humans and predators are estimated from environmental concentrations and bioconcentration factors. Validation of bioconcentration factors was described in section 3.1.5. Since the bioconcentration factors are defined as the concentration in the organisms, divided by the concentration in the exposure medium, the 'model' $Corganism = BCForganism \cdot Cmedium$ does not need to be validated. In this section the main point is operational and conceptual validation to check if the use of the BCFs is appropriate and if the assumptions are acceptable. Furthermore, BCFs are usually derived under laboratory conditions with relative high concentrations. It is not clear beforehand if these factors are still applicable in field situations. It may be especially interesting to see if the kinetics of uptake and translocation are rapid enough, with respect to short emission episodes, to reach a steady state. This problem of bioconcentration kinetics will be investigated in 1995, as part of the USES project.

The following sub-modules are distinguished: drinking water, fish, earthworms (for predating birds and mammals only), plants (root crops and leaf crops), cattle (meat and milk), and the total daily intake module (where all contributions are summed). The concentration of the contaminant in air, leading to human exposure through inhalation, is taken directly from the distribution module (section 3.3.2).

3.5.1. Concentration in drinking water

Drinking water is prepared from groundwater or purified surface water. The purification process can not be accurately predicted from physico-chemical properties, therefore, the purification factors have been conservatively chosen (Hrubec & Toet, 1992). Validation of this module by Toet *et al.* (1991) showed that the agreement with measured data was fairly good (in most cases within a factor of 10). This was despite the fact that the system at this point assumed no purification at all. This validation can be performed again with the version of the module in USES 1.0 on the same data set.

Due to the conservative approach, extensive validation might not be very effective. More in-depth research in the treatment process is required.

Assumptions in the standard scenario:

- Drinking water will be prepared exclusively from contaminated surface water (at 1000 m from STP) or from contaminated groundwater (from agricultural soil on which sludge was applied).
- No further purification will occur for groundwater.
- For surface water, conservative purification factors are applied.

Input	Symbol	Output	Symbol
conc. in surf. water	$Cdiss_{surf,arm}$	frac. removal	$FPUR$
conc. in groundw.	C_{grw}	conc. drinking w.	C_{drw}
Kow	Kow		
Henry coeff.	$HENRY$		
half life for degr.	$DT50bio_{water}$		

References

Hrubec, J. and C. Toet (1992). Predictability of the removal of organic compounds by drinking water treatment. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 714301007.

Toet, C., A.C.M. de Nijs, T.G. Vermeire, P. van der Poel and J. Tuinstra. Risk Assessment of New Chemical Substances; System Realisation and Validation II. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102004.

3.5.2. Concentration in fish

Fish, for human consumption and predators, is swimming in the contaminated surface water and is assumed to reach equilibrium with the water. This assumption is questionable, especially for substances only emitted during short episodes as equilibration may take up to several months for lipophilic substances (estimated with relations given by Spacie & Hamelink, 1982). The consequences, and possible solutions, of this problem will be investigated in 1995.

Assumptions in the standard scenario:

- Fish will be in equilibrium with the annual average concentration at 1000 m from the STP. This assumption will be investigated in 1995.

Input	Symbol	Output	Symbol
conc. in surf. water	$Cdiss_{surf}$	conc. in fish	C_{fish}
bioconc. fact. fish	BCF_{fish}		

References

Spacie, A. and J.L. Hamelink (1982). Alternative models for describing the bioconcentration of organics in fish. Environ. Toxicol. Chem. 1, 309-320.

3.5.3. Concentration in earthworms

The earthworms, for consumption by predators, are exposed to the concentration in agricultural soil. Only uptake from the soil-water is accounted for. The results of Belfroid (1994), as discussed in section 3.1.5.2, support this assumption. Furthermore, experimental *BCF*s were measured by Belfroid of chlorobenzenes in earthworms, in water and soil. The time for reaching an equilibrium was fast (7 days for the most lipophilic compound tested: log *Kow* of 5.7).

Assumptions in the standard scenario:

- The worms will be in equilibrium with the average concentration in agricultural soil (top layer of 20 cm) over a period of 180 days (starting with the moment of sludge application). The results of Belfroid (1994) indicate the applicability of this assumption. The time necessary for equilibrium was short (within 7 days).

Input	Symbol	Output	Symbol
conc. in soil	$Ctot_{agr}$	conc. in worm	C_{worm}
bioconc. fact. worm	BCF_{worm}		

References

Belfroid, A.C. (1994). Toxicokinetics of hydrophobic chemicals in earthworms. Validation of the equilibrium partitioning theory. Phd. Thesis. Utrecht University, The Netherlands.

3.5.4. Concentration in plants

Plants are grown on soil where sludge is applied once a year. Chemical are taken up by the plant via the root, subsequently, the substance may be translocated to the shoots. The plants are simultaneously exposed to the annual average air concentration and aerial deposition. The consequences of the kinetics of these processes will be investigated within the USES project in 1995.

The validation activities of Toet *et al.* (1991) reveal a huge discrepancy between calculated and measured concentrations in plants. It should be noted that many field data were derived for substances that were applied directly as pesticide (this was not accounted for in the risk assessment system). Furthermore, the route from air to plant was not yet incorporated in the system. The data gathered by Toet and co-workers can be re-examined with the present version of USES.

Assumptions in the standard scenario:

- The plants are in equilibrium with the concentration in the porewater, and with the concentration in air. Also, deposition on the leaf surface is in equilibrium with the removal processes.
- The exposure concentration can be assumed to be constant during the exposure period.
- Annual average air-concentrations and half-year average soil-concentrations are relevant with respect to indirect exposure of humans through crop consumption.
- The contribution to the concentration in stems of translocation from the roots, aerial deposition, and gas uptake can be summed. This assumption is questionable, and will be examined in 1995.

Input	Symbol	Output	Symbol
conc. in soil	$Ctot_{agr}$	conc. in root crops	C_{root}
conc. in air	C_{air}	conc. in leaf crops	C_{stem}
frac. ass. aerosol	$Fass_{aer}$		
bioconc. root	$BCFroot_{plant}$		
bioconc. stem	$BCFstem_{plant}$		
bioconc. air	$BCFair_{plant}$		

References

Toet, C., A.C.M. de Nijs, T.G. Vermeire, P. van der Poel and J. Tuinstra. Risk Assessment of New Chemical Substances; System Realisation and Validation II. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102004.

3.5.5. Concentration in cattle meat and milk

The results of the USES module may be compared with a kinetic model as for instance the PB-PK model of Derks *et al.* (1994) for dioxines in cows, to check whether the assumption of steady state is valid. This can be done in the planned project within USES in 1995.

The validation activities of Toet *et al.* (1991) for this module are not very satisfactory. Only a few measured data were available which showed huge deviations from expected values. It

should be noted that concentrations in food crops where taken as input of the module for validation. These could very well differ from concentrations in grass, and were probably also measured on a different location. Furthermore, as discussed in section 3.1.5.4, the uncertainties in the biotransfer factor are very large, therefore adding to the inaccuracy of this module.

Assumptions in the standard scenario:

- The period of exposure is sufficient to reach equilibrium between the cows daily intake of the substance and the concentrations in meat and milk. This assumption will be investigated in 1995.
- The exposure concentration can be assumed to be constant during the exposure period.
- Annual average air-concentrations and half-year average soil-concentrations are relevant with respect to indirect exposure of humans through meat and milk consumption.

Input	Symbol	Output	Symbol
conc. in soil	$Ctot_{agr}$	conc. in meat	C_{meat}
conc. in air	C_{air}	conc. in milk	C_{milk}
conc. in grass	C_{grass}		
biotransfer to meat	BTF_{meat}		
biotransfer to milk	BTF_{milk}		

References

Derks, H.J.G.M., P.L.M. Berende, M. Olling, H. Everts, A.K.D. Liem and A.P.J.M. de Jong (1994). Pharmacokinetic *modelling of polychlorinated dibenzo-p-dioxines (PCDDs) and furans (PCDFs) in cows. Chemosphere* 28,711-715.

Toet, C., A.C.M. de Nijs, T.G. Vermeire, P. van der Poel and J. Tuinstra. Risk Assessment of New Chemical Substances; System Realisation and Validation II. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102004.

3.5.6. Total daily intake

Humans are exposed via the environment through consumption of food products (crops, meat, dairy products, fish), drinking water, and inhalation of air. The scenario seems very worst case, but it should be noted that, usually, only one or two routes dominate the exposure. This approach indicates the routes for potential hazardous exposure in a transparent way, and makes the results readily interpretable.

The intake rates for humans where derived from a large scale survey, and were harmonised between several risk assessment systems (Heijna-Merkus & Hof, 1993). In the framework of the development towards a European risk assessment system, these values will have to be reexamined for the European situation.

Surprisingly, Toet *et al.* (1991) found good agreement between measured and calculated total daily intakes. In view of the deviations observed for the concentrations in food media, this agreement was judged as artificial.

For some substances, human exposure through food products is very well examined. As an example, dioxines are thoroughly studied (Liem *et al.*, 1991). However, actual validation of this model is difficult, since relevant data for the exposure scenario will be scarce. Therefore, it is advised to aim at a thorough operational and conceptual validation of the exposure

scenario.

Assumptions in the standard scenario:

- All of the consumption of air, drinking water, crops, meat, milk, fish is derived from the contaminated area. With this worst case approach, the main routes of potential importance are shown.
- Average consumption rates and bodyweight of the Dutch population are used. These values were harmonised. More discussion will take place in the framework of the EU-project.
- Exposure via ingestion of soil is neglected. The intake through this route is usually small, nevertheless, this route needs some more specific investigation.
- Only adults are assessed. This needs further examination since children often have a higher exposure than adults.
- The humans assessed will be exposed to the annual or semi-annual average concentrations in media and products. This is a median case assumption.

Input	Symbol	Output	Symbol
Concentration in food products		Total daily intake	*DOSEtot*

References

Heijna-Merkus, E. and M. Hof (1993). Harmonization of model parameters. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102022.

Liem, A.K.D., R.M.C. Theelen, W. Slob and J.H. van Wijnen. Dioxinen en planaire PCB's in voeding. Gehalten in voedingsproducten en inname door de Nederlandse bevolking. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 730501034. *(Dioxines and planar PCBs in food. Levels in food products and intake by the Dutch population)*

Toet, C., A.C.M. de Nijs, T.G. Vermeire, P. van der Poel and J. Tuinstra. Risk Assessment of New Chemical Substances; System Realisation and Validation II. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102004.

3.5.7. Consumer exposure

The consumer exposure module offers several exposure scenarios from which the user can choose. Each scenario describes the magnitude of exposure and uptake that is expected if the behaviour of compound matches that assumed in the scenario. Two validation questions can be put forward:

- Is the set of exposure scenarios adequate to describe consumer exposure?
- Does each exposure scenario adequately describe exposure?

The first question is difficult to answer, but the RIVM project Human Exposure sub-project Consumer Exposure aims at answering it (see Van Veen *et al.*, 1994). The second question is also not easy to answer. A major difficulty is the lack of experimental data, both in the literature and at the RIVM. A first step can be taken by performing uncertainty analysis by assessing how variability in a single parameter propagates through the model. The tools to execute this analysis are available in the form of the CONSEXPO program (Van Veen, manual in prep.) to estimate consumer exposure. This procedure will reveal the most important parameters and model parts. Then, the validity of the parameter defaults and the model parts can be assessed further.

At this moment the approach for consumer exposure in USES is quite rough. On the basis of the work performed by Van Veen *et al.* (1994) and future work planned, it is foreseen that the module as incorporated in USES 1.0 will be changed or amended.

Assumptions in the standard scenario:

- The set of exposure scenarios available in USES are sufficient to evaluate the risks of consumer exposure

References

Van Veen, M., T.G. Vermeire and M. Olling (1994). Consumentenblootstelling: een overzicht van blootstellings- en opname-modellen. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 612810001. (in Dutch). *(Consumer exposure: an overview of exposure and uptake models)*

3.6. Effect module

In the effect module, No-Effect-Concentrations (NEC) and No-Effect-Levels (NEL) are derived from single species toxicity tests. The extrapolation is performed with (conservative) extrapolation factors of 10, 100, 1000 or 10000. If a sufficient number of NOECs is given, a statistical procedure is applied, estimating the concentration at which 95% of the species in the ecosystem is protected.

Validation of these extrapolation procedures has been performed by Emans *et al.* (1993). The results of this study can be directly translated to USES. This validation did not cover the entire effect module as incorporated in USES. The authors compared extrapolated single species toxicity tests to the results of multiple species (semi-) field experiments. Only freshwater organisms were examined. The results indicate the validity of the modified EPA method for preliminary effects assessment as it usually arrives at a safe level. However, when only one single species test was used, the probability of underestimating the safe level for ecosystems increased. The best estimates of the ecosystem 'safe levels' were obtained with the statistical extrapolation method of Aldenberg & Slob (1993) as applied in USES 1.0.

The EU recently proposed different assessment factors for the extrapolation of single species tests to ecosystem level (EC, 1993). Usually, this approach will give a more conservative estimate of the ecosystem NEC. In the EU proposal, the Aldenberg & Slob method is not applied.

The equilibrium partitioning method is an accepted method for indicating toxicity to sediment organisms (see for example DiToro *et al.*, 1991). In soil, the applicability of this theory was investigated by Van Gestel & Ma (1988, 1990) and Belfroid (1994), indicating the validity of the concept for the soil organisms.

Assumptions in the standard scenario:

- Protection of the most sensitive species would immediately protect the structure and functioning of the ecosystem or population.
- No-Effect Levels for ecosystems, predators, and humans can be derived from laboratory LC50, NOEC, LD50 and NOAEL values.
- Soil-dwelling organisms are equally sensitive to the concentration in the porewater as aquatic organisms to the concentration in the water column.

Input	Symbol	Output	Symbol
toxicity data single species		no-effect levels	$NECaqua_{ass}$
			$NECterr_{ass}$
			$NECterr_{EP}$
			$NECfood_{pred}$
			NEL_{man}

References

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Belfroid, A.C. (1994). Toxicokinetics of hydrophobic chemicals in earthworms. Validation of the equilibrium partitioning theory. Phd. Thesis. Utrecht University, The Netherlands.

DiToro, D.M., C.S. Zarba, D.J. Hansen, W.J. Berry, R.C. Swartz, C.E. Cowan, S.P. Pavlou, H.E. Allen, N.A. Thomas and P.R. Paquin (1991). Technical basis for establishing sediment quality criteria for nonionic organic

chemicals using equilibrium partitioning. Environ. Toxicol. Chem. **10**, 1541-1583.

EC (1993). Risk assessment of notified new substances; Technical Guidance Document. Brussels, Commission of the European Communities, Directorate-General Environment, Nuclear Safety and Civil Protection.

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Van Gestel, C.A.M. and W. Ma (1988). Toxicity and bioaccumulation of chlorophenols in earthworms in relation to bioavailability in soil. Ecotox. Environ. Saf. **15**, 289-297.

Van Gestel, C.A.M. and W. Ma (1990). An approach to quantitative structure-activity relationships (QSARs) in earthworm toxicity studies. Chemosphere **21**, 1023-033.

3.7. Evaluation module

In the evaluation module, PEC/NEC ratios are calculated for the groups to be protected. Unfortunately, PEC/NEC ratios cannot be measured, therefore, other validation activities must be developed. One method to validate the risk estimates of USES, in a more relative way, with the experts opinion is described in chapter 4.

Another, more absolute, method is to investigate substances with *known* adverse effects in the field for a group to be protected. Properties of these substances can be entered in USES. USES should, at least, predict a PEC/NEC ratio > 1 for this substance and this group to be protected. The other way around is also possible, taking substances with no known adverse effects whatsoever. For these substances, USES should predict a PEC/NEC ratio < 1. This procedure requires further elaboration, but may provide a means for validating the ultimate ability of USES to predict adverse effects. Furthermore, if this procedure is performed extensively, it may help the interpretation of the hazard and risk levels given by USES.

Assumptions in the standard scenario:

- The PEC/NEC ratio as derived with USES is a measure of the potential risk of the substance
- The probability that a PEC/NEC ratio of 1 is exceeded gives additional information on the amount of uncertainty that has to be taken into account in the decision making process

Input	Symbol	Output	Symbol
'Expert opinion' or		Hazard ratios	*HAZARD, MOS*
'Known hazard'		Probability	*PROBpecnec*

3.8. Specific routes/scenarios for pesticide application

The application and subsequent distribution of pesticides is handled in application-specific scenarios. Many distribution models are shared by the pesticide assessment and the new/existing chemicals assessment (e.g., OPS, PESTLA). Others are specific for pesticides (e.g., the SLOOTBOX model for calculating concentrations in a ditch due to drift and drainage). The pesticide assessment makes use of empirical relations and tables which are useful, but not easily validated.

The SLOOTBOX model is based on measured drift to the ditch, as far as application to fruit trees, higher (>25 cm) and lower crops (<25 cm) is concerned. Other input data are measured data from the registration base set. Therefore, SLOOTBOX can be considered as partially validated. Its successor (TOXSWA) will undergo the same validation process as was carried out for PESTLA. By the EU, a working group on groundwater and surface water model validation is established. The results from this group are expected in 1995.

The assumptions for the emission to air are questionable when looking at spraying of pesticides. The air module of USES is currently being analyzed. This includes the numerical models, as well as relevance of the exposure scenario. This could well lead to a different air module for pesticide application.

For pesticides, many different PEC/NEC ratios are calculated that are used as input for so-called decision trees (which are not part of USES). The additional work on the decision trees of birds and mammals will be finished in 1995.

No further validation activities are performed or planned for 1995.

Assumptions in the standard scenario:

- The standard environment is a plot of agricultural soil of 1 hectare, surrounded by a typical ditch.
- For emission to air during spraying of pesticides, a fixed fraction of 0.10 is taken. The plot of agricultural soil is modelled as a point source (same choices as for industrial chemicals are applied, see page 25, 26).
- If the substance is mixed with soil, a soil layer of 20 cm is considered, otherwise a depth of 5 is applied.
- Concentrations in soil will decrease, over the time period considered, through biodegradation only.
- Terrestrial organisms are exposed to the concentration averaged over a period equivalent to the duration of the toxicity test for this organism.
- Aquatic organisms are exposed in the ditch surrounding this area (again with the concentration averaged over a period equivalent to the duration of the toxicity test for this organism).
- Humans are exposed through drinking water derived from groundwater or surface water from this area, but crops, meat, and milk are derived from a neighbouring plot.
- On the regional scale, emissions are set at 80% of the production volume to soil, 10% to air, and 10% to surface water.

3.9. Specific scenarios for biocide application

The distribution of biocides (non-agricultural pesticides) is handled in application specific scenarios. All scenarios are part of the emission module. In these scenarios, a large amount of expert judgement is applied. The scenarios can be judged on their relevance. However, as this module is still in development, and their is little experience with the use of this module, validation activities might be postponed.

In 1994 additional work on this module was reported by Luttik *et al.* (in prep.). This report includes scenarios for disinfectants for swimming water, leaching from impregnated wood to soil and groundwater, and household products used for fogging. Additionally, a concept is presented to describe the diffusion of metal ions from the water phase to the sediment. Extension of the module to other application types is planned within the USES project for 1995.

Assumptions in the standard scenario:

- The scenarios as applied in USES 1.0 are realistic worst case situations, and are sufficient to evaluate exposure to these chemicals

References

Luttik, R., P. van der Poel and M.A.G.T. van den Hoop (in prep.). Supplement to the Evaluation System for PEsticides (ESPE) 2. Non-agricultural pesticides. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report No. 679102xxx.

4. AN EXPERIMENT WITH 'RISK VALIDATION'

Risks or hazards cannot be measured in the field. However, the aim of USES is to predict risks of substances. Validation activities of USES sofar, were only based on validating the accuracy of individual exposure models. The main assumption made is, that the more accurate the exposure of the target organisms is estimated, the more accurate the risk estimate. This is of course an acceptable assumption, but the value of the risk estimate of USES remains untouched, and the benefit may not justify the efforts. The experiment described in this chapter is an attempt to address this problem. It should be stressed that this experiment was not meant as an 'ultimate validation', but to examine the possibilities of this approach to validation.

4.1. Design of the experiment

To investigate the possibilities of validating risks, a small experiment was set up with 39 members of the Dutch Society of Toxicology during a meeting at the RIVM. For this experiment, 10 well known substances were selected from the list of attention chemicals. The participants were asked to make a selection in this list of substances, based on perceived risk. This selection could then be compared to the ranking made by USES.

The question asked was: "Which of these substances are candidates for further investigation and risk evaluation, based on the toxic risk they pose to man and other organisms?" Each of the participants was asked to select two different substances with the highest perceived risk (using stickers). From the reactions of the participants, it was clear that the question should be defined very strictly. The choice should be made on the basis of perceived risks, and not based on measures planned. It should also be avoided that people do not select a certain hazardous chemical because there is already enough information on that substance. The question should be as close as possible to the purpose and possibilities of USES.

The following substances were chosen for the experiment:

- **Pentachlorophenol** was applied broadly as biocide, particularly in the wood industry. At this moment, only the application of PCP-laurate is allowed in the textile and fibre industry.
- **Dioxines (based on TEQs)**, a group of 210 different substances. De toxicity is attributed to 17 congeners, and expressed as equivalents of 2,3,7,8-TCDD. Dioxines are formed as a waste product at, for instance, waste incinerators.
- **Benzene** is used predominantly as a intermediate for the formation of other substances. It is a ingredient of gasoline, which makes traffic the largest emission source at this moment.
- **Benzo[a]pyrene** is a PAH (polychlorinated, aromatic hydrocarbon), formed by combustion, but also emitted by creosoting of wood.
- **Methylbromide** is only allowed as fumigant for stored supplies, quarantine materials, and objects as planes and buildings. The potential for ozone depletion should not be taken into account in the selection procedure of this experiment.
- **Ethene** is used as intermediate for the formation of other substances (e.g., polyethylene). Traffic and chemical industry are the main emission sources.
- **Di(2-ethylhexyl)phthalate** is one of the commonest members of the phthalates, a group of

substances, applied as plasticizer in a.o., carpets, paints, rubber, glues, and PVC-products.
- **Trifenyltinaceticacid** is used as agricultural pesticide, but also as biocide in anti-fouling paints for ships.
- **Phenol** is used for the production of phenol derivates and phenol resin and for production of isolating materials, chipboard, and paints.
- **Formaldehyde** is a volatile organic substance, emitted by traffic, at industrial production processes, and from fireplaces. The substance is applied in a.o., glue and plastics production, as preservative and disinfectant.

After selection by the participants, the resulting list could be compared to the list prepared by USES. The data were mainly obtained from a project at the RIVM where several attention substances are prioritised with USES. These data were collected from readily available secondary literature sources (e.g., integrated criteria documents). In the process of data selection, we encountered the following problems:
- USES only allows *one* use pattern of the substance. This means that the entire production volume must be set on one type of use. For many substances (especially with high production volumes) this is not very relevant.
- For substances as dioxines and benzo[a]pyrene, it is impossible to select a production volume and a use pattern as these substances are emitted unintentionally during combustion processes. We had to make use of emission estimations from the integrated criteria documents.
- It is not allowed to change intermediate results during prioritisation. For many of these substances, relative good emission estimates have been made. However, these cannot be used in standard prioritisation.
- For relevant, and comparable, toxicity data, we made use of MTR (maximum tolerable risk level) values for ecosystems, and TDI (tolerable daily intake) values for humans. This was mainly done to avoid the effort of toxicity data selection. USES however, does not allow input of MTR values. These values were entered as a single LC50 value multiplied by 1000 (in this way, the resulting NEC will equal the MTR level).
- The use (processing step) of non-agricultural pesticides is only defined at a local scale. At the regional scale, only production and formulation can be assessed. These options were calculated both. It should be noted that the scenarios for non-agricultural pesticides are relatively worst case compared to the scenarios for industrial chemicals.
- The use scenario for methylbromide (as fumigants) is not yet implemented in USES. Therefore, this substance could only be assessed for production and formulation.
- USES gives many priority lists (for each group to be protected on local and regional scale) whereas the participants constructed only one list. USES does not construct *one* final priority list since this cannot be done in a scientific way.

The data used as input for USES are summarised in the appendix. All the individual priority lists are also given in this appendix. The final aggregation of the lists prepared by USES was done on the basis of the average position on the lists. Each list of USES was analyzed, the substance on top of a list received 10 points, the one at the bottom 1 point. The points for each substance were summed over all the lists (10 lists in total). The resulting list is displayed in Table 2 together with the 'expert-list'. Another aggregation protocol is displayed in Table 3. Here, for each substance, all lists are examined to find the list where the substance has its highest PEC/NEC ratio. This ratio (only at the regional scale in this case) is put in the list. The relation between the lists is plotted in Figure 8 and Figure 9.

Table 2 *Expert ranking (number of stickers) and the USES ranking (position scored over all lists).*

Expert list		**USES average ranks**	
Benzene	16	Ethene	81
Trifenyltinaceticacid	15	Trifenyltinaceticacid	69
Dioxins	13	Benzo[a]pyrene	67
Benzo[a]pyrene	13	Benzene	65
Formaldehyde	8	Dioxins	57
Di(2-ethylhexyl)phthalate	7	Di(2-ethylhexyl)phthalate	52
Methylbromide	4	Formaldehyde	51
Pentachlorophenol	1	Phenol	41
Ethene	1	Pentachlorophenol	41
Phenol	0	Methylbromide	24

Table 3 *Expert list (number of stickers) and USES ranking (maximum PEC/NEC ratio over all regional lists).*

Expert list		**USES maximum reg. risk**	
Benzene	16	Dioxins	1887
Trifenyltinaceticacid	15	Benzo[a]pyrene	210
Dioxins	13	Trifenyltinaceticacid	9.7
Benzo[a]pyrene	13	Ethene	7.4
Formaldehyde	8	Formaldehyde	0.15
Di(2-ethylhexyl)phthalate	7	Benzene	0.14
Methylbromide	4	Phenol	0.08
Pentachlorophenol	1	Di(2-ethylhexyl)phthalate	0.02
Ethene	1	Pentachlorophenol	4.6e-3
Phenol	0	Methylbromide	1.3e-4

In the following figures, the results from Table 2 and Table 3 are expressed graphically. The substance on top of the list receives a ranking of 10, the substance on the bottom 1. When a position is shared, the rankings are averaged. In this way, the substances are put on an ordinal risk-scale.

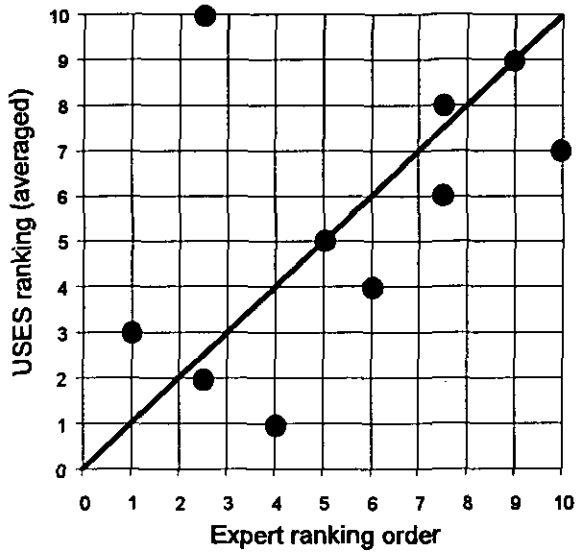

Figure 8 *Expert ranking compared to the 'average' ranking made by USES.*

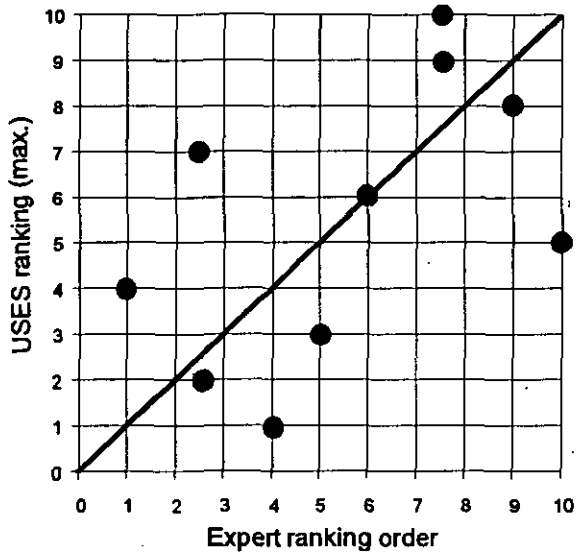

Figure 9 *Expert ranking compared to the ranking of USES based on highest PEC/NEC ratio.*

4.2. Conclusions from the experiment

The results from Table 2 and Table 3, and Figure 8 and Figure 9, should be analyzed with care. It is not possible to validate USES with expert opinion since both are prone to errors. Risk perception in the experts view might differ from the actual risks of substances. They may rank risks based on hard facts (e.g., expected numbers of deaths per unit time), but may also take into account how well the process in question is understood, how the risk is distributed over a population, how personal exposure can be controlled, and whether risk is assumed voluntarily (Morgan, 1993). Substances that enjoy major media coverage may receive excessive attention. This indicates that it is difficult to obtain an objective answer from experts (which is one of the advantages of USES).

Therefore, this experiment cannot give more than an indication of the 'validity' of USES in estimating risks from a small set of data. The main value of comparison with the experts opinion is to see whether the outcome of USES is comparable to the risk perception of the expert. It must be kept in mind that USES is meant as a system to *support* decision-making, and not to replace the experts opinion. Despite all these difficulties, an approach like this can give more insight in the value of the hazard quotients of USES, which facilitates interpretation and appreciation of the system's results.

The similarity in the ranking order of the experts and USES (Figure 8) is striking. Only the

estimated rank of ethene clearly differs between USES and the experts. The reasons for this deviation are not entirely clear. The main reason is probably that the production volume of ethene is extremely high (4.3 million tonnes per year in the Netherlands). For these production volumes, the emission estimates may turn out as an extreme worst case for this substance. Also, one application of the substance (as intermediate) is though to be relevant for the entire production volume, which is clearly not correct.

If an experiment like this is carried out more extensively, and more scientifically, this will yield valuable information on the performance of the system. One has to keep a few point in mind:

- The selected substances have to be well known to all participants in the experiment.
- The question posed should be clear and relevant with respect to the assessment of USES.
- Data gathering and evaluation should be done more extensively.
- The participants should be experts in the field of risk assessment of substances.
- It must be clear beforehand which list of USES is used to compare with the expert opinion.

References

Morgan, M.G. (1993). Risk analysis and management. Scientific American, July 1993, 24-30.

5. CONCLUSIONS AND RECOMMENDATIONS

Model analysis provides valuable information on the performance of a model. It is important that models that are used in processes, as important as risk assessment of substances, are thoroughly analyzed. Risk assessors should be able to take the performance of the model into account in their decisions. Validation and uncertainty analysis are an important part of model analysis. Validation efforts of USES and its predecessors (DRANC, ESPE, PRISEC, USES prototype II) have been insufficient sofar.

This report shows that a proper validation of USES in the strictest sense is not possible. USES predicts PEC/NEC ratios which, unfortunately, cannot be measured. A pragmatic solution is to validate separate models or sub-modules. This procedure should meet no particular problems. Validation of a 'chain' of models is not so easy: this requires a data set with measurements relevant for a larger part of the exposure scenario as defined in USES. For some substances (e.g., dioxines), measurements were performed in several parts of the chain from emissions to human exposure which makes these substances candidates for such a validation attempt.

Numerical validation of separate models is not sufficient to ensure the validity of a risk assessment system. Conceptual and operational validation should be an important part of a proper validation. No matter how good a model performs numerically, if it is not appropriate for the system, or if its assumptions are not compatible with the risk assessment system, it is not 'valid'. For instance, if the model for uptake by plants is derived on experiments with barley, it might not be valid to use for other crops and grass. Furthermore, the assumptions made in the exposure scenario should be subject to conceptual validation. The assumptions should be supported by a discussion on the relevance of the assumption for the type of assessment that is aimed at. The entire local exposure scenario should be investigated in more detail. This is especially important in the development of USES towards a European system since the exposure scenario should be agreed upon by all member states. Therefore, it is expected that some form of 'conceptual validation' of the exposure scenario will automatically take place in 1995.

This report describes the validation status for *each* sub-module or model, this is summarised at the end of this chapter. For many parts of USES, validation activities have been performed or initiated, often outside the framework of the USES project. A thorough operational and conceptual validation is still lacking. As an example: the soil and groundwater model PESTLA, has been extensively validated. The implementation in USES and the appropriateness of the associated assumptions need further attention.

A boundary condition for validation is the ongoing development of USES. The development of a European risk assessment system is planned for 1995/1996. The present version of USES will form the basis for this system, but this does not mean that modules will remain unchanged. An extensive validation of the present USES system is clearly not advisable. When this European risk assessment system is finalised, there lies an excellent opportunity to validate this system extensively, based on the recommendations of this report. Furthermore, this report is helpful in the development of the European system since the validation status

of each separate model and the associated assumptions are discussed.

Data collection and validation for *all* the models in USES requires a lot of effort. From the summary at the end of this chapter, it is clear where actions should be initiated. The data entry/filling module requires relatively little attention. The validity of the QSARs can usually be derived from the article in which they where published, and the uncertainty in the estimate can be quantified in an uncertainty analysis. Furthermore, these estimation routines are only used when measured data are lacking. It should however, be investigated if QSARs are applied properly and not used outside their working range (operational validation).

The case study with the regional model of HAZCHEM, as described in section 3.4, indicates the need for a careful interpretation of the regional risks as estimated by USES. The case study also shows the difficulties involved in validation of these types of models. It is especially important to note that there is a danger in taking absolute values from regional models of the Mackay type. Serious underestimations of risk levels may occur. Even if regional models as HAZCHEM and SimpleBox are not adequate to predict environmental concentrations, they are still extremely useful if their *relative* concentration predictions are accurate. A more in-depth validation of these models is necessary to facilitate the interpretation of the regional risk levels.

Validation of the evaluation module is addressing the purpose of USES directly. The purpose of USES is, in the first place, making a risk statement of a substance, based on a limited data set. The approach of comparing the results of USES with expert judgement, as described in chapter 4, is promising despite its limitations. With the recommendations given, the experiment can be refined. Experiments like this can give better insight in the functioning of risk assessment systems and their place in the risk assessment process. Unfortunately, the purpose of the system is often overlooked in validation activities as the main effort is usually placed on developing better numerical models. USES was not developed to calculate extremely accurate exposure levels, it is meant to support decision-making by screening chemicals rapidly and efficiently for potentially hazardous ones.

A complete validation of USES is not planned for 1995. Since many activities for numerical validation or investigation are planned, and since a European system will be developed, numerical validation seems not urgently needed. It is important that all individual efforts (often outside the framework of the USES-project) are finally bundled to gain insight in the degree of accuracy USES is able to give. However, the implementation of these models in USES and the validation status of the exposure scenario needs more attention.

Overview validation status of USES submodules:

Data entry/data filling	
Physico-chemical	requires no immediate validation
Char. environment	requires no immediate validation
Intermedia part.	requires no immediate validation
Biodegradation	the approach will be discussed in 1995
Bioaccumulation	validation is done for plant uptake from soil, validation of the route air-plant is planned, the applicability of the other QSARs needs further investigation (especially for biotransfer to meat and milk, other approaches need to be investigated)
Emission module	no validation activities, however, work is done to obtain better estimates, conceptual validation of emission scenario is required
Local distribution	conceptual validation of exposure scenario is required
SimpleTreat	extensive validation initiated
Air module	further investigation initiated
Surface water	requires no immediate validation for the Dutch situation since the estimate of dilution is based on measurements
Soil-groundw.	validation of the original model is performed, the implementation in USES needs further investigation
Regional distribution	no validation activities planned, case study with HAZCHEM suggest that serious underestimations of absolute risk levels may occur
Intake module	research to the applicability of the steady-state assumption is planned for 1995, however, conceptual validation with regard to exposure scenario is required
Effect module	partial validation has been done, no further activities planned
Evaluation module	validation required, the approach to validate this module needs more elaboration
Agricultural pesticides	SLOOTBOX model is partially validated and further validation is initiated, validation of scenarios and other models required
Non-agricult. pesticides	validation of scenarios and models required, the approach is relatively new and still under development

APPENDIX: Risk validation, inputs and results

Emission data substances:

Name	Tonnage NL t/year	Tonnage EU t/year	Industrial Category	Use Category	prod Mn Cat	form Mn Cat	proc Mn Cat
Pentachlorophenol	30 (laurate)	8000	13 textile	39 non-agr.p.	no	yes III	yes text.
Benzene	0.93 e6	4.2 e6	3 synthesis	33 intermed	yes Ic	no	yes III
Methylbromide	2000	*20000*	15 others	39 non-agr pest	yes III	no	no
Ethene	4.3 e6	17.2 e6	3 synthesis	33 intermed	yes Ic	no	yes III
Di-(2-ethylhexyl) phthalaat	12700	*127000*	11 polymer	47 softeners	no	no	yes III
Trifenyltin acetic acid	230	*2300*	15 *others*	39 *non-agr.p.*	yes III	yes III	yes *a.f.*
Phenol	0.188 e6	1.0 e6	3 synthesis	33 intermed	yes Ic	no	yes III
Formaldehyde	0.311 e6	*3.11 e6*	3 synthesis	33 intermed	yes Ic	no	yes III

Name	region. air	region. water	region. soil	W.Eur. air	W.Eur. water	W.Eur. soil	Frac. main source
Dioxins	600 g/y	4 g/y	3 g/y	2000 g/y	*13* g/y	*10* g/y	*35* % air
Benzo[a]pyrene	2.8 t/y	0.5 t/y	1.1 t/y	200 t/y	*35* t/y	*80* t/y	*5* % air

Values in italics are estimated values.

Physico-chemical properties substances:

Name	Molw. g/mol	Melt.pt. C	VP Pa	log Kow	Sol. mg/l	readily biodeg.
Pentachlorophenol	266.4	189	0.013	4.8	0.14	no
Dioxins (TCDD)	321.97	306	2e-7	6.8	0.2e-3	no
Benzens	78.11	5.533	1.333e4	2.13	1800	yes
Benzo[a]pyrene	252		*1.3e-8*	*6.0*	*0.15*	*no*
Methylbromide	95	-93.7	1.89e5	1.19	1.5e4	no
Ethene	28.1	-169.2	*1e6*	*3.0*	160	yes
Di-(2-ethylhexyl) phthalaat	390.5	-50	0.00086	5.24	0.045	yes
Trifenyltin acetic acid	409.6	124	0.000176	3.2	15	no
Phenol	94.11	40.9	30	1.5	6.7e4	yes
Formaldehyde	30.03	-92	170	0.35	*3.97e5*	yes

Toxicitity data substances:

Naam	Aquatic mg/l (dissolved)	Terrestrial mg/kg (wetweight)	Mammal Tox. mg/kgBW/day	Human Tox. mg/kgBW/day
Pentachlorophenol	MTR: 0.002	MTR: 0.14	NOAEL: 3	TDI: 0.030
Dioxins (TCDD)	MTR: 1.2e-9	MTR: 0.36	NOAEL: 1e-6	TDI: 1.0e-8
Benzeen	MTR: 2.4	MTR: 6.8	NOAEL: 1	TDI: 4.3e-3
Benzo[a]pyrens	GW: 2e-6	SW: 0.018	indic.NOAEL: 0.02	indic.NEL: 0.002
Methylbromide	NOECf: 0.3 NOECa: 3.2 NOECc: 1.7	Int.W.: 7.1	NOAEL: 0.4	ADI: 1.0
Ethene	MTR: 8.5	LC50p: 115 NOECp: 12	default: NOAEL: 1	MTRinh: 2 ug/m3
Di-(2-ethylhexyl) phthalaat	MTR: 0.008	MTR: 1.8	NOAEL: 2.5	TDI: 0.025
Trifenyltin acetic acid	MTR: 5e-6	C: 7.1	LOAEL: 0.3	TDI: 0.5e-3
Phenol	GW: 0.002	Int.W.:28.6	NOAEL: 5	TDI: 0.060
Formaldehyde	MTR: 4e-3	Indic. MTR: 0.00122 (eq.p.)	NOAEL: 10	TDI: 0.15

Values in italics are estimated values.

Priority lists of USES 1.0.

Current hazard	Aquatic Local
Trifenyltinacetaat (prod/form)	305354
Benzo[a]pyreen	149680
Dioxine (I-TEQ's)	86954.2
Trifenyltinacetaat	19491.5
Formaldehyde	1149.31
Fenol	1109.95
Methylbromide	11.5475
Benzeen	8.1917
Etheen	7.45229
Pentachloorfenol (formulation)	3.11166
Pentachloorfenol	1.24964
Di(2-ethylhexyl)ftalaat (DEHP)	0.11016
Dioxine (I-TEQ's) (emissie)	0
Benzo[a]pyreen (emissie)	0

Current hazard	Aquatic Regional
Trifenyltinacetaat (prod/form)	9.69116
Benzo[a]pyreen (emissie)	0.6305
Benzo[a]pyreen	0.322051
Formaldehyde	0.148347
Fenol	0.0813536
Dioxine (I-TEQ's)	0.019627
Dioxine (I-TEQ's) (emissie)	0.009006
Benzeen	0.000207433
Etheen	0.000161931
Methylbromide	0.000130451
Di(2-ethylhexyl)ftalaat (DEHP)	0.000125062
Pentachloorfenol (formulation)	2.84713e-05
Pentachloorfenol	??
Trifenyltinacetaat	??

Current hazard	Terrestrial Local
Etheen	6737.71
Benzo[a]pyreen	1538.25
Formaldehyde	133.383
Pentachloorfenol	11.3066
Benzeen	3.61517
Pentachloorfenol (formulation)	2.53679
Di(2-ethylhexyl)ftalaat (DEHP)	1.10419
Benzo[a]pyreen (emissie)	1.001
Trifenyltinacetaat (prod/form)	0.251533
Fenol	0.0158036
Dioxine (I-TEQ's)	0.0103291
Methylbromide	0.00295818
Dioxine (I-TEQ's) (emissie)	7.492e-5
Trifenyltinacetaat	0

Current hazard	Terrestrial Regional
Benzo[a]pyreen	47.2515
Benzo[a]pyreen (emissie)	7.943
Formaldehyde	0.0120697
Etheen	0.00408938
Pentachloorfenol (formulation)	0.00337132
Dioxine (I-TEQ's)	0.00197039
Di(2-ethylhexyl)ftalaat (DEHP)	0.000902758
Dioxine (I-TEQ's) (emissie)	0.0001785
Trifenyltinacetaat (prod/form)	2.27577e-05
Benzeen	1.17998e-05
Fenol	3.80373e-08
Methylbromide	4.33798e-09
Trifenyltinacetaat	??
Pentachloorfenol	??

Current hazard	Indirect Exposure Local
Etheen	33240.2
Benzeen	630.202
Benzo[a]pyreen (emissie)	88.65
Benzo[a]pyreen	45.4587
Dioxine (I-TEQ's) (emissie)	28.6369
Trifenyltinacetaat (prod/form)	17.4129
Dioxine (I-TEQ's)	15.388
Trifenyltinacetaat	7.8269
Formaldehyde	3.84944
Di(2-ethylhexyl)ftalaat (DEHP)	2.33266
Fenol	1.02898
Pentachloorfenol	0.0626945
Pentachloorfenol (formulation)	0.0152466
Methylbromide	0.0133356

Current hazard	Indirect Exposure Regional
Etheen	7.40696
Dioxine (I-TEQ's)	0.344427
Benzo[a]pyreen (emissie)	0.200
Benzeen	0.141015
Benzo[a]pyreen	0.139575
Dioxine (I-TEQ's) (emissie)	0.034447
Trifenyltinacetaat (prod/form)	0.00592081
Di(2-ethylhexyl)ftalaat (DEHP)	0.00156797
Formaldehyde	0.000617454
Fenol	0.000134318
Pentachloorfenol (formulation)	1.47805e-05
Methylbromide	2.46825e-06
Pentachloorfenol	??
Trifenyltinacetaat	??

Current hazard	Aquatic Predators Local
Dioxine (I-TEQ's)	83895.9
Benzo[a]pyreen	17166.2
Etheen	2612.96
Benzeen	101.385
Trifenyltinacetaat (prod/form)	23.64
Trifenyltinacetaat	19.6389
Di(2-ethylhexyl)ftalaat (DEHP)	2.34187
Pentachloorfenol	1.64795
Fenol	0.536725
Pentachloorfenol (formulation)	0.450332
Methylbromide	0.410232
Formaldehyde	0.0393448
Benzo[a]pyreen (emissie)	0
Dioxine (I-TEQ's) (emissie)	0

Current hazard	Aquatic Predators Regional
Dioxine (I-TEQ's)	6.91189
Dioxine (I-TEQ's) (emissie)	3.172
Benzo[a]pyreen (emissie)	2.932
Benzo[a]pyreen	1.49791
Etheen	0.0690788
Trifenyltinacetaat (prod/form)	0.0119066
Di(2-ethylhexyl)ftalaat (DEHP)	0.00323471
Benzeen	0.00312357
Pentachloorfenol (formulation)	5.57028e-05
Fenol	4.78628e-05
Methylbromide	7.04806e-06
Formaldehyde	6.17875e-06
Pentachloorfenol	??
Trifenyltinacetaat	??

Current hazard	Terrestrial Predators Local
Dioxine (I-TEQ's)	109213
Benzo[a]pyreen	40659.6
Etheen	23030.4
Dioxine (I-TEQ's) (emissie)	792.2
Benzeen	578.175
Trifenyltinacetaat (prod/form)	171.215
Benzo[a]pyreen (emissie)	26.45
Di(2-ethylhexyl)ftalaat (DEHP)	23.3455
Pentachloorfenol	12.7022
Pentachloorfenol (formulation)	3.47511
Fenol	1.28804
Methylbromide	0.486979
Formaldehyde	0.0298639
Trifenyltinacetaat	0

Current hazard	Terrestrial Predators Regional
Dioxine (I-TEQ's)	20833.4
Benzo[a]pyreen	1248.97
Dioxine (I-TEQ's) (emissie)	1887
Benzo[a]pyreen (emissie)	209.9
Di(2-ethylhexyl)ftalaat (DEHP)	0.0190866
Trifenyltinacetaat (prod/form)	0.0154908
Etheen	0.013978
Pentachloorfenol (formulation)	0.00461833
Benzeen	0.00188714
Fenol	3.10015e-06
Formaldehyde	2.70237e-06
Methylbromide	7.14123e-07
Trifenyltinacetaat	??
Pentachloorfenol	??