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Uncertainty Analysis of the Uniform System for the Evaluation of Substances (USES)

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	108	Projecten- en rapportregistratie
109 -	110	Bibliotheek RIVM
111 -	150	Reserve exemplaren

CONTENTS

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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 risk assessments of chemical substances during their life-cycle. Risk assessment is an inherently uncertain process due to the limited data availability and lack of knowledge. Furthermore, many model parameters exhibit natural variability (e.g., the flow rate of a river). Therefore, a thorough model analysis is advisable. Uncertainty analysis shows the user of a model what amount of uncertainty accompanies the model's results (the risk quotients or PEC/NEC ratios). In this manner, the uncertainty can be taken into account in decision-making by indicating the probability that a wrong decision is made. An additional benefit is that uncertainty analysis can steer data gathering or research by pointing out the main sources of uncertainty in the model's results. This can be used effectively, to refine a risk assessment.

Version 1.0 of USES already contained a limited uncertainty analysis for the aquatic organisms and the micro-organisms in the sewage treatment plant. In this report, the uncertainty analysis is extended to the other groups to be protected (humans, terrestrial organisms, predating birds and mammals). In this report, only the local exposure model is examined. Due to its technical nature, this report is primarily meant for the further development of USES.

The described simple analytical method to combine uncertainties is limited to multiplicative models and lognormal uncertainties. The advantage of this method is that an exact answer can be calculated very rapidly. However, not all calculations are multiplicative. Therefore, we have to resort to Monte Carlo approaches for several parts of the system. One single uncertainty analysis of USES is not possible as the uncertainty in the model's result will vary for different substance properties. Therefore, the analysis must be performed 'on-line' by the user, for each substance to be assessed. Naturally, this poses restrictions on the computer time required for the uncertainty calculations.

Each calculation or model of USES 1.0 is discussed separately with respect to uncertainty. Furthermore, uncertainties in parameters are quantified. In many cases, this is done by a thorough data analysis, in some cases by expert judgement. Not all sources of uncertainty can be quantified. Only uncertainty and/or variability in model parameters is taken into account. Uncertainty due to the exposure scenario cannot be quantified. Furthermore, the uncertainties in the extrapolation procedure of No-Effect Concentrations (NECs) for ecosystems, need further examination. Therefore, the absolute value of the uncertainty in the model's result must not be exaggerated. In the interpretation of risk quotients with their uncertainties, the limitations mentioned need to be taken into consideration. A thorough testing of the proposed uncertainty analysis is therefore, advisable (testing may take place in 1995).

SAMENVATTING

UBS, het Uniforme Beoordelingssysteem Stoffen (in het engels: USES), is een beslissingsondersteunend gereedschap voor een snelle, kwantitatieve risico-analyse van een chemische stof gedurende zijn levenscyclus. Risico-analyse is een inherent onzeker proces door de beperkte beschikbaarheid van invoergegevens, en gebrek aan kennis. Verder vertonen veel modelparameters natuurlijke variatie (zoals bijvoorbeeld de stroomsnelheid van een rivier). Een grondige modelanalyse is daarom aan te bevelen. Onzekerheidsanalyse toont de gebruiker van een model de onzekerheidsmarge van het eindresultaat (de risicoquotiënten of PEC/NEC ratio's). Zo kan de onzekerheid worden meegenomen in de te nemen beslissing door de kans op een verkeerde beslissing aan te geven. Een bijkomend voordeel is de mogelijkheid tot sturing van verder onderzoek door de grootste bronnen van onzekerheid in het eindresultaat te identificeren. Dit kan effectief gebruikt worden om een risico-analyse te verfijnen.

Versie 1.0 van UBS bevatte reeds een beperkte onzekerheidsanalyse voor de aquatische organismen en de micro-organismen in de rioolwaterzuivering. In dit rapport wordt de onzekerheidsanalyse uitgebreid naar de andere beschermingsdoelen (mensen, terrestrische organismen, vis- en wormetende vogels en zoogdieren). Alleen het lokale blootstellingsmodel is onderzocht. Door het technische karakter is dit rapport met name bedoeld ten behoeve van de verdere ontwikkeling van UBS.

De beschreven simpele analytische methode is beperkt tot multiplicatieve modellen met lognormale onzekerheden. Het voordeel van deze methode is dat een exact antwoord op een snelle manier berekend kan worden. Niet alle berekeningen zijn echter multiplicatief. Daarom moet voor verscheidene delen van het systeem Monte Carlo methoden worden toegepast. Een eenmalige onzekerheidsanalyse van UBS is niet mogelijk omdat de onzekerheid in het eindresultaat anders zal zijn bij verschillende stofeigenschappen. De analyse moet dus door de gebruiker van UBS gedaan kunnen worden bij elke stof die doorgerekend wordt. Dit stelt natuurlijk beperkingen aan de computertijd die nodig is voor de onzekerheidsberekeningen.

Elke berekening of model van UBS 1.0 wordt apart besproken voor wat betreft de onzekerheden. Verder worden de onzekerheden gekwantificeerd. In veel gevallen is dit door een nauwkeurige gegevensanalyse gebeurd, in een aantal gevallen werd gebruik gemaakt van expert judgement. Niet alle bronnen van onzekerheid kunnen worden gekwantificeerd. Alleen de onzekerheid en/of variabiliteit in modelparameters is meegenomen. De onzekerheid ten gevolge van het blootstellingsscenario kan bijvoorbeeld niet worden gekwantificeerd. Verder dienen de onzekerheden in de extrapolatie van No-Effect Concentrations (NEC's) voor ecosystemen nader onderzocht te worden. Daarom moet de absolute waarde van de onzekerheid in het eindresultaat niet overschat worden. Bij de interpretatie van de risicoquotiënten met hun onzekerheidsmarge dienen de genoemde beperkingen in overweging te worden genomen. Grondig testen van de voorgestelde onzekerheidsanalyse is daarom aan te raden (testen kan mogelijk in 1995 plaatsvinden).

1. INTRODUCTION

The Uniform System for the Evaluation of Substances (USES, RIVM *et al.*, 1994) is a general risk assessment system for chemical substances. In principle, this system should perform a risk assessment for all organic, non-ionic, non dissociating substances. This immediately introduces the problem of uncertainty. If a system must work for this broad range of substances, one will inherently have to deal with uncertainty in the model's results. More specific models may produce less uncertain results, at a price of describing only specific groups of substances. Furthermore, the amount of data available for risk assessment is small (e.g., the EC Base Set), which makes uncertainty an important property of risk assessment in this framework.

The modelling process may proceed through a number of predefined steps, as for example shown in Figure 1. Uncertainty analysis is an important aspect of the analysis of a model's performance. The other important aspect, validation, is subject of a separate report discussing the feasibility of validating USES (Jager, 1995).

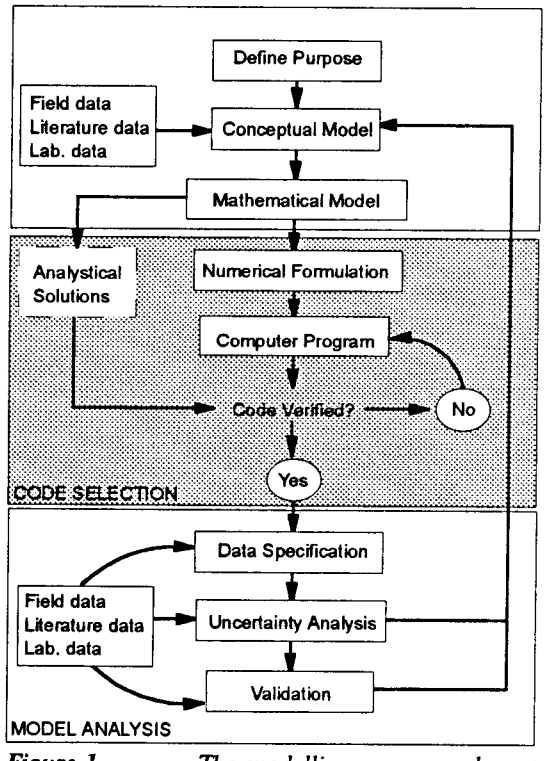

Figure 1 *The modelling process relevant to USES (adapted from Anderson & Woessner, 1992)*

Uncertainty analysis is an instrument to show users of a model what amount of uncertainty accompanies the model's results. The decision makers may take the amount of uncertainty in the model's result into account in the decision-making process because it indicates the probability that a wrong decision is made. Uncertainty analysis also offers the possibility to reward input of measured data by diminishing uncertainty in the system's risk estimate. Furthermore, uncertainty analysis can steer data gathering and future research by identifying the main sources of uncertainty in model results. Research will be most efficient if it aims at diminishing these main sources of uncertainty. If the identification of these sources can be performed on-line, risk assessors will have the opportunity to ask for specific data that are most effective in the refinement of the risk assessment.

The aim of this report is to develop a framework for a complete uncertainty analysis for the local exposure model of USES. The first thought was to aim at an analysis for human exposure through the environment. When an uncertainty analysis for human exposure is completed, uncertainty analysis for the other groups to be protected (predators, terrestrial organisms) can easily be added, as it already covers all relevant routes. This report will deal with the following steps:

- Defining the purpose of the analysis.
- Defining the conceptual framework (e.g., what kinds of uncertainties are included).
- Per separate model: definition of scenario choices and parameters for which uncertainty/variability must be quantified.
- Quantifying an uncertainty/variability distribution for each parameter.
- Developing calculation methodology to efficiently calculate uncertainty in the final results.

The uncertainty analysis as proposed in this report, will focus on uncertainties in the exposure side of the hazard quotient. The derivation of No-Effect Levels (NECs) with extrapolation factors is, at this moment, a worst case approach (because the NECs represent a safe level). Other scientists at RIVM are investigating the possibilities of adapting the extrapolation factor approach to include a more stochastic approach. The possibility to add this to USES can be investigated at a later stage.

Some choices must be made to restrict the analysis. This is necessary because of the limited resources available for this subject. Furthermore, it is not advisable to make the analysis very detailed at this stage, because the development of a European risk assessment system, based on USES 1.0, is planned for 1995/1996.

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 also 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. Model analysis 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. Calculation 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, generic 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 average Dutch situation.
- Continental scale: emissions are regarded as diffuse; the spatial scale is that of 'Western Europe'. No targets are considered, the only purpose is to compute continental concentrations as background concentrations 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 scenario assumed with this exposure, is given in Table 1. It includes aspects of the spatial and temporal scales. USES calculates the continental and regional computations sequentially, using the model SimpleBox (Van de Meent, 1993), which is a model of the so-called 'Mackay-type'. The continental concentrations are used as background conditions for 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.

1.2. Introduction to uncertainty analysis

> **Uncertainty analysis** is the study for the uncertain aspects of a model and their influence on the model's results.
>
> From: Janssen *et al.* (1990)

A model is never an exact representation of reality. This is, among others, caused by the complexity of reality, and lack of knowledge of it. Furthermore, required data are often incomplete and contain measurement errors (Janssen *et al.*, 1990). In risk assessment, we are typically confronted with this situation as data are usually scarce, and mechanisms often poorly understood. Therefore, a model like USES can only give an approximation of the true exposure. Clearly, it is important to have an impression of the quality of this approximation.

USES version 1.0, which was completed this year, contains an uncertainty analysis for the exposure concentration of the aquatic ecosystem, and for the micro-organisms in the sewage treatment plant (Slob & De Nijs, 1989). The model's parameters related to emission to wastewater, sewage treatment, and dilution, were taken as probability distributions, instead of fixed values. These are not all uncertainties involved in the surface water concentration, but it is safe to assume that they constitute by far the largest ones. The purpose of this report is to expand the uncertainty analysis to the exposure of humans, predators, and the terrestrial ecosystem.

A common practice is to perform a sensitivity analysis before an uncertainty analysis is done. When the most sensitive parameters have been selected, these can be subjected to uncertainty analysis. USES however, should be able to handle, in principle, all chemicals. USES has many compound-specific input parameters, covering wide ranges (e.g., log Kow usually lies between -2 and 8). Additionally, there are many fixed model parameters that are related to the environment or the exposure scenario. The sensitivity of the model's output for a parameter will depend on the *value* of these input parameters. Therefore, the sensitivities will vary for different compounds. A limited uncertainty analysis, performed specifically for each substance, will be more useful as it is not hampered by this problem. It can show the influence of the main uncertainties in the model on the final results. Furthermore, it may be possible to locate some of the main sources of uncertainty. These will also vary for different substances, but identifying them is a powerful too to refine a specific risk assessment.

The main purpose of an uncertainty analysis is to show the user of the system what amount of uncertainty accompanies the model's results. This is particularly important if information is poor and in inherently uncertain situations. From a scientific point of view, it is not advisable to draw conclusions from models without taking the uncertainties and assumptions of the model into account. Uncertainty analysis is helpful in this process as it can indicate the probability that a wrong decision is made (e.g., the probability that PEC/NEC exceeds 1 even though the median ratio is lower than 1). An additional benefit of an on-line analysis is, that it may reward input of more and/or better data by reducing the uncertainty in the final results. Measured bioconcentration factors, for instance, will

not decrease the risk estimate if they are not lower than the value estimated by USES. Nevertheless, measured data may decrease the probability that a wrong decision is made. The way in which the decision maker may deal with these probabilities still requires further elaboration.

Uncertainty in the model's results can be caused by uncertainty in parameters due to lack of knowledge (e.g., in the case of emission estimates) and natural variability in parameters (a parameter can vary in the natural environment and be well known, e.g., temperature) or a combination of both. Uncertainties attached to scenario choices are extremely difficult, or even impossible, to assess. Therefore, the analysis we propose is restricted to the model's parameters not set in the scenario at a particular value. This requires a list of parameters judged to belong to these scenarios. This choice for a parameter between scenario specific and not scenario specific is, more or less, arbitrary. For instance, 'density of soil' can be defined as a model parameter with an amount of variability, or as a fixed property of the standard environment in the scenario.

Which uncertainties should be taken into account in the analysis?

Parameter uncertainty due to lack of knowledge
Natural variability in a parameter only when:
- the parameter is *not* defined in the exposure scenario to have a particular value, *and*
- when this variability is *not* averaged out by subsequent parts of the system (as is the case for instance, with the consumption habits of individual cows; humans consume meat and milk from different cows, not from one individual, therefore, this variability can be ignored)

The distinction between uncertainty and variability needs some elaboration. Parameter uncertainty due to lack of knowledge can often be decreased by research (e.g., measurements can improve the emission estimates). Variability, however cannot be decreased as it is an inherent property of the process under consideration.

Consider a parameter that is part of the exposure scenario, e.g., the exposure location of fish at 1000 m downstream of the STP. Naturally, fish will not stay at one location, and the fixed exposure location of 1000 metres is an arbitrary assumption. This variability is extremely difficult to quantify. What we need for this quantification would be the swimming habits of fish and the concentration in surface water as a function of the location. The concentration in surface water depends on the dilution factor (which itself is highly variable between different locations). It may be clear from this example that quantifying the variability or uncertainty in these scenario parameters is not practically feasible. For pragmatic reasons, we propose to ignore this source of uncertainty. This implies that the uncertainty as calculated in the risk estimates, is a measure of the uncertainty *given* the scenario-defined standard environment. Nevertheless, the validity and relevance of the scenario choices should be analyzed as well. This will be done as part of the validation project for which a feasibility study is in preparation (Jager, 1995).

We may ignore variability when subsequent parts of the system tend to average them out. This is the case, for instance, with the concentration in fish. Properties of fish (e.g., percentage fat) will vary between and within species. Humans however, will usually consume different fish and therefore, differences between fish will tend to average out. This means that the variability in the annual average concentration in fish, as exposure level for humans, will be smaller than the variability in concentrations between individual fish. On the other hand, variability of the dilution rate of the STP effluent should be considered since the effluent always enters the same surface water, which is usually unknown beforehand.

Definition of **scenario** in this context:

The set of fixed parameters and assumptions that define the environment and conditions for which the risk assessment is performed.

The result of an analysis as proposed here might answer the following question: "If a random adult is placed in the standard environment (as defined in the exposure scenario), what is the probability that a certain reference criterion (e.g., NEL, ADI, TDI) is exceeded?". One should always keep in mind that the model's structure and the simplifications made influence this probability, which therefore, does not strictly relate to the real world situation. However, this analysis still provides an opportunity to deal with uncertainties in a quantitative way.

2. IMPLEMENTATION OF THE ANALYSIS

The uncertainty analysis will be implemented as an 'on-line' calculation module. This enables the user to perform an uncertainty analysis for each particular substance. The aim of the analysis is to indicate the amount of uncertainty for the particular substance in the final result (the PEC/NEC ratio). This immediately puts restrictions on the calculation time needed for each assessment. If the time needed for an uncertainty analysis is unacceptable, the analysis might be included as a separate option in the program.

2.1. Quantifying uncertainties in parameters

For each, not scenario specific, parameter, it should be investigated whether it is prone to uncertainty or variability. Secondly, we must choose the type of distribution. A simple analytical method of uncertainty analysis, explained in the next section, requires lognormal distributions of parameters. Fortunately, many processes in nature are well described by lognormal distributions (see Slob, 1987). Lognormal distributions have another convenient property, in that the uncertainty can be quantified with a 'dispersion factor' (here called 'uncertainty factor' or k). It indicates how much a stochastic variable X may deviate from the median value (M) (Slob, 1994):

$$probability\left(\frac{M}{k} < X < k \cdot M\right) = 0.95$$

This approach is especially useful when data are scarce and the magnitude of the uncertainty can only roughly be quantified using expert judgement. For these reasons, lognormal parameter distributions are suitable for our purpose.

Information on the distribution of the uncertainties and variability can be obtained by:
- Expert judgement
- Using measured data

Measured data can be used to estimate the uncertainty factor k. When assuming lognormal distribution of uncertainties, the factor k can be derived from the experimental data from the standard deviation of the distribution on log scale (σ) (Slob, 1994):

$$k = \exp\left(1.96 \cdot \sigma \ln b\right)$$

where b denotes the base of the logarithm used. As an example, consider the QSAR (Quantitative Structure Activity Relationship) that estimates the bioconcentration factor of fish (BCF_{fish}) from the log Kow (the octanol-water partitioning coefficient):

$$\log BCF = \alpha \cdot \log Kow + \beta$$

The two parameters α and β can be estimated with linear regression on a data set containing measured BCF values in fish. The deviations from this line quantify the

uncertainty in the estimate of BCF. Of course, in this process, we have quantified the uncertainty of the bioconcentration factor of a fish, randomly drawn from the training set of data. This includes the inter- and intra-species variation obviously present in the experimental data set. This differs from the objective of the uncertainty analysis for human exposure through fish, as discussed in 1.2. Humans do not take *one* fish from the distribution but, as we are examining chronic exposure, many different fish are consumed. It is however, very difficult to distinguish between the sources of uncertainty from the data given. Furthermore, we do not know the consumption habits of humans with respect to species of fish eaten (which may be far from a random selection of fish from the training set). Therefore, we propose to ignore this difficulty at this moment and, as a pragmatic approach, take the entire uncertainty in the estimation of BCF as the relevant uncertainty. Of course, this is a conservative approach, overestimating the true uncertainty. This problem also illustrates that a measured BCF will not necessarily give a better estimation of the 'real' BCF of fish. The inter- and intraspecies variation included in the QSAR-estimation are also present in the measured values. This means that there is a danger of underestimation, by ignoring the uncertainty when a measured BCF of one fish species is used as an estimate.

The error in the estimate of BCF is assumed to be normally distributed around the median and constant (we are already on a logarithmic scale because of the model formulation used; on the original scale, the error would be assumed lognormal). The validity of this assumption can be checked by making plots of the residuals and see that they do not exhibit a systematic pattern, and that the normal distribution applies. The standard deviation of the residuals is σ in the formula above, which yields a value of k. If the plot of the residuals against the predicted BCF reveals a pattern, the regression model used was not appropriate, or the data set might have been inhomogeneous. In this case, one may choose a different regression model, or another data set. The choice of the regression model is arbitrary: as the model is only used to interpolate an estimate, it does not necessarily require a mechanistic background. The only advice is the economy principle: when you have to choose between models that describe the data equally well, choose the simplest one. However, it is not the intention of this report to thoroughly examine the models applied in USES 1.0. This approach can be used for all of the QSAR estimation routines in the data/filling module where data are available.

McKone (1993) quantifies uncertainty in several QSAR estimation routines, also applied in USES. McKone uses mean values and the coefficient of variation (CV) or the geometric standard deviation (GSD) to characterize the distribution. The GSD and the CV of a certain parameter X, are related to the standard deviation on log-scale (σ_{lnX}) by the following relations (Slob, 1994):

$$\sigma_{lnX} = \ln GSD$$

$$\sigma^2_{lnX} = \ln (CV^2 + 1)$$

The standard deviation on log-scale can then be related to the uncertainty factor k by the following relation (Slob, 1994):

$$k = e^{1.96 \cdot \sigma_{ln}}$$

2.2. Technical implementation

Calculation of uncertainty in the final result as a consequence of uncertainty and variability in underlying models can be performed in several ways (for a more extensive methodological discussion see Janssen *et al.*, 1990). In the uncertainty analysis for USES, two methods are important:

- Analytically, as described by Slob (1994) and as applied by Slob & De Nijs (1989) in an uncertainty analysis for the exposure of the aquatic ecosystem in the predecessor of USES, DRANC. This method is restricted to lognormal distributions in multiplicative models (since the product or quotient of two lognormal distributions is, again, a lognormal distribution). Furthermore, correlation cannot be taken into account.
- Numerically, the use of Monte Carlo analysis does not put any limitations on the type of distributions assumed (as long as they can be characterized), nor on the model equations. This method requires extensive calculations and therefore, will consume more time than the analytical method.

These methods will be described in more detail in the following sections.

2.2.1. The analytical method

The simple analytical method will be followed as far as possible. Fortunately, lognormal distributions occur frequently in the real world, and USES is for a large part a multiplicative model. From theoretical and empirical considerations, it may be concluded that the lognormal distribution is very appropriate as a default distribution for most non-negative physical entities (see Slob, 1994). This approach has a serious advantage in that it allows for a rapid and accurate uncertainty analysis.

The analytical solution can be used for a model of the form:

$$Y = \frac{X_1 \cdot X_2}{X_3}$$

The uncertainty in Y can be quantified from the uncertainty factors (k_1, k_2, k_3) of X_1, X_2, and X_3 as follows (Slob, 1994):

$$k_Y = \exp\left[\sqrt{(\ln^2 k_1 + \ln^2 k_2 + \ln^2 k_3)} \right]$$

2.2.2. Monte Carlo techniques

There are however, several steps in the exposure model of USES where additions take place (as for instance, the addition of the contributions of several food products to the total daily intake of humans). In these cases, the simple method of the previous section cannot be performed. In these calculations, the simple analytical method can be combined with a Monte Carlo analysis. First, all possible analytical calculations of uncertainties are done, followed by Monte Carlo analysis for the summations and subsequent calculations.

The use of Monte Carlo analysis has recently become popular in health and environmental risk assessment (see for example Thompson *et al.*, 1992; Copeland *et al.*, 1993; McKone & Ryan, 1989; McKone & Bogen, 1991). It is a transparent method which sets no restrictions to model formulation or parameter distributions. However, the results will always be approximate (the accuracy depending on the number of runs) and the analysis will take some time (depending on the hard- and software).

When the parameter distributions are characterized with a probability distribution, parameter values are drawn from the distributions (Monte Carlo sampling). Subsequently, for each series of values drawn, the matching model's result is calculated by running the model (Monte Carlo simulations). From the obtained model's results, the median, variance, percentiles, probability distribution etc. are derived. For each simulation, the entire model has to be run. Therefore, the number of required model runs should be restricted. The use of efficient sampling techniques (e.g., Latin Hypercube sampling) can be helpful to reduce the number of model runs. Through use of statistical techniques, the contribution of the separate parameters to the total uncertainty can be estimated (Janssen *et al.*, 1990).

2.3. Provisional solution for some summations

The simple method of the previous section does not work for summation of parameters. Consider a calculation of the following form, which occurs several times in the USES calculations:

$$b = 1 + a$$

where a is lognormal distributed, and the value of 1 is without uncertainty. The resulting parameter b follows a distribution which is not lognormal (in fact it is lognormal, but shifted to the right). The deviation from the (unshifted) lognormal distribution will depend on the value of a compared to 1. If a is much larger than 1, the resulting distribution in b will be indistinguishable from a lognormal distribution. The uncertainty in b will be close to the uncertainty in a. If a is small compared to 1, the distribution will diverge from the lognormal distribution. However, in the latter case, the uncertainty in b will be very small since the uncertainty in a will only contribute slightly to the total uncertainty.

Parameter a follows a lognormal distribution characterized by its median value (M_a) and an uncertainty factor k_a. Parameter a therefore lies for 95% between M_a/k_a and $M_a \cdot k_a$. This implies that b lies for 95% between:

$$\frac{M_a}{k_a} + 1 \; < \; b \; < \; M_a \cdot k_a + 1$$

If we estimate the distribution of b with a lognormal distribution, we will make an error. The magnitude of this error depends on the value of k_a and M_a. As a provisional solution we propose to use the following approach. The median of b is given by $M_a + 1$. The distance between median and the 95% boundaries cannot be quantified with a single k value because the distribution of b is not symmetrical on a logarithmic scale.

The following example acts as an illustration:

$b = a + 1$

$M_a = 1$ $\qquad$ $k_a = 10$

$M_b = 2$ $\qquad$ 95% boundaries: $\qquad$ $1.1 < b < 11$

Two values of k_b can be quantified from the left and from the right boundary:

left $k_b = 2/1.1 = 1.8$ and $\qquad$ right $k_b = 11/2 = 5.5$

The ratio of the two k values is a measure of the error made when assuming a lognormal distribution. The closer this ratio is to 1, the smaller the error. It can be calculated that this ratio is largest when M_a equals 1. We propose to take the largest of the two k_b values for the resulting variable b. It is advisable to give the user of the system a warning when the two values of k are differing too much. In that case, the final uncertainty in the hazard quotient will be overestimated. It is not clear beforehand whether this leads to a larger exceedance of a PEC/NEC ratio of 1 since only the lower tail of the distribution is extended. In our example, this would mean that the resulting distribution of b will be described as:

$M_b = 2$ $\qquad$ $k_b = 5.5$ $\qquad$ 95% boundaries: $\qquad$ $0.36 < b < 11$

ratio of the k values = $5.5/1.8 = 3.1$

This is illustrated in Figure 2 where both the true distribution and the estimated (non-shifted) lognormal distribution are drawn.

In a more general form, the relations can be written as:

$$M_b = M_a + c$$

$$left\ k_b = \frac{M_a + c}{\frac{M_a}{k_a} + c} \qquad right\ k_b = \frac{M_a \cdot k_a + c}{M_a + c}$$

The right k_b is the largest, and will be used in the subsequent calculations. The ratios between the two values of k_b is given by:

$$ratio = \frac{M_a^2 + M_a \cdot c \cdot k_a + \frac{M_a \cdot c}{k_a} + c^2}{(M_a + c)^2}$$

At this stage, a cut-off point may be selected where the user is warned that the simplification may have consequences for the result. We propose, as an initial value, to take a *ratio* of 2 as acceptable. The criterium will then be:

if *ratio* >= 2 then
[warning to the user]

This approach allows us to extend the use of the analytical method of the previous section without sacrificing too much of the realism of the analysis.

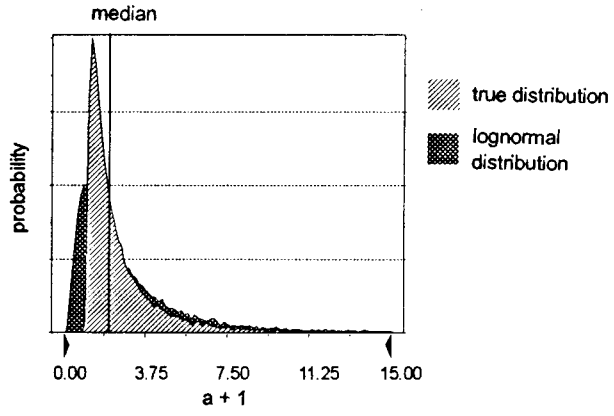

Figure 2 *Approximation of a shifted lognormal distribution with an unshifted lognormal distribution*

2.4. Presentation of uncertainty in the final results

Another point to consider is the presentation of the results of the analysis: the uncertainty in the hazard quotient. Several possibilities are:

- the probability distribution of the values (graphically)
- the probability that PEC exceeds NEC
- the x-th percentile of the distribution of PEC/NEC values (e.g., 95%)
- the 95% interval (upper and lower boundary)

This point needs examination, with the demands of the primary users of the results of the risk assessment (the decision makers) in mind, and needs more elaboration. The main criterium will be the interpretability of the results. It should be noted that the distribution of several hazard quotients will not be lognormal and therefore cannot be described with

an uncertainty factor. Most important, it should be avoided to give the appearance that uncertainty in the hazard quotients is totally quantified. The uncertainties are only quantified to a limited extent, and should not be interpreted as an absolute 'confidence level'. The outcome should be interpreted more in a relative way. Sometimes the risk level can be estimated with more confidence than in other cases. E.g., if the main exposure route of humans is by inhalation of contaminated air, the risk can be estimated with greater confidence than when the main exposure route is formed by an entire food chain of STP to sludge to soil to grass to cattle to meat. Therefore, the most appropriate use of the outcome of the uncertainty analysis, is to indicate the probability of making the wrong decision: the probability of PEC/NEC>1 when the ratio is below one, and the probability that PEC/NEC<1 when the ratio is larger than one. This results may show when one substance can be assessed with greater confidence than another.

3. QUANTIFICATION OF UNCERTAINTIES

In this chapter, the details of the proposed uncertainty analysis are worked out per sub-module. For each sub-module, the input parameters are listed, with their uncertainty factors, and the calculation routine is elucidated. The calculations given are mainly used to illustrate the structure of the formulas, sometimes conversion of units etc. is necessary. This is part of the USES program but will not be reiterated here. For a more extensive discussion and background of the model calculations, the reader is referred to the USES 1.0 documentation (RIVM *et al.*, 1994).

For each sub-module, the problems of the module in the uncertainty analysis are also discussed. As much as was possible, the analytical approach was followed, as discussed in section 2.2. Whenever a calculation does not agree with a multiplicative model and lognormal uncertainties, this will be discussed. Figure 3 shows the main modules of USES and their relations.

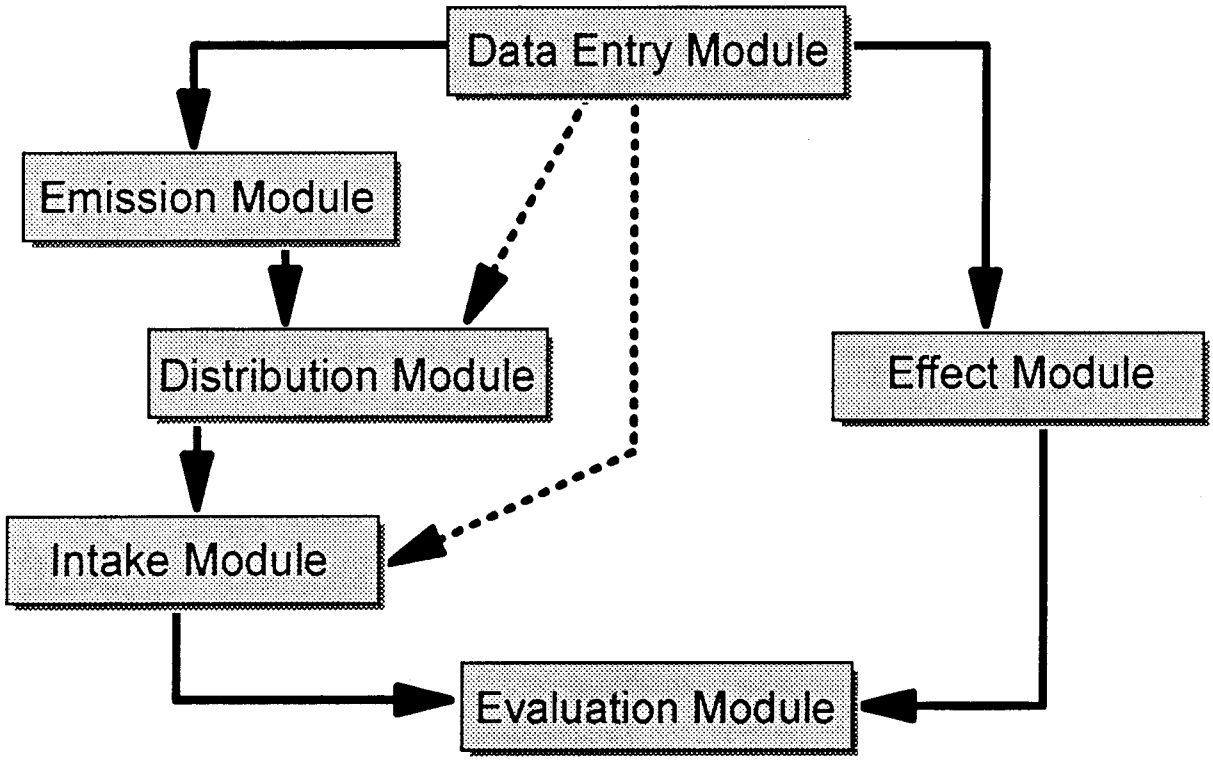

Figure 3 *The main modules of USES 1.0. and the flow of data between them.*

As discussed in section 1.2, the scenario concept of USES restricts the uncertainty analysis. The relevance of the exposure scenario should be assessed, but this should be done in a validation of the system. An extensive list of all scenario choices and assumptions is given in the report on the feasibility of validating USES (Jager, 1995). In the present report, scenario choices are only discussed when they are relevant for the *value* of a model parameter.

With respect to the uncertainty analysis, for each (sub-) module the following items will be discussed:

- Scenario choices, if relevant for the value of a parameter.
- A short description of the (sub-) module.
- A table, showing the input parameters of the calculation and their uncertainties*. For several parameters, the uncertainty is denoted as *L* or *M*. This means that this parameter is output of another calculation and the uncertainty is calculated from uncertainties in other parameters with the analytical approach (yielding a *L*ognormal distribution) or *M*onte Carlo approach (yielding a distribution other than lognormal) respectively.
- The model calculations (sometimes simplified to facilitate reading).
- A discussion of this calculation with respect to the uncertainties in the results, and the possibilities to apply the simple analytical method of section 2.2.1.
- If relevant, a table with intermediate or output parameters for which uncertainties are defined (e.g., for QSARs where uncertainties in the estimate are not calculated from uncertainties in the input parameters, but quantified from the residuals of the regression).

* It should be noted that lognormal parameter distributions are characterized with an uncertainty factor, as explained in section 2.1. In the tables these are mentioned in the column named 'UF'.

3.1. Data entry and filling module

The calculation of USES starts with the data entry and the filling procedure for missing values. Missing data are filled with estimation routines, adding uncertainty to the parameter. Of course, this offers an excellent opportunity for rewarding additional input data by lowering the overall uncertainty in the risk estimate. When the user enters data in the system, no uncertainty is assumed for this parameter. In a future version of USES, the possibility may be added to allow input of the uncertainty of the parameter together with the parameter value.

Many uncertainty factors are difficult to estimate, for instance when estimation routine represents a worst case situation (e.g., biodegradation rates). The consequences of these difficulties will be discussed per estimation routine. Many missing parameters can be estimated with QSARs. Usually, these QSARs are a (linear or log-linear) regression on a set of measured values. The divergence from the regression can be quantified as the uncertainty in the estimate. This is not entirely correct because this uncertainty is only representing the substances in the training set of data used. If we assume that the training set is randomly drawn from all substances, this difficulty can be ignored. However, for other (classes of) chemicals, not present in the training set, the uncertainty may be much larger.

With QSARs, it is usually difficult to take uncertainty in *input* parameters (e.g., the octanol-water partitioning coefficient, *Kow*) into account. Since analytical combination of uncertainties is preferred, often only the uncertainty in the estimate of the QSAR will be taken into account. This ignores the possible uncertainties in the input parameters of the QSAR, and therefore underestimates the true uncertainty. If we decide to apply Monte Carlo analysis for the entire USES, it would be possible to take these uncertainties into

account. However, at this moment, we propose to use the analytical approach whenever possible.

3.1.1. Estimation of water solubility

The QSAR applied in USES to estimate the water solubility from the octanol-water partitioning coefficient was derived by Isnard & Lambert (1989). The authors derived the relations by performing log-linear regression on a data set containing values of 300 substances. For solids, a correction on the melting point is performed. Another regression was made without the use of the melting point. It should be noted that the approach given below differs to some extent from the one applied in USES. In USES, the interpretation of the results of Isnard & Lambert (1989) was incorrect. This also implies that the formulas of USES have to be corrected.

input parameters

Model parameter	Symbol	Unit	UF	Status
Octanol-water partition coefficient	Kow	[-]	1	Data entry
Molecular weight	MOLW	[kg.mol^{-1}]	1	Data entry
Melting point	TEMPmelt	[K]	1	Data entry

model calculations

if TEMPmelt is given:

$$\log SOL = 2.90 - 1.18 \log Kow - 0.0048 (TEMPmelt-298) \qquad \sigma = 0.560$$

if substance is liquid (TEMPmelt < 298) then TEMPmelt should be entered in the formula as 298

if no TEMPmelt is given:

$$\log SOL = 3.05 - 1.29 \log Kow \qquad \sigma = 0.631$$

uncertainty in model results

The uncertainty in the first estimates of solubility can be quantified from the data set collected by Isnard & Lambert (1989). The authors report the standard deviation of the residuals (denoted above as σ), which can be translated to uncertainty factors according to section 2.1.

Model parameter	Symbol	Unit	UF	Status
Water solubility	SOL	[kg.m^{-3}]	13	if TEMPmelt is given
			17	if no TEMPmelt given
				from Isnard & Lambert (1989)

3.1.2. Estimation of the octanol-water partitioning coefficient

The relation between *Kow* and *SOL* is derived by Isnard & Lambert (1989) for the same 300 chemicals for which they derived the reciproke relations from the previous section.
As with the previous QSAR, it should be noted that the approach given below differs to some extent from the one applied in USES. This implies that the formulas of USES have to be corrected for these formulas also.

input parameters

Model parameter	Symbol	Unit	UF	Status
Solubility	SOL	[kg.m^{-3}]	1	Data entry
Melting point	TEMPmelt	[K]	1	Data entry

model calculations

if TEMPmelt is given:

$$\log Kow = 4.81 - 0.77\ [\log (SOL \cdot 1000) + 0.0032\ (TEMPmelt - 298)] \qquad \sigma = 0.453$$

if substance is liquid (TEMPmelt < 298) then TEMPmelt should be entered in the formula as 298

if no TEMPmelt is given:

$$\log Kow = 4.62 - 0.72 \log (SOL \cdot 1000) \qquad \sigma = 0.474$$

uncertainty in model results

The uncertainty in the estimates of Kow can be quantified from the data set collected by Isnard & Lambert (1989). The uncertainty factors are quantified from the standard deviation of the residuals (σ) as given by the authors.

Model parameter	Symbol	Unit	UF	Status
Octanol-water part. coeff.	Kow	[-]	7.7	if TEMPmelt is given
			8.5	if no TEMPmelt is given
				from Isnard & Lambert (1989)

3.1.3. Characterization of the environment

Scenario	*Comments*
By default, typical soil characteristics of a Dutch agricultural soil are taken.	Median case assumption.

In this sub-module, bulk densities of the environmental compartments are derived. Furthermore, volumes of the compartments of the regional and continental models are derived. For the uncertainty of the local model, only the derivation of bulk density of soil is important.

input parameters

Model parameter	Symbol	Unit	UF	Status
Fraction air in soil	$Fair_{soil}$	$[m^3.m^{-3}]$	1	Defined in scenario
Fraction water in soil	$Fwater_{soil}$	$[m^3.m^{-3}]$	1	Defined in scenario
Density of air	RHOair	$[kg.m^{-3}]$	1	Defined in scenario
Density of water	RHOwater	$[kg.m^{-3}]$	1	Defined in scenario
Density of solids	RHOsolid	$[kg.m^{-3}]$	1	Defined in scenario

At this moment, we propose to define soil characteristics in the exposure scenario. This might be changed in the future.

model calculations

$$Fsolids_{soil} = 1 - Fair_{soil} - Fwater_{soil}$$

$$RHO_{soil} = Fair_{soil} \cdot RHOair + Fwater_{soil} \cdot RHOwater + Fsolid_{soil} \cdot RHOsolids$$

uncertainty in model results

Due to the scenario definition, there will be no uncertainty in the results of this sub-module. The calculations of the sub-module are solely based on default parameters. This means that, if the uncertainty in soil characteristics is taken into account, the calculation of the uncertainty in bulk density of soil from the input parameters can be completed 'off-line'.

3.1.4. Intermedia partitioning

3.1.4.1. Air-water partitioning

The partitioning between air and water is described with the Henry coefficient and the dimensionless Henry coefficient ($K_{air\text{-}water}$).

Scenario	*Comments*
Typical characteristics of the (by default) Dutch environment are taken	Median case assumption.

input parameters

Model parameter	Symbol	Unit	UF	Status
Vapour pressure	VP	[Pa]	1	Data entry
Molecular weight	MOLW	[kg.mol^{-1}]	1	Data entry
Solubility	SOL	[kg.m^{-3}]	1/L	Data entry/filling
Gas constant (8.314)	R	[Pa.m^3.mol^{-1}.K^{-1}]	1	Constant
Temperature air-water interface	TEMP	[K]	1	Scenario defined

It should be noted that the vapour pressure is temperature dependent. Therefore, if we propose to add uncertainty to the temperature, we may also need to relate vapour pressure to the temperature.

Model calculations

$$HENRY = \frac{VP \cdot MOLW}{SOL}$$

$$K_{air\text{-}water} = \frac{HENRY}{R \cdot TEMP}$$

uncertainty in model results

Uncertainties in *HENRY* and $K_{air\text{-}water}$ can be calculated analytically because the calculation is strictly multiplicative.

3.1.4.2. Fraction associated with aerosol

The aerosol-air partitioning is estimated according to Junge (1977).

input parameters

Model parameter	Symbol	Unit	UF	Status
Constant of Junge equation	CONjunge	[Pa.m]	3	Temporary, estimated roughly from Noordijk & De Leeuw (1991)
Surface area aerosol particles	SURFaer	[m^2.m^{-3}]	2	Temporary, estimated roughly from Noordijk & De Leeuw (1991)
Vapour pressure	VP	[Pa]	1	Data entry

Uncertainty of the product of *CONjunge* and *SURFaer* can be calculated analytically since both uncertainties are assumed lognormal, and not correlated. This leads to an uncertainty factor of 3.7 for the product, using the formula in section 2.2.

model calculations

$$Fass_{aer} = \frac{CONjunge \cdot SURFaer}{VP + CONjunge \cdot SURFaer}$$

This formula gives some problems. Due to its form, analytical combination of uncertainties is not possible. If *VP* is large compared to the product of *CONjunge* and *SURFaer*, the resulting uncertainty in $Fass_{aer}$ will equal the uncertainty in the product. The other way around, if *VP* is small compared to the product, uncertainty will disappear since the values in the nominator and denominator will be nearly equal. In section 2.3, a provisional solution to this problem is discussed. This makes it possible to approach the distribution of $Fass_{aer}$ with a lognormal distribution. To facilitate this calculation, the formula can be rewritten as:

$$Fass_{aer} = \frac{1}{\frac{VP}{CONjunge \cdot SURFaer} + 1}$$

3.1.4.3. Partitioning between soil and water

Scenario	*Comments*
By default, typical soil characteristics of a Dutch agricultural soil are taken.	Median case assumption.

Of the many regression formulas that have been reported for different classes of organic compounds, the equation proposed by Karickhoff (1981) is chosen. The factor *a* is an empirical regression coefficient that is different for different types of substances. This estimation method is valid for all non-ionic organic chemicals. This partition model is not to be applied for all other chemicals:

- acidic or basic chemicals that to some extent occur in an ionic form;
- anionic and cationic surfactants;
- metals.

input parameters

Model parameter	Symbol	Unit	UF	Status
Fraction organic carbon in soil	Foc_{soil}	$[kg.kg^{-1}]$	1	Scenario defined
Octanol-water part. coeff.	Kow	[-]	1/L	Data entry/filling
Regression coeff.	a	$[m^3.kg^{-1}]$	5.1	From McKone (1993)
Density of the solid phase	RHOsolid	$[kg.m^{-3}]$	1	Scenario defined
Volume fraction water of soil	$Fwater_{soil}$	$[m^3.m^{-3}]$	1	Scenario defined
Volume fraction solids of soil	$Fsolid_{soil}$	$[m^3.m^{-3}]$	1	Scenario defined

Uncertainty in *a* is derived from the data set collected by Karickhoff (1981). McKone (1993) estimated a coefficient of variation of 1 for this estimation routine. Using the relations given in section 2.1, an uncertainty factor of 5.1 is calculated.

Model calculation

$$Kp_{soil} = \frac{a \cdot Foc_{soil} \cdot Kow}{1000}$$

$$K_{soil-water} = Fwater_{soil} + Fsolid_{soil} \cdot Kp_{soil} \cdot RHOsolid$$

$$Fdiss_{soil} = \frac{Fwater_{soil}}{K_{soil-water}}$$

Uncertainty in model result

Uncertainty in Kp_{soil} can be calculated analytically. Uncertainty in $K_{soil-water}$ can also be calculated analytically. $Fwater_{soil}$ is scenario-defined and therefore uncertainty is ignored, therefore, the simplification of 2.3 can be applied for the summation. Finally, the uncertainty in $Fdiss_{soil}$ can also be derived analytically. The uncertainty in Kow can be taken into account in this estimation.

3.1.4.4. Partitioning between suspended matter-water

Scenario	*Comments*
Typical characteristics of suspended matter are taken.	Median case assumption.

Estimation of suspended matter-water equilibrium constants is performed in the same way as demonstrated for soil-water equilibrium. For suspended matter in the sewage treatment plant's primary solver and solids-liquid separator/aeration tank, separate values for Kp_{susp} are calculated because of the different organic carbon content of the suspended matter.

input parameters

Model parameter	Symbol	Unit	UF	Status
Regression coefficient	a	$[m^3.kg^{-1}]$	5.1	From McKone (1993)
Fraction organic carbon in susp.	Foc_{susp}	$[kg.kg^{-1}]$	1	Scenario defined
Frac. oc in susp. STP prim. solver	Foc_{suspPS}	$[kg.kg^{-1}]$	1	Scenario defined
Frac. oc in susp. of AT and SLS	$Foc_{suspATSLS}$	$[kg.kg_{-1}]$	1	Scenario defined
Octanol-water part. coeff.	Kow	[-]	1/L	Data entry/filling
Density of the solid phase	RHOsolid	$[kg.m^{-3}]$	1	Scenario defined
Volume fraction water of susp.	$Fwater_{susp}$	$[m^3.m^{-3}]$	1	Scenario defined
Volume fraction solids of susp.	$Fsolid_{susp}$	$[m^3.m^{-3}]$	1	Scenario defined

Model calculation

Suspended matter in surface water

$$Kp_{susp} = \frac{a \cdot Foc_{susp} \cdot Kow}{1000}$$

Suspended matter in STP primary solver and aeration tank/solids-liquid separator

$$Kp_{suspPS} = \frac{a \cdot Foc_{suspPS} \cdot Kow}{1000}$$

$$Kp_{suspATSLS} = \frac{a \cdot Foc_{suspATSLS} \cdot Kow}{1000}$$

uncertainty in model results

The calculations above are strictly multiplicative. Therefore, analytical combination of uncertainties is possible. Uncertainty in *Kow* can be taken into account analytically.

3.1.5. Biodegradation

3.1.5.1. Biodegradation in soil

Scenario	*Comments*
By default, typical soil characteristics of a Dutch agricultural soil are taken.	Median case assumption.

If no biodegradation half-life in soil is given, the biodegradation in soil is obtained by means of the scaling procedure proposed by Struijs & Van den Berg (1992, 1995).

input parameters

Model parameter	Symbol	Unit	UF	Status
Conc. of bacteria in the test water	$BACT_{test}$	[cfu.m^{-3}]	1	Scenario defined
Result of a standard screening test	PASSreadytest	[yes/no]	n.a.	Data entry
Frac. of chemical dissolved in soil	$Fdiss_{soil}$	[-]	L	Output filling
Conc. of bacteria reported in soil	$BACT_{soil}$	[cfu.kg^{-1}]	1	Scenario defined
Bulk density of soil	RHO_{soil}	[kg.m^{-3}]	1	Scenario defined
Volume fraction water in soil	$Fwater_{soil}$	[-]	1	Scenario defined

Model calculation

$$kdeg_{test} = \frac{\ln 2}{5 \cdot 24 \cdot 3600} \; s^{-1} \quad \text{if} \quad PASSreadytest = yes \quad \text{(half-life of 5 days)}$$

$$kdeg_{test} = \frac{\ln 2}{1000 \cdot 24 \cdot 3600} \; s^{-1} \quad \text{if} \quad PASSreadytest = no \quad \text{(half-life of 1000 days)}$$

$$BACTporew_{soil} = \frac{BACT_{soil} \cdot RHO_{soil}}{Fwater_{soil}} \quad \text{rescale to bacteria in porewater}$$

$$kdeg_{soil} = kdeg_{test} \cdot \frac{BACTporew_{soil}}{BACT_{test}} \cdot Fdiss_{soil}$$

uncertainty in model results

The conservatively chosen default degradation rates severely hamper the uncertainty analysis. If uncertainty in the degradation rate is to be quantified, median case defaults have to be chosen instead of 5 and 1000 days, together with an uncertainty factor. Uncertainty due to the scaling procedure can be quantified analytically. At this moment however, this problem is not urgent since the uncertainty in the degradation rate in soil cannot be taken into account in the soil-groundwater module. In this module, $kdeg_{soil}$ is used to derive a fraction accumulation and concentration in groundwater from a table (see section 3.6).

3.1.5.2. Biodegradation in the sewage treatment plant

When no value is given in the input data set, a value has to be estimated from the ready biodegradability test. According to Struijs & Van den Berg (1992, 1995) the degradation rate constant in the water phase of activated sludge can be taken as 3 hr^{-1} for all chemicals that are positive in a readily biodegradability test.

input parameters

Model parameter	Symbol	Unit	UF	Status
Result of a standard screening test	PASSreadytest	[yes/no]	n.a.	Data entry

Model calculation

$$kdeg_{stp} = 3 \cdot \frac{1}{3600} \; s^{-1} \quad \text{if} \quad PASSreadytest = yes$$

$$kdeg_{stp} = 0 \; s^{-1} \quad \text{if} \quad PASSreadytest = no$$

uncertainty in model results

The default biodegradation rates are conservatively chosen. This severely hampers the uncertainty analysis. If uncertainty in the degradation in the STP is to be quantified,

median case defaults have to be chosen, together with an uncertainty factor.

For this moment, uncertainty in this biodegradation rate may be ignored, as the STP module itself is simplified. In the STP module, uncertainty in input parameters (apart from the emission rate) is not taken into account.

3.1.6. Bioconcentration factors

3.1.6.1. Bioconcentration in fish

Bioconcentration factors for fish are, in the present version of USES, calculated as follows:

$$BCF_{fish} = \frac{Ffat_{fish} \cdot Kow}{RHO_{bio}}$$

This equation however, describes a passive partitioning process, it does not take into account any metabolism or active excretion. This kind of, rather worst case, estimation is difficult to translate to a parameter distribution. Therefore, we change this approach to a less mechanistic, but more descriptive linear regression.

input parameters

Model parameter	Symbol	Unit	UF	Status
Octanol-water part. coeff.	Kow	[-]	1/L	Data entry/filling

model calculations

It should be noted that the unit of *BCFfish* is taken as l/kg as this is the unit applied in the data set by Veith & Kosian (1983). A conversion to m^3/kg is necessary in USES.

$$\log BCF_{fish} = \alpha_{fish} \cdot \log Kow + \beta_{fish}$$

where α and β are derived from a regression on a set of measured data including values of metabolised and non-metabolised substances.

uncertainty in model results

The uncertainty can be quantified from the residuals of the regression, using the formula from section 2.1. We performed a linear regression to estimate α and β, and quantified the deviations from the regression line. The data set collected by Veith & Kosian (1983) was taken as a representative set, consisting of different classes of chemicals and several fish species. Figure A1 in Appendix 1 shows the data with the linear regression. Table 2 gives the results of the regression. The uncertainty factor k was derived using the equation in section 2.1.

It is clear from Figure A1 in Appendix 1 that the data are well described with linear

regression. The plot of residuals is shown in Figure A3, the frequency distribution of the residuals in Figure A2.

The uncertainty in the input parameter Kow cannot be taken into account analytically.

Table 2 Linear regression log $K_{fish\text{-}water}$ vs. log Kow

Parameter α	0.7879
Parameter β	-0.3948
r^2	0.8567
Number of data	122
SD of resid.	0.49025
Var. of resid.	0.24034
k	9.1

Model parameter	Symbol	Unit	UF	Status
Bioconc. factor for fish	BCF_{fish}	[l.kg^{-1}]	9.1	derived from regression on data set of Veith & Kosian (1983)

3.1.6.2. Bioconcentration in earthworms

The bioconcentration process in earthworms can, according to equilibrium partitioning theory, be seen as a two-step process: partitioning between soil particles and interstitial water, followed by partitioning between worm and interstitial water.

The relation between soil-water and worm, as applied in USES, is taken from Connell & Markwell (1990). The relation is a linear regression (on a logarithmic scale), on 100 data points for 30 substances (mainly pesticides). The residues of this fit give us a measure of the uncertainty in the BCF for worms. This includes variability between individual worms. This variation is averaged out, however, since we consider the exposure of worm-eating predators. As in the estimation of BCF_{fish} in the previous section, the present data set does not allow this variability to be distinguished from the other sources of uncertainty.

input parameters

Model parameter	Symbol	Unit	UF	Status
Octanol-water part. coeff.	Kow	[-]	1/L	Data entry/filling
Soil-water part. coeff.	$K_{soil\text{-}water}$	[m^3.m^{-3}]	L	Data entry/filling
Density of soil	RHO_{soil}	[kg.m^{-3}]	1	Scenario defined

It should be noted that uncertainties in *Kow* and $K_{soil\text{-}water}$ will be correlated. At this moment, this will not pose any problems, since Kow is used in the regression and its uncertainty therefore ignored.

model calculations

It should be noted that the unit of $K_{worm\text{-}porewater}$ is taken as l/kg as this is probably the unit used by Connell & Markwell (1990). The authors did not mention the unit of their bioconcentration factors. The factor of 1000 in the equation below is applied to convert the unit of BCF_{worm} to m^3/kg for subsequent calculations.

$$\log K_{worm\text{-}porewater} = \alpha_{worm} \cdot \log Kow + \beta_{worm}$$

$$BCF_{worm} = \frac{K_{worm\text{-}porewater} \cdot RHO_{soil}}{1000 \cdot K_{soil\text{-}water}}$$

uncertainty in model results

Table 3 Linear regression log $K_{worm\text{-}porewater}$ vs. log Kow

Parameter α	1.001
Parameter β	-0.5528
r^2	0.8260
Number of data	100
SD of resid.	0.63244
Var. of resid.	0.40000
k	17

The data set for $K_{worm\text{-}porewater}$ was taken from Connell & Markwell (1990), mainly consisting of pesticide data. The parameters α and β were estimated and the residuals analyzed. The table below gives the results of the regression and analysis of the residuals.

From Figure A4, Figure A5, and Figure A6 in Appendix 1 the appropriateness of a linear model may be questioned. Nevertheless, for the purpose of this report, the linear model is maintained. This will however, increase the uncertainty as the fit is not very satisfactory. The results from Table 3 show that the resulting uncertainty factor is large, compared to the estimation of the BCF for fish. Maybe the estimation can be improved by developing a more mechanistic model or by expanding the data set.

Uncertainty in the input parameter *Kow* is not taken into account into $K_{worm\text{-}porew}$. However, uncertainty in $K_{soil\text{-}water}$ is accounted for in the final result of BCF_{worm} (this can be calculated analytically).

Model parameter	Symbol	Unit	UF	Status
Part. coeff. worm-porewater	$K_{worm\text{-}porew}$	[l.kg^{-1}]	17	Derived from regression on data set of Connell & Markwell (1990)

3.1.6.3. Bioconcentration plant from soil

Bioconcentration to roots and stems of plant from soil is estimated with the relations of Briggs *et al.* (1982, 1983).

input parameters

Model parameter	Symbol	Unit	UF	Status
Octanol-water part. coeff.	Kow	[-]	1/L	Data entry/filling
Bulk density of soil	RHOsoil	[kg.m^{-3}]	1	Scenario defined
Soil-water part. coeff.	$K_{soil-water}$	[-]	L	Data entry/filling

model calculations

$$TSCF = 0.748 \cdot e^{-\frac{(logKow - 1.78)^2}{2.44}}$$

$$SCF = \frac{0.82 + 10^{0.95 \cdot logKow - 2.05}}{1000}$$

$$BCFstem_{plant} = SCF \cdot TSCF \cdot \frac{RHO_{soil}}{K_{soil-water}}$$

$$K_{root-porew} = \frac{0.82 + 10^{0.77 \cdot logKow - 1.52}}{1000} \quad [m^3.kg^{-1}]$$

$$BCFroot_{plant} = K_{root-porew} \cdot \frac{RHO_{soil}}{K_{soil-water}}$$

uncertainty in model results

Uncertainties in the estimations of *SCF*, *TSCF* and $K_{root-porew}$ can be estimated using the data set collected by Polder *et al.* (1994). It should be noted that the *SCF* used here is defined as the ratio between concentration in stem and the concentration in *transpired* water. The experimental *SCF*s as collected by Polder and coworkers is relative to the concentration in soil solution. Therefore, the uncertainty estimated from this data set should be applied to *SCF* • *TSCF*. The data of Polder and coworkers have not been analyzed in detail yet, therefore, temporary uncertainties are given (estimated by eye from the data).

Uncertainty in *Kow* can not be taken into account. However, uncertainty in $K_{soil-water}$ can be accounted for analytically.

Model parameter	Symbol	Unit	UF	Status
Transp. stream conc. factor	TSCF	[-]	1	Ignored (incorporated into SCF)
Stem conc. factor	SCF	[m^3.kg^{-1}]	6	Temporary, estimated roughly from Polder *et al.* (1994)
Root-porew. part. coeff.	$K_{root-porew}$	[m^3.kg^{-1}]	6	Temporary, estimated roughly from Polder *et al.* (1994)

3.1.6.4. Bioconcentration plant from air

Bioconcentration in plants from air is divided into two separate processes; deposition onto the leaves and gas absorption. Deposition is described according to McKone & Ryan (1989), equilibrium between gas and plant according to Riederer (1990).

input parameters

Model parameter	Symbol	Unit	UF	Status
Aerosol-plant part. coeff.	$K_{aerosol-plant}$	$[m^3.kg^{-1}]$	8.4	From McKone (1993)
Fraction air in plant	$Fair_{plant}$	$[m^3.m^{-3}]$	n.a.	Incl. in UF $K_{gas-plant}$
Fraction water in plant	$Fwater_{plant}$	$[m^3.m^{-3}]$	n.a.	Incl. in UF $K_{gas-plant}$
Fraction lipids in plant	$Flipid_{plant}$	$[m^3.m^{-3}]$	n.a.	Incl. in UF $K_{gas-plant}$
Bulk density of plant	RHO_{plant}	$[kg.m^{-3}]$	1	Temporary
Octanol-water part. coeff.	Kow	[-]	1/L	Data entry/filling
Air-water part. coeff.	$K_{air-water}$	[-]	L	Output filling
Frac. ass. aerosol	$Fass_{acr}$	[-]	L	Output filling

McKone (1993) estimates coefficients of variations for several QSARs, including the estimations of aerosol-plant partitioning coefficient. Using the relation between CV and *k*, given in section 2.1, the CV of 1.5 (as estimated by McKone) can be translated to an uncertainty factor.

model calculations

$$K_{aerosol-plant} = 3300 \qquad \text{(constant)}$$

$$K_{gas-plant} = \left[Fair_{plant} + (Fwater_{plant} + Flipid_{plant} \cdot Kow) \cdot \frac{1}{K_{air-water}} \right] \cdot \frac{1}{RHO_{plant}}$$

$$BCFair_{plant} = Fass_{acr} \cdot K_{aerosol-plant} + (1 - Fass_{acr}) \cdot K_{gas-plant}$$

uncertainty in model results

Table 4 Analysis of difference between $K_{gas-plant}$ from literature and USES estimate

Number of data	10
SD of resid.	0.708783
Var. of resid.	0.502374
k	25

The uncertainty in $BCFair_{plant}$ can be calculated from the uncertainty in the input parameters. It should be noted that the model is not longer multiplicative, thus requiring Monte Carlo analysis. However, it is possible that this approach will be adapted in the near future as summation of deposition and gas-uptake might not be very relevant.

Uncertainty in the gas-plant partitioning coefficient can be estimated from the experimental results of Bacci *et al.* (1990). Even though the authors tested only 10 substances, this gives sufficient

information for a temporary estimate of the uncertainty. The comparison between measured and calculated values is graphically shown in Appendix 1, Figure A7.

The possible uncertainty in RHO_{plant} is not taken into account, but can easily be added.

Model parameter	Symbol	Unit	UF	Status
Gas-plant part. coeff.	$K_{gas\text{-}plant}$	$[m^3.kg^{-1}]$	25	Derived from analysis of data Bacci *et al.* (1990)

3.1.6.5. Bioconcentration meat and milk from uptake by cow

The bioconcentration factors between the cows daily intake and the concentrations in meat and milk were derived by Travis & Arms (1988). Log-linear regressions were performed on values for 36 substances for biotransfer to meat (log *Kow* between 1.3 and 6.9), and 28 substances for biotransfer to milk (log *Kow* between 2.8 and 6.9).

input parameters

Model parameter	Symbol	Unit	UF	Status
Octanol-water part. coeff.	Kow	[-]	1/L	Data entry/filling

model calculations

$$\log BCF_{meat} = -7.6 + \log Kow$$

$$\log BCF_{milk} = -8.1 + \log Kow$$

uncertainty in model results

Table 5 *Linear regression log BCF_{meat} vs. log Kow*

Parameter α	0.8344
Parameter β	-6.8870
r^2	0.808
Number of data	36
SD of resid.	0.9201
Var. of resid.	0.8466
k	64

Uncertainty in the estimates for the bioconcentration factor can be derived from analysis of the residuals of the regression. Uncertainty in *Kow* will not be taken into account.

It may be clear from Table 5 that the relation between *Kow* and BCF_{meat} is not very satisfactory, resulting in a very high uncertainty factor. Interestingly, our regression gives different coefficients then the regression of Travis & Arms. The value of r^2 is equal, and the plot of the regression in Appendix 1 (Figure A8) is close to the figure given by the authors.

Table 6 shows the results of the regression of BCF_{milk} versus *Kow*. Again, the coefficients

Table 6 Linear regression log BCF_{milk} vs. log Kow

Parameter α	0.7309
Parameter β	-6.7856
r^2	0.737
Number of data	28
SD of resid.	0.7917
Var. of resid.	0.6267
k	36

differ from the original authors, without effecting r^2 very much. Figure A10 in Appendix 1 shows the plot of the regression.

The origin of the deviation of the regression coefficients from the original publication requires more detailed examination.

Model parameter	Symbol	Unit	UF	Status
Bioconc. factor for meat	BCF_{meat}	[d.kg^{-1}]	64	Calculated from Travis & Arms (1988)
Bioconc. factor for milk	BCF_{milk}	[d.kg^{-1}]	36	Calculated from Travis & Arms (1988)

3.2. Emissions

Scenario	*Comments*
The emission is averaged over the year in case of human and soil organism exposure assessment.	Averaging over the year may not be very valid (it may be best case), as many substances are only produced during short episodes.

From the table above it may be concluded that, although uncertainty factors for the emissions to water and air have been assessed, the *scenarios* are not median case. In the scenario a standard, main source of the substance is assessed.

Emissions are given as tables, together with the uncertainty factors (lognormal distributions are assumed). It should be noted that measured emission data are preferred above use of these tables. It should therefore also be possible to enter uncertainty in the measured data.

input parameters

Model parameter	Symbol	Unit	UF	Status
Production volume	TONNAGE	[kg.s^{-1}]	1	Data entry
Fraction of tonnage to air	$Fair_{release}$	[-]	L	From tables
Fraction of tonnage to wastew.	$Fwater_{release}$	[-]	L	From tables
Fraction from main source	$F_{mainsource}$	[-]	L	From tables

model calculations

Local, annual averaged, emissions from the main point source are calculated as:

$$Edirect_{air} = F_{mainsource} \cdot Fair_{release} \cdot TONNAGE \qquad [kg.s^{-1}]$$

$$Edirect_{water} = F_{mainsource} \cdot Fwater_{release} \cdot TONNAGE \qquad [kg.s^{-1}]$$

The number of emission days is used to calculate the emission flux during an emission episode. This is in USES 1.0 the output of the emission module. For human exposure, this is not relevant, as only chronic exposure is considered. It is better to adapt USES, to make the *annual average* emission from a point source *and* the number of days output of the emission module. With this number of days, annual average surface water concentrations can be translated to episode concentrations.

uncertainty in model results

Since the parameters from the emission table are assumed to be distributed lognormally, uncertainty in this module's results can be calculated analytically.

3.3. STP model

Scenario	*Comments*
The STP is modelled as, by default, an average Dutch plant with SimpleTreat. Characteristics of the 'average' plant are assumed.	Median case. Perhaps USES should allow more specific tuning of the STP.

For the purpose of uncertainty analysis, the STP-model is simplified to 4 fractions of the emission to wastewater (air, water, sludge and degraded). This way, the STP module gives less difficulties in the proposed analysis. The modelling is more or less median or average. Uncertainty factors can probably be derived from expert judgement or validation studies. Of course, the fractions of the substance degraded, to air, to water, and to sludge, are correlated (due to conservation of mass). The sum of these fraction cannot exceed 1. This makes the simplification difficult to combine with lognormal distribution of uncertainties as lognormal distributions do not have an upper boundary, whereas the fractions have. For now, this complication will be ignored.

input parameters

Model parameter	Symbol	Unit	UF	Status
Octanol-water part. coefficient	Kow	[-]	1/L	Data entry/filling
Henry's law constant	HENRY	[Pa.m^3.mol^{-1}]	L	Data entry/filling
Solids-water part. coeff. in PS	Kp_{suspPS}	[m^3.kg^{-1}]	L	Data entry/filling
Solids-water part. coeff. AT/SLS	$Kp_{suspATSLS}$	[m^3.kg^{-1}]	L	Data entry/filling
Emission to wastewater	$Edirect_{water}$	[kg.s^{-1}]	L	Output emission
First order degr. rate constant STP	$kdeg_{stp}$	[s^{-1}]	n.a.	ignored in calculations
[Characteristics of the average STP]			1	Scenario defined

model calculations

With these fractions, indirect emissions via the STP can be calculated to air, surface water and sludge:

$$Estp_{air} = Edirect_{water} \cdot F_{air} \qquad [kg.s^{-1}]$$

$$Estp_{tot,surf} = Edirect_{water} \cdot F_{tot,surf} \qquad [kg.s^{-1}]$$

$$Estp_{sludge} = Edirect_{water} \cdot F_{sludge} \qquad [kg.s^{-1}]$$

uncertainty in model results

With this simplification of the STP model, analytical combination of uncertainties is possible. However, this will underestimate the true uncertainty since only uncertainty in emission is taken into account with the input parameters. The other input parameters are ignored. On the other hand, uncertainties may also be overestimated since a lognormal distribution is assumed for the fractions, and correlations are ignored.

Model parameter	Symbol	Unit	UF	Status
Fr. of emission redirected to air	F_{air}	[-]	1.5	Estimated from Struijs *et al.* (1991)
Fr. of emission to surf. water	$F_{tot,surf}$	[-]	2	De Greef & De Nijs (1990)
Fr. of emission to sludge	F_{sludge}	[-]	2	Estimated from Struijs *et al.* (1991)
Fr. of emission degraded	$F_{degraded}$	[-]	1	Not used in calc.

3.4. Surface water

Scenario	*Comments*
Dilution factor at 1000 m from the STP is used.	Chosen as representative location for exposure of the aquatic ecosystem.
Average characteristics of the receiving surface water are assumed (esp. concentration of suspended matter).	Median case assumption.

The dissolved concentration in surface water is calculated by dividing the emission to surface water by the effluent discharge and the dilution factor, and multiplying with the fraction of the chemical present in the water phase (i.e. not sorbed to particles).

input parameters

Model parameter	Symbol	Unit	UF	Status
Emission from STP to effluent	$Estp_{tot,surf}$	[kg.s^{-1}]	L	Output STP
Number of emission days	$T_{emission}$	[d]	L	Output emission
Solids-water part. coeff. in susp.	Kp_{susp}	[m^3.kg^{-1}]	L	Data entry/filling
Concentration susp. in surf. water	$SUSPCONC_{surf}$	[kg.m^{-3}]	1	Scenario defined
Dilution factor in surface water	DILUTION	[-]	148*	Research De Greef & De Nijs (1990)
Effluent discharge of STP	$EFFLUENT_{stp}$	[m^3.s^{-1}]	1	Included in UF dilution

*This value includes the uncertainty in effluent discharge

model calculation

$$Ctot_{surf} = \frac{Estp_{tot,surf}}{EFFLUENT_{stp} \cdot DILUTION}$$

$$Cdiss_{surf,ann} = \frac{Ctot_{surf}}{1 + Kp_{susp} \cdot SUSPCONC_{surf}}$$

$$Cdiss_{surf,epi} = Cdiss_{surf,ann} \cdot \frac{365}{T_{emission}}$$

uncertainty in model results

Uncertainty in $Ctot_{surf}$ can be calculated analytically. The derivation of $Cdiss_{surf,ann/epi}$ requires summation. in 2.3, a provisional solution to this problem is discussed. This makes it possible to approach the distribution of $Cdiss_{surf,ann}$ with a lognormal distribution.

3.5. Air concentration and deposition fluxes

Concentrations in air and deposition fluxes of gasses and aerosols are calculated using results from the OPS-model. These results were obtained with standard source characteristics.

Scenario	*Comments*
Only annual average concentrations are generated by averaging emissions over the year.	Thought to be relevant with respect to chronic human exposure. Questionable for substances only emitted for several days.
Standard source characteristics and environmental and meteorological data were used to derive the standard concentrations and standard fluxes.	Probably median case assumption.

General values for uncertainties can probably be extracted from the RIVM reports concerning the OPS model and its implementation into USES. A large part of the uncertainties will be caused by uncertainty in environmental parameters (particle size aerosol, meteo data, etc.) and source characteristics (source height, heat content of plume, etc). It is important to define which parameters must be seen as part of the (fixed) scenario, and which parameters contain the uncertainty we search to quantify.

input parameters

Model parameter	Symbol	Unit	UF	Status
Emission to air direct	$Edirect_{air}$	[$kg.s^{-1}$]	L	Output emission
Emission to air via STP	$Estp_{air}$	[$kg.s^{-1}$]]	L	Output STP
Standard conc. from OPS model	$Cstd_{air}$	[$kg.m^{-3}$]	2	Temporary, estimated from Noordijk & De Leeuw (1991)
Standard dep. flux aerosols OPS	$Dstd_{aer}$	[$kg.m^{-2}.s^{-1}$]	10	Temporary, estimated from Noordijk & De Leeuw (1991)
Standard dep. flux gas from OPS	$Dstd_{gas}$	[$kg.m^{-2}.s^{-1}$]	10	Temporary, estimated from Noordijk & De Leeuw (1991)
Frac. of chem. sorbed to aerosol	$Fass_{aer}$	[-]	L	Data entry/filling

model calculations

The concentration in air will be calculated as:

$$C_{air} = \max \left[Estp_{air} , Edirect_{air}\right] \cdot Cstd_{air}$$

The total deposition flux will be calculated as:

$$Dtot = [Estp_{air} + Edirect_{air}] \cdot [Fass_{aer} \cdot Dstd_{aer} + (1-Fass_{aer}) \cdot Dstd_{gas}]$$

uncertainty in model results

The uncertainties in the air concentration can be assessed analytically. The deposition flux however, requires summation of several uncertain components. For this calculation, Monte Carlo analysis cannot be avoided.

3.6. Soil and groundwater

Scenario	*Comments*
Sludge is applied once each year (the maximum amount of 2000 $kg.ha^{-1}.yr^{-1}$).	Worst case assumption. Sludge from industrial plants is not applied as fertilizer.
The concentration in sludge, that is used on agricultural land, is calculated with annual average emissions.	Median case assumption, the concentration will be higher if sludge from an emission episode is used, and zero if sludge outside an emission episode is used.
Typical dutch soil characteristics are applied in PESTLA (density, fraction organic matter, etc.). The soil type is more or less best case with respect to accumulation, but worst case with respect to leaching to groundwater.	This soil type is common for agricultural soils in the Netherlands.
A top-soil layer of 20 cm is assumed relevant for uptake by plants, cattle. This layer is regarded homogeneous.	Probably median case.
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.	More or less median case. This value may be too long to protect soil organisms, but is appropriate with respect to chronic human exposure. This time period needs more investigation (also with respect to EU guidelines for sludge application).

For the calculation of concentrations in soil and groundwater due to sludge application and aerial deposition, results from the model PESTLA are used. The numerical PESTLA model was simplified to two tables (giving the fraction of the substance remaining in the top soil layer after one year, *Facc*, and the maximum concentration in groundwater, $Cgrw_{table}$). Only the two most important input parameters are used in these tables: the half-life time for biodegradation in soil and the sorption to organic matter (*Kom*, derived from *Kow*). The fraction accumulated in the soil layer is recalculated to a first order 'disappearance' rate constant, assuming first order kinetics. With this constant, the concentration in soil due to yearly application of sewage sludge and continuous aerial deposition can be assessed. The concentration that is used for further calculations, is the

concentration averaged over 180 days, in the 'steady-state year' (the year in which no further accumulation takes place).

Uncertainty in the PESTLA model used for USES is difficult to assess. PESTLA has many parameters and assumptions that are hidden in USES (e.g., type of crops grown, meteo data, soil characteristics). These parameters are therefore incorporated in the exposure scenario.

input parameters

Model parameter	Symbol	Unit	UF	Status
Emission from STP to sludge	$Estp_{sludge}$	[kg.s^{-1}]	L	Output STP
Rate of sludge production	$SLUDGE_{stp}$	[kg.s^{-1}]	1	Scenario defined
Total deposition flux	Dtot	[kg.m^{-2}.s^{-1}]	M	Output air
Amount of sludge applied	$APPL_{sludge}$	[kg.ha^{-1}.yr^{-1}]	1	Scenario defined
Mixing depth of soil	$DEPTH_{soil}$	[m]	1	Scenario defined
Density of soil	RHO_{soil}	[kg.m^{-3}]	1	Scenario defined
Exposure period considered	EXP	[d]	1	Scenario defined

The rate of sludge production is calculated in the STP module. The uncertainty is ignored for the time being (the parameter is taken as part of the exposure scenario), as the uncertainty cannot be quantified in the STP module without the use of Monte Carlo analysis.

model calculations

PESTLA is incorporated in USES in the form of tables. These tables give for an application of 1 kg/ha the concentration in groundwater ($Cgrw_{table}$) and the fraction of the substance accumulated in one year (*Facc*). Input for the tables are the organic matter-water partitioning coefficient (*Kom*) and the half-life for biodegradation ($DT50_{soil}$).

The concentration in dry sludge can be calculated as:

$$C_{sludge} = Estp_{sludge} / SLUDGE_{stp}$$

The maximum concentration in groundwater is calculated as:

$$Cgrw = Cgrw_{table} \cdot (C_{sludge} \cdot APPL_{sludge} + Dtot) \quad [kg_{chem}.m^{-3}]$$

All parameters should be converted to suitable units (conversions are not shown here).

$$kdis_{soil} = \frac{1}{365} \cdot \ln\left[\frac{1}{Facc}\right] \qquad [d^{-1}]$$

The soil concentration due to aerial deposition only, is calculated as:

$$Csoil_{dep} = \frac{Dtot}{DEPTH_{soil} \cdot kdis_{soil} \cdot RHO_{soil}}$$

The average concentration of the exposure period due to sludge use is calculated as:

$$Csoil_{sludge} = \frac{C_{sludge} \cdot APPL_{sludge}}{DEPTH_{soil} \cdot kdis_{soil} \cdot RHO_{soil}} \cdot \frac{1 - e^{-kdis_{soil} \cdot EXP}}{EXP \cdot (1-Facc)}$$

$$Ctot_{agr} = Csoil_{dep} + Csoil_{sludge}$$

It should be noted that this procedure pictured above is likely to change depending on the outcome of the intended changes of the PESTLA implementation in USES.

uncertainty in model results

Calculating concentration in groundwater requires summation of two uncertain processes; sludge application and deposition. Therefore, an analytical solution is not possible. The calculation of $Ctot_{agr}$ also requires summations, but also an exponential factor. This module requires Monte Carlo analysis for a part of the calculations. Furthermore, it is not possible to attach a lognormal uncertainty to *Facc*. Lognormal distributions do not have an upper boundary and value of *Facc* > 1 would lead to negative rate constants. As a pragmatic solution, uncertainty is attached to $kdis_{soil}$. Pending the development of the European risk assessment system, at this moment, only temporary uncertainty factors are set.

Model parameter	Symbol	Unit	UF	Status
Disappearance rate constant	$kdis_{soil}$	[-]	5	Temporary, initial guess by expert
Maximum conc. in groundwater	$Cgrw_{table}$	[kg.m^{-3}]	10	Temporary, initial guess by expert

3.7. Concentration in intake media humans and predators

In this module, concentrations in the intake media for humans and predating birds and mammals are calculated. These calculations exclude air, which is calculated in section 3.5. The exposure scenario chosen is a location in the vicinity of a source *and* an STP.

3.7.1. Purification of drinking water

Scenario	*Comments*
Conservative purification factors. No purification by groundwater treatment.	Worst case.

Drinking water is prepared from surface water or groundwater. Surface water purification is modelled by means of a purification factor. These factors are chosen quite conservatively due to the limited prediction ability from physico-chemical properties. Due to these worst case assumptions uncertainty in purification of drinking water is difficult to take into account.

Only surface water will be purified, purification factors are dependent on *Kow*, Henry coefficient and DT50 in water.

input parameters

Model parameter	Symbol	Unit	UF	Status
Conc. dissolved in surface water	$Cdiss_{surf,ann}$	[kg.m^{-3}]	L	Output surface water
Purification factors	PURF	[-]	1	Scenario defined (worst case)
Concentration in groundwater	C_{grw}	[kg.m^{-3}]	M	Output soil/groundw.

model calculations

$$C_{drw} = \max (Cdiss_{surf,ann} \cdot PURF , C_{grw})$$

uncertainty in model results

If the purification factors are seen as a worst case scenario, the resulting uncertainty in drinking water is the uncertainty in surface water *or* groundwater concentration. If surface water is used, the uncertainty in drinking water can be quantified analytically. However, if groundwater is used, Monte Carlo analysis must be applied.

3.7.2. Concentration in fish

The fish are assumed to be in equilibrium with the annual average surface water concentration.

input parameters

Model parameter	Symbol	Unit	UF	Status
Conc. dissolved in surface water	$Cdiss_{surf,ann}$	$[kg.m^{-3}]$	L	Output surf. water
Bioconcentration in fish	BCF_{fish}	$[m^3.kg^{-1}]$	L	Data entry/filling

model calculation

$$C_{fish} = Cdiss_{surf} \cdot BCF_{fish}$$

uncertainty in model results

Uncertainty in the concentration of fish can be assessed analytically.

3.7.3. Concentration in earthworms

The earthworms are assumed to be in equilibrium with the concentration in agricultural soil.

input parameters

Model parameter	Symbol	Unit	UF	Status
Concentration in agricultural soil	$Ctot_{agr}$	$[kg.kg^{-1}]$	M	Output soil/groundw.
Bioconcentration in worm	BCF_{worm}	$[kg.kg^{-1}]$	L	Data entry/filling

model calculation

$$C_{worm} = Ctot_{agr} \cdot BCF_{worm}$$

uncertainty in model results

The uncertainty in the concentration in worms cannot be calculated analytically because the concentration in soil is not lognormally distributed. Therefore, Monte Carlo analysis needs to be applied for this calculation.

3.7.4. Concentration in crops

Roots are assumed to be in equilibrium with the soil concentration. The above-ground parts of plants are in equilibrium with soil and air (it should be noted that their contributions are summed).

input parameters

Model parameter	Symbol	Unit	UF	Status
Concentration in agricultural soil	$Ctot_{agr}$	[kg.kg^{-1}]	M	Output soil/groundw.
Concentration in air	C_{air}	[kg.m^{-3}]	L	Output air module
BCF from soil to plant stem	$BCFstem_{plant}$	[kg.kg^{-1}]	L	Data entry/filling
BCF from air to plant stem	$BCFair_{plant}$	[m^3.kg^{-1}]	M	Data entry/filling
BCF from soil to root	$BCFroot_{plant}$	[kg.kg^{-1}]	L	Data entry/filling

model calculation

$$C_{stem} = Ctot_{agr} \cdot BCFstem_{plant} + C_{air} \cdot BCFair_{plant}$$

$$C_{root} = Ctot_{agr} \cdot BCFroot_{plant}$$

uncertainty in model results

Uncertainties in root and stem concentrations cannot be assessed analytically because $Ctot_{agr}$ and $BCFair_{plant}$ are not distributed lognormally. Furthermore, for concentrations in stem, a summation is necessary.

3.7.5. Concentration in meat and milk

Scenario	*Comments*
Typical characteristics of a (by default) Dutch Agricultural soil are taken	Median case assumption
Average characteristics of plants are taken	Median case assumption

For cattle, the situation is somewhat more complex. Cows will be exposed by eating grass and adhering soil, and breathing polluted air. All these contributions are summed. The concentration in meat and milk is assumed to be in equilibrium with the cow's daily intake of the substance.

input parameters

Model parameter	Symbol	Unit	UF	Status
Concentration in agricultural soil	$Ctot_{agr}$	[kg.kg^{-1}]	M	Output soil/groundw.
Concentration in air	C_{air}	[kg.m^{-3}]	L	Output air module
Concentration in stems of plants	C_{stem}	[kg.kg^{-1}]	M	Output food module
Conversion dry to fresh wt. plant	CF_{plant}	[kg.kg^{-1}]	1	Scenario defined
Density of soil	RHO_{soil}	[kg.m^{-3}]	1	Scenario defined
Density of solids in soil	RHOsolids	[kg.m^{-3}]	1	Scenario defined
Fraction solids in soil	$Fsolid_{soil}$	[-]	1	Scenario defined
Daily intake of grass	IC_{plant}	[kg.d^{-1}]	n.a.	Variab. ignored
Daily intake of soil	IC_{soil}	[kg.d^{-1}]	n.a.	Variab. ignored
Daily intake of air	IC_{air}	[m^3.d^{-1}]	n.a.	Variab. ignored

The inter-individual variability in the cow's daily intake can be ignored. Humans consume products from many cows. Therefore, this variability tends to average out.

model calculation

$$CONVsoil = \frac{RHO_{soil}}{RHOsolid \cdot Fsolid_{soil}}$$

$$C_{meat} = BCF_{meat} \cdot (C_{stem} \cdot IC_{plant} \cdot CF_{plant} + Ctot_{agr} \cdot IC_{soil} \cdot CF_{soil} + C_{air} \cdot IC_{air})$$

$$C_{milk} = BCF_{milk} \cdot (C_{stem} \cdot IC_{plant} \cdot CF_{plant} + Ctot_{agr} \cdot IC_{soil} \cdot CF_{soil} + C_{air} \cdot IC_{air})$$

uncertainty in model results

Due to several summations, analytical calculation of uncertainties is not possible.

3.8. Total daily intake

Scenario	*Comments*
Only adults are assessed, therefore, all physiological parameters and consumption patterns are relevant for adults.	Best case. Exposure assessment for children may be added in the future.
The human assessed will only be exposed to 'yearly average' concentrations in media and products.	Median case, the influence of peak concentrations on chronic exposure cannot be predicted in general.

In this sub-module, the contributions of the chemicals in the intake media for humans are summed to derive a total daily intake. The uncertainties in intake rates may very well be correlated (e.g., a person consuming more fish, is likely to consume less meat). The scenario looks more worst case than it is, as usually, only one or two routes make up 95% of the total human exposure.

input parameters

Model parameter	Symbol	Unit	UF	Status
Conc. in drinking water	C_{drw}	[kg.m^{-3}]	L/M	Output food module
Conc. in fish	C_{fish}	[kg.kg^{-1}]	L	Output food module
Conc. in leaf crops	C_{stem}	[kg.kg^{-1}]	M	Output food module
Conc. in root crops	C_{root}	[kg.kg^{-1}]	M	Output food module
Conc. in meat	C_{meat}	[kg.kg^{-1}]	M	Output food module
Conc. in milk	C_{milk}	[kg.kg^{-1}]	M	Output food module
Conc. in air	C_{air}	[kg.m^{-3}]	L	Output air module
Daily intake of drinking water	IH_{drw}	[m^3.d^{-1}]	2	Temporary value
Daily intake of fish	IH_{fish}	[kg.d^{-1}]	2	Temporary value
Daily intake of leaf crops	$IH_{leaf\ crops}$	[kg.d^{-1}]	2	Temporary value
Daily intake of root crops	$IH_{root\ crops}$	[kg.d^{-1}]	2	Temporary value
Daily intake of meat	IH_{meat}	[kg.d^{-1}]	2	Temporary value
Daily intake of dairy products	IH_{dairy}	[kg.d^{-1}]	2	Temporary value
Daily ventilation rate	IH_{air}	[m^3.d^{-1}]	2	Temporary value
Bioavailability for inhalation	BIO_{air}	[-]	1	Temporary value
Average human bodyweight	BW	[kg]	1.5	Temporary value

Uncertainties in intakes for the Dutch population can be derived from the extensive research of the ministry of Public Health (WVC, 1992). This was not yet performed, therefore, temporary, rough estimates are given.

model calculations

Dosages in $kg.kg^{-1}.d^{-1}$ can be calculated for each medium as follows:

$$DOSE_i = \frac{C_i \cdot IH_i \cdot BIO_{route}}{BW}$$

with i ∈ {drinking water,fish,root crops,leaf crops,meat,milk,air}

Uncertainty in bioavailability through the oral route will be ignored. Bioavailability through the oral route is considered to be comparable to the bioavailability encountered in the toxicity test with the experimental animals.

The total dose can than be calculated as:

$$DOSE_{tot} = \sum_{for\,all\,i} DOSE_i$$

uncertainty in model results

It is clear from the calculations above that this module uses summations extensively. Therefore, Monte Carlo analysis cannot be avoided. It can be expected that intake rates are correlated with each other and with the body weight of humans.

3.9. Effects assessment

In this module, No-Effect-Concentrations (NECs) are derived from single species toxicity tests. Unfortunately, the extrapolation procedures applying fixed safety factors are worst case, aiming to protect the entire ecosystem. As a consequence, uncertainty analysis for this module will be postponed until more information on distribution of sensitivities of organisms in an ecosystem can be incorporated. The NEC is a very important part of the hazard ratio, just as important as the PEC. Therefore, research for the uncertainties involved in this extrapolation procedure is required.

When a sufficient number of NOECs (at least 4 for different taxonomic groups) is given in the data set, a statistical extrapolation procedure is applied to arrive at an NEC (Aldenberg & Slob, 1993). This approach offers the possibility for calculating the uncertainty in the NEC. However, because the data set available for risk assessment is usually too small to apply this method, this option will not be worked out in this report.

When no terrestrial toxicity data are given, equilibrium partitioning theory is applied to translate aquatic toxicity data to indicative terrestrial toxicity values. In this method, the soil-water partitioning coefficient ($K_{soil\text{-}water}$) is used. Uncertainty in this parameter may be taken into account.

input parameters

Model parameter	Symbol	Unit	UF	Status
Aquatic LC50 for each species	$LC50aqua_{species}$	$[kg.m^{-3}]$	n.a.	Data entry
Aquatic NOEC for each species	$NOECaqua_{species}$	$[kg.m^{-3}]$	n.a.	Data entry
Soil-water part. coeff.	$K_{soil-water}$	$[m^3.m^{-3}]$	L	Data entry/filling
Bulk density of soil	RHO_{soil}	$[kg.m^{-3}]$	1	Scenario defined

model calculation

$$LC50terr_{species} = \frac{K_{soil-water}}{RHO_{soil}} \cdot LC50aqua_{species}$$

$$NOECterr_{species} = \frac{K_{soil-water}}{RHO_{soil}} \cdot NOECaqua_{species}$$

uncertainty in model results

Uncertainty in the resulting terrestrial NEC will simply be equal to the uncertainty in the soil-water partitioning coefficient.

3.10. Risk characterisation

In this module, the final calculation of the PEC/NEC quotients for the different endpoints takes place.

input parameters

Model parameter	Symbol	Unit	UF	Status
Conc. in STP aeration tank	$Ctot_{AT}$	[kg.m^{-3}]	L	Output STP
Conc. surf. water during episode	$Cdiss_{surf,epi}$	[kg.m^{-3}]	L	Output surf. water
Concentration in agricultural soil	$Ctot_{agr}$	[kg.kg^{-1}]	M	Output soil/groundw.
Concentration in fish	C_{fish}	[kg.kg^{-1}]	L	Output food module
Concentration in earthworms	C_{worm}	[kg.kg^{-1}]	M	Output food module
Total dose for humans	DOSEtot	[kg.kg^{-1}.d^{-1}]	M	Output tot. daily intake
NEC for micro-organisms STP	NEC_{micro}	[kg.m^{-3}]	1	Output effects ass.
NEC aquatic organisms	$NECaqua_{ass}$	[kg.m^{-3}]	1	Output effects ass.
NEC terrestrial organisms	$NECterr_{ass}$	[kg.kg^{-1}]	1	Output effects ass.
NEC terr. org. equilibrium part.	$NECterr_{EP}$	[kg.kg^{-1}]	L	Output effects ass.
NEC for predators in food	$NECfood_{pred}$	[kg.kg-1]	1	Output effects ass.
NOAEL for mammals (rat)	$NOAEL_{mammal,oral}$	[kg.kg-1.d-1]	1	Data entry

model calculations

$$HAZARD_{micro} = \frac{Ctot_{AT}}{NEC_{micro}}$$

$$HAZARD_{aqua} = \frac{Cdiss_{surf,epi}}{NECaqua_{ass}}$$

$$HAZARD_{terr} = \frac{Ctot_{agr}}{NECterr_{ass}}$$

$$HAZARD_{terrEP} = \frac{Ctot_{agr}}{NECterr_{EP}}$$

$$HAZARDaqua_{pred} = \frac{C_{fish}}{NECfood_{pred}}$$

$$HAZARDterr_{pred} = \frac{C_{worm}}{NECfood_{pred}}$$

$$MOS = \frac{NOAEL_{mammal,oral}}{DOSEtot}$$

The hazard quotients for aquatic organisms and the micro-organisms in the STP can be calculated analytically. For the other endpoints, Monte Carlo methods are required.

4. SUMMARY OF UNCERTAINTIES

In the table below, all the uncertain parameters are displayed with the (provisional) uncertainty factors (UF) and comments as discussed in the previous chapter. This simplifies the incorporation in the USES system, and reveals where further investigation should be done.

Model parameter	Symbol	Unit	UF	Comments
Molecular weight	MOLW	[kg.mol^{-1}]	1	Data entry
Production volume	TONNAGE	[kg.s^{-1}]	1	Data entry
Melting point	TEMPmelt	[K]	1	Data entry
Vapour pressure	VP	[Pa]	1	Data entry
Octanol-water partition coeff.	Kow	[-]	1	Data entry
Octanol-water partition coeff.	Kow	[-]	7.7	if TEMPmelt is given
			8.5	if no TEMPmelt is given from Isnard & Lambert (1989)
Water solubility	SOL	[kg.m^{-3}]	1	Data entry
Water solubility	SOL	[kg.m^{-3}]	13	if TEMPmelt is given
			17	if no TEMPmelt given from Isnard & Lambert (1989)
Result of standard screening test	PASSreadytest	[yes/no]	n.a.	Data entry
Const. of Junge equation	CONjunge	[Pa.m]	3	Temporary, estimated roughly from Noordijk & De Leeuw (1991)
Surface area aerosol particles	SURFaer	[m^2.m^{-3}]	2	Temporary, estimated roughly from Noordijk & De Leeuw (1991)
Uncertainty of the product of *CONjunge* and *SURFaer* can be calculated analytically since both uncertainties are assumed lognormal, and not correlated. This leads to an uncertainty factor of 3.7 for the product, using the formula in section 2.2.				
Regression coeff.	a	[m^3.kg^{-1}]	5.1	From McKone (1993)
Bioconc. factor for fish	BCF_{fish}	[l.kg^{-1}]	9.1	derived from regression on data set of Veith & Kosian (1983)
Part. coeff. worm-porewater	$K_{worm\text{-}porew}$	[l.kg^{-1}]	17	Derived from regression on data set of Connell & Markwell (1990)
Transp. stream conc. factor	TSCF	[-]	1	Ignored (incorporated into SCF)
Stem conc. factor	SCF	[m^3.kg^{-1}]	6	Temporary, estimated roughly from Polder *et al.* (1994)
Root-porew. part. coeff.	$K_{root\text{-}porew}$	[m^3.kg^{-1}]	6	Temporary, estimated roughly from Polder *et al.* (1994)
Aerosol-plant part. coeff.	$K_{aerosol\text{-}plant}$	[m^3.kg^{-1}]	8.4	From McKone (1993)
Fraction air in plant	$Fair_{plant}$	[m^3.m^{-3}]	n.a.	Incl. in UF $K_{gas\text{-}plant}$
Fraction water in plant	$Fwater_{plant}$	[m^3.m^{-3}]	n.a.	Incl. in UF $K_{gas\text{-}plant}$
Fraction lipids in plant	$Flipid_{plant}$	[m^3.m^{-3}]	n.a.	Incl. in UF $K_{gas\text{-}plant}$
Bulk density of plant	RHO_{plant}	[kg.m^{-3}]	1	Temporary
Gas-plant part. coeff.	$K_{gas\text{-}plant}$	[m^3.kg^{-1}]	25	Derived from analysis of data Bacci *et al.* (1990)
Bioconc. factor for meat	BCF_{meat}	[d.kg^{-1}]	64	Calculated from Travis & Arms (1988)
Bioconc. factor for milk	BCF_{milk}	[d.kg^{-1}]	36	Calculated from Travis & Arms (1988)

Model parameter	Symbol	Unit	UF	Comments
Fraction of tonnage to air	$Fair_{release}$	[-]	L	from tables
Fraction of tonnage to wastew.	$Fwater_{release}$	[-]	L	from tables
Fraction from main source	$F_{mainsource}$	[-]	L	from tables
First order degr. rate constant STP	$kdeg_{stp}$	[s^{-1}]	n.a.	ignored in calculations
Fr. of emission redirected to air	F_{air}	[-]	1.5	Estimated from Struijs *et al.* (1991)
Fr. of emission to surf. water	$F_{tot,surf}$	[-]	2	De Greef & De Nijs (1990)
Fr. of emission to sludge	F_{sludge}	[-]	2	Estimated from Struijs *et al.* (1991)
Fr. of emission degraded	$F_{degraded}$	[-]	1	Not used in calc.
Dilution factor in surface water	DILUTION	[-]	148*	Research De Greef & De Nijs (1990)
Effluent discharge of STP	$EFFLUENT_{stp}$	[$m^3.s^{-1}$]	1	Included in UF dilution
*This value includes the uncertainty in effluent discharge				
Standard conc. from OPS model	$Cstd_{air}$	[$kg.m^{-3}$]	2	Temporary, estimated from Noordijk & De Leeuw (1991)
Standard dep. flux aerosols OPS	$Dstd_{aer}$	[$kg.m^{-2}.s^{-1}$]	10	Temporary, estimated from Noordijk & De Leeuw (1991)
Standard dep. flux gas from OPS	$Dstd_{gas}$	[$kg.m^{-2}.s^{-1}$]	10	Temporary, estimated from Noordijk & De Leeuw (1991)
Disappearance rate constant	$kdis_{soil}$	[-]	5	Temporary, initial guess by expert
Maximum conc. in groundwater	$Cgrw_{table}$	[$kg.m^{-3}$]	10	Temporary, initial guess by expert
Daily intake of grass	IC_{plant}	[$kg.d^{-1}$]	n.a.	Variab. ignored
Daily intake of soil	IC_{soil}	[$kg.d^{-1}$]	n.a.	Variab. ignored
Daily intake of air	IC_{air}	[$m^3.d^{-1}$]	n.a.	Variab. ignored
Daily intake of drinking water	IH_{drw}	[$m^3.d^{-1}$]	2	Temporary estimate
Daily intake of fish	IH_{fish}	[$kg.d^{-1}$]	2	Temporary estimate
Daily intake of leaf crops	$IH_{leaf\ crops}$	[$kg.d^{-1}$]	2	Temporary estimate
Daily intake of root crops	$IH_{root\ crops}$	[$kg.d^{-1}$]	2	Temporary estimate
Daily intake of meat	IH_{meat}	[$kg.d^{-1}$]	2	Temporary estimate
Daily intake of dairy products	IH_{dairy}	[$kg.d^{-1}$]	2	Temporary estimate
Daily ventilation rate	IH_{air}	[$m^3.d^{-1}$]	2	Temporary estimate
Bioavailability for inhalation	BIO_{air}	[-]	1	Temporary estimate
Average human bodyweight	BW	[kg]	1.5	Temporary estimate

n.a. : not applicable

L : value is variable, but follows a lognormal distribution

In the following table, all of the parameters are show which are defined by the exposure scenario, and are therefore without uncertainty. In further research it can be examined whether uncertainty in these parameters can be accounted for.

Model parameter	Symbol	Unit	UF	Comments
Fraction air in soil	$Fair_{soil}$	$[m^3.m^{-3}]$	1	Defined in scenario
Fraction water in soil	$Fwater_{soil}$	$[m^3.m^{-3}]$	1	Defined in scenario
Volumefraction solids of soil	$Fsolid_{soil}$	$[m^3.m^{-3}]$	1	Scenario defined
Density of air	RHOair	$[kg.m^{-3}]$	1	Defined in scenario
Density of water	RHOwater	$[kg.m^{-3}]$	1	Defined in scneario
Density of solids	RHOsolid	$[kg.m^{-3}]$	1	Defined in scenario
Gas constant (8.314)	R	$[Pa.m^3.mol^{-1}.K^{-1}]$	1	Constant
Temperature air-water interface	TEMP	[K]	1	Scenario defined
Fraction organic carbon in soil	Foc_{soil}	$[kg.kg^{-1}]$	1	Scenario defined
Fraction organic carbon in susp.	Foc_{susp}	$[kg.kg^{-1}]$	1	Scenario defined
Frac. oc in susp. STP prim. solver	Foc_{suspPS}	$[kg.kg^{-1}]$	1	Scenario defined
Frac. oc in susp. of AT and SLS	$Foc_{suspATSLS}$	$[kg.kg_{-1}]$	1	Scenario defined
Volumefraction water of susp.	$Fwater_{susp}$	$[m^3.m^{-3}]$	1	Scenario defined
Volumefraction solids of susp.	$Fsolid_{susp}$	$[m^3.m^{-3}]$	1	Scenario defined
Conc. of bacteria in the test water	$BACT_{test}$	$[cfu.m^{-3}]$	1	Scenario defined
Conc. of bacteria reported in soil	$BACT_{soil}$	$[cfu.kg^{-1}]$	1	Scenario defined
[characteristics of the average STP]			1	Scenario defined
Concentration susp. in surf. water	$SUSPCONC_{surf}$	$[kg.m^{-3}]$	1	Scenario defined
Rate of sludge production	$SLUDGE_{stp}$	$[kg.s^{-1}]$	1	Scenario defined
Amount of sludge applied	$APPL_{sludge}$	$[kg.ha^{-1}.yr^{-1}]$	1	Scenario defined
Mixing depth of soil	$DEPTH_{soil}$	[m]	1	Scenario defined
Exposure period considered	EXP	[d]	1	Scenario defined
Purification factors	PURF	[-]	1	Scenario defined (worst case)
Conversion dry to fresh wt. plant	CF_{plant}	$[kg.kg^{-1}]$	1	Scenario defined

5. DISCUSSION

In risk assessment we are dealing with inherently uncertain situations. From a scientific point of view, it is advisable that this uncertainty is taken into account in the decision-making process. Furthermore, an uncertainty analysis can identify the main sources of uncertainty in the risk estimate, which is extremely helpful in the refinement of the risk assessment. This clearly shows the need to extend the present uncertainty analysis of USES for the aquatic organisms and micro-organisms to other end-points. In the previous chapters, enough work has been described to implement an uncertainty analysis, covering the entire local exposure model, into USES. This analysis proposed here, is limited due to pragmatic choices made. It only covers the exposure part of the hazard quotient, many uncertainties are not taken into account (e.g., parameters defined by scenario choices), correlations between parameters are ignored, lognormal distributions are assumed, several uncertainties are only provisionally quantified. However, this analysis is a starting point, already showing several aspects of uncertainties in the risk assessment process with USES in a simple and straightforward manner. Depending on the developments of USES, the analysis of uncertainties can be more extensively examined in the future.

For human risk assessment, the outcome of an uncertainty analysis as proposed here would be the uncertainty attached to placing a random, adult individual in a strictly defined (realistic worst case) exposure situation. The described approach is practically feasible on a short term. In 1995 and 1996, a European risk assessment system will be developed, based on USES 1.0. A detailed uncertainty analysis of USES 1.0 is not advisable as model calculations may change. The approach described in this report can be implemented relatively easily in this European system. In view of these rapid developments it is advisable, from a scientific point of view, that any new model to be incorporated into the system is accompanied by a quantification of the uncertainties in that calculation.

The boundary conditions for the analysis are:
- Short time for calculations so it can be applied in routine assessments.
- Results must be easily interpretable for non-experts.
- The analysis must be done on-line for each substance assessed.

Some work has already been done by Slob & De Nijs (1989), completing an uncertainty analysis for the local aquatic ecosystem and micro-organisms in the sewage treatment plant. Uncertainties in emission, treatment, and dilution where taken into account. This analysis was incorporated into USES 1.0. The calculations for this part of the model are strictly multiplicative, no summations occur. Lognormal uncertainties where assumed to facilitate the analytical uncertainty approach.

As discussed in section 2.2, a multiplicative model with lognormal uncertainties has advantages for an uncertainty analysis: the calculation can be done analytically (Slob, 1994). This means that an exact answer can be derived with a simple calculation. Monte Carlo analysis puts no restrictions on model formulation and uncertainty distribution, but is relatively time-consuming, and the result will always be an approximation of the true parameter distribution. Luckily, many parameters in the real world can be accurately

described with lognormal distributions (Slob, 1987). In view of the boundary conditions posed to the analysis, we propose to use the analytical method as much as possible. Furthermore, we will restrict the analysis to the parameters not defined in the exposure scenario of USES. Uncertainties due to the scenario choices made will be extremely difficult (or even impossible) to take into account. Due to this choice, it is important to explicitly define the list of scenario conditions (which parameters are part of the definition, and which not). In the course of the development of the EU risk assessment system, as planned for 1995/1996, it is advisable to critically discuss the realism of this exposure scenario. The scenario does not necessarily have to be median or average case. A realistic worst case scenario is very useful, as long as it is clear for the user *how* realistic or unrealistic it is. This procedure is seen as a conceptual validation of USES, and is elaborated in a separate report (Jager, 1995), together with a discussion of the scenario choices and other assumptions.

Unfortunately, USES is not entirely a multiplicative model, summations are present in several calculations. This makes a simple analytical combination of all uncertainties impossible. However, the analytical method can be used for many of the calculations. For the summations we must use numerical methods (Monte Carlo sampling), but some summations can be solved (see section 2.3). A combination of these methods must be implemented in USES. As discussed in the previous chapters, the search for lognormal distributions leads to several points of attention in the analysis:

- Uncertainties in input parameters can sometimes not be taken into account (e.g., uncertainty in *Kow* in deriving *BCF*s, uncertainty in input parameters STP).
- Sometimes, lognormal distributions are not a very appropriate choice (e.g., for fractions, which have an upper boundary of 1, whereas lognormal distributions do not have an upper boundary at all).
- For several summations with one fixed parameter, and one parameter with a lognormal distribution, an approach is used to estimate the resulting distribution with a lognormal one.

We recommend that these 'attention points' are kept in mind when interpreting the resulting uncertainty in the hazard quotient. Nevertheless, the proposed analysis offers the possibility to roughly assess uncertainties in the entire local exposure model in a quick and transparent manner. If the analysis of this report is implemented in a following version of USES, and when experience is gained, a more extensive analysis can be developed. It should especially be stressed that when *Kow* is estimated, instead of measured, the uncertainty in the hazard quotients is underestimated. In many of the estimation routines, *Kow* is prominently present, but uncertainty cannot be taken into account without a full scale Monte Carlo analysis. A solution to this potential problem is to implement two separate uncertainty approaches in USES:

- A combination of analytical calculations with Monte Carlo analysis for a quick routine assessment of the uncertainties in the PEC/NEC ratio.
- A full scale Monte Carlo analysis for a more in-depth assessment of the uncertainties in the cases where there is an indication of unacceptable risks (this could include identification of the main sources of uncertainty).

It should however, be noted that *Kow* and water solubility are required parameters in the data sets for new and existing chemicals and also in the base set for pesticides. Therefore, the estimation routines for *Kow* and water solubility will seldom be necessary. However, measured *Kow* values will likely have a substantial measurement error. The influence of

measurement errors needs further investigation.

Collection of uncertainty factors does not form a major problem. Many of these values can be estimated from literature, validation attempts, or by expert judgement. Especially the link with validation offers interesting opportunities. When a large amount of experimental data is gathered to validate parts of the system, these data can also be used to fine-tune QSARs, and to derive uncertainty distributions for a given parameter. Validation will also benefit from uncertainty analysis since uncertainty analysis can serve to set priorities for validation activities. The parts of the system which contribute the most to the overall uncertainty, are the first to be subjected to validation.

Uncertainty analysis offers the possibility to take the uncertainty in the results of data gap filling (e.g., estimation of *BCFs*) into account. This could provide a stimulus for the notifier to submit measured data, thus diminishing the uncertainty in the final results (even if the hazard quotient increases). In this report, we have ignored uncertainty in input parameters for the time being. The possibility should be examined for the user to enter or change uncertainties for a parameter. This approach needs some further discussion because uncertainties in measured data can also be very large. The way in which the decision-maker can handle uncertainty also needs elaboration. Too avoid too much fixation on the quantitative value of the uncertainty analysis, we propose to show only the probability that PEC exceeds NEC. This information shows the decision-maker the (at least relative) probability that a wrong decision is made.

In this report, we have only addressed uncertainty in the exposure levels (the nominator). The denominator of the risk quotient, the NEC, remains untouched. It may be a good idea to try to say something more about this uncertainty, and maybe quantify it. This quantification should be addressed separately by experts in the field of (eco)toxicology. As these uncertainties will have a large influence on the total uncertainty in the risk quotient (being the ratio of PEC and NEC), quantification of these uncertainties is required. This is difficult because the extrapolation of NECs, using extrapolation factors, is relatively worst case. The uncertainty in the margin of safety (MOS), as done for humans, can be addressed more accurately since no extrapolation to a safe level is performed. The use of statistical extrapolation methods, as the method of Aldenberg & Slob (1993), offers the possibility to more accurately assess uncertainties, since the distribution of sensitivities of organisms in the ecosystem is estimated. However, the applicability of this method is limited because it requires at least 4 NOEC values. It is concluded that uncertainty analysis of the effects assessment needs further elaboration. Much work is already done at the RIVM, but this information still needs to be assessed for its applicability in USES.

Uncertainty analysis of the consumer exposure module is not discussed in this report. This module is currently examined in the framework of the RIVM project Human Exposure subproject Consumer Exposure (see Van Veen *et al.*, 1994). The tools to estimate consumer exposure are available in the form of the CONSEXPO program (Van Veen, manual of CONSEXPO in prep.). This package also includes the possibility to perform an uncertainty analysis (using Monte Carlo analysis). Therefore, analysis of uncertainties can be performed outside USES.

As a last warning, uncertainty analysis is important, but the relevance should not be

exaggerated. The attention points as mentioned above, should be taken into account when interpreting the uncertainty in the final results. Furthermore, uncertainty analysis gives little insight in the uncertainty caused by improper model formulation or model use. Only uncertainty in parameters is accounted for, and not uncertainty in the structure and linking of the models. When QSARs are applied outside of their ranges and boundary conditions, uncertainty may be much larger. This also clarifies the link between uncertainty analysis and validation. Conceptual validation should indicate the validity of model use and relevance of the model assumptions (for a more in-depth discussion of validation of USES, see Jager, 1995). Validation activities can also be used to assess 'overall' uncertainties for a model or a parameter. The other way around, uncertainty analysis can identify the parameters responsible for a large contribution to the uncertainty in the final results, and therefore, steer validation.

Testing of the uncertainty analysis could not be finished in the framework of this report. For this testing, USES was programmed in Microsoft Excel®. With this spreadsheet version of USES, uncertainty analysis can be performed rapidly and transparently with Crystal Ball® (using Monte Carlo analysis). Several substances with different properties need to be selected, as it can be expected that uncertainties in the risk estimate depend strongly on the properties of the substance. The physico-chemical properties and the emission pattern of the substance govern the distribution routes of the substance. The uncertainties in the risk estimate will be different for each route (e.g., it can be expected that the uncertainties in human exposure will be small when inhalation of air is the main exposure route, but much larger when intake of meat or milk is most important). Testing of this uncertainty analysis gives more insight in the functioning of the analysis and the main sources of uncertainty. If proper testing can take place in 1995, the results will be reported as an annex to the current report. Extensive testing is advisable before this analysis is implemented in the European risk assessment system.

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APPENDIX 1: Derivation of uncertainty factors from data sets, figures

A1.1. Bioconcentration in fish

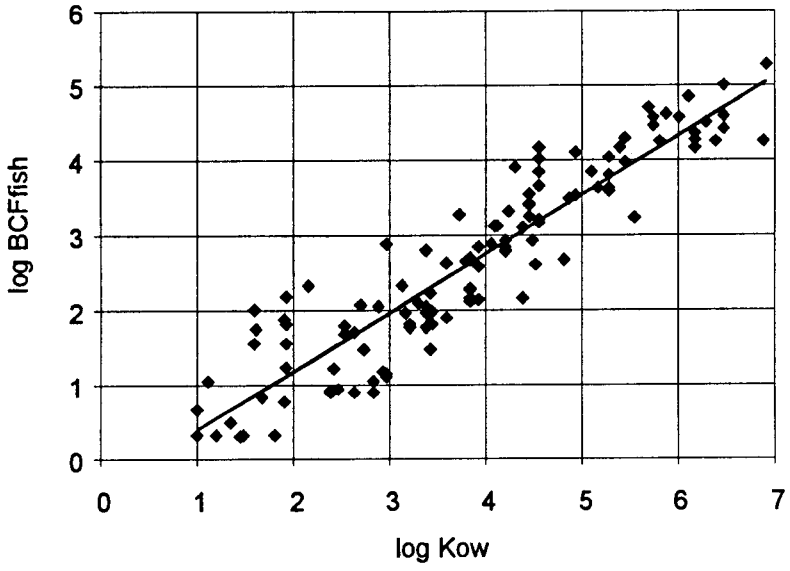

Figure A1 *Linear regression of log BCF for fish from the data set of Veith & Kosian (1983) against log Kow.*

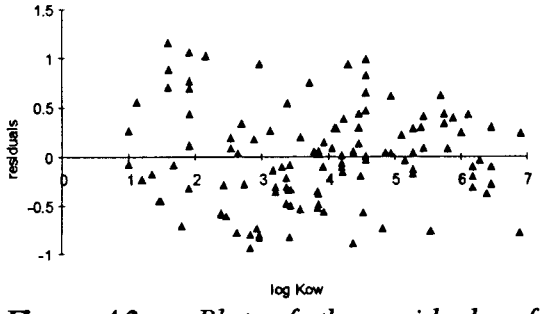

Figure A3 *Plot of the residuals of the linear regression against Kow.*

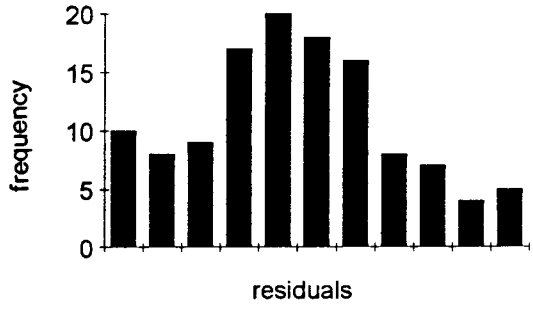

Figure A2 *Frequency distribution of the residuals of the linear regression.*

A1.2. Bioconcentration in earthworms

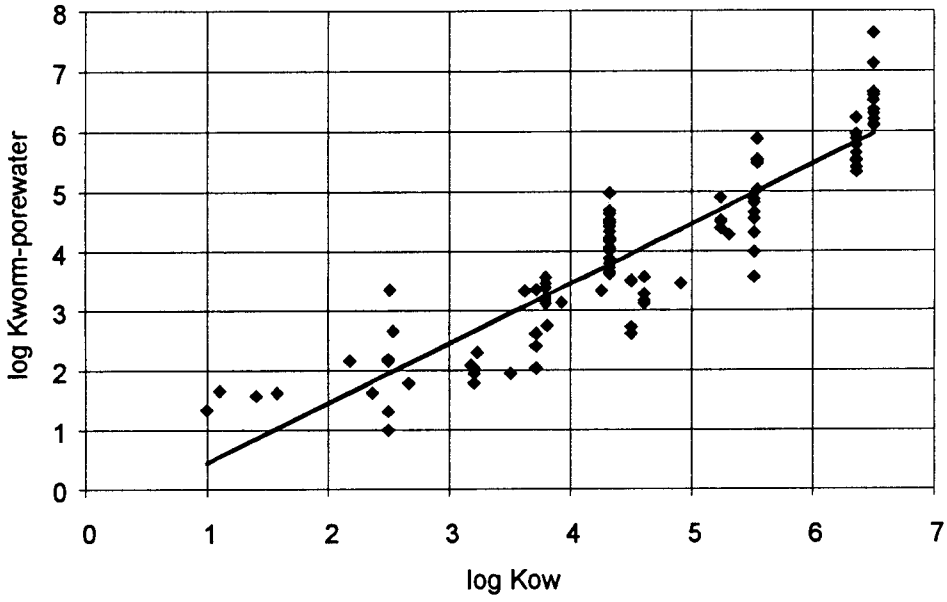

Figure A4 *Linear regression of log $K_{worm\text{-}porew}$ from the data set of Connell & Markwell (1990) against log Kow.*

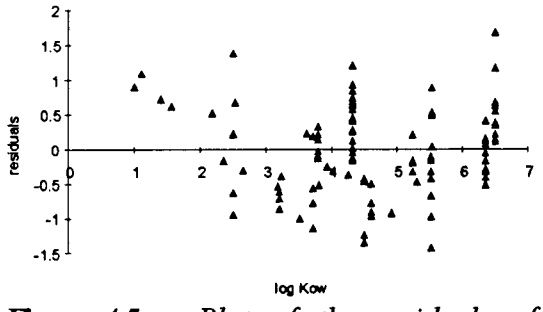

Figure A5 *Plot of the residuals of the linear regression against Kow.*

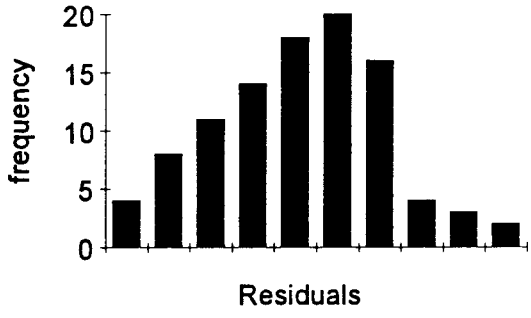

Figure A6 *Frequency distribution of the residuals of the linear regression.*

A1.3. Uptake of plants from air

In the following figure, BCF is expressed as $[m_{air}^{3}.m_{leaf}^{-3}]$

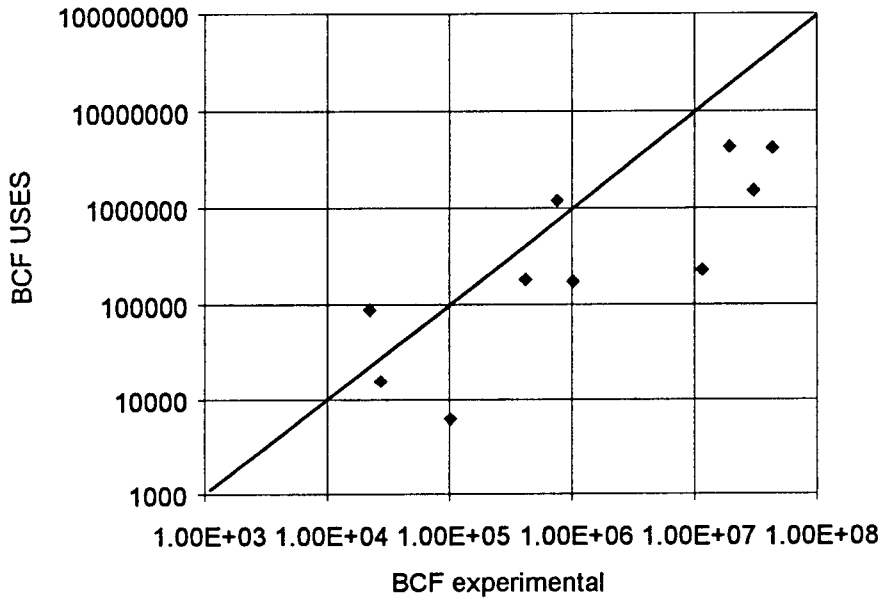

Figure A7 *The BCF between gas-phase and plant leafs estimated by USES, compared to experimental results of Bacci et al. (1990).*

A1.4. Biotransformation from uptake cow to meat

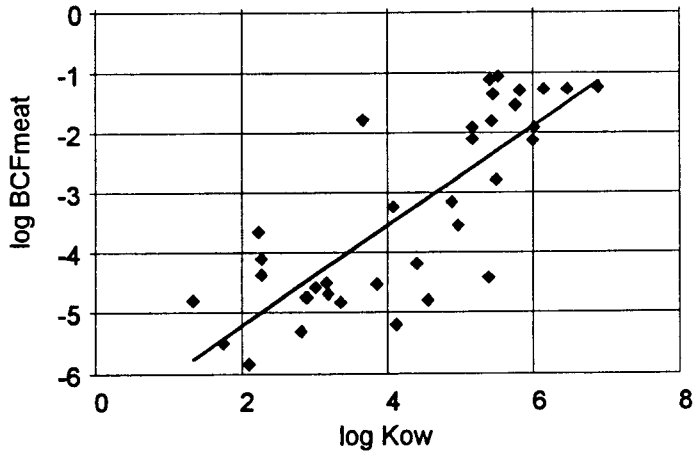

Figure A8 *Linear regression of log BCF_{meat} for cattle from the data set of Travis & Arms (1988) against log Kow.*

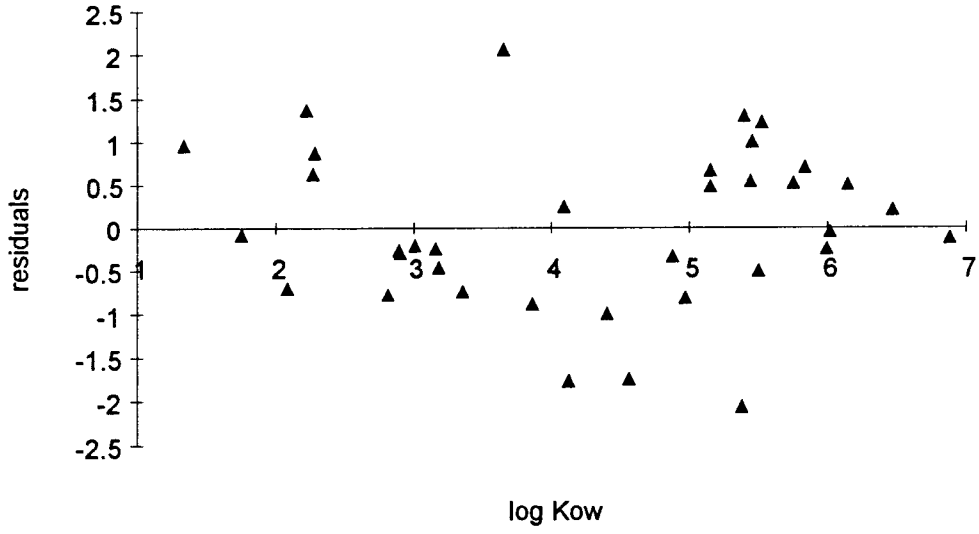

Figure A9 *Plot of the residuals of the linear regression against Kow.*

A1.5. Biotransformation from uptake cow to milk

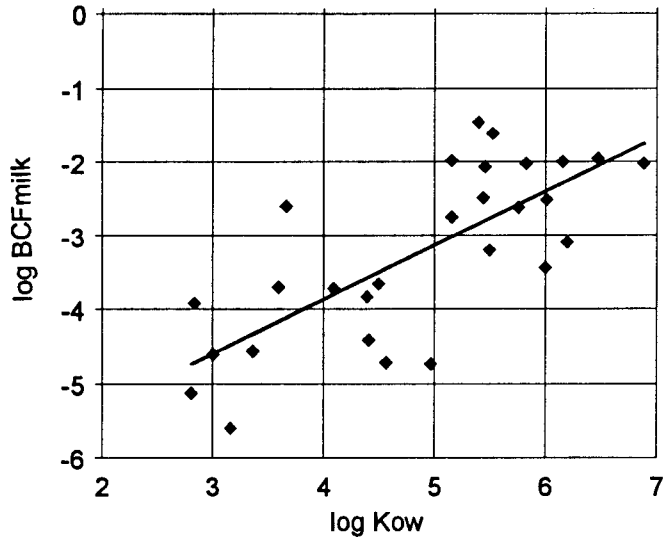

Figure A10 *Linear regression of log BCF_{milk} for cattle from the data set of Travis & Arms (1988) against log Kow.*

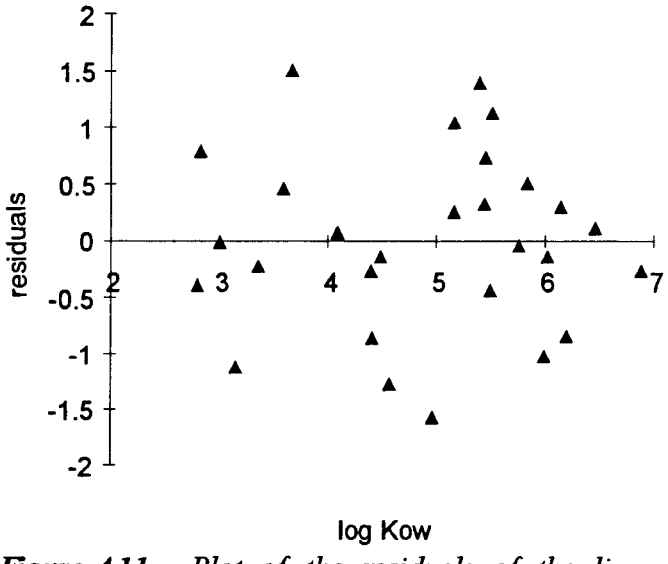

Figure A11 *Plot of the residuals of the linear regression against Kow.*