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**Evaluation of EUSES: inventory of experiences
and validation activities**

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Abstract

This report discusses the validation status of the European Union System for the Evaluation of Substances (EUSES). The individual models implemented in EUSES are discussed, as well as the problems encountered when applying the system in daily practice. EUSES can be concluded to deliver normally conservative estimates for a standard exposure scenario not usually directly comparable to measured data. Several modules, particularly release estimation, biodegradation, the exposure scenario, workplace exposure and environmental effects assessments, can be characterised as conservative. EUSES is not particularly suited for the assessment of chemicals outside the neutral organic compounds.

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Samenvatting

Het “European Union System for the Evaluation of Substances” (EUSES) wordt door de meeste EU-lidstaten gebruikt om de potentiële risico’s van nieuwe en bestaande industriële chemicaliën in te schatten. Ondanks dat het systeem uitgebreid toegepast wordt, blijft de validiteit onduidelijk. Dit rapport onderzoekt de validatiestatus van de individuele modellen die in EUSES geïmplementeerd zijn en bespreekt de problemen die in de dagelijkse praktijk optreden bij het gebruik van het systeem. Dit rapport kan dus risicobeoordelaars helpen bij het interpreteren en waarderen van de resultaten van het systeem en het rapport kan gebruikt worden bij de discussies rond updates van EUSES en de EU technische leidraad (TGD). Het valideren van een systeem als EUSES is niet recht-toe-recht-aan, omdat het systeem een conservatieve schatting geeft voor een standaard blootstellingsscenario welke meestal niet direct vergelijkbaar is met meetwaarden. Gezien de beschikbare data mag geconcludeerd worden dat de EUSES resultaten aanzienlijk kunnen afwijken van de werkelijkheid. Verscheidene modules kunnen als conservatief gekarakteriseerd worden, m.n.: emissieschattingen, biodegradatie, het blootstellingsscenario, blootstelling van werknemers en de effectbeoordeling voor het milieu. De schatting van partiticoëfficiënten en bioconcentratiefactoren is mediaan omdat meestal log-lineaire regressies toegepast worden. Het regionale verspreidingsmodel lijkt waarden op te leveren die aan de onderkant van de range aan meetgegevens liggen. De meeste problemen liggen in de emissieschatting. Dit wordt gedeeltelijk veroorzaakt door de beperkte flexibiliteit van de user-interface waardoor voor een aantal typen beschikbare gegevens handmatige berekeningen noodzakelijk zijn. Verder zijn de schattingen van de algemene tabellen nogal ruw en hun onzekerheid beïnvloedt de hele opvolgende modelketen. EUSES is niet direct toepasbaar voor de beoordeling van andere stoffen dan neutrale organische stoffen. EUSES is toegepast bij het maken van een risicobeoordelingsrapport voor zink, maar daarbij waren een groot aantal extra aannamen noodzakelijk.

Summary

The European Union System for the Evaluation of Substances (EUSES) is used by most EU Member States to estimate potential risks of new and existing industrial chemicals. Although the system is being used extensively, its validity remains unclear. This report investigates the validation status of the individual models implemented in EUSES and discusses the problems encountered when applying the system in daily practice. The current report may thus help risk assessors with the interpretation and appreciation of the results of the system and this report also provides input for the discussion on updates of EUSES and the EU-Technical Guidance Documents. Validating a system like EUSES is not straightforward as the system delivers a conservative estimate for a standard exposure scenario which is usually not directly comparable to measured data. From the available data, it is concluded that the degree of deviation from reality can be substantial for the EUSES results. Several modules can be characterised as conservative, especially: release estimation, biodegradation, the exposure scenario, workplace exposure, and the environmental effects assessments. The estimation of partition coefficients and bioconcentration factors is median case because a log-linear regression is usually applied. The regional distribution model seems to provide estimates on the lower end of the range of measured values. Most problems are encountered with the release estimation. Partly because of the limited flexibility of the user interface which requires manual calculation for several types of available inputs, partly because the estimates from the general tables are quite rough and their uncertainty affects the entire subsequent model chain. EUSES is not particularly suited for the assessment of chemicals other than neutral organic compounds. EUSES has been applied to produce a risk assessment report for zinc, but extra assumptions were required.

1. Introduction

Chemical risk assessment tries to protect humans and the environment from the possible adverse effects of substances. The methods for risk assessment of new and existing chemicals are harmonised between the EU Member States and laid down in Technical Guidance Documents (TGD) (EC, 1996). To ensure rapid and transparent assessments, the methodology of the TGD is implemented in a computerised system: the European Union System for the Evaluation of Substances (EUSES) (EC, 1996; Vermeire *et al.*, 1997). With this system, calculations can be performed for, in principle, all chemicals, based on a relatively limited amount of available data (e.g. the EC Base Set for new chemicals). The assessment should protect ecosystems and human populations but, for pragmatic reasons, several groups are defined for which a risk estimate is made; the so-called protection targets or endpoints as summarised in Table 1.

Table 1 protection targets in EUSES.

<p>Human populations:</p> <ul style="list-style-type: none"> • Workers • Consumers • Humans exposed via the environment <p>Ecological systems and populations</p> <ul style="list-style-type: none"> • Micro-organisms in sewage treatment systems • Aquatic ecosystems • Terrestrial ecosystems • Sediment ecosystems • Top predators
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EUSES became available in April of 1997 and is now extensively used in European risk assessment practice. It is important that the user of (results of) EUSES is aware of the "validity" of this system (see Table 2). It is difficult to specify the degree of certainty that a decision-maker needs when assessing the risks associated with chemicals¹. Furthermore, the degree of certainty depends heavily on the amount and quality of the input data: no system may be expected to provide accurate estimates of exposure and effects on the basis of base-set data alone. Nevertheless, the user of a system should be aware of the *degree* of (in)accuracy of the model so that this information can be taken into account (quantitatively or qualitatively) in the decision-making process. Therefore, the principle aim for validation of these types of systems should be to transparently show how well the model represents a part of reality (Jager, 1995). It is up to the decision maker to judge whether or not this accuracy is sufficient to justify risk reduction measures. Furthermore, it is important to indicate for *which* part of reality the model provides adequate results (Schwartz, 1997).

Table 2 Definitions on model validation (Van der Giessen (ed.), 1997).

<p>Validation: Proving the reliability, accuracy and usefulness of the model within the specified field of use.</p> <p>Validation should consist of:</p> <p>Conceptual validation: Are assumptions, choices and theories correct (or appropriate)? Mainly qualitative and referring.</p> <p>Algorithm validation/verification: Is the conceptual model translated correctly in mathematical formulations?</p> <p>Software validation/evaluation: Correctness and efficiency of the software code, quality of interfaces and documentation.</p> <p>Functional validation: Do model results sufficiently correspond with independent measurements, theoretical analysis, or other models?</p>
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A strict validation of systems like EUSES is not possible. Firstly, following Popper, it is only possible to *invalidate* a hypothesis. Secondly, the result of EUSES is a risk estimate²: a PEC/PNEC quotient (quotient of the Predicted Environmental Concentration and the Predicted No-Effect Concentration for an endpoint) or a Margin Of Safety (MOS). Both are designated by the term RCR (Risk Characterisation Ratio). These risk estimates are abstractions and cannot be determined in the real world. Nevertheless, an evaluation in a less strict manner should be performed to clarify the degree of

¹ Additionally, a model does not necessarily need to be accurate as long as the uncertainty in it is quantified and can be taken into account in decision-making (see Chapter 1.3).

² Strictly speaking, these quotients are not risk estimates as they do not quantify the incidence and severity of toxic effects. They are merely surrogate indicators for the unknown risk.

confidence in the final results. Parts of the system (modules or models) can be validated numerically. Exposure concentrations can be measured but one has to realise that measured data are usually not representative for the situation described by EUSES for two reasons:

1. In the absence of specific data, several chemical-specific parameters are set to worst-case values (e.g. release rates, degradation rates) and the assessment is performed for a worst-case exposure scenario, the so-called "standard environment". Measured field data will invariably be non-representative for this situation. The concept of a standard scenario clearly plays a crucial role in the assessment and its applicability and appropriateness should be considered in a model validation.
2. Most variations in time and space are averaged out in EUSES. It is not abnormal for the concentration of a chemical in sediment samples from within the same square meter to vary by more than a factor 10 or even 100 (ECETOC, 1992). This variation cannot be described by EUSES.

The use of a standard scenario does not mean that EUSES is "not valid". In fact, the purpose of EUSES is not to predict actual effects or concentrations occurring in the environment. In fact, the system will provide the user with a conservative estimate for a non-existing standard environment, based on limited data requirements. There are much better models or systems for the purpose of exposure prediction but they operate at much higher data needs and only for specific locations. The main purpose of EUSES is to distinguish potentially risky chemicals from "safe" chemicals based on a limited amount of data and to indicate where further data are needed to reach confident decisions. Naturally, this purpose will be served by appropriate and numerically valid sub-models but this should not be seen as a prerequisite for validity of the system as a whole. A more "holistic" form of system validation was investigated in an experiment with the "expert opinion" from a group of toxicologists (Jager, 1995) (discussed in more detail in Section 4.11). Although the results of this form of evaluation must be carefully interpreted, attempts like this may shed more light on the actual validity of EUSES.

1.1 Whole-system approaches

The purpose of this evaluation is to clarify the degree of accuracy of EUSES and to indicate fields of future work. Several validation activities have already been initiated or performed for parts of the system (SimpleBox, SimpleTreat, bioaccumulation, effects assessment, etc.). For the whole system, several validation projects need be mentioned. The predecessor of EUSES, USES 1.0 (RIVM *et al.*, 1994), was critically evaluated by Devillers *et al.* (1995). They recognised the considerable amount of work put into USES 1.0 but concluded that it could not be seen as more than a preliminary ("beta") release. Their main points of criticism were:

1. The documentation is unclear, difficult to read and understand.
2. Uncertainty analysis is required.
3. For several QSAR routines better alternatives are available. With the QSARs, no statistical parameters are provided to allow users to judge the accuracy.
4. The local models for air, surface water and soil/groundwater are insufficient.
5. Numerous small errors (e.g. in the emission tables).

Most of these points of criticism have been fixed in EUSES. However, uncertainty analysis was investigated (Jager & Slob, 1995; Jager, 1995; Jager *et al.*, 1997; Jager, in prep.) but is not yet implemented, and the local models for air and water were hardly changed. Jager (1995) discussed the validation status of the modules of USES 1.0 in detail. Validation has been fragmented, and insufficient so far. Especially a more conceptual validation is lacking. It should be noted that all errors, bugs, and "wishes" are being gathered in a so-called "blacklist" by the EUSES working group. This list will be used to update the system and is added to this report as Appendix 2.

Recently, a detailed three-year study was started to validate EUSES at the University of Osnabrück. The following items are planned in the project:

1. Quality of the software and documentation. Are models from the literature implemented correctly, are the model concepts and assumptions applicable. How are the user friendliness, error messages, transparency and documentation.
2. For which chemical classes and environmental sections does the model provide realistic estimates. For which chemical classes is the system (or parts thereof) not applicable.
3. Comparison with measured data for several chemicals from different chemical classes (especially field data).
4. Uncertainty and sensitivity analysis. Show model uncertainty given the uncertainty in the input parameters and show important input parameters.
5. Comparison with other models (e.g. CemoS, HAZCHEM, CalTOX). Check whether simpler models can be applied (e.g. a level II fugacity model instead of SimpleBox).

Recently, provisional results were presented (Schwartz *et al.*, 1997; Schwartz *et al.*, Accepted). After testing the software and reviewing the documentation, the authors considered EUSES to be a modern product which basically fulfilled the postulated quality criteria. Particularly with regard to correctness and stability no errors were found. Nevertheless, to use the program, a thorough understanding of the theory and applicability of the implemented models is necessary. This means that EUSES is targeted towards experts in risk assessment of chemicals. The evaluation was hampered by the fact that the source code of EUSES is not publicly available. EUSES contains some features which are not common in these types of programs: the possibility to use different units for input, testing plausibility of input values according to an advised range. However, the high complexity (multitude of dialogues and parameters), low modularity (fixed linear structure, it is very difficult to run models in isolation), and incomplete documentation (especially for SimpleBox and SimpleTreat) results in insufficient transparency and are emphasised as major point of criticism. The lack of a possibility for uncertainty analysis and assessment of ionising substances were also recognised as disadvantages. Some specific proposals for improvement of EUSES were given which should be entered in the discussion on future updates (the project will be finished by October 1999). Within this project, the food chain was validated (Schwartz, 1997). Considerable, but explicable, deviations from measured values were found (especially for metabolisable and very hydrophobic chemicals).

1.2 Criteria for validity

It is difficult to judge what degree of validity is required for EUSES and for its models. There are no explicit specifications of the risk assessors or risk managers what degree of accuracy is necessary for decision making. The "Kerngroep UBS" has selected several criteria which can be used in the discussion on implementation of new models in USES (see Table 3). These were not binding criteria but depend upon the state of the art and the availability of alternatives. Nevertheless, these criteria may serve to discuss a model's performance.

1.3 Relationship with uncertainty analysis

Currently, decisions on chemical safety are made on the basis of point estimates (PEC/PNEC and MOS). It is, however, advisable to take uncertainties in the risk assessment into account in the stage of decision making (at least from a scientific point of view). Furthermore, uncertainty analysis can also facilitate the question of "validity". When an uncertainty analysis is routinely applied to assessments, even generally applicable models with a poor performance can be applied as long as their uncertainty is quantified and accounted for in decision making. A procedure for probabilistic risk assessment in EUSES was outlined by Jager *et al.* (1997), discussing possibilities, options for risk characterisation

etc. This report was discussed with several representatives from the EU Member States and industry to investigate to which degree these proposals agree with their needs (Jager, in prep). Generally, there was sufficient interest in this field to try to develop it further. Nevertheless, more work needs to be done before an uncertainty analysis can be implemented in EUSES.

1.4 About this report

In this report, we will not attempt to validate EUSES in a detailed manner. Clearly, the university of Osnabrück is performing a more detailed study than we can do in this project. We therefore restrict this study to an inventory of the validation status of each module, investigate current experiences and problems, discuss the exposure scenario, and provide advice for future studies. Chapter 2 discusses experiences with EUSES so far for new and existing chemicals and Chapter 3 for metals, using the example of zinc. In Chapter 4, the separate modules of EUSES are discussed individually regarding their validation status. Conclusions and recommendations are given in Chapter 5.

Table 3 Suggested criteria for implementation of new models in USES (Kerngroep UBS, 1997).

<p>Does the model fit the purpose of USES? Sub-criteria:</p> <ul style="list-style-type: none"> • Is there a (policy) need for implementation of the product in USES? • Models must be suitable for general assessment of a wide range of chemicals. • The general assessment uses generic scenarios and a standard environment. • The model must fit into one or more of the time and spatial scales of USES. • The model must aim for risk assessment of one or more of the protection targets of USES. <p>Is there a description of the model? This description must include:</p> <ul style="list-style-type: none"> • Purpose of the model, importance for USES, policy relevance. • The application range of the model. • The mathematical relations. • The theoretical backgrounds and the limitations of these relations. • Support for the assumptions and advised parameter values. • Results of model analysis. • If a computer program is available: a user manual. • Proposal for implementation in USES. <p>Has model analysis been sufficient? Sub-criteria:</p> <ul style="list-style-type: none"> • Correctness of theories, concepts and assumptions. • Correctness of mathematical or numerical expressions. • Representativeness of assessment scenarios and relevance of parameter values, and the expected degree of uncertainty. • Degree of model evaluation (validation status). • Sensitivity of the model for input. <p>Status of the model:</p> <ul style="list-style-type: none"> • Support of the model (national and international). • Maintenance and updating of the model.

2. Experiences from users: problems and solutions

In this chapter, experiences from users with EUSES will be presented. An inquiry into these experiences resulted in an inventory of problems and omissions which occurred over a period of one year (April 1997- April 1998). Each (sub)module of EUSES was checked for major and minor problems and omissions. This chapter concentrates on major problems and the solutions which came up until now. The minor problems have been collected on a Blacklist, which is being generated by RIVM and the EUSES Help Desk of the European Chemicals Bureau (ECB) since April 1997. This Blacklist (Doc. ECB/4374/CH/ch; see Appendix 2) is distributed by the EUSES Working Group. The participants of the EUSES Working Group are from industry and EU member states and their purpose is to generate proposals for further development and improvement of EUSES to the EC Technical Committee of New and Existing Substances. The Blacklist contains the following categories: bugs, suggestions for improvement and omissions, and inconsistencies in EUSES 1.00. All users have the opportunity to report bugs or problems to the EUSES Help Desk of the ECB or to RIVM. Besides a description of major problems and omissions in EUSES, the experience from the risk assessment of veterinary medicines in using the sub-module for the calculation of drinking water concentrations is discussed.

2.1 Release estimation

In general, generic scenarios (default emission calculations) are very little used for existing chemicals because site-specific emission data are often available (especially for the stage of production). Besides site-specific emission data from intentional sources, data are often available on emissions from unintentional sources (which can be industrial or not). For example, a chemical may be formed and emitted unintended as a by-product during industrial production (for instance, in the surfactant industry 1,4-dioxane can be formed as a by-product during ethoxylation reactions). Non-industrial sources are for example traffic and cigarette smoke: these types of diffuse sources produce, among others, acrolein as a result of combustion. At the moment, no guidance exists on how to incorporate these data in EUSES. In this section, the problems and possible solutions are described as well as the use of the "10% rule".

2.1.1 Estimation of the continental emission from regional emission

Problem: In EUSES, the regional model is nested within the continental model. How to take this into account in estimating the continental emission rate from a known regional emission rate?

Solution: For the estimation of the continental emission rate the regional emission rate is multiplied manually by a factor of 10 (inverse use of 10% rule, see 2.1.6.). After this calculation the regional emission rate should be subtracted from the estimated continental emission (see Example 1).

2.1.2 Site-specific scenarios (intentional sources)

Problem: A measured emission rate (kg/d) is available for a specific local source (i.e. industrial plant). The number of emission days and the fraction of release are unknown. The fraction of the main source is one.

a) How to incorporate the measured emission rate into EUSES?

b) How to derive regional and continental emission rates (kg/d) from a local emission rate and how to enter these data into EUSES?

Solution: Ad a) Via the interactive or outline mode of EUSES the following screens have to be accessed: "Use patterns", "Emission input data", "Release fractions and emission days" and "Local emission" (See Example 2).

Ad b) The local emission rate is manually calculated to the annual average regional emission rate. For the estimation of the continental emission rate the calculated regional emission rate is multiplied

manually by a factor of 10 (inverse use of 10% rule, see 2.1.6). The manually calculated regional and continental emission rates should be used as input in the following EUSES screens: "Regional releases" and "Continental releases". These manually calculated rates are automatically summed up for the total regional and continental emission rate.

Remark: The manual calculations and input are sometimes time consuming and mistakes are easily made.

Example 1		
Regional emission rate Measured emission rate to air for chemical X in DE ^a (regional scale): 100 kg/d		
Problem	Solution (e.g. pre-calculations)	Solution in EUSES
How to estimate the continental emission rate from the regional emission rate?	The continental emission rate = regional emission rate x 10 ^b - regional emission rate (=900 kg/d).	-screen "Continental emission" input of 900 kg/d.

^a The regional scale of Germany is different from the size of the regional scale in EUSES (200 X 200 km²). A pragmatic approach will be followed and the different regional scale size is not taken into account.

^b Inverse use of 10% rule (TGD'96).

Example 2		
Local plant (paint industry) Measured emission rate to water: 10 kg/d Fraction of main source (one site): 1 Number of emission days ^a : 300 days Industry/Use category: 14/48 Life cycle step: formulation of paint		
Problem	Solution (e.g. pre-calculations)	Solution in EUSES ^e
a) How to enter 10 (kg/d) in EUSES?	-	screen ^f : "Use pattern" -"Emission input data" -"Release fractions and emission days [1, IC=2/UC=48]" -"Local emission"
b) How to derive regional and continental emission rates and how to enter these in EUSES?	regional (kg/d): 10 x 300/365 ^b = 8 continental ^c (kg/d): (8 x 10 ^d) - 8 = 72	screen ^f : "Regional releases" and "Continental releases" [1, IC14/UC48] formulation

^a The number of emission days and fraction of release are unknown. A number of 300 emission days has been assumed because this leads to a high annual concentration in air (*C_{local,air,ann}*).

^b Number of days

^c See Example 1 for calculation of the continental emission rate from the regional emission rate.

^d Inverse use of a factor of 0.1 which is derived from the TGD.

^e Overwrite defaults via interactive or outline mode

^f Input for each screen:

screen "Use pattern": insert use pattern

screen "Emission input data": input Industry/Use category and life cycle step

screen "Release fractions and emission days [1, IC=2/UC=48]: input fraction of main local source and number of emissions days per year, screen "Local emission": via edit, input of emission (kg/d).

screen "Regional releases" and "Continental releases" [1, IC14/UC48] formulation: input of regional emission rate (local emission rate back calculated to annual average) and continental emission rate (see Example 1 for calculation of continental emission rate from regional emission rate).

2.1.3 Generic scenarios and site-specific scenarios

Problem: Several site-specific scenarios (e.g. emission data) and generic scenarios (default calculations) are combined within one EUSES-calculation. Which generic and site specific scenarios should be taken into consideration for the total regional emission? How to calculate the total regional emission and how to use EUSES?

Solution: All specific and generic sites are put in one region, despite the different EU countries (worst-case approach). The local emission rates for site specific scenarios are all back-calculated to annual averages. The regional emission rates for each scenario are automatically summed up by EUSES. In Example 3, the screens of EUSES are described which must be used for this type of calculation.

Example 3		
Data on the number and type^a of local sites		
1. production site no.1 in NL	emission rate to water is 100 kg/d	site-specific scenario
2. production site no.2 in GE	emission rate to water is 50 kg/d	site-specific scenario
3. production site no.3 in GE	no data ^c on volume or emission	generic ^d scenario
4. formulation site no.1 in DK	emission rate to water is 15 kg/d	site-specific scenario
5. formulation sites (>1) in Eu ^b	no data on volume or emission	generic scenario
6. processing sites (>) 1in EU	no data on volume or emission	generic scenario
Problem	Solution	Solution in EUSES
Which generic and site-specific scenarios should be taken into consideration for the total regional emission rate (kg/d)? How to solve this with EUSES?	-worst-case approach: all site-specific site and generic sites are put in one region, despite the different countries. -The local emission rates are all back-calculated to annual averages.	screen ^e : -“Use pattern” -“Emission input data” -“Regional releases” [1-6, IC14/UC48] for the relevant life cycles (production 1, production 2 etc.).

^a The production sites produce a chemical which will be used as solvent in paint. Industry and Use category is 14/48. Relevant life cycle steps are production, formulation and processing (use of paint by industry).

^b There are more formulation sites in the EU besides DK (Denmark). For these sites no emission rates are available. For pragmatic reasons the regional emission rate (formulation) of site no.1 in DK is not subtracted from the generic or default estimated emission rate.

^c It is possible that volume (tonnes/year) for a specific site is known. This tonnage might be higher than the default tonnage given by EUSES (EU-tonnage x 0.10).

^d Generic: model calculations are carried out with defaults because no data are available on a specific site

^e Input for each screen:

screen “Use pattern”: insert and edit six use patterns. For reasons of clarity each use pattern represents a scenario. It should be noted that less use pattern could be selected.

screen “Emission input data”: input Industry/Use category and life cycle step

screen “Regional releases” [1,2,3., IC14/UC48] production etc.: input of regional emission rate (local emission rates are back-calculated to annual averages and must be entered manually)

2.1.4 Full picture of site-specific data

Problem: Site-specific emission data are available for all EU production sites for a certain existing chemical. There are too many local emission data (i.e. emission rates) which can be used as input for EUSES. How to make a proper estimation for the local, regional and continental emission?

Solution: There are two option for the solution to this problem (see Example 4):

1) Estimation of an *average local emission rate* which is based on the total emission rate (kg/d) of all production sites and the total number of the sites. The regional and continental emission rate are manually calculated as presented in Example 1 and 2.

2) Estimation of an *average release fraction* which is based on the total emission (i.e. release kg) from all sites and the total amount of all these sites.

The regional and continental emissions are automatically calculated by EUSES.

Remark: There are more solutions to this problem:

- Select a known region (i.e. EU country) with the highest regional emission. The local emission rates (back-calculated to annual average) are summed up for the regional emission. The area of the regional system (default in EUSES: 200X200 km) will not be changed, irrespective the area of the EU-country.

- Or, select the highest emission source within this EU (local scale).

For all solutions: all local emission rates are summed up for the total continental emission rate.

Example 4

Site specific data on production for whole EU

Number of production sites in EU: 25
 Emission rate to water (kg/d): range: 10-100
 Total emission to water from site 1-25 (kg/d): 1100
 Amount of tonnage (T/year): range: 100-2000
 Total amount of tonnage from site 1-25 in EU (T/year): 26,000

Problem	Solution (e.g. pre-calculations)	Solution in EUSES
How to make a proper estimation for local, regional and continental scale and how to enter the data in EUSES?	<p>1. Estimate an average emission rate^a by dividing the total emission with number the of production sites. Average local emission rate is 44 kg/d (=1100/25). Regional emission rate is 10% of continental emission rate: 110 kg/d. Continental emission rate: 990 kg/d (1100-110 kg/d).</p> <p>2. Estimate an average release fraction. A number of emission days of 300 will be assumed. The total emission from site 1-25 is multiplied with 300 (days) and divided by the total amount of tonnage from site 1-25. Average release fraction is 0.013 (= 1100 kg/d x 300 d / 26,000E+3 kg)</p>	<p>1. screen^b: -"Use pattern" -"Emission input data" -"Release fractions and emission days [1, IC=x/UC=y]" -"Local emission" - "Regional releases" and "Continental releases" [1, ICx/UCy] production</p> <p>2. screen^c: -"Use pattern" -"Emission input data" -"Release fractions and emission days [1, IC=x/UC=y]"</p>
Remark	Solution 2: EUSES calculates the output automatically.	

^a Other options are possible. For example a realistic worst case approach could be followed by selecting a production site with the highest local emission rate (100 kg/d).

^b Input for each screen:

screen "Use pattern": insert and edit one use pattern

screen "Emission input data": input Industry/Use category and life cycle step

screen "Release fractions and emission days [1, IC=x/UC=y]: input fraction of main local source of 1 and number of emissions

days per year (300). See also Example 1.

screen "Local emission": via edit, input of emission 44 (kg/d).

screen "Regional releases" and "Continental releases" [1, ICx/UCy] production: input of region emission rate (110 kg/d) and continental emission rate (990 kg/d). See example 1 for calculation of continental emission rate from regional emission rate.

^c Input for each screen:

screen "Use pattern": insert and edit use pattern

screen "Emission input data": input Industry/Use category and life cycle step

screen "Release fractions and emission days [1, IC=x/UC=y]: input of fraction of release to waste water (0.06), fraction of main local source is 1 and number of emissions days per year (300).

Local emission (kg/d), Regional releases and Continental releases are automatically calculated by EUSES.

2.1.5 Actual-emission data from non-intentional sources

Emissions of existing chemicals may include emissions from unintentional point and diffuse sources (e.g. formation of acrolein by traffic, waste). There is no guidance on how to incorporate these data in EUSES.

Actual emission data from non-intentional point sources

Problem: A substance is emitted as a by-product from an industrial point source. Local emission rates (kg/d) are available for several point sources in different European countries.

- a) How to enter local emission rates from unintentional point sources(kg/d) in EUSES?
- b) How to derive regional and continental emission rates (kg/d) from these local emission rates and how to use EUSES?
- c) How to estimate the total regional and continental emission of intentional en non-intentional point-sources? How to use EUSES?

Solution: For a) and b) a similar approach is followed, as described in 2.1.2.

Ad c) For the total regional emission from all site-specific sites, intentional as well as unintentional, and generic sites at a local scale are placed in one region (this is a worst-case approach). See Example 2 for the estimation of the continental emission rate. The regional and continental emission rates are automatically summed up for the total regional and continental emission rates.

Remark: The manual calculations and the use of EUSES are sometimes time consuming and mistakes are easily made.

Example 5		
Industrial site which produces a chemical unintentionally or as a by-product		
Emission rate to water site no.1: 200 kg/d		
Emission rate to water site no.2: 10 kg/d		
Problem	Solution (e.g. pre-calculations)	Solution in EUSES
a) How to enter 200 and 10 (kg/d) in EUSES?	-	See Example 2.
b) How to derive regional and continental emission rates and to incorporate in EUSES?	-The local emission rates from unintentional sites are all back calculated to annual averages. See for further details example 2.	See Example 2.
c) How to estimate the total regional and continental emission of intentional and non-intentional point-source and how to use EUSES?	-worst case approach: all available site specific sites, generic sites and unintentional sources/sites are put in one region, irrespective of the different countries.	See Example 3 (input total regional) ^a

^a There is no specific option in EUSES for point-sources which forms a chemical unintentionally. So there is not an appropriate Industry/Use category or life cycle step available. For reasons of clarity 15/55 (i.e. other/other) and life cycle step production could be selected.

Actual emission data from unintentional diffuse sources

Problem: A substance is emitted from an unintentional, diffuse sources (e.g. traffic). A measured regional emission rate is available for one EU-country.

- a) How to incorporate the regional emission rate from an unintentional diffuse source into EUSES?
- b) How to estimate a continental emission rate from regional emission rate and how to use EUSES?
- c) How to estimate the total regional and continental emission of intentional (local) point sources and an unintentional diffuse source and how to use EUSES?

Solution: Ad a) Via ~~interactive~~ or the outline mode of EUSES the following screens have to be entered: "Use patterns", "Emission input data", "Release fractions and emission days" and "Regional releases". The input for local emission rate is not relevant for this type of source.

Ad b) The regional emission rate is multiplied manually by a factor of 10 (see Example 1). Another and more realistic approach is estimating a factor which is based on the number of inhabitants or cars in the region and the number of inhabitants or cars in Europe.

Ad c) For the total regional emission, all site-specific sites, intentional as well as non-intentional, and generic sites at local scale are placed in one region. This is a worst case approach. See Example 1 for the estimation of the continental emission rate for the industrial sources. The regional and continental emission rates will be automatically summed up for the total regional and continental emission rates.

Example 6

Traffic (formation of a chemical unintentionally)

Measured emission rate from diffuse sources, such as cars, to air in the Netherlands (region)^a: 100 kg/d

Problem	Solution (e.g. pre-calculations)	Solution in EUSES
a) How to incorporate 100 kg/d in EUSES?	-	Screen: "Regional Releases" ^b .
b) How to estimate a continental emission rate from regional emission rate and how to incorporate in EUSES?	1. Regional emission rate ^a multiplied with factor of 10 (see Example 1). 2. Realistic approach ^a will be followed for the estimation of a multiplication factor. Estimated factor of 24 is based on number of inhabitants or cars in the EU divided by the numbers of these in the region (350 million inhabitants in EU/15 million inhabitants in NL). The continental emission rate is: regional emission rate x 24 - regional emission rate (2376 kg/d).	1. See Example 1. 2. See Example 1.
c) How to estimate the total regional and continental emission of intentional and non-intentional diffuse source and how to incorporate these data in EUSES?	For the total regional emission from all available site-specific sites, unintentional sources, and generic sites at local scale are placed in one region (worst case approach). See Example 1 for total continental estimation rate (inverse use 10% rule).	See Example 3.

^a The regional scale of other countries (e.g. Germany) can be different than the size of the regional scale in EUSES (200 X 200 km²). A pragmatic approach will be followed and the different regional scale size is not taken into account. However, in solution 2 specific continental estimate can be made by changing the number of inhabitants.

^b There is no specific option in EUSES for diffuse sources which produces a chemical unintentionally. So there is not an appropriate Industry/Use category or life cycle step available. For reasons of transparency 15/55 (i.e. other/other) and life cycle step production may be selected.

Continental emission data from unintentional diffuse sources

Problem: A “realistic” worst-case estimate is available, in a review, for the continental scale. How to estimate the regional emission rate?

Solution: The regional emission rate is derived from the continental emission rate by making use of the 10% rule (see 2.1.6.).

Example 7

Continental emission rate

Estimated emission rate from diffuse sources, such as cars, to air in Western EU (continent): 2000 kg/d

Problem	Solution (e.g. pre-calculations)	Solution in EUSES
-How to derive the regional emission rate from the continental emission rate?	Regional emission rate: 2000×0.10^a = 200 kg/d	-Screen: “Regional releases”.

^a a 10% rule which is derived from TGD'96.

2.1.6 The use of the 10% percent rule in emission estimations

A discussion paper is written by the Netherlands for the first Technical Meeting for the Risk Assessment of Existing Chemicals (TM I, March 1998) on the use of the “10% percent rule” for release estimations. The contents of this section mainly refers to this discussion paper (NL/01/98 of TMI, 1998). A number of questions came up regarding the 10% rule in emission estimation during the discussions at TM level. From these discussions it has become clear that:

- 1) different countries make different choices,
- 2) the current text in the TGD does not give enough guidance, and
- 3) the 10% rule is currently implemented as a default in the EUSES program.

The background of the 10% rule is not theoretical but is historical. Hence, it is clear that for risk assessments of both new and existing substances a common understanding on the 10% rule needs to be developed that can be implemented in the TGD by a technical recommendation, and, if necessary, can be followed by a change in the EUSES software when the next version will be released. In several risk assessment reports the 10% rule has been applied to calculate the emission input for the exposure models. The use of this rule may lead to discrepancies between the different reports:

- In case of production, of the existing substances in almost all cases site-specific information has been delivered thereby making the use of the 10% rule redundant. Either this information is used directly or specific assumptions based on the production volume ranges given in HEDSET are made. For new substances the default should be overwritten anyway because it may be assumed that in most cases just one or at the most a few producers exist. Therefore the factor of 0.1 should be changed to one (assuming that all production sites are located within one region).
- In case of formulation and processing of substances the question how and when to use the 10% rule becomes more apparent. Some Member States have applied the 10% rule directly, others only in case information was available that a large number of formulation/processing sites exist in Europe, thereby underpinning the assumption that the use is reasonably spread over Europe, and finally some Member States, in absence of further information, have not applied the rule at all. On the other hand, where information on the number of sites was available this number (N) has been used directly in some reports to calculate the fraction of main source (as 1/N), thereby ignoring the variation in the size of the sites.

These different ways of applying the 10% rule on the one hand demonstrate the confusion and lack of clear guidance but on the other hand also demonstrate the need for expert judgment both in applying the emission tables from the TGD as well as in the interpretation of the outcome. In some cases the 10% rule may be reasonable but the result from the calculation may not be in accordance with the specific knowledge of the use of the substance. In other cases, because of lack of information or because information on regional differentiation is available, the 10% rule needs to be overruled and

the fraction of main source may be specifically selected. Despite this need for expert judgment the following general guidelines for the emission estimation for new and existing substances are proposed:

- For production, the input for the regional production volume is by default set at the EU production volume, which is also used as input for the B-tables. Based on the information available to the rapporteur on the number of production sites, size distribution and geographic distribution it can be decided to apply the 10% rule, to use another percentage or to use specific values as input for the regional model (e.g. the emissions from the largest source or the emissions from the largest emitter). Similarly, this information can be used to set the fraction of main source for the local exposure calculation.
- For formulation and processing (industrial use) a similar approach is used: by default the EU volume is used as input for the region as well as for the B-tables *unless* it can be shown/is known that a large number of sites with a reasonable European distribution exists for the specific formulation/processing step of the substance involved. In that case again it can be decided to apply the 10% rule, to use another percentage or to use specific values. Whether or not the available information is sufficient for a specific substance will depend on the expert judgement by the rapporteur.
- For private use, the 10% rule is applied automatically both for the input of the regional volume and for the input volume for the B-table (assuming an even distribution over Europe).

It must be realised that depending on the IC/UC combination this approach may in some cases lead to unreasonable worst-case assumptions, especially for the estimation of the emissions during formulation/processing. Hence, a case-by-case assessment using expert judgement remains warranted. Furthermore it should be noted that in case real data on regional and continental emissions are available these should be used to overwrite the default assumptions.

2.2 Distribution module

2.2.1 Partition coefficients

For surface active compounds, organo-metallic compounds and inorganic compounds (e.g. metals and metal compounds) the octanol-water partition coefficient is not an accurate predictor for estimating the partition coefficients (solids-water partitioning).

Problem: The substance has surface active properties (< 0.05 N/m). No adsorption test is available. An estimated log *K_{ow}* is available. However, for surface-active compounds the log *K_{ow}* may not be an accurate predictor for estimating partition coefficients (i.e. solid-water partitioning in soil, sediment and suspended matter). How to make a proper estimation with EUSES?

Solution: The estimated log *K_{ow}* will be used and one or two qualitative remarks are made on the outcome of EUSES:

- “the estimated risk for aquatic organisms might be lower because of more adsorption to sludge”;
- and when a substance is readily degradable: “However, on the other hand, due to adsorption, less biodegradation may occur”.

Similar qualitative remarks could be made on the estimated risk for terrestrial and sediment organisms.

Problem: Metal, metal compounds and organo-metal compounds with a bioavailable metal-ion. No adsorption test is available. How to make a proper estimation with EUSES?

Solution: An assumption is made for fate of chemicals in a sewage treatment plant (STP). In EUSES the fraction of emission in a STP can be estimated on the basis of log *K_{ow}* (adsorption to sludge), Henry's Law constant (volatilisation) and the results of biodegradation tests. This estimation is not applicable for metal compounds. The following assumption is made: the emission of metal-ions to a STP are all (i.e. 100%) directed to the water phase. This will lead to a worst-case approach for the

aquatic environment (i.e. surface water concentration). A risk assessment for the terrestrial compartment cannot be made. See also Section 2.3.

Remark: For organo-metal compounds an EUSES-calculation will also be conducted on the organic part of the compound.

2.2.2 Sewage treatment

Input of “number of inhabitants” and “Effluent discharge of this STP”

Problem: The effluent discharge of a site-specific STP is always submitted by the industry as a flow rate (m^3/day). No data on the number of inhabitants is given because the site-specific STP often concerns an industrial installation.

Solution: Until now the number of equivalents/inhabitants must be derived from the default parameter of EUSES (200 L/d per equivalent) and the flow rate of the specific STP (equivalents = specific flow rate L/d divided by 200 L/d). The default “number of inhabitants feeding this STP” (equivalents) is overwritten for generating a site-specific “Effluent discharge of this STP” (L/d). A direct input of the site-specific flow rate of a STP in the field “Effluent discharge of this STP” should be allowed.

Fate of chemicals in a STP based on Simple Treat model

Problem: The fractions of emission directed to air, water and sludge by a default STP ($2000 \text{ m}^3/\text{d}$) are different between local, regional and continental scale. According to TGD the fraction differs with the size of STP. Why do these fractions differ?

Solution: The STPs on the regional and continental scales are modelled as one very large STP on each scale (with 20 and 370 million inhabitant equivalents, respectively). This is actually not correct although the quantitative consequences are minor. A better option would be to take the fractions from the local STP and use these for the regional and continental estimates also.

2.2.3 Local environmental distribution

Calculation of concentration in groundwater

Problem: The groundwater concentration ($PEC_{local,grw}$) for veterinary medicines is often above $0.1 \mu\text{g/L}$ which is the limit value (Dutch regulation) for drinking water. This is also observed for new chemicals (5 notifications in 1997).

Solution: For veterinary medicines the limit value of $0.1 \mu\text{g/L}$ is used as a trigger for identifying potential risks for the drinking water consumption. Specific test reports are asked from the notifier when the groundwater concentration exceeds this limit value. The data from these specific test reports are used as input for another model (PESTLA). There is no limit value available for new chemicals. No research has been carried out whether new chemicals with a $PEC_{local,grw} > 0.1 \mu\text{g/L}$ are problematic.

2.3 Exposure module

2.3.1 Bioconcentration factor (BCF)

For exposure of humans and predators through the environment, an estimate of the concentration in their food and drinking water must be made. This is done by multiplying the concentration in the environment (from the distribution module) with the measured or estimated BCF (BioConcentration Factor) or BAF (BioAccumulation Factor) or a purification factor in the case of drinking water. These bioconcentration factors are for example used for secondary poisoning ($BCF_{fish/worm}$) and for indirect exposure for humans ($BAF_{milk/meat}$).

Problem: For surface active compounds, organo-metallic compounds and inorganic compounds (e.g. metals and metal compounds) the octanol-water partition coefficient (e.g. $\log K_{ow}$) cannot be experimentally determined or is not representative for its behaviour in the environment. The estimation of most BCFs or BAFs is highly dependent on K_{ow} and is therefore only valid for organic, non-ionised or non-dissociating chemicals. Furthermore, the BCF_{fish} estimation is not applicable for compounds with high molecular weight (> 700 g/mol).

Solution: For substances with surface active properties (< 0.05 N/m), a risk assessment on secondary poisoning and indirect human exposure cannot be performed. Further investigation should be done on the relation between the solid-water partition coefficient (K_p) and the experimental BCF (D. Sijm, RIVM, pers. comm.).

For metals, metal compounds and organo-metal compounds, a risk assessment on secondary poisoning cannot be performed. For human exposure, only the drinking water exposure route is taken into account (see also 2.2.1). For organo-metal compounds, an EUSES-calculation can also be conducted on the organic part of the compound.

For substances with a high molecular weight (> 700) the QSAR for BCF_{fish} is not valid (see also the blacklist, Appendix 2, item II.4). When bioaccumulation is expected and no experimental data on BCF_{fish} is available, the input of molecular weight is set to 699 to allow the calculation of secondary poisoning and human exposure to proceed. The outcome of this risk assessment should be used carefully. For existing chemicals with a high molecular weight, the use of monitoring data should be considered. A low indication of bioaccumulation potential may be inferred when the chemical is never detected in biota.

2.3.2 Indirect exposure of humans via the environment

Indirect exposure of humans via food products

Problem: Chemicals with high $\log K_{ow}$, low water solubility and low vapour pressure show high accumulation in roots of plants (fraction $> 90\%$). For this estimation, the approach of Trapp and Matthies (1995) is used. The estimated concentration in roots and the daily intake of root crops results in a high total daily intake for humans which may indicate a potential risk, even though the chemical has a high NOAEL-value (e.g. > 1000 mg/kg bw).

Solution: The performance of the model needs investigation for these compounds. Other possible solutions can be found under Section 2.5.2.

Consumer exposure

Problem: For existing chemicals the consumer model in EUSES only concerns a screening stage and is therefore often skipped in favour of the more elaborate models of CONSEXPO.

Solution: CONSEXPO also contains the EUSES screening model. More models from CONSEXPO may be implemented in EUSES in the future.

2.4 Effect module

Problem: For the risk assessment for existing chemicals, data on protozoan species are sometimes used for the derivation of the $PNEC_{stp}$. There is already discussion on this topic (i.e. which protozoans and which assessment factors should be used) in the Technical Meeting and a special working group is installed (DOC. ECB 4/42/97). It has been agreed in this group that protozoans have to be regarded as additional species and not as additional trophic level. The same assessment factors as for "specific bacterial populations" can be used (H. Loonen, RIVM, pers. comm.).

Solution: In the near future, the effects assessment for protozoans should be incorporated in EUSES.

2.5 Risk characterisation module

Problem: In the risk characterisation table there are only two Margins of Safety (MOS) presented: MOS_{total} and MOS_{air} . According to the TGD a MOS has to be determined for each of the relevant endpoints (e.g. general toxicity and developmental toxicity).

Solution: The risk characterisation should be extended in the future.

Problem: In the human risk assessment an attempt is made to identify the hazards of the substances and to relate them to exposure. For those substances for which a threshold for toxicity is assumed to exist, a No-Observed-Adverse-Effect Level (NOAEL) has to be derived or, if this is not possible, a Lowest-Observed-Adverse-Effect Level (LOAEL). The risk is characterised by comparing estimated (or measured) concentrations in air or on skin or total daily intakes to the results of the effects assessment. This Margin Of Safety (MOS) has to be determined separately for each population potentially exposed and for each effect. Another widely used approach is the explicit derivation of a Human Limit Value (HLV³) from experimental or epidemiological toxicity data by dividing the NOAEL or LOAEL by an overall assessment factor. This overall assessment factor is a multiple of several factors, accounting among others for inter- and intraspecies variations, differences in exposure time scales, the nature of the adverse effects and the adequacy of the database. Comparing the Margin of Safety approach of the current TGD to the assessment factor approach, it has been noted that the current TGD does not provide any quantitative guidance on the size of the Margin of Safety (Vermeire *et al.*, 1998).

Solution: Vermeire *et al.* (1998) concluded that decision criteria for human risk characterisation need to be made explicit. This could be achieved by establishing a formal, harmonised set of default assessment factors accompanied by elaborate guidance. The default set should only be applied in the absence of data which permit a more substance-specific, scientific choice. The default set should allow for differentiation with regard to exposure scenarios, including groups at risk, and the toxicological database. Proposals have been made to achieve this goal.

³ HLV: general term covering various limit values such as the ADI, RfD, PNAEL and HBORV

3. Risk assessment for metals, the case of zinc

EUSES is not especially targeted to perform risk assessments for metals and metal compounds. Most estimation routines and QSARs only work properly for neutral organic compounds (because they rely heavily on *Kow*). The TGD provides some qualitative guidance for these compounds, but the approach retains a high “case-by-case” character. In the existing substances program, the Netherlands are the rapporteur for zinc. This Chapter describes the procedure that was followed to make a risk assessment of zinc with EUSES and may serve as illustration how to deal with those compounds.

For the exposure assessment of zinc, the predicted environmental concentration (PEC) for the different environmental compartments are calculated using the EU-Technical Guidance document (EC, 1996) and EUSES 1.0 (EC, 1996). For zinc a distinction is made between the approach for the local and the regional exposure assessment. The presence of zinc in the environment due to natural processes (resulting in a natural background concentration of zinc in all environmental compartments, incl. organisms), the chemical processes that will affect the speciation of zinc in the environment, and the fact that zinc is an essential element have implications for the environmental exposure and effect assessment of zinc and thus for the risk characterisation of zinc (see also the section “difficulties”).

Since the Technical Guidance Document (TGD) does not provide detailed information on how to deal with (essential) elements that have a natural background concentration in the environment, such as zinc, the “added risk approach” (Struijs *et al.*, 1997; Crommentuijn *et al.*, 1997) has been used for the risk assessment report on zinc. In this approach both the Predicted Environmental Concentration (PEC) and the Predicted No Effect Concentration (PNEC) are determined on the basis of the added amount of zinc. The use of the added risk approach (a method that in principle can be used for all naturally occurring substances) implies that only the anthropogenic amount added to the natural background concentration is considered to be relevant for effect assessment (bioavailable), i.e. that the possible effects of the (bioavailable fraction of the) natural background may be ignored.

In the present environmental exposure assessment, the use of the added risk approach implies that the PEC (for each compartment, either local or regional) is calculated from zinc emissions due to anthropogenic activities. This results in an “added Predicted Environmental Concentration” (PEC_{add}), which is the anthropogenic part of the zinc concentration in the environment. By focusing only on the anthropogenic part of zinc, the problem of the considerable variation of natural background levels of zinc over the different geographic regions is eliminated. It is noted, however, that comparison of the PEC_{add} with the monitoring data must thus take into account that the latter values comprise the a natural background *and* the anthropogenic part. In the environmental effect assessment, the use of the added risk approach implies that the PNEC is derived from toxicity data that are based on the added zinc concentration in the tests. This results in an “added Predicted No Effect Concentration” (PNEC_{add}). Finally, in the environmental risk characterisation, the use of the added risk approach implies the evaluation of the PEC_{add} / PNEC_{add} ratio⁴.

⁴ In the current local risk characterisation of zinc and zinc compounds the local PEC_{add} values (thus without the regional PEC_{add}) is compared with the PNEC_{add}. The local risk characterisation thus primarily focuses on the contribution of point sources to the potential risks, thereby neglecting the contribution of diffuse sources (and of course the natural background). If the regional PEC_{add} would have been added for water, all local scenarios would have resulted in PEC/PNEC ratios larger than 1 (water). This because the calculated regional PEC_{add} already exceeds the PNEC_{add}. It is not clear yet how the issue of adding the regional PEC_{add} will be dealt with in the next draft/final report of zinc and zinc compounds.

3.1 Local exposure assessment

The entry for estimating the environmental concentrations is the submitted industrial information (when available) like local emission values, effluent discharge rates, efficiency of local STP, flow rate of receiving water and the concentration in effluent. More than 80 production sites submitted site specific information. Because of this quantity, EUSES itself was not used for the local assessment but a spreadsheet version was used for the necessary calculations:

1. air (100 m) as annual average,
2. effluent water of local STP,
3. STP sludge concentration (according to the TGD, page 292),
4. surface water during emission episode,
5. sediment during emission episode,
6. agricultural soil.

For modelling the behaviour of zinc in the environment the octanol-water partitioning coefficient (K_{ow}) and the solubility are not appropriate. Measured K_p values were used instead for sediment and suspended matter (TGD, Ap. VIII). The vapour pressure was fixed at a low value of 1.10^{-10} Pa. and the biotic and abiotic degradation rates were minimised (TGD, Ap. VIII). For some generic scenarios (A-tables, TGD) the solubility is required. The water solubility for zinc chloride and zinc sulphate is about 5000 g/L and 500 g/L respectively. All other zinc compounds were considered to be insoluble.

Depending on the information submitted, the PEC calculations start at different levels. The different levels are presented in the flowchart of Figure 1. A generic scenario was used when no specific industrial emission information was available. In that case the EU (production) tonnage is the starting point for calculating the PEC (entry 1). When a regional tonnage or an EU emission is available, which is possible for the formulating and processing stages, the starting point is 2 or 3. With a regional tonnage regional emissions can be derived by multiplying it with the appropriate release fractions (A-Tables of the TGD). An EU emission is divided by 10 to derive a regional emission⁵. Also a submitted regional emission can be an entry for the PEC_{add} calculation (entry 4). With this regional emission a local emission can be derived by multiplying it with the appropriate fraction of main source (B-Tables of the TGD). With a local tonnage (entry 5) also local emissions can be derived by multiplying it with the appropriate release fractions (A-Tables). A site specific scenario can be used when local emissions are submitted by the industry (entry 6). The risk characterisation, i.e. the comparison of the PEC_{add} with the corresponding PNEC, should be based on the most realistic exposure information. For this, the calculated local PEC_{add} values are compared with measured local concentrations, if available (entry 7)

⁵ Recently (EU Technical Meeting (TM), March 1998) a discussion was held about the use of the 10% rule in the emission estimations. This because the rule was interpreted in several ways by the different member states. Until that time The Netherlands mostly used the 10% rule in their risk assessment reports. Also in the present report on zinc and zinc compounds the 10% rule was applied, i.e. the regional production/processing tonnages are set at 10% of the EU-volume if site-specific data are lacking. However, at the above-mentioned TM it was decided that for production and processing the EU tonnages (100%) should be used as input for the regional exposure assessment (conservative approach). This *unless* it can be shown that the 10% estimate is appropriate by providing the rapporteur with data on the number of production/processing sites, size distribution of the sites and their geographic distribution. Currently the exposure assessment is not (yet) changed on the basis of the TM decision. This because it is thought that in a number of cases the 10% rule is justified as the process is known to be spread over a large number of sites throughout the EU (e.g. galvanising). But in other cases it is less evident and industry has to submit data to support the choice of the 10% rule! Industry is requested to submit information for each life cycle stage where the 10% rule is applied.

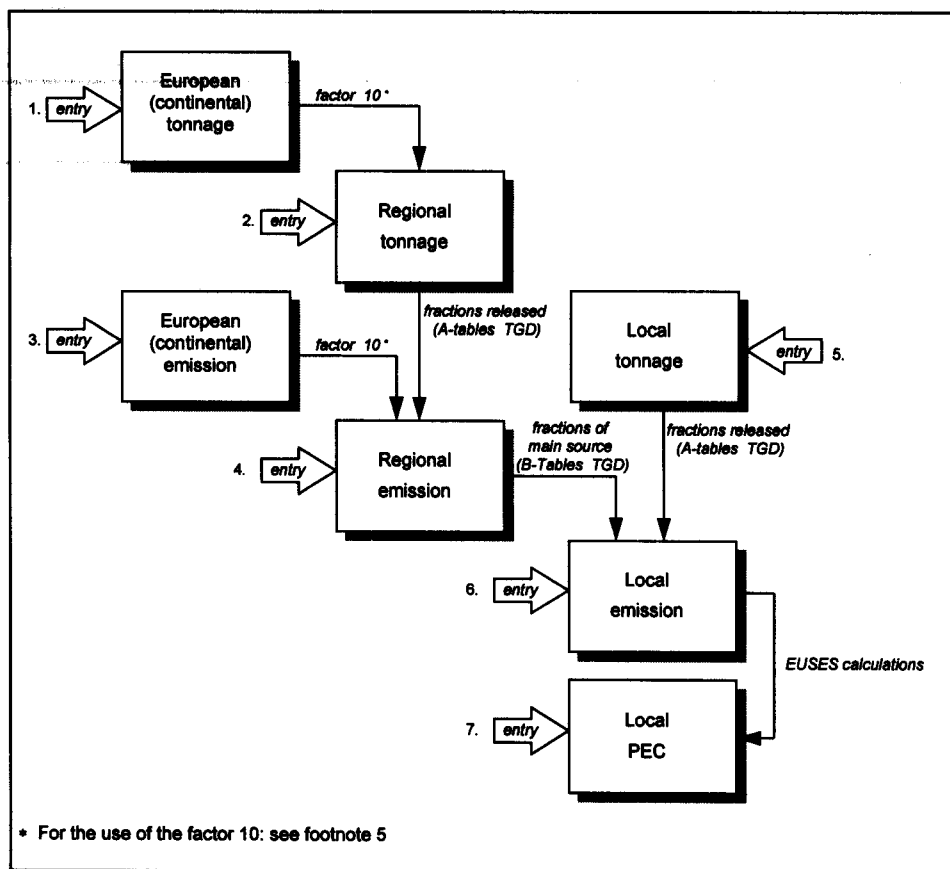


Figure 1 Flowchart for calculating the PEC_{add} : the entry for the calculations is depending on the submitted information.

3.2 Regional exposure assessment

For the regional scale not only point sources but also diffuse emissions are taken into account. In accordance with Appendix VIII of the TGD, it is assumed that the individual zinc compounds are all transformed into the ionic species. Another assumption for the regional exposure assessment is that all emissions are diffuse. As mentioned, EUSES 1.0 was used to calculate the regional PEC values for each environmental compartment. The input for the regional assessment are the emissions to air, wastewater, surface water and agricultural soil. Emission data are available for the Netherlands (1995), Belgium (1995) en Sweden (1990). On the basis of the available emission data it is difficult to make a choice for the appropriate regional input data. Nevertheless data of the Netherlands was used, because the data set of Belgium is incomplete and the Swedish data set is rather dated and incomplete compared to that of the Netherlands. Furthermore, the reason for using the emission data of the Netherlands as regional input is that this information is the most recent, extended and detailed available. The area of the Netherlands corresponds with the area of a regional system (40,000 km²).

For a regional exposure assessment, continental emissions are also necessary for the determination of the regional (ambient) background levels. The emissions used for the continental scale (foreign emissions) are estimated according to the "10% rule" (see Section 2.1.6). With EUSES, the regional environmental concentrations are directly calculated from the regional and continental emission input. It must be noted that according to this method the PEC values are not corrected for the *natural* background concentrations in surface water, sediment and soil.

Difficulties

1. Natural origin, what is the natural background concentration of zinc and which K_p values must be used? For the zinc risk assessment report, the values are adopted from Cleven *et al.* (1993) and Crommentuijn *et al.* (1997).
2. Historical pollutions, natural occurrence: it is difficult to compare measured and calculated data.
3. Lack on information on processes in STPs. For most production and processing stages, no information was available on the adsorbed fraction of zinc in waste water from a particular process. Additionally, specific information was lacking about the processes in an STP which may have been useful to determine the adsorbed fraction of zinc. Because of this lack of information, one rate of removal of zinc in an STP has been applied to the concerned life stages and zinc compounds. It was assumed that 80% of the total emission to waste water is directed to sewage sludge. This percentage is based on measured influent and effluent concentrations of communal STPs (Pers. Comm. L.V.M. Teurlinkx, RIZA, Lelystad, The Netherlands). In the absence of specific information it was assumed that this value is also representative for the removal in industrial STPs. The removal rate of 80% was used for calculating the PEC water for the production sites for which no submitted emissions are available. The removal rate of 80% was further used for calculating the PEC in water from the calculated waste water emissions (formulation and processing stages).
4. Availability of zinc will vary from site to site and is highly dependent on the speciation. Speciation was not taken into account: for the STP it was assumed that the adsorbed fraction is removed and that the remaining zinc in effluent water is completely available.
5. Knowledge about the emitted substances for the different processes at industrial sites. No information was available.
6. Are the emissions of the Netherlands for the regional scale representative for the EU? Emission data were also available for Belgium and Sweden. It is not always possible to compare these data, because of the format of the available information and because of the specific information in the different countries.
7. How must the exposure be estimated? Can EUSES be used? See local and regional exposure assessment before.

Comparison of measured and calculated data on a regional scale

The risk characterisation should be based on the most realistic exposure information. Hence, it must be decided whether calculated regional concentrations or monitoring data are more useful for the exposure assessment. It must be noted that measured concentrations can only directly be compared with calculated concentrations when the natural background concentration is added to the calculated values. The natural background value for surface water was assumed to be 12 µg/L and for soil and sediment 140 mg/kg_{dwt}.

	calculated background values)	(excl. measured
water	13.7 µg/L	4-41 µg/L
sediment	567 mg/kg dwt	10-1300 mg/kg
air	0.019 µg/m ³	0.037-0.054 µg/m ³
soil: agricultural	72 mg/kg dwt	10-320 mg/kg (avg. 50 mg/kg)
natural	1.8 mg/kg dwt	10-190 mg/kg (avg. 50 mg/kg)

Comparison of measured and calculated data on a local scale was not possible, because representative measured local concentrations were not available.

water

The calculated regional concentration of zinc in surface water is 13.7 µg/L, excluding a natural background level of 12 µg/L. The annual mean dissolved concentrations measured in the Netherlands from 1988-1993 in the rivers Meuse, Rhine and Lake IJssel are not larger than 41, 10 and 3.6 µg/L

respectively. A comparison of measured and calculated data is possible, because monitoring data of dissolved and total concentrations of zinc in surface water are sufficiently available. From this comparison it can be concluded that in general the measured and calculated data are in the same order of magnitude.

sediment

The calculated regional concentration of zinc in sediment is 567 mg/kg_{dwt} (218 mg/kg_{wwt}), excluding a natural background level of 140 mg/kg_{dwt}. Monitoring data of sediments in the rivers of Europe, measured until about 1989, are generally found to be in the same order of magnitude. The annual mean concentrations in the rivers Rhine and Meuse at the Dutch border are higher with values of about 1300 mg/kg. For the Rhine even a 90th percentile value of 3300 mg/kg is reported.

air

The calculated regional concentration of zinc in air is 0.019 µg/m³. Recent monitoring data of the Netherlands (0.037-0.054 µg/m³) are found to be in the same order of magnitude: the difference is not more than a factor 2. In General, the measured values are higher than the calculated PEC_{add} for air.

soil

The calculated regional concentrations (PEC_{add}) of zinc in agricultural and natural soils are respectively 72 mg/kg_{dwt} (63 mg/kg_{wwt}) and 1.8 mg/kg_{dwt} (1.6 mg/kg_{wwt}), excluding a natural background level of 140 mg/kg_{dwt}. Considering a natural background concentration of 140 mg/kg_{dwt}, the calculated agricultural soil and natural soil concentrations are found to be in the same order of magnitude as the measured values. The measured mean agricultural and natural soil concentration in the Netherlands are about the same, with a value of about 50 mg/kg. In the Integrated Criteria Document Zinc (Cleven *et al.*, 1993) it is also stated that the observed mean concentrations of various arable soil studies lie in the range of the nature reserves in The Netherlands. According to that document the observed maximum values measured in arable soils are nevertheless markedly higher. The calculated difference between agricultural and natural soil concentrations is not clearly visible in the measured values.

4. Validation status EUSES modules

In this chapter, an inventory is presented of the validation status of each sub-module of EUSES. Literature sources which are relevant to parts of EUSES are summarised. This chapter is mainly concerned with conceptual and functional validity (see Table 2) and provides recommendations for further study. Whenever possible, a quick comparison with measured data is presented.

4.1 Emission

When no specific information on chemical release is available, standard tables are used based on the use pattern of the chemical. The values in these tables are partly based on in-depth studies but also on professional judgement. For some groups, use category documents are available.

Standard-scenario assumptions

1. 10% of the European production volume is used for the standard region. This assumption is not appropriate for new chemicals which are usually produced in one or a few plants (see Section 2.1.6).
2. The local releases are calculated from this 10%.
3. For the local situation a large point source is considered (the "main source").

Emission factors concern the size (capacity) of the main source and the activity level (number of emission days). At generating these factors, the aim was to obtain estimates which were within an acceptable range of the expected level, although it is difficult to specify these ranges. For emission factors, it is important to know if the fractions emitted are far below 1, several percent or several tens of percents, etc. Nevertheless, large inaccuracies may occur in some situations as the tables must cover all possible applications in all different branches of society. Clearly, expert judgement and common sense are always needed for classification and interpretation in EUSES, overruling values provided by the tables. For estimates based on e.g. use category documents, better values may be expected with an estimated accuracy within a factor 2. Some studies used to derive emission factors for the tables, are over 10 years old, but it is likely that the estimates are still realistic for the present situation.

1. Production

A) Production is the stage where each substance begins. The emissions of substances varies considerably, because of differences in the way they are produced (dedicated equipment, multi-purpose equipment, continuous process) and the steps involved (e.g. reaction media, number of washings with solvent or water, distillation processes, etc.). Furthermore, emissions from production may be treated with end of pipe measures because of regulations or common practice. The first element, the type of equipment used, was considered in the tables for the emission factors, together with an assumed dependence on vapour pressure and water solubility. For the emission factors at this stage, no profound basis exists. During the discussions on the Technical Guidance Documents, representatives of the chemical industry generally agreed with the proposed values, where a dependence on vapour pressure and water solubility was assumed. Only for the releases with waste water the values were adapted, considering a dependence in tonnage for these emission factors instead of water solubility. There is no scientific evidence in daily practice for this assumption but this procedure is based on expert opinion.

- For dyestuffs used for the dyeing of textile, paper and leather the emission factors at the stage of production are based on a use category study (Ros, 1985). So for this category of substances (Use Category 10 'colorants') a better estimation with the default values from the specific table (Table A1.3) may be expected.

For specific substances, producers will normally know at least the order of magnitude of the emissions. In this case the default values from the table will be overruled, leading to more accurate values.

B) For the size of the main source, i.e. the source where the largest part of the substance is produced in this stage of the life cycle, expert judgement has formed the basis for the values used. A distinction between different Use Categories is made to obtain a realistic estimate, apart from the concept of 'high production volume'. Also in this case producers usually know exactly how much of a substance they produce or may produce (production capacity). With this information, the defaults of the tables may be overruled.

2. Formulation

A) This is the stage of the life cycle where a substance is mixed with other substances to obtain a preparation which is applied in a process later on in the life cycle. As no studies on emissions were available, expert judgement was used for most tables. Only for one specific formulation process, the emission factors are based on a use category study: Industry Category 10 'Photographic industry' for the formulation of photographic paper and film (Ros & Bogte, 1985).

B) For the source where the largest fraction of a substance is formulated, expert judgement was used also for the values in the tables. In some cases, the Use Category is used for a discrimination between values. A correction is made automatically by the program to avoid unrealistic values in case a substance is used at a very low level in a formulation (the fraction of the substance in the formulation can be entered). In some cases producers of a substance or the formulation know the fraction of the substance formulated by a single formulator.

3. Processing

For almost every Industrial Category a specific table with emission factors was generated for this stage of the life cycle, i.e. the stage where the substance (as such or in a formulation) is applied industrially. Therefore every Industrial Category will be treated separately.

3.1. IC=1 Agricultural industry

The emission factors have been generated by expert judgement. It was tried to limit inaccuracies by considering the purpose of the substance in agriculture. So for those use categories, specific estimates were introduced. For the number of days substances will be used in agricultural industry again discrimination between several Use Categories was assumed (e.g. a feedstuff additive will be used almost daily where a fertiliser is applied only several times a year).

3.2. IC=2 Chemical industry: basic chemicals

There was no study available on emissions of basic chemicals such as acids and alkalis used in chemical industry. Tables were based on expert judgement, assuming a dependence on vapour pressure and water solubility. Expert judgement was also used for the size of the main source and the number of days per year that the substances is applied.

3.3. IC=3 Chemical industry: chemicals used in synthesis

For intermediates, the estimates are based on experiences in a study in the pharmaceutical industry. For other UCs see 3.2.

3.4. IC=4 Electrical/electronic industry

For the emission factors, only Main Category 2 (inclusion into/onto a matrix) and 3 (non-disperse) were used in the table based on expert judgement. There may be large inaccuracies in the estimates as there is no consideration with respect to specific processes (e.g. application in a semiconductor, in an etching bath, to produce printed circuit boards, as an insulating agent in a capacitor or a transformer, etc.). For the size of the main source and the number of days a general table (expert judgement) is used.

3.5. IC=5 Personal/domestic

Not applicable

3.6. IC=6 Public domain

The table (based on expert judgement) only recognises two specific Use Categories (9 'cleaning/washing agents' and 39 'pesticides, non-agricultural'). Rather large inaccuracies may occur for all other Use Categories. The same holds for the number of days substances are applied in this Industrial Category. As application in this Industrial Category is very diffuse, only the STP (sewage treatment plant) is considered as point source for the local scale. Assuming a safety factor of 4 (to account for differences between STPs) it is assumed that the application of the substance will be the same in every region. This approach is used in all other tables where diffuse use occurs (IC=5, 10, 13, 14, 16 and 0 for the stage of private use).

3.7. IC=7 Leather processing industry

The table for the emission factors is based on expert judgement. For emissions into waste water, a distinction was made between Main Category 2 (inclusion into/onto a matrix) and 3 (non-disperse). In this way, serious mistakes between substances used to remain in the leather (such as dyes) and substances used to produce leather (such as tanning agents) are avoided. For the size of the main source and the number of days a general table (expert judgement) is used.

3.8. IC=8 Metal extraction, refining and processing industry

Whereas the previous Industrial Category was confined to a very limited number of process steps where chemicals are involved (e.g. tanning and dyeing), this Industrial Category consists of several separate industrial branches. The activities involved consist of mining activities, the extraction or separation of metals from the ore (e.g. by means of flotation), the production of primary metals (often with characteristic processes for every metal considered), and all kinds of metal processing steps (ranging from metal removing operations to galvanic treatment and degreasing). A table with general estimates was made trying to encompass almost the whole range of possible processes and purposes. Hence large mistakes may be encountered here. Only for one specific Use Category, a specific study formed the bases for a more reliable estimate: for substances used in metalworking fluids (Van der Poel & Ros, 1987). For the size of the main source and the number of days, a general table is used for most applications of substances. Only for the Use Category combination describing the application of substances in metalworking fluids a specific table is used, making a distinction between primary steelworks and factories, shipyards, etc. where metalworking (rolling, cutting, etc.) is carried out.

3.9. IC=9 Mineral oil and fuel industry

A very general table (with possibly large inaccuracies for specific substances) was generated. No distinction has been made between lubricants based on mineral oil for all kinds of (industrial) application and fuels and fuel additives. Also for the main source, a rough estimate was made on the base of the tonnage involved and application assumed evenly spread over the year.

3.10 IC=10 Photographic industry

For the emission factors the specific study as mentioned before at the stage of formulation was available (Ros & Bogte, 1985). The table was based on the results from this study. Where appropriate, the specific Use Category for this Industrial Category (42 'photochemicals') was considered at the level of its specific function in photography. For the size of the main source, a distinction was made between application by only one company (1 source), and large (at most one third of the substance at one site) and small (at most 5% of the substance at one site) companies (expert judgement).

3.11 IC=11 Polymers industry

Two sets of tables for emission factors were generated as polymers are numerous and processing takes place in many branches of industry. The first table concerns the production of polymers. Taking into account the main types of substances involved in the production of polymers (according to the relevant Use Categories) estimates were generated by expert judgement considering vapour pressure and water solubility. There were no use category documents available for the different processes in such way that emission factors could be derived from the data. The second table deals with the processing of thermoplastics (shaping into the desired article) and thermosetting resins. Several types of chemicals were distinguished

- (considering the relevant Use Categories) and emission factors assigned by expert judgement (assuming dependence on vapour pressure/water solubility in many cases). For the size of the main source and the number of days for processing expert judgement was used again.
- 3.12 IC=12 Pulp, paper and board industry
Also for this Industrial Category, two tables with emission factors were generated. As the process of printing was not covered in another industrial category specifically, a table based on expert judgement was generated discriminating between the main Use Categories (e.g. 10 'colouring agents' for inks and 45 'reprographic agents'), assuming dependence on vapour pressure/water solubility in most cases. The other table contains the emission factors for the actual process of paper and cardboard making (including pulping). Emission factors were generated by expert judgement assuming a dependence on vapour pressure/water solubility. For the process of paper colouring (by adding dye to the pulp mass at paper making) a use category study was used (Ros & Berns, 1988). For the size of the main source and the number of processing days, a general table based on expert judgement was made, only taking into account three levels of company size (one company, large and small companies).
- 3.13 IC=13 Textile processing industry
Only for textile dyeing, emission factors for specific types of dyes and dyeing techniques were used in the tables, due to the availability of a use category study (Ros, 1985). Estimates by expert judgement were generated for all other Use Categories. Also for this Industrial Category, general estimates were generated by expert judgement for the size of the main source and the number of processing days.
- 3.14 IC=14 Paints, lacquers and varnishes industry
Formulation of paints (i.e. mixing and blending of substances resulting in paint products) is the only activity which belongs to this Industrial Category, strictly speaking. The application of paints (where the main emissions take place usually) may take place in many branches of industry at a wide range of scales (very diffuse, e.g. painting of lamp posts or at large point sources, e.g. motor car factories). A general table based on expert judgement was generated often using vapour pressure/water solubility for a range of Use Categories and for water and solvent based systems. For specific paint applications, large deviations in emission factors seem possible. Also for this Industrial Category, general estimates were generated by expert judgement for the size of the main source and the number of processing days.
- 3.15 IC=16 Engineering industry: civil and mechanical
In fact this is an Industrial Category with very different processes. It concerns e.g. building construction and motor car manufacture (including metalworking activities and paint spraying amongst others). Very general emission factors were generated (assuming a dependence on vapour pressure/water solubility) by expert judgement as no specific studies were available. Also for the main source and number of processing days expert judgement was used to generate estimates.
- 3.16 IC=0 Others
This is an even more "diffuse" Industrial Category than the previous one (IC=16). The same tables were used, possibly leading to large deviations from reality.

4. Private use

Only for some Industrial Categories, this stage of the life cycle has been considered (in many cases substances as such or in a preparation are not used by the public at large). The main Industrial Category is of course 5 'Personal/domestic'. Emission estimates were generated on the basis of expert judgement (assuming a dependence on vapour pressure/water solubility in many cases) for a whole range of Use Categories. For the number of days it has been assumed that the emissions are evenly spread over the year (though products as sun milk are mainly used in summer). For the local situation, only the STP is considered as a point source for which a fraction has been calculated including the safety factor of 4 (see also item 3.6).

- For Industrial Category 9 (Mineral oil and fuel industry) private use is considered because of the use of engine oil and fuels. Emission factors have been generated by expert judgement. The same table is used for the number of days as for Industrial Category 5 (Personal/domestic).
- For Industrial category 10 (Photographic industry) a fraction of the substance used by the public at large may be specified in the program. There is a general estimate for the emission factor, whereas for the local situation the approach of the STP with a safety factor of 4 has been used.
- For Industrial Category 13 (Textile processing industry), private use is covered in the same way as described for the previous Industrial Category.
- This has also been done for the application of paint products by the public at large in Industrial Category 14 (Paints, lacquers and varnishes industry). The emission factors however were generated for appropriate Use Categories and for water and solvent based systems by expert judgement.
- For Industrial Categories 16 (Engineering industry) and 0 (Others) the same tables have been used as for paints.

5. *Recovery*

- For Industrial Category 10 (Photographic industry) emission factors for the recovery of silver have been generated. For the emission to waste water the estimate is derived from a specific study (Ros & Bogte, 1985). For the size of the main sources and the number of emission days expert judgement was used.
- For Industrial Category 12 (Pulp, paper and board industry) for both the emission factor table and the main source and number of days, estimates were based on a specific study (Ros & Berns, 1988). The report reflects the Dutch situation at that time and different results may occur in some cases and in other countries (regions).

Comparison with measured data

The EU Technical Guidance Document (TGD) prescribes that the release of a substance at different stages of its life cycle should be estimated by order of preference from:

- 1) specific release information for the given substance (e.g. from producers or open literature);
- 2) specific information from the emission scenario documents (ESD) which are available for a number of industry categories;
- 3) emission factors as presented in the A-tables of the TGD

Unfortunately, the current experience in the EU work on Existing Chemicals (Regulation 793/93) has shown that, except for production, specific release information (1) is very difficult to obtain. As the ESD (2) are only available for a limited number of industrial categories, in most cases, the exposure assessment is carried out with the TGD-default emission factors (3). These TGD-defaults are based on very generic assumptions and are thus a potential source of uncertainty in the risk assessment. The present EU risk assessment reports on existing chemicals were screened on the use of site-specific release estimates to quantify this uncertainty. These specific release estimates are then compared with the TGD-defaults for the corresponding life cycle stage. For 20 chemicals, site-specific release factors could be found for various life cycle stages (Table 4). The correlation between site specific emission factors versus the defaults from the A-tables in the TGD for the 20 compounds is shown in Figure 2. The scatter plot comprises the data (water and air) for all available life cycle stages.

The general conclusion from this limited survey is that the TGD-defaults are generally higher, i.e. more conservative, than the site-specific release factors. In some cases the difference between site-specific and default is up to three, in extreme cases up to four, orders of magnitude. In other cases, the estimate is quite accurate. The current TGD-defaults can thus be considered as a precautionary estimate which is in most, but not all cases, quite conservative.

Table 4 EU priority list chemicals for which site-specific release factors were found or could be derived.

1	styrene	production
	styrene	processing polystyrene
2	naphthalene	production
	naphthalene	processing phthalic anhydride
3	trichloroethene	production
	trichloroethene	processing intermediate
4	1,3-butadiene	production
	1,3-butadiene	processing intermediate (polybutadiene)
	1,3-butadiene	processing intermediate (styrene-butadiene)
5	nonylphenol	production
	nonylphenol	processing intermediate
6	acrylonitrile	production
	acrylonitrile	processing acrylamide/adiponitrile
	acrylonitrile	processing acrylic fibres
	acrylonitrile	processing ABS/SAN
7	tetrachloroethene	production
8	propylene oxide	production
	propylene oxide	processing
9	acrolein	production
10	HF	production
11	DEGME	production
12	DEGBE	production
13	1,4-dichlorobenzene	production/processing
	1,4-dichlorobenzene	production
	1,4-dichlorobenzene	processing
14	benzene C10-13 alkyl der.	production/processing
15	C10-C13 Chloro alkanes	production
16	o-anisidine	production
	o-anisidine	processing
17	4,4-MDA	production
18	pentabromobiphenyl	production
19	octabromobiphenyl	production
20	decabromobiphenyl	production

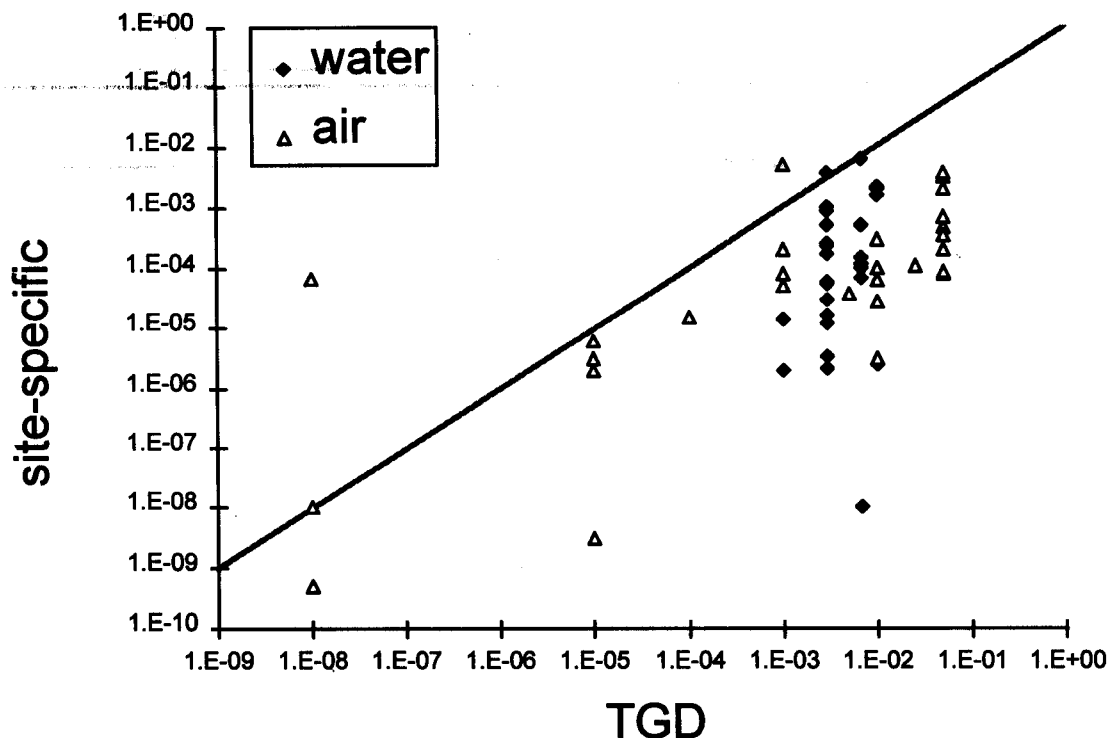


Figure 2 Scatterplot of site-specific emission factors vs. TGD defaults (production and processing). The 1:1 line is shown.

Conclusions

In the Technical Guidance Document (EC, 1996), emission scenarios are included which may be used for improvement of the A-tables. However, these documents often deal with only one compartment, one or two stages of the life cycle, and either the local or the regional situation (Van der Poel, 1997). In order to obtain better estimates for emissions, many studies will have to be performed, considering all processes and specific applications/purposes of substances. In order to reach such a goal, a strategy should be followed where the most urgent studies are performed first. The priority will have to be based on items such as number of substances notified for a specific process/use (see e.g. Table 2 of Umweltbundesamt, 1997), the amounts involved in important processes and the importance of processes (for a process directed approach Nelson -1990- may be useful). An aspect which considers attention in near future is the fact that many substances in articles may emit in a diffuse way over the life time of those articles. These emissions will increase every year new articles are manufactured that include these substances (an example are plasticisers in plastic articles). At the moment a report on emissions from automotive lubricants and fuels, and additives for these products, is prepared at the RIVM. This report will suggest emission tables to be used for Industrial Category 9 'Mineral oil and fuel industry'. Expansion of tables for specific processes within the Industrial Categories and for specific Use Categories may lead to the need of a separate data base and calculation program; the output of such a program then can be used for the assessment program. However, expert judgement can and should never be replaced completely.

4.2 Sewage treatment

The multi-media model SimpleTreat 3.1 is applied in EUSES. This model is a multi-media box model of the Mackay-type.

Standard-scenario assumptions:

1. In the local assessment, all of the wastewater is treated in an STP.
2. In the regional assessment, 70% of the water is treated. The remainder is discharged directly into the surface water. This is an optimistic estimate of the EU average.
3. The number of inhabitants on the local scale is 10,000. On the regional and continental scale 20 million and 370 million, respectively.
4. All emissions are treated in a municipal STP with standard characteristics. Many industrial plants have their own dedicated STPs which are usually considerably larger and usually more efficient.

Source: Struijs *et al.*, 1991

Description: Describes SimpleTreat 1.0 and compares the model to field data for LAS and to data for 5 chemicals from a municipal STP in Chicago (using the operating parameters of the plant). The model is able to simulate field data (within a factor 1.5).

Source: Temmink & Klapwijk, 1997

Description: Extensive validation study for STP models using a pilot-scale activated sludge plant. Unfortunately, it was not the main aim to test existing models. Instead, a new model was developed (DynTreat) which was calibrated and tested. The preface of the report states that existing models are applicable for a screening stage assessment (although no details are found in the text). Biodegradation kinetics are the most important bottleneck in the application of models as linear kinetics are insufficient. Monod kinetics, or similar models, are needed although the Monod parameters are not constants but seem to increase at decreasing influent chemical concentrations.

Source: Toet *et al.*, 1991

Description: Validation study for DRANC which contains SimpleTreat 1.0. For a wide range of substances and situations, the model reasonably predicts effluent concentrations and sludge concentrations (generally within a factor of 10) with the standard scenario.

Conclusion: More work is needed before validity can be shown. Especially the implementation of degradation kinetics needs further consideration. Monod kinetics is already optional in EUSES but guidance on selection of parameter values is lacking. Nevertheless, the limited validation so far suggests that the model is reasonably reliable.

4.3 Partition coefficients

Partition coefficients between environmental media are estimated from physico-chemical properties. A QSAR is used for *K_{oc}* based on experimental data. From this *K_{oc}*, soil-water partition coefficients (*K_p*) in the environmental compartments are calculated based on the amount of organic carbon in the medium.

Standard-scenario assumptions:

1. All sorption is related to organic carbon. This is generally appropriate for neutral organic compounds.
2. "Typical" environmental characteristics are used (e.g. fraction organic carbon, fraction solids).

Source: Sabljic *et al.*, 1995

Description: QSAR for *K_{oc}* are presented, based on experimental data. Calculated uncertainty factors are a factor 3.2 for the log *K_{ow}* range 1-4, and a factor of 14 for the log *K_{ow}* range 4-7 (Jager *et al.*, 1997). Only one QSAR from this source is implemented for the group "predominantly hydrophobics". Other QSARs for different groups are available and are also mentioned in the TGD but not implemented in EUSES (the results in EUSES can be overwritten by manually calculated data).

Source: Temmink & Klapwijk, 1997

Description: Validation study for STP models using a pilot-scale activated sludge plant. For sludge-water distribution, *Koc* can be related to *Kow* when a relatively low accuracy is sufficient. For more detail, sorption isotherms are required. Furthermore, the reversibility of sorption needs to be further investigated.

Source: Schwartz, 1997

Description: The estimation of the particle-bound fraction in air can be improved by using different values for the surface area and the Junge constant ($1.5 \cdot 10^{-6} \text{ m}^2/\text{m}^3$ and 17.2 Pa.m, respectively).

Conclusion: The QSAR for *Koc* seems sufficiently descriptive to use in risk assessment, especially when also the formulas for other groups of chemicals are implemented. For dissociating chemicals and metal compounds, no quantitative guidance is available.

4.4 Degradation rates

Unless kinetic data from simulation tests are available, first-order rate constants are based on the results of standard biodegradability tests (OECD, 1993). These "ready" or "inherent" tests are conducted in artificial systems and no attempts are made to reflect the real world. Rate constants from real world studies, however, are scarce and usually there is no alternative for applying results of those artificial standard tests. Due to the low predictive power of these tests, worst-case rates are assigned to results which have been categorised based on expert judgement (VROM, 1995). This extrapolation procedure represents a consensus, yielding rather conservative rate constants as defaults for aerobic biodegradation in water and soil.

Standard-scenario assumptions

1. A rate constant for aerobic biodegradation can be derived from the standard test results.
2. Degradation in soil and sediment is inversely related to sorption.
3. The upper 10% of the sediment layer is aerated and is considered microbially equivalent to soil. There is no degradation assumed in the remaining fraction.

Water, soil and sediment

A first attempt to evaluate results from OECD tests to biodegradation in aerobic compartments of the real world was made by Struijs & Van den Berg (1994). This approach, modified by experts (VROM, 1995), was supported in a preliminary validation exercise by comparing results of reported field studies on biodegradation of 20 chemicals with positive results in OECD Ready Biodegradability tests. From a biodegradation database (ECETOC, 1994) 36 substances were retrieved with results from screening, soil and surface water biodegradation tests. During the EU Expert Meeting (VROM, 1995), these substances were classified according to the EUSES categories "ready", "ready without 10 d window", "inherent" and "persistent". For the latter category, a half-life in surface water equal to 50 years was assumed, which is at least two orders of magnitude longer than "inherent". Figure 3 compares measured half-lives reported (ECETOC, 1994; Struijs & Van den Berg, 1994) with half-lives obtained from OECD standard tests results categorised according to EUSES. For the soil compartment, such a comparison is based only on the ECETOC data (see Figure 4). Further quantitative validation is needed as real world biodegradation rates may differ from rates obtained according to the EUSES approach by several orders of magnitude. EUSES is generally on the conservative side (up to a factor of 100) but, in a few cases, the measured degradation rates are slower than the estimates.

For the sediment compartment, such a comparison is not yet possible due to the lack of field data on *aerobic* biodegradation. Anaerobic biodegradation, especially reductive dehalogenation, has been

reported for reasonable number of compounds. However, data based on a standardised biodegradation test for anaerobic biodegradation is the limiting factor to develop an extrapolation routine for EUSES.

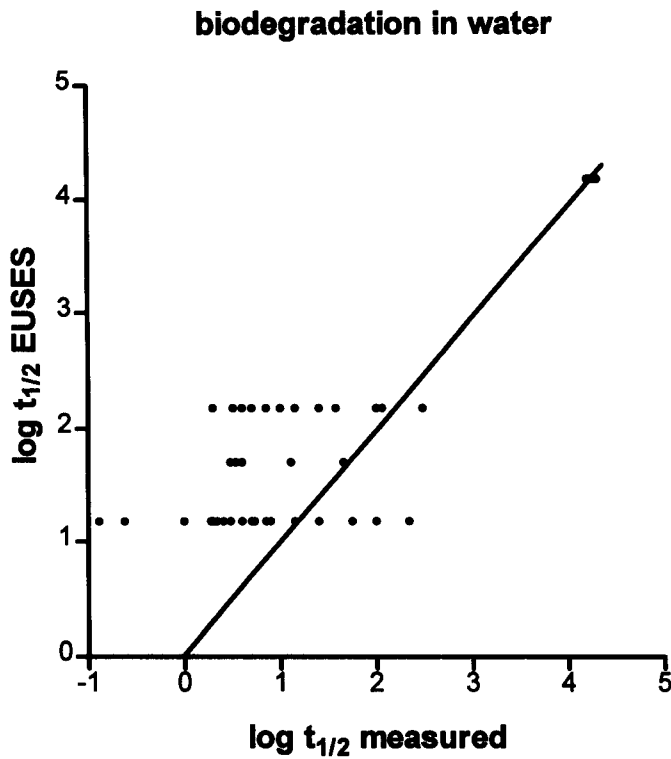


Figure 3 Measured vs evaluated (according to EUSES) logarithmic half-lives in surface water. Data of ECETOC (1994) and Struijs & Van den Berg (1994) are combined. The 1:1 line is shown.

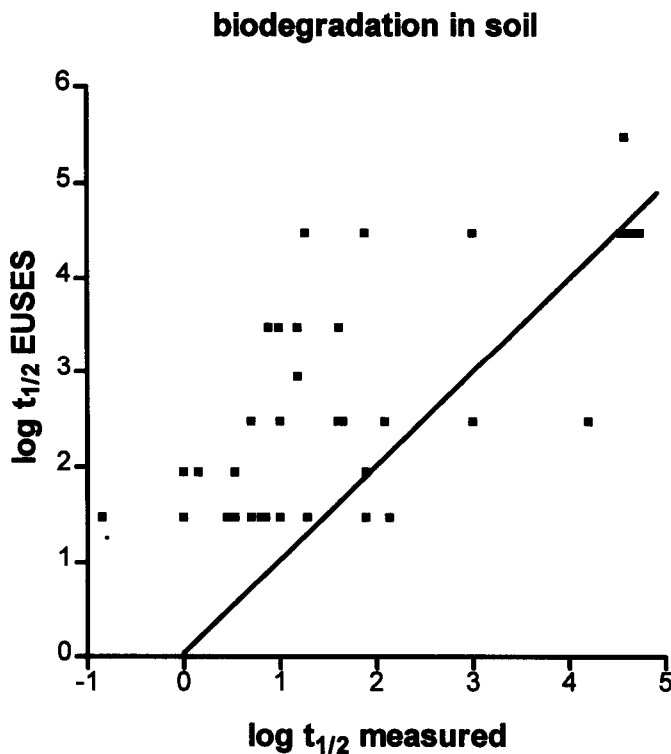


Figure 4 Measured vs evaluated (according to EUSES) logarithmic half-lives in the (aerobic) soil compartment. Data from ECETOC (1994). The 1:1 line is shown.

Sewage treatment plants

Temmink & Klapwijk (1997) conducted a validation study on models to predict the fate of organic chemicals in biological wastewater treatment plants. It was shown that an increasing loading rate of a compound is counteracted by an increased biodegradation capacity of the activated sludge. This indicates Monod kinetics rather than a first order rate constant which in EUSES is applied as a default for positive chemicals in OECD biodegradability tests. However, the validation study was limited to only a few easily biodegradable substances and further work needs to be done.

Conclusion: EUSES will usually provide a worst-case estimate of biodegradation, based on the standard test results. Nevertheless, the deviation may be up to a factor of 100, indicating the low predictive value of the standard tests for the situation in the environment.

4.5 Local distribution

The local distribution module of EUSES consists of separate models for air, water/sediment and soil/groundwater. These models are not generally linked (e.g. chemicals volatilising from soil do not lead to increased air concentrations), only deposition is linked to the soil model. An alternative would be to extend SimpleBox with a box on the local scale. An advantage would be that all processes are linked and consistency between the different scales. This could be investigated in the future.

4.5.1 Air distribution

EUSES does not contain an air distribution model but applies standard concentrations calculated with the model OPS at a standard source strength. These standard concentrations are multiplied with the true release estimate.

Standard-scenario assumptions:

1. Standard source characteristics: height 10m, no heat content of gases, source area 0 (ideal point source). These characteristics may not be representative for large producers (high sources) and ground sources (e.g. traffic and leakages).
2. Standard weather conditions for the Netherlands are applied. This may not be representative for other EU countries.
3. The PEC in air is taken as the highest resulting from source and STP; for deposition, the contributions of STP and source are summed.
4. Air concentrations are calculated at 100 m from the source, deposition flux averaged over a circle with 1000m radius around source. This spatial scale seems rather arbitrarily chosen and 100m is not necessarily a worst case (with higher sources, the plume can reach the ground much further away from the source).
5. Annual average concentration are assumed to be most representative.

Source: Van Jaarsveld (1989)

Description: This report describes and evaluates the OPS model. Validation was only performed for the regional scale calculations (not included in EUSES) which showed excellent agreement for long-term average (deviation in concentrations 10%, in deposition 15%). On the local scale, validation was not performed, but a comparison with a different Dutch model was performed, showing differences smaller than 35%.

Source: Van Jaarsveld (1995)

Description: This PhD thesis concerns the description and evaluation of OPS. Chapter 5 deals with model validation. Experiments with SO₂ showed that OPS was able to accurately describe the concentrations around a point source (note that the model in this case was parameterised to the site-specific conditions). 90% of the data were within a factor of 2.

Source: Teeuwisse & Bakker (1996)

Description: TNO presents an alternative model for implementation in EUSES. No comparison with the current model is made but the advantage is that the source characteristics and environmental parameters can be changed.

Conclusion: Although the underlying model seems well-described and validated, the current implementation with "standard concentrations" is inflexible and includes Dutch weather assumptions. Other simple models (e.g. as described by TNO) can be investigated, especially when they allow to adapt the scenario to site-specific situations (e.g. the height of the source).

4.5.2 Water and sediment distribution

The distribution in water only considers dilution and sorption to suspended organic matter. The sediment concentration is calculated from solids-water partition coefficient.

Standard scenario assumptions:

1. The relevant water concentration used for the PEC is calculated at the point of complete mixture of effluent and river water. The fact that aquatic organisms move and therefore exposure and risk are variable is ignored.
2. A dilution factor of 10 is assumed. This dilution factor is quite worst case. Production sites are usually located on larger rivers, but on the other hand, in Mediterranean countries, rivers may run dry in summer (thereby effectively concentrating the chemical instead of diluting).
3. For the aquatic ecosystem, the average concentration during an emission episode is taken, for predators and human exposure the annual average is used. It is assumed that annual averages are more representative for chronic exposure.
4. Volatilisation, degradation (biotic and abiotic) and sedimentation are ignored as loss terms. This seems usually valid for short time scales as dilution tends to dominate.
5. Sediment is in continuous equilibrium with overlying water. This may not be appropriate for very hydrophobic chemicals.
6. "Typical" properties of suspended matter are assumed.

Source: De Nijs & De Greef (1992).

Description: The dilution of effluents from the majority of STPs in the Netherlands was estimated. The median dilution is a factor of 30 but ranges are from 1 (polder water) to 100.000 (the river Rhine).

Source: Jager (1995).

Description: RIVMODEL was examined as described in the report on HAZCHEM (ECETOC, 1994). It was concluded that generally sedimentation, degradation, and volatilisation are insufficiently rapid to influence concentration in surface water. It seems acceptable to assume dilution as the main removal mechanism.

Conclusion: More elaborate river models may be pursued for more site-specific assessments, although the effect on concentrations is expected to be limited. More is to be gained by using alternative scenarios. The model for sediment may be too simple as the kinetics of this compartment are ignored.

4.5.3 Soil and groundwater distribution

EUSES applies a one-compartment model with sludge application and continuous deposition as inputs, and volatilisation, degradation and leaching as outputs. Exchange rates are based on SimpleBox routines.

Standard scenario assumptions:

1. Standard soil characteristics. These characteristics will not only vary between Member States, but also within countries. The chosen values are "not atypical" for European soils.
2. The maximum amount of sludge is used on agricultural and grassland soils each year. It should be noted that in many countries sludge is not used as fertiliser.
3. Sludge is taken from the STP during an emission episode (worst-case assumption).
4. Ten years of accumulation are accounted for. This is a pragmatic choice. Because the degradation rates are quite worst case, chemicals may accumulate for thousands of years leading to unrealistic high concentrations.
5. Only the top 20 cm are considered. These are assumed to be homogeneously mixed. For arable soils, this is defensible as this more or less covers the ploughing depth. For other soils, 5 cm is taken.
6. Soil concentrations are averaged over 30 days for ecosystem exposure and 180 days for crops. For crops this is probably too long (Jager & Hamers, 1997).
7. "Typical" weather conditions and soil properties are assumed.
8. Volatilisation is calculated from a two-film resistance model which assumes two well-mixed layers. This may not be appropriate for soil as soil is not vigorously stirred.
9. Groundwater concentrations are assumed equal to soil water in the top 20 cm.

Source: Jager (1995)

Description: The EUSES model was compared to the extensive soil/groundwater model PESTLA (Van der Linden & Boesten, 1989) (for the comparisons, no volatilisation is assumed in the box model, and degradation is scaled to temperature as in PESTLA). A quick comparison revealed very similar results (difference never more than a factor of 1.5).

Conclusion: The leaching and degradation behaviour in the one-compartment model seems to be similar compared to a more complicated model although the comparison can not give more than an indication. The validity of the volatilisation rate is not tested. The validity of taking soil water as groundwater is questionable, but it is unlikely that another generic model is capable of better predictions.

4.6 Regional distribution

For regional and continental distribution a multi-media box model of the "Mackay-type" is used (a simplified version of SimpleBox 2.0).

Standard scenario assumptions:

1. Region and continent are made up of 6 well-mixed compartments (air, water, sediment, and three soils).
2. All emissions are treated as continuous and diffuse.
3. The region is 200x200 km with averaged EU properties, the continent has the size of all EU Member States plus Norway.
4. Steady-state concentrations are calculated. For some chemicals this may take several hundreds or thousand years. The SimpleBox 2.0 spreadsheet also allows quasi-dynamic calculation which are very interesting to understand the dynamics of the accumulation.

Source: RIVM report validation SimpleBox (in prep.)

Description: The main aim of this project was to validate the use of SimpleBox to evaluate the consistency of environmental quality objectives. Therefore, emphasis is placed on validating concentration *ratios* between compartments. This study is therefore not directly applicable to EUSES. The main problem identified in this study is the lack of good quality data. The

available data are usually not representative for SimpleBox and the model predicts long-term average concentrations which cannot usually be measured. Only for a few chemicals, sufficient consistent data were available to make a comparison between the measured and calculated concentration ratios. The computed water-sediment and air-water concentration ratios were in good agreement with measured ratios. The measured air-soil ratios were consistently lower than computed ones. Furthermore it seemed that the measured concentration ratios have a higher variability than the computed ones (uncertainty analysis was performed for computed ratios).

Source: Klepper & Den Hollander (in prep.)

Description: In this paper, comparison is made between SimpleBox and a spatially explicit model for water, air and soil. The spatially explicit model is based on the same model formulation as SimpleBox but uses maps of emission patterns and environmental properties instead of average values. The results are expressed on a 25 by 25 km scale over Europe. For soil and air, the value provided by the SimpleBox model is close to the calculated average of the spatially explicit model. The maximum values were within a factor of 10 of this average. For the water compartment, a large difference between the model approaches was found. The concentration in the water compartment of SimpleBox may considerably underestimate average concentrations. Furthermore spatial variability is high: maximum values may be a factor of 100 to 1000 above the average.

Source: ECETOC (1994)

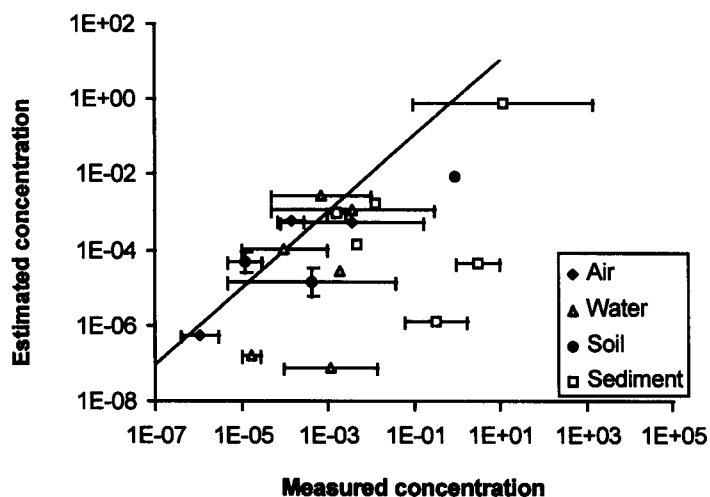


Figure 5 Comparison between estimated and measured (background) concentrations of chemicals. Error bars indicate ranges. The 1:1 line is shown.

Description: Measured data were taken from EU risk assessment reports and compared to EUSES estimates on regional and continental scales. It is difficult to draw definite conclusions on this limited verification but it may serve to get an impression of the order of magnitude. The SimpleBox estimate is usually on the lower end or below the reported values (Figure 6). The maximum reported values (usually close to sources) can however be much higher (up to a factor of 10^7 !). The modelled air concentration seems most representative for the measured values which is not surprising as this compartment can be described as well-mixed. Soil concentrations are reported for one chemical only. Sediment and groundwater seem usually under-estimated. This may be caused by the fact that these are usually measured at polluted locations.

Description: ECETOC gathered measured data from existing literature and ECETOC reports. Wherever possible, background data were selected, although measurements are often made near pollution sources or contaminated sites. Data were compared to HAZCHEM, a multi-media fate model largely comparable to SimpleBox. Generally, the measured data are higher than expected by the model (Figure 5). This may be expected when measurements are conducted when and where a pollutant is expected.

Source: Risk assessment reports on five existing substances.

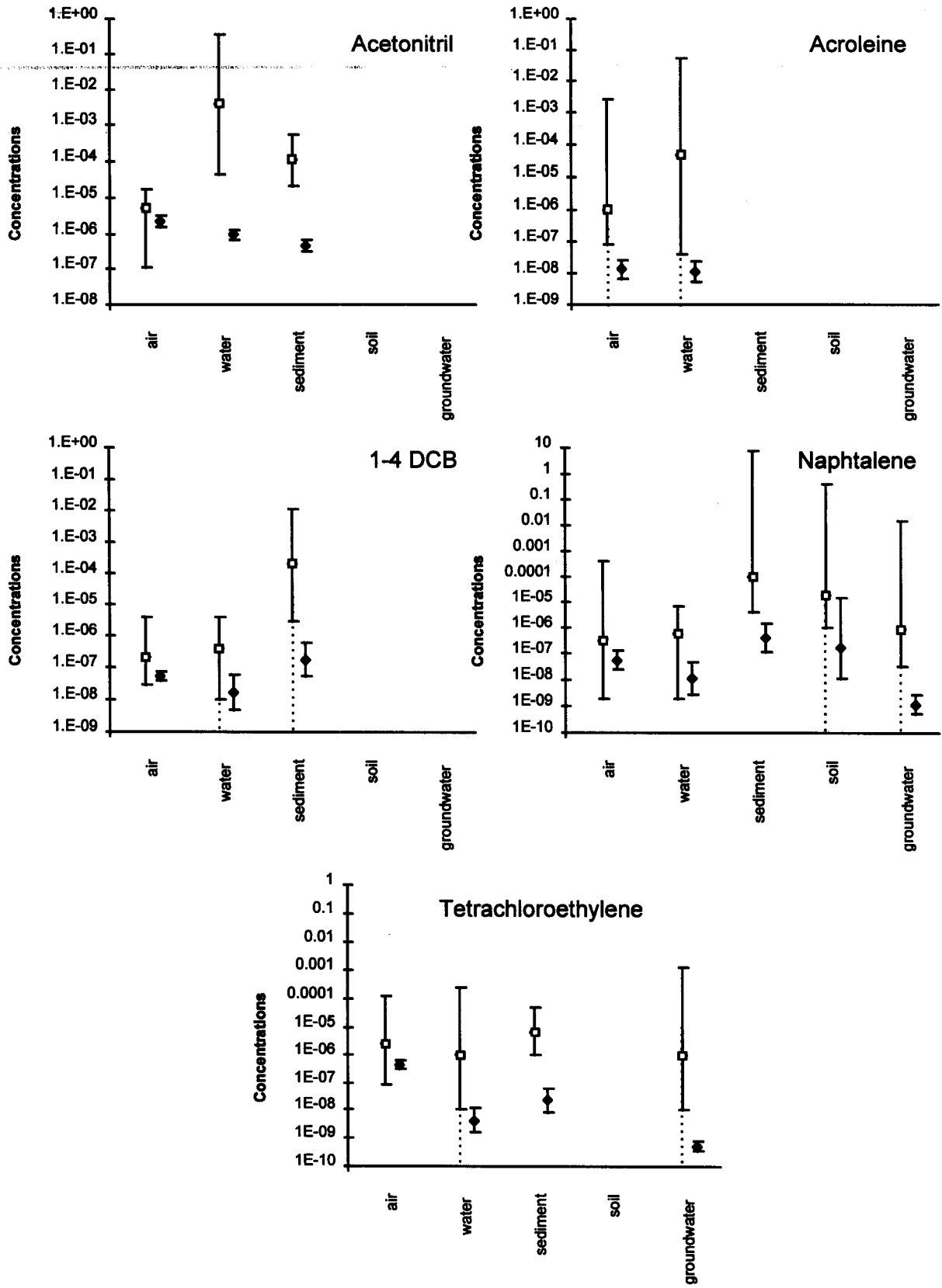


Figure 6 Comparison of measured (open squares) and estimated (closed symbols) environmental concentrations). The measured data point is a "typical value" the range represents the minimum reported value (a dotted line means lower than detection limit) and the maximum point source-related value.

Conclusion: Due to the assumptions, the model is not easily validated. The parameter values for the average EU environment need reconsideration. Nevertheless, the limited data suggest that the user should be aware that SimpleBox will usually give an estimate at the lower end of the range. It should be investigated whether another definition of the standard region will affect the model results in a significant manner (e.g. a Scandinavian or southern-Europe scenario).

4.7 Exposure

Currently, the QSARs for bioconcentration are mostly in the form of empirical regressions. Only for plants, the TGD proposes a mechanistic model. Disadvantages of regressions are:

1. Regressions are only valid within the chemical and biological domain of the training set. Different data sets will yield different regressions. Extrapolation outside the domain should be discouraged (especially for polynomial models).
2. Regressions provide little insight in the process of bioconcentration and the role of the chemical, biological and environmental characteristics in the process.

Jager & Hamers (1997) propagate the use of mechanistic model approaches for fish, worms and plants. These approaches are successful in describing bioconcentration and allow for more insight in the mechanism.

4.7.1 Bioconcentration factor for fish

A linear QSAR is applied in the range log *Kow* 1-6, a polynomial relation for the range log *Kow* 6-10.

Standard scenario assumptions:

1. Fish will reach equilibrium with the annual average water concentration. This is a reasonable assumption (Jager & Hamers, 1997). These authors demonstrated that equilibrium with the annual average water concentration is comparable to the annual average concentration in a dynamically modelled fish.
2. For predators, the concentration in fish is averaged over local and regional scale. This is done to account for the fact that these species are generally mobile and may source food from different areas.

Source: Schwartz (1997)

Description: This author investigated the food chain modelling of EUSES. For hydrophilic compounds, the TGD model provides good results (within a factor of 10). For more hydrophobic chemicals, the variation increases. Generally, PCBs seemed to be underestimated and PCDDs and DEHP overestimated. The deviations were up to a factor of 1000. Eel seems to have much higher measured concentrations than other species due to their much larger fat content. Field data for PCBs were consistently underestimated by the model (up to a factor of 100). This may be related to food chain accumulation.

Source: Jager & Hamers (1997)

Description: The QSARs are quite uncertain, especially the fundamental uncertainty about behaviour of very hydrophobic compounds (it may be better to assume a constant BCF at log *Kow* > 6). Furthermore, these authors showed that a mechanistic approach gives comparable results and that it may be possible to distinguish fatter fish like eel specifically.

Source: Jager *et al.* (1997)

Description: Uncertainty in the calculated BCF for the log *Kow* range 1-6 is 20, for log *Kow* 5-10, the uncertainty is factor of 185.

Conclusion: The QSAR seems sufficiently valid for use in EUSES although variation remains large. For very hydrophobic compounds, the variation is very large. It may be possible to decrease

variation by distinguishing groups of compounds. Because eel is much fatter than other species, this species may be considered specifically. Furthermore, food chain accumulation may be considered more specifically.

4.7.2 Bioconcentration in earthworms

Linear QSAR in the range log *Kow* 1-6.5, based on collected experimental data.

Standard scenario assumptions:

1. The worm reaches equilibrium with the 180-day averaged soil concentration. This assumption is reasonable as the kinetics of bioaccumulation in the earthworm are relatively fast (Jager & Hamers, 1997).
2. The only route of uptake is from the porewater phase. Although earthworms do take up chemicals from food, their total body residues can be described by uptake from the water phase (Jager, 1998).

Source: Jager & Hamers (1997)

Description: The available experimental data were not properly evaluated by the original authors of the QSAR. Equilibrium in worms seems to be fast in relation to the kinetics in soil.

Source: Jager (1998)

Description: This author collected and evaluated BCFs from the literature and compared them to a theoretical model. The QSAR from the TGD overestimates the data. The theoretical model predicts the data from worms exposed in water very well but overpredicts data from soil exposure. This is most likely caused by non-equilibrium conditions in the soil-porewater-worm system.

Conclusion: The current QSAR requires reconsideration as it is too conservative and based on an inappropriate data set. The approach given by Jager (1998) provides an alternative.

4.7.3 Bioconcentration in plants

For assessing the concentrations in above-ground plant material, a one-compartment model is used. The concentration in roots is described by a partition process between water and the phases in the root.

Standard scenario assumptions:

1. Plants are in steady-state with 180-day average porewater concentration and the annual average air concentration.
2. All above-ground parts are treated as one, well-mixed compartment. Roots are assumed to be in direct equilibrium with the soil solution. This assumes a large surface area, therefore, root crops may behave quite differently.
3. Deposition on leaves is ignored. This assumption needs further consideration.
4. A generic leafy crop is taken for the entire plant/fruit consumption.
5. Exponential growth is assumed. Only valid for plants that are harvested before maturation (e.g. lettuce).
6. The parameter values for a "generic crop" are taken. These values need reconsideration (Jager & Hamers, 1997) and seems to characterise grasses (Schwartz, 1997).
7. The standard environmental temperature is 12 °C while plants mainly grow in spring and summer (Schwartz, 1997).

Source: Polder *et al.* (1995)

Description: Validation work to evaluate the route soil to plant as implemented in USES 1.0. Main conclusions were that the root partitioning performs reasonably well. The QSAR for TSCF was

found to be questionable. For above-ground plant parts, the estimate failed (not used in EUSES anymore).

Source: Polder *et al.* (1997)

Description: Validation work to evaluate the route air to plant. The estimator on the basis of the phases in the leaf is generally valid (within a factor of 5).

Source: Trapp & Matthies (1995)

Description: Partly validated the one-compartment model by comparing the results to a more elaborate model and field data for TCDD.

Source: Jager & Hamers (1997)

Description: These authors also investigated this module and also selected the approach of Trapp and Matthies as appropriate. They proposed different properties for plant material (distinction between root tissue and leaf tissue). This requires some more detailed investigation (possibly distinguish between several plant species). Different parameters for roots and leaves are appropriate and the 180 days growing period is too long.

Source: Versluijs *et al.* (1998)

Description: Examines the route soil to crops for the model CSOIL. This model is used to derive soil quality criteria for humans. The model of Trapp and Matthies for plants is also advised for this framework. In this project, it will also be investigated what the main uncertain parameters are and if it is necessary to identify different types of crops.

Source: Trapp & Matthies (1994)

Description: These authors provide some equations to include dry and wet deposition fluxes onto plants (analogous to the formulas of SimpleBox). This procedure, however, does not account for the effect of weathering and assumes that the deposited chemicals are taken up in the well-mixed leaf compartment.

Source: Schwartz (1997)

Description: The model usually underestimates concentrations in plants (up to a factor of 100). Particle deposition is insufficient to completely explain this. Other factors may be the route soil to air to plant and exposure via dust or rainsplash.

Conclusion: It may be possible to make better estimates for specific plant species like root crops. Deposition on the leaf surface must be added but the most appropriate ways to do it need further study. Plant-specific parameters and the exposure scenario need further consideration. Furthermore, particles from soil may attach to the plants (e.g. rainsplash). This route also requires further consideration.

4.7.4 Biotransfer to meat and milk

EUSES contains a linear QSAR in the range $\log K_{ow}$ 1.5-6.5 for meat and 3-6.5 for milk, based on collected experimental data.

Standard scenario assumptions:

1. Steady-state is assumed between the daily intake and the concentrations in meat and milk. A steady state for meat may take a long time to achieve (Van Eijkeren *et al.*, 1998).
2. All milk products are represented by milk. This is not valid as cheese and butter are much fatter. Maybe it is better to relate concentrations to fat content (the original authors of this QSAR assumed 3.68% fat).
3. Fat percentage of meat is assumed 25%, of milk 3.68%. The value for meat seems quite high, 4.4-16.5% is more reasonable (Schwartz, 1997).
4. The cow is exposed by eating grass with adhering soil, inhaling air, and drinking water. Other feed stuffs are ignored (since grass is usually more polluted, this assumption represents a worst case).

Source: Van Eijkeren *et al.* (1998)

Description: A more in-depth investigation has been performed at the RIVM (Laboratory for Exposure Assessment) to investigate the possibility of PB-PK modelling. The main problem seems to be that metabolism and absorption play important roles for many chemicals but they are poorly related to available physico-chemical properties. A generic PB-PK model is therefore not feasible for the first stages of an assessment.

Source: Schwartz (1997)

Description: Validation of the food chain of the TGD/EUSES. The model works very well for low chlorinated PCDDs (within factor 10). Hepta- and octa-chlorinated dioxins were overestimated. For PCBs the model underestimates meat concentrations by a factor of 100. The model for milk seems to go for overestimation. For the PCDDs, TCDD seems reasonably well predicted, but the higher chlorinated PCDDs are overestimated (up to a factor of 100).

Source: Jager *et al.* (1997)

Description: Uncertainty factors calculated for milk: 36, for meat a factor of 64.

Conclusion: The predictability of biotransfer factors from *Kow* is quite poor. There seems to be little room for improvement of the models on the basis of the available data in the base set.

4.7.5 Drinking water

Purification factors are roughly based on the chemical properties *Kow*, Henry's law constant and biodegradation.

Standard scenario assumptions:

1. Drinking water is produced from surface water (locally: annual average concentration at the point of complete mixing) or groundwater (in fact: the porewater concentration under agricultural soil).
2. Groundwater is not purified but used directly as drinking water.

Source: Jager *et al.* (1997)

Description: Purification seems to depend very little on physico-chemical properties. It seems better to take a value for all chemicals. Uncertainty was calculated as a triangular distribution between 0 and 65% with a mode of 15%.

Conclusion: Predictability of removal from physico-chemical properties seems to be low. More investigation is needed unless the degree of uncertainty is acceptable.

4.7.6 Total dose

The total dose for human exposure is calculated by combining the concentrations in food products with a standard consumption pattern.

Standard scenario assumptions:

1. Humans are only exposed to food, air, and drinking water. Dermal exposure and soil ingestion are not accounted for although these sources seem to influence exposure only in specific cases of pollution.
2. Only freshwater fish is consumed which is not likely as mainly sea fish is consumed.
3. All meat is cow meat. Other meat types (chicken, pork) are not considered explicitly. This is reasonable as long as the concentrations are comparable.
4. A standard worst-case consumption pattern is taken: the highest country-average of the EU is taken for each food source.
5. Only adults are considered. Children have a different consumption pattern and body weight.

Source: Schwartz (1997)

Description: EUSES does not consider uptake directly from soil, through the skin or via package materials. This author compared the TGD estimates with other estimates (based on measured concentrations). Generally, the TGD is on the conservative side but most datapoints are within a factor of 100. This conservatism is caused partly by the very high intake rates. Nevertheless, for specific groups (workers, infants, smokers, etc.), higher exposures may be encountered.

Source: Van Veen & Kroese (1998)

Description: The approaches of USES 1.0 were compared with an actual detailed risk assessment for PAHs. The USES intakes were one order of magnitude higher than the detailed study. Food is the main source of exposure although the relative contributions is estimated differently (USES estimates food attributes over 90% of the intake, the detailed study showed over 50%).

Conclusion: Due to the conservative consumption pattern, the EUSES estimate will usually provide a conservative estimate of total exposure.

4.7.7 Example validation study: Risk assessment for BBP

Effting & Van Veen (1998) assessed the human health risk of butylbenzyl phthalate (BBP) in the Netherlands. Indirect environmental exposure was estimated with use of EUSES. The regional compartment in EUSES was regarded as the Netherlands with the continental scale being all other EU Member States. Since most BBP emissions are diffuse, the regional assessment is appropriate for predicting environmental concentrations. BBP is a plasticiser for PVC and is mainly applied in vinyl products like flooring and wall paper (Polymers Industry -IC 11-, softeners -UC 47-). BBP can also be found in smaller amounts in consumer products like adhesive, sealant, paint and lacquers (Paint, lacquers and varnishes industry, IC 14; softeners UC 47). The substance flow of BBP for every relevant life-cycle stage was estimated using data on production, import and export, and consumption of products containing BBP. Releases for every life stage of vinyl products were estimated with use of specific literature for vinyl products and the default emission scenario for the painting industry. Abiotic and biotic degradation rates in air, soil, sediment, surface water and STPs were derived from a recent literature review of the environmental behaviour of phthalates (Staples *et al.*, 1997). Bioaccumulation parameters are also derived from this review.

Predicted surface water concentrations (i.e. $1.7 \cdot 10^{-6}$ mg/L continental and $2.9 \cdot 10^{-6}$ mg/L regional) are compared with water concentrations measured by RIWA (department IMLO) at different locations in the Netherlands. BBP could be detected in 8 out of 107 surface water samples. BBP is only detected at the borders of the Netherlands in rivers Meuse and Rhine (1995-1997), measured surface water concentrations can be compared with continental predicted concentrations as well. Assuming concentration in samples below the detection limit to be between 1/100 and 1/2 of the detection limit (Staples *et al.*, 1997), the average concentration is between $2.7 \cdot 10^{-6}$ and $7.1 \cdot 10^{-6}$ mg/L. This compares well to the predicted values.

In Table 5, predicted food concentrations are compared with measured concentrations in meat and milk in the United Kingdom (MAFF, 1996a). The predicted regional food concentrations are far below the measured values. A local assessment was also made for the major vinyl flooring manufacturer in the Netherlands and a paint manufacturer. The predicted food concentrations are comparable with these figures, indicating that the measured data in the UK may be more representative of local exposure. It should be noted that measured concentrations are also uncertain because it is unknown whether the concentration in the samples are representative of average concentrations. In addition, there is an extra uncertainty whether Dutch food samples contain comparable amounts of BBP as UK food samples. Comparing concentrations measured in infant formulae in both countries, Dutch samples seem to contain considerably less phthalate (Heisterkamp & Van Veen, 1997; MAFF, 1996b) (about 30 times). Therefore it is possible that Dutch food samples contain less phthalate than measured in the United Kingdom.

Table 5 Comparison of measured and calculated data for BBP.

	Regional	Local Vinyl manufacturer	Local Paint manufacturer	(MAFF, 1996a) (measured)
meat [mg/kg ww]	$2.8 \cdot 10^{-5}$	0.087	0.0182	0.09
milk [mg/kg ww]	$8.5 \cdot 10^{-6}$	0.0275	$5.74 \cdot 10^{-3}$	$2.0 \cdot 10^{-3}$

4.8 Consumer exposure

The consumer exposure models aim at describing reasonable worst case exposure. They adopt an exposure scenario and apply it using reasonable worst case parameter estimates. For example, a scenario is a volatile compound that evaporates immediately in a room, achieving the concentration that otherwise would be established over some period of time. The amount of product used will be worst case and acts as a parameter in the scenario. These worst case models aim at the upper limit of exposure. Their message is that the exposure will certainly not be larger than estimated by the model.

Remark: The inhalatory model does not account for saturation in air. The model should be extended to prohibit concentrations larger than the saturation.

Source: Van Veen *et al.* (Subm.)

Description: The indoor application of paint was modelled and validated by Van Veen *et al.* (submitted). The paint model explained the data very well with preset parameter values. The mean concentration during the day of application was 75.6 mg/m^3 . The corresponding EUSES model assuming a constant concentration would predict 753 mg/m^3 . This figure is a factor 10 larger than the measurements.

4.9 Workplace exposure

EASE was specifically developed by the UK Health and Safety Executive for the purpose of modeling inhalation and dermal workplace exposure. EASE is based on measured data which are assigned to specific scenarios. Numerical ranges have been assigned to these fields using measured data contained within the UK National Exposure Database for inhalation exposure, and experimental data and expert judgement for dermal exposure. The experimental data gathered in the validation efforts described below are plotted in figures. These should be interpreted with care as the data are usually not very representative. Nevertheless, these figures may serve to put the model results in the right perspective.

Source: Vincent et al. (1996)

Description: Evaluation of EASE 2.0. EASE produces reliable results in different situations. Several problems and shortcomings were identified: good modelling practice was not followed and numerous gaps were found in the user's guide and software. The program requires bug check and further refinement. The collected data are shown in Figure 7.

Source: Van Amelsfort et al. (1997)

Description: The main target of this report was to study the literature to see whether the EASE model is appropriate to assess inhalation exposure to auxiliary substances, used in small amounts. Based on the available information, it could be concluded that the terms of choices to be made in EASE do not correspond with the terms used in practice; comparing data with EASE is therefore very difficult. The results of the exposure assessments for auxiliary substances made with EASE overestimates exposure levels found in the literature for those situations where a comparison could be made (Figure 8). The validation of EASE for auxiliary substances is severely hampered by a lack of useful measured data. It was therefore concluded that EASE can only be used indicatively for the assessment of inhalation exposure to substances, used in relatively small amount (and with very low vapour pressure). In such cases the overestimation by EASE leads to a relatively high degree of conservatism.

Source: Lansink et al. (1997)

Description: This literature study was performed to obtain dermal exposure data on industrial activities. These data were compared to results of EASE. Only 18 publications contained dermal exposure data, of which only four could be used in a comparison with EASE (shown in Figure 9). Due to the limited amount of data no definite conclusions could be drawn.

Source: H. Marquart, TNO (pers. comm.)

Description: TNO and a number of other institutes are developing a European study to validate parts of EASE with data from a number of sources, including exposure databases. A publication reviewing EASE with regards to dermal exposure is submitted to Risk Analysis.

Conclusion: Based on these very preliminary results, it may be concluded that EASE currently works reasonably well to provide a conservative estimates of workplace exposure. Nevertheless, the observed variation in measured data and estimates is considerable (measured data may deviate up to a factor of 1000 or more from the estimate). Further work is needed but will be coordinated by TNO.

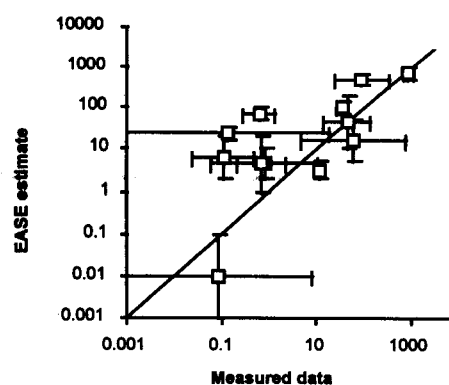


Figure 7 Comparison of EASE with measured data Vincent et al. (1996)

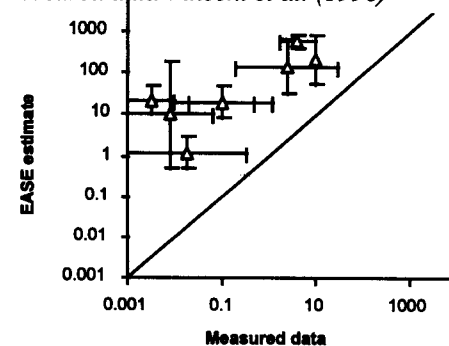


Figure 8 Comparison of EASE with measured data Van Amelsfort et al. (1997).

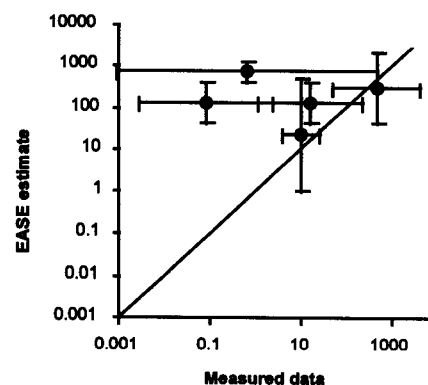


Figure 9 Comparison of EASE with measured data Lansink et al. (1997).

4.10 Effects assessment

4.10.1 Ecological effects assessment

In this module, no-effect concentrations (PNEC) for ecological endpoints are derived by applying fixed assessment factors to the results of single-species laboratory tests. Soil and sediment PNECs are derived through equilibrium partitioning.

Standard scenario assumptions:

1. Protection of the most sensitive species will also protect ecosystem structure and function.
2. Laboratory animals are representative for field species.
3. Soil and sediment organisms are equally sensitive as water organisms and are exposed through porewater. At $\log K_{ow} > 5$ an extra assessment factor of 10 accounts for ingestion of particles.

Source: Emans *et al.* (1993)

Description: Compared data of multiple-species experiments with results of extrapolation methods. The best estimates of "safe levels" were derived using the statistical extrapolation method of Aldenberg & Slob (1993). The EPA assessment factors were more conservative, but usually safe enough. The data are collected in Figure 10.

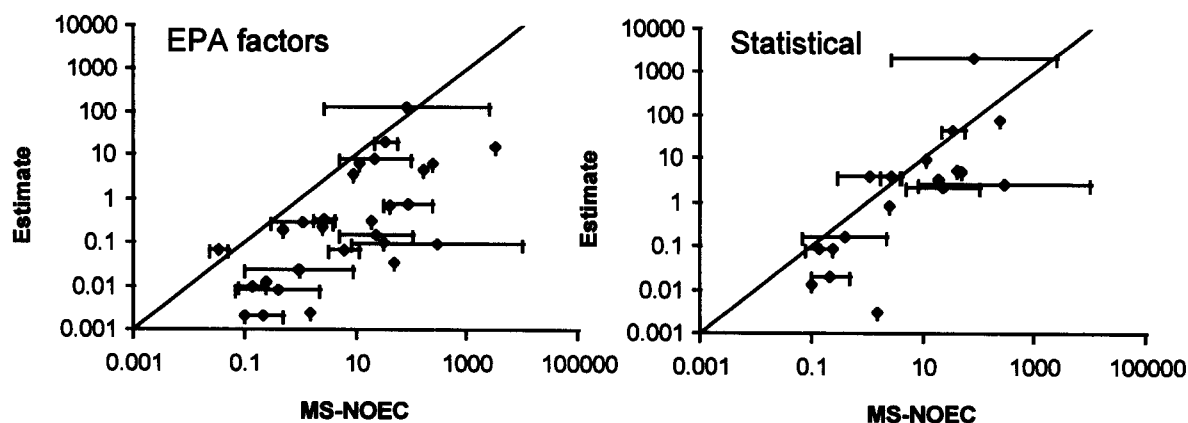


Figure 10 Comparison of estimated PNECs with NOEC from multiple-species (mesocosm) experiments (MS-NOEC). Two estimation approaches are shown: EPA assessment factors and the statistical extrapolation according to Aldenberg & Slob (1993).

Source: Jager *et al.* (1997)

Description: Proposal for data-based assessment factors. There is a considerable amount of data to derive probability distributions for the extrapolation steps (especially the acute-chronic ratio). Nevertheless, the uncertainties remain high.

Source: Belfroid *et al.* (1996)

Description: In this review, it was concluded that the main route of uptake of hydrophobic chemicals in invertebrates from soil and sediment is through interstitial water. For compounds with a $\log K_{ow} > 5$, uptake from particles becomes important, although the quantitative impacts are not clear.

Source: Di Toro *et al.* (1991)

Description: Provides the basis for the application of Equilibrium Partitioning (EP) for sediment quality criteria. Biological effects occur at the same concentrations (within a factor of 2) in different sediments when expressed on porewater basis or organic carbon basis (for chemicals that are not highly hydrophobic). Furthermore, effects concentrations in sediment could be predicted from water-only exposure systems.

Source: Power & McCarthy (1997)

Description: Critical discussion on ecological effects assessment. The three basic assumptions (most sensitive species, chronic data are better than acute, laboratory data can be extrapolated to the field) may be useful from a policy perspective but are not scientifically valid. Alternatives are, however, not available.

Source: Posthuma *et al.* (1989)

Description: This project was a corporation between the RIVM, the free University of Amsterdam and TNO and was performed in the period of 1992-1997. The project was initiated by questions raised about validity of the ecotoxicological risk levels as derived from laboratory toxicity data. The project focused on two aspects: how representative are laboratory toxicity data for field situations, and what is the ecological significance of risk levels. The validity of the extrapolation methods were not discussed. Many factors may cause differences between field and laboratory conditions e.g. differences in the availability, mixtures of contaminants, differences in species and endpoints. Experiments were carried out with different species into laboratory as well as of research carried out in field contaminated sites, focusing on heavy metals. Some of the general conclusions on the field relevance of laboratory toxicity data:

- Bioavailability is an important factor affecting the extrapolation of toxicity data for metals. Soil acidity and contaminant aging are important factors influencing bioavailability.
- Expression of toxicity data on the basis of 0.01M CaCl₂ exchangeable or water soluble concentrations reduces differences between metal toxicity data in different soils.
- Multiple substances can be evaluated assuming additivity unless strong evidence for other responses exists.
- The current short-term toxicity tests do not allow conclusions about long-term population effects. Toxic levels from laboratory-bred species cannot be directly extrapolated to other species.
- Many studies reveal similar ranking of toxicities of metals and pesticides in laboratory and the field.

Conclusion: Based on the limited data, the assessment factor approach seems to provide a safe, but worst-case, estimate. It is possible to derive data-based assessment factors or use statistical approaches, but these methods are not yet acceptable for all Member States (Jager, in prep.).

4.10.2 Human effects assessment

Currently, the effects assessment for humans is limited to route-to-route extrapolation. The data are used without further extrapolation in a margin of safety (MOS).

Standard scenario assumptions:

1. Effects data can be extrapolated between different routes of uptake accounting for availability (only for systemic effects).

Source: Vermeire *et al.* (1998)

Description: Presents a proposal for data-based assessment factors for various extrapolation steps. This approach may be used to help interpretation of the MOS. Vermeire and co-workers summarise a TNO study on route-to-route extrapolation. It was concluded that scientific justification for this extrapolation was not possible due to a lack of adequate experimental data.

Conclusion: Data-based assessment factors may be used instead of the MOS or as support for its interpretation. The route-to-route extrapolation procedure remains difficult to validate.

4.11 Risk characterisation

Risk Characterisation Ratio (RCR) is the general name for the quotient of an exposure and an effects parameter (either a PEC/PNEC ratio or a MOS). RCRs are not parameters that can be actually measured for a chemical. Numerical validation is therefore impossible in the strictest sense. It is possible to get indirect evidence of the validity of an RCR to indicate risky chemicals. It could for instance be attempted to check what RCRs EUSES will predict for known "dangerous" chemicals and known "harmless" compounds.

Source: Jager (1995)

Description: Describes an experiment with risk validation using a group of 39 toxicologists (members of the Dutch Society of Toxicology). For this experiment, 10 well-known substances were selected from a list of attention chemicals. The participants were asked to select two chemicals, based on perceived risk. This selection was compared to the results of USES 1.0. There seemed to be some agreement between the averaged USES ranking and the participants ranking but no definite conclusions could be drawn.

Conclusion: An indication of validity of the risk characterisation is very difficult to obtain but is in fact the most important module for the user. It should be noted, however, that perceived risk may be different from actual risk. People may rank risks on the basis of hard facts (e.g. expected deaths per time unit), but may also take into account how well a process is understood, how the risk is distributed over the population, how personal exposure can be controlled, and whether risk is assumed voluntary (Morgan, 1993). If an experiment like this is to be carried out, the following points must be kept in mind (Jager, 1995):

- The selected chemicals must be well known to the participants. In that way, it is possible for them to make an expert judgement of "risk".
- It should be clear to the participants on what basis they have to make their judgement. It should, for example, be avoided that participants give PCBs a low priority just because they are not produced anymore.
- A representative base-set for these chemicals must be collected.
- The participants must be true "experts" in the field of risk assessment.
- Which RCRs must be used or how should they be combined to give a ranking which can be compared to the expert ranking?

5. Conclusions

Because of the nature of the system and the concept of a "standard environment" one cannot expect EUSES to predict the spatially and temporally varying concentrations in the environment with a great degree of accuracy. The model's outcome is a conservative estimate to support decision making on chemical safety based on the legally restricted minimum requirements of the base-set data. Because of the worst-case assumptions and scenarios, a numerical validation is not easily achieved as the measured data are not usually representative for the model scenario. The system should, however, be able to distinguish potentially risky chemicals from harmless substances. This was recognised in an earlier report (Jager, 1995) but is often overlooked when validity is discussed. Nevertheless, an evaluation as this may not be easy to realise and it is more pragmatic to focus on the performance of the individual models.

Due to the generic nature of EUSES, the applied models usually have a low degree of detail. It is therefore tempting to apply more site-specific models in the assessment (e.g. a more detailed air-distribution model). However, this will inevitably lead to large data needs and results with limited general applicability. Implementation of an uncertainty analysis in EUSES may be more useful in this respect. In that way, poor but general models can be maintained (e.g. the QSAR for the biotransfer to meat and milk) as long as the uncertainty is transparently accounted for. The analysis of the main sources of uncertainty will afterwards reveal where further model or data refinement is needed. This procedure leaves the models simple and thus allows for a more transparent assessment. The acceptability of a probabilistic risk assessment has been investigated in a series of interviews (Jager, in prep.) and will be further developed in 1999. The main application of uncertainty analysis may be to indicate where the main sources of uncertainty are and where model refinement and further guidance are required.

Currently, the validation status of EUSES as a whole leaves much to be desired. Validation activities for individual models are performed but are seldom directly applicable to EUSES. The limited validation status of EUSES does not mean that the system should not be used in risk assessment. It represents a "state-of-the-art" in generic risk assessment and Member States as well as the European Chemical Industry have reached consensus over its contents. Nevertheless, the user of (results from) EUSES should be aware of the degree of accuracy and precision of the specific models to fully appreciate the results. This report aims to clarify this degree of accuracy and precision to facilitate interpretation of the model results (the results of Chapter 4 are simplified and summarised in Table 6). For 1999, an update of the TGDs is planned and this document may serve as input for the upcoming discussions.

Clearly, the degree of deviation from reality may be substantial for the EUSES results. Several modules can be characterised as conservative: release estimation, biodegradation, the exposure scenario, workplace exposure, and the environmental effects assessments. The estimation of partition coefficients and BCFs is median case because a log-linear regression is usually applied. The regional distribution model may be characterised as quite optimistic as it usually seems to provide estimates on the lower end of the range of measured values. It is hoped that the German validation project can evaluate EUSES in a more detailed manner and that they are able to find representative data to compare to the model results.

An important limitation of EUSES is the use of a fixed, "standard", exposure scenario. The model results represent this standard situation but the influence of these scenario assumptions on the risk estimates remains unclear. This may be one of the most important sources of uncertainty. Perhaps it is possible to allow for alternative scenarios in EUSES to make the interpretation of variability for the user easier (Jager, in prep.). From the experiences of the users of EUSES (Chapter 2), it is clear that

most difficulties are encountered in using the emission module. Manual calculations outside EUSES are often necessary to obtain reliable model results. In terms of flexibility, this module needs more work. Another important point is that EUSES is clearly not aimed at the assessment of "difficult substances" like surfactants, dissociating compounds and metals. The TGD also lacks quantitative guidance for these compounds. As illustrated in Chapter 3, the assessment of metals is possible but requires a lot of extra effort and additional assumptions. Since it may be expected that future new chemicals are less straightforward compounds, this remains a point of concern.

Table 6 Summary of the validation status of the EUSES sub-modules.

Module	Conservatism	Indication of possible deviation from measured values
Release estimation	Worst case	1 - 1000
Environmental distribution <i>partition coefficients</i> <i>biodegradation rates</i> <i>sewage treatment</i> <i>local distribution</i> <i>regional distribution</i>	median estimate generally worst case median case largely unknown, scenario w.c. optimistic case	up to factor of 15 for high <i>Kow</i> 0.1 - 100 within factor of 10 unknown 0.001-10
Exposure <i>BCFs</i> <i>drinking water</i> <i>total dose</i>	usually median case worst case worst case	within a factor of 100 unknown unknown
Consumer exposure	worst-case scenario	unknown
Workplace exposure	generally worst-case	0.1-1000
Effects assessment <i>environment</i> <i>human</i>	generally worst case unknown	0.5-1000 unknown

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Appendix 1 Mailing list

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- 2 Directoraat-Generaal Milieubeheer, Directeur Drinkwater, Water en Landbouw, t.a.v. dr. J. Al
- 3 Plv. Directeur-Generaal Milieubeheer
- 4 Drs. M.A. van der Gaag, DGM/SVS, SG UBS
- 5 Drs. A.W. van der Wielen, DGM/SVS, SG UBS
- 6 - 15 EU-OECD Commissies d.t.v. Prof. Dr.C.J.van Leeuwen
- 16 - 35 OECD-RAAB d.t.v. Prof. Dr.C.J.van Leeuwen
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- 38 Ing. R. Faassen, RIZA, SG UBS
- 39 Dr. M. Lans, CTB
- 40 H. Roelfzema, VWS/IGZ, SG UBS
- 41 Ir. D.J. Bakker, TNO
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- 75 - 88 Beoordelingsgroepen H en H/M d.t.v. Drs.A.G.A.C. Knaap
- 89 - 94 Beoordelingsgroep M d.t.v. Ir.J.B.H.J. Linders
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- 97 - 98 Laboratorium voor Ecotoxicologie
- 99 Dr. J.H.M. de Bruijn, CSR
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- 105 Dr. M.P. van Veen, LBO
- 106 Dr. H. Loonen, ECO
- 107 Dr. D. Van de Meent, ECO
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Appendix 2 Blacklist of EUSES 15 June 1998

Contents

I. Bugs

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In each category the entries are numbered. The number between brackets refers to the Blacklist EUSES 1.00 as discussed at the EUSES Working Group Meeting of 23/23 October 1997. An asterix is an additional item also discussed at this meeting. New entries are shown in italics.

I. Bugs

Ia. Bugs which can be circumvented

1. (5)

Source: K. den Haan, ECETOC/Shell

Date: 27 March 1997

After clicking the "finish" button the program does not always present the risk characterisation table, but falls back to the outline. Usually a second trial is successful.

2. (9)

Source: T. Vermeire, RIVM

Date: 23 April, 1997

The screen "Risk characterisation [...]" only appears in the outline mode, but not in the interactive assessment. Normally this is no problem, since the interactive mode does show the summary risk characterisation table. However, the parameters "Intermittent release" and "Extra factor applied to PEC" (applied for PEC soil/sediment in case $\log K_{ow} > 5$) only appear in the detailed screen and not in the summary table. In this way the user is not made aware in the interactive mode that the emission pattern is "intermittent" and that the PEC is increased with a factor of 10.

3. (10)

Source: M. Rikken, RIVM

Date: 23 April, 1997

Printing a full report following a preview is not possible. The "Print" button on the preview screen shows the "Customise Print" screen. However, no output is obtained from the printer following the choice "Full document". A full document can be obtained, however, by choosing "Select pages to print" and entering the full page range of the document. The "Current page" command also works without problems.

4. (19)

Source: M. Mons, RIVM

Date: 10 July, 1997

Error: The summary report does not contain the risk characterisation results for consumers. These results can only be found in the full report and in the compact report.

5.*

Source: B. Scharenberg, UBA

Date: 22 October 1997

In case of IC/UC 3/33 and "Substance not processed elsewhere" the "Fraction of the main source" for production and processing are now different, whereas they should be the same. At present, the user has to overwrite the estimated values.

6.*

Source: B. Scharenberg, UBA

Date: 22 October 1997

The compact report does not contain any PECs. The full and summary report do contain PECs.

7.*

Source: S. Bintein, Ministère de l'environnement

Date: 22 October 1997

Emission factor in TGD and EUSES manual for IC 4, processing, soil, MC 3 is 0.01. EUSES gives 0.001. This has to be corrected manually.

For HPVC, IC = 16, no emission fractions are given by EUSES for formulation, whereas Table B2.3 should have been implemented. These fractions now have to be put in manually.

8.*

Source: S. Bintein, Ministère de l'environnement

Date: 22 October 1997

Emissions for type of dyes used for continuous dyeing are implemented in EUSES during private use, but in the TGD emissions during private use must be considered only for type of dyes used for batch dyeing.

9.

Source: Theo Vermeire, RIVM

Date: 1 November 1997

Emission edit screen: if "production" is switched off the corresponding MC-box does not become grey. Switching production on again results in the MC box becoming grey. However, after going to the next screen and subsequently returning to the edit emission screen it turns out that the MC-box has the right colour.

For IC/UC 3/33 the MC shows a default Ic, which should be III.

10.

Source: Tjalling Jager, RIVM

Date: 10 November 1997.

Changing the dilution factor in the defaults section does not influence the assessment. The dilution factor has to be changed for each life cycle stage in the screen "Local STP input and configuration".

11.

Source: Margreet Mons, RIVM

Date: 20 November 1997

The summary report does not include the inhalatory NOAEL, whereas it does include the oral NOAEL.

12.

Source: EUSES Short Course, Helsinki

Date: 14 November 1997

Consumer inhalatory exposure: if the C_{air} is set, the intake is not recalculated and has to be adapted manually.

13.

Source: Paul van der Poel, RIVM

Date: 6 April 1998

If a substance has more than one use pattern, the estimated emission rate for production may depend on the IC to which this stage has been assigned in EUSES (Screen "use patterns"). This is due to the fact that the B-tables have been designed considering that "typical" chemicals can be used for certain ICs with a specific production regime. However, for substances such as pigments it does not matter whether they are used in printing inks, plastics or paints: the production takes place in chemical industry specialised in pigment production and not in chemical industry specialised in chemicals for a specific branch. In this example the production would give rise to the application of the following tables of EUSES depending on the IC to which the production stage is assigned to:

IC	Table NSEC	Table HPVC	default tonnage (t)
11	B1.9	B1.4	3000
12	B1.8	B1.4	2500
14	B1.2	B1.6	7000

This can lead at lower tonnages to considerable differences in the "fraction of the main sources" (fms) and "number of processing days" (nd). To avoid this two strategies may be followed

This problem could be solved by

1. inserting an extra use pattern IC2 (chemical industry: basic chemicals) and UC 0/55 with the fraction of application set at 1. (this should be the last use pattern inserted since EUSES always automatically calculated the default value for the remaining use patterns by subtracting the sum of the use patterns input from 1; the total fraction in the end will be 2).
2. assigning the stage of production to the main use pattern. This should for instance be chosen in the case of dyes for leather, paper and/or textile industry because a specific A-table exists for dyes.

14.

Source: Charles Bodar, RIVM

Date: 18 June 1998

The STP can be switched off. However, in that case EUSES still calculates a PEC/PNEC for STP micro-organisms. This should be ignored.

Ib. Bugs which cannot be circumvented

1. (2)

Source: P. Gingnagel, RIVM

Date: 13 March 1997

Mammalian effects input: once input is given, e.g. a NOAEL, this value can be replaced by another value as expected, but it cannot be erased (e.g. by replacing it with '??'). EUSES always "remembers" the input. This error is probably related to the gap filling behaviour in this screen and therefore this error also occurs in the screen "Human effects input".

2. (6)

Source: L. Verdam, RIVM

Date: 7 April 1997

New substance, very low vapour pressure, category 4/55, tonnage EU and regional 0.35 tonnes.year⁻¹, resulted in emission to waste water for production of 7 kg.d⁻¹ production for 1 day. File subsequently saved as export file. After importing this file the emission rate remained unchanged (i.e. at 7 kg.d⁻¹) after increasing the production volume to 999 tonnes/year and keeping the number of emission days at 1. The emission fractions are OK. For other life cycle stages there was no problem.

After starting the assessment from scratch no more problems were encountered. The emission rate increased, as expected, linearly with the production volume.

3. (12)

Source: C. Heidorn, ECB

Date 4 June, 1997

In the default screen "Regional and continental distribution defaults" the continental area is given as 3.52E+8 km², whereas it should be 3.52E+6 km² (i.e. Eu area - Regional area = 3.56E+6 km² - 4E+4 km²). In the export file the value is correct and the calculations performed also use the right value. Probably the wrong value on the screen is caused by a faulty unit conversion.

4. (13)

Source: C. Heidorn, ECB

Date 4 June, 1997

In the Help-screen "Regional and continental system definition" the number of EU-inhabitants incorrectly given as 3.8E+6 instead of 3.7E+8. This does not influence any calculation.

5. (20)

Source: E. van der Plassche, RIVM

Date: 15 August, 1997

On screen, in the program reports and in the background report the concentration in earthworms for secondary poisoning is indicated as "Local concentration in earthworms from agricultural soil". This should be "Concentration in earthworms from agricultural soil", which is the average of the local and the regional concentration in agricultural soil. The calculation is correct.

6.*

Source: S. Bintein, Ministère de l'environnement

Date: 22 October 1997

EASE in EUSES does not produce correct results for an aerosol. Whatever the class of volatility is, the ability to become airborne is chosen as high, whereas other options (moderate) should be available (TGD, page 171; EUSES-report, appendix V, page 3; it is also noted that page 3 in the EUSES-report is different from page 171 in the TGD in that an additional class "volatility very low" is shown for which, in case of an aerosol, TBA appears to be high?).

7.*

Source: S. Bintein

Date: 22 October 1997

Import of data into EUSES directly from SNIF or HEDSET is not possible.

8.

Source: J. de Bruijn, RIVM

Date: 1 November 1997

The parameter "Equilibrium Partitioning used for PNEC in soil" always has the value "yes". It should change to "no" in case more than 1 toxicity value for terrestrial organisms is entered.

9.

Source: EUSES Short Course, RIVM

Date: 6 November 1997

In case of IC/UC 3/33, substance not processed elsewhere and production only, the results are reported under processing.

10.

Source: EUSES Short Course, RIVM

Date: 6 November, 1997

Consumer exposure, dermal scenarios: the parameter "duration of contact" is presented as a parameter for both scenarios A and B. However, it only applies to scenario B and should therefore move to the specific entry screen.

11.

Source: EUSES Short Course, RIVM

Date: 6 November, 1997

If only consumer and worker exposure assessment are selected the "human" defaults cannot be approached.

12.

Source: EUSES Short Course, Helsinki

Date: 14 November, 1997

In case a dermal or inhalatory LOAEL or a dietary LOEC for mammals or man is set, any value of the NOAEL or NOEC which has been calculated from the oral NOAEL via route to route extrapolation should not be used in the risk characterisation: a measured LOAEL or LOEC is preferred above a calculated NOAEL or NOEC.

13.

Source: Theo Vermeire, RIVM

Date: 22 December 1997

The ratios between brackets in the screens "Risk characterisation for consumers" for oral and dermal exposure should be reversed, e.g. $N(L)OAEL/uptake$ instead of $uptake/N(L)OAEL$.

14.

Source: Theo Vermeire, RIVM

Date: 22 December 1997

In the case of assessment types III, IV or V, EUSES still presents the input screens for the environmental effects assessment. This is not necessary except for the mammalian toxicity data input screen.

15.

Source: Theo Vermeire, RIVM

Date: 18 March 1998

It was reported that the yes/no switch for "Exceeds solubility limit" did not work. An export file was sent to me in which this was indeed the case. Is this problem related to no. 8?

16.

Source: Paul van der Poel, RIVM

Date: 6 April 1998

As soon as IC8 is chosen in the "emission input data" window the first grey field for "extra data on use category" turns white and shows as default "Pure oils" with the alternatives "Water based" and "Unknown". This box should be grey, however, for IC8; it is only relevant for UCs 29 and 35. Though it will not affect the outcome of the emission estimation, it is confusing especially when you have to consider usage as a solvent (e.g. for a vapour degreasing installation).

17.

Source: Theo Vermeire, RIVM

Date: 1 June 1998

Saving a non-standard default set leads to another default filename in the statusbar as expected. However, a reset does not lead to a reset of this filename. This name only changes back after choosing default - edit - ok.

18.

Source: Stefan Schwartz, Universität Osnabrück

Date: 16 June 1998

Entering extreme values may give problems: e.g. entering $\log Kow < -308$ gives ,1.234; entering $Kow > 308$ gives ??

19.

Source: Stefan Schwartz, Universität Osnabrück

Date: 16 June 1998

The program stops at "Degradation and transformation input" after entering 0 in the field "Fraction connected to sewer systems" in the dialogue "Defaults/Release estimation".

II. Suggestions for improvement and omissions

1. (3)

Source: M. Rikken, CSR, RIVM

Date: 18 February 1997

Separate reporting of PECair,point source and PECair,STP. EUSES now just shows the highest of the two which is used for the risk characterisation.

2. (7)

Source: T. Vermeire, RIVM

Date: 7 April, 1997

Contrary to the Specifications for EUSES (January 1996), the program does not offer a qualitative risk assessment according to the TGD (chapter 3, section 4.5) in case no $PNEC_{water}$ can be calculated (no-effects in short term tests). The program is able to recognise > values for toxicity in the environmental effects assessment input fields. However, in case of no values for aquatic toxicity of limit values such as $> 100 \text{ mg.l}^{-1}$, the program should ask whether a qualitative assessment should be performed and, if the answer is "yes", should calculate a substitute PNEC by dividing the aqueous solubility by 100 and flag this one (only in case $\log Kow > 3$ or $BCF_{fish} > 100$).

3. (8)

Source: T. Vermeire, RIVM

Date: 21 April, 1997

The full report of EUSES does not report regional and continental emission rates for agricultural soil for the individual life cycle steps. However, it does report the total emission rate for agricultural soil.

4. (11)

Source: L. Wijkhuizen-Maslankiewicz, RIVM

Date: 15 May, 1997

In case the molecular weight of a substance is > 700 the BCF_{fish} is not calculated because the QSAR is not valid any more. The user, however, does not get a warning and is left in doubt about the cause of the problem that no $PEC_{oral, fish}$ and C_{fish} are calculated and consequently not intakes for predators and humans.

Solution: In case the user would like to have a maximum estimate he has to lower the molecular weight to 700.

5. (14)

Source: E. van de Plassche, RIVM

Date: 11 June, 1997

According to the TGD ecotoxicological data for soil organisms should be normalised for the standard soil containing 2% organic carbon. These ecotoxicological tests can be performed with a variety of soils. This normalisation is not performed by EUSES and should be done by the user before input. The normalisation can only be applied in case of organic substances, assuming these mainly adsorb to organic matter. It is further noted that this normalisation will lead to errors in case of very low (< 2%) or very high (>30%) content of organic matter.

6. (15)

Source: E. van de Plassche, RIVM

Date: 11 June, 1997

In de output screen "Local concentrations and depositions" the user is not informed that the concentrations in surface water are dissolved concentrations as is shown in the background report page III-51 and in the output files.

7. (16)

Source: E. van de Plassche, RIVM

Date: 11 June, 1997

The PEC_{local} concentrations are only shown for the dissolved fraction. Since the total concentrations are not shown the amount adsorbed to suspended matter cannot be derived directly. The amount adsorbed can be calculated using formulae 58 (regional) and 64 (local).

8. (17)

Source: E. van de Plassche, RIVM

Date: 27 June 1997

In some cases the levels of the substance in sewage sludge applied to agricultural soil are known. EUSES allows to overwrite the estimated levels in sludge by these measured ones at the local scale. However, this is not possible at the regional and continental scales. This problem can be solved in EUSES by overwriting the regional and continental emission rate to agricultural soil by this rate multiplied with the ratio between C_{sludge} estimated and C_{sludge} measured.

9. (18)

Source: E. van de Plassche, RIVM

Date: 27 June, 1997

The estimation of the K_{oc} from K_{ow} in EUSES is performed according to the default QSAR for the domain "predominantly hydrophobics" (TGD section 2.3.5. and section 4.3). However, the user is not warned that other QSARs are available for specific chemical classes. These QSARs should be used, if appropriate, and the general EUSES estimate needs to be overwritten in such cases.

10. (21)

Source: C. Bodar/M. Rikken/T. Vermeire, CSR, RIVM and B. Scharenberg, UBA

Date: 15 August, 1997 and 22 October 1997

In case emission rates from part or all sources of a substance are known and used to overwrite the generic estimates for the local average emission rates during emission episodes, both the TGD and EUSES still calculate a generic total regional annual average emission rate. However, the sum of all site-specific and generic local releases, back-calculated to annual averages, should be a better estimate of the total continental annual average emission rate and should also be the basis for the calculation of the total regional emission rates. At present this can only be done manually and the result can be used to overwrite the generic estimates. Note that in the case of the calculation of regional emission rates from 'real' continental emission rates one cannot use the default assumption that the regional emission rate is 10% of the continental emission rate. If the geographic location of all sources is known, one should take account of this somehow.

11. (23)

Source: G. Janssen, RIVM

Date: 14 October 1997

Consumer exposure assessment: EUSES does not automatically check whether the estimated daily uptake exceeds the theoretical maximum as can be derived from the amount of product used, the concentration of the substance in the product and the use frequency. Example: facial cream, 800 mg with 1% substance, 1 time per day. Maximum uptake is 8 mg/70 kg per day or $0.1143 \text{ mg.kg}_{\text{bw}}^{-1}.\text{d}^{-1}$. EUSES calculates a potential uptake of $1.69 \text{ mg.kg}_{\text{bw}}^{-1}.\text{d}^{-1}$.

12. (24)

Source: Theo Vermeire, RIVM

Date: 14 October 1997

The risk characterisation for man is performed for each population potentially exposed and for each relevant route of exposure, but not separately for each effect as is indicated in TGD.

13.*

Source: Dr. G. Heinemeyer, BgVV

Date: 22 October 1997

Consumer exposure assessment: EUSES only allows consideration of one exposure scenario per exposure route in one run. In case more scenarios per route have to be considered, this calculation needs another EUSES-file. This should be possible in one run with no limit in the number of scenarios. It would be very useful then to have an extra field for a description of each use scenario.

14.*

Source: Dr. G. Heinemeyer, BgVV

Date: 22 October 1997

Consumer exposure assessment: a discussion is needed on the inclusion of models for higher tier consumer exposure assessments in EUSES

15.*

Source: B. Scharenberg, UBA

Date: 22 October 1997

In case of wrong input of a number as 0,2 or 1,6 etc., EUSES should warn the user, that this is illegal. Presently EUSES accepts such values (as 0 and 1, respectively).

16.*

Source: M. Palmquist, KEMI

Date: 22 October 1997

The output could be improved by replacing the number of the use pattern in the headings by text, specifying the use pattern.

17.*

Source: EUSES WG, Ispra

Date: 22 October 1997

Updates of EUSES should include a helpscreen with information on the changes made.

18.*

Source: EUSES WG, Ispra

Date: 22 October 1997

The output for the regional model could be improved by presenting the % distribution.

19.*

Source: EUSES WG, Ispra

Date: 22 October 1997

The options to select the output to the printer (now possible in different ways via the Assess-Select screen, the RCR-table [not explained in manual] and the File/Print Setup) could be improved.

20.

Source: T. Vermeire, RIVM

Date: 20 November 1997

Terrestrial effects assessment: In case only one test is available EUSES calculates a PNEC both from this value after application of an assessment factor and via the equilibrium partitioning method. Subsequently the lowest of the two is reported and used in the risk characterisation. This is as expected. However, EUSES should report as intermediate result both PNECs.

21.

Source: M. Palmquist, KEMI

Date: 28-10-97

Edit emission screen: No main categories should be shown in case the corresponding life cycle stage is not checked. In case information on all or specific main categories is not needed according to the A-Tables, no value should be given either. The default main category should be shown.

22.

Source: EUSES Short Course, RIVM

Date: 6 November 1997

Text improvements:

- Consumer exposure input - inhalation: "Amount of product released" = "Amount of product used"
- Worker exposure input -dermal: "Amount of dermal contact" = "Frequency of dermal contact".

23.

Source: Tjalling Jager, RIVM

Date: 11 November 1997

The Previous Button in the Interactive and Direct Modes also cancels the input just made. The input is only confirmed after going to the next screen with the Next Button. It may be considered to change this behaviour: once an input is set (s) by the user it should be considered as confirmed.

24.

Source: Tjalling Jager, RIVM

Date: 11 November 1997

The guidance concerning the Tonnage used to access the A and B Table can be improved.

25.

Source: Charles Bodar, RIVM

Date: 20 November 1997

It would be helpful if a free text field is added under Study in which detailed information on the use pattern can be stored for the first page of the report.

26.

Source: EUSES Short Course, Helsinki

Date: 13 November, 1997

Working in the outline it would be helpful to indicate in the status bar where you are.

27.

Source: P. Gingnagel, RIVM

Date: 21 January 1998

For the physical-chemical property of vapour pressure only one unit (Pascal at 25 °C) is available. The data set of existing chemicals can also include data of vapour pressure with different units e.g. atmosphere. More units should be allowed for the input of vapour pressure.

28.

Source: P. Gingnagel, RIVM

Date: 21 January 1998

There is no warning when an user select an invalid industry and use category combination. The appendix VI. "Valid IC/UC combinations" of the EUSES-report should be incorporated in EUSES.

29.

Source: P. Gingnagel, RIVM

Date: 21 January 1998

The TGD indicates that a low-flow rate of a river (or 10-percentile) should be used for calculating the actual dilution factor at the point of complete mixing. However when an average flow is given one third of this average should be taken for calculating the dilution factor (TGD page 303). No information on this calculation is available in the EUSES help function. This calculation should be (1/3 of average flow rate) incorporated in EUSES.

30.

Source: P. Gingnagel, RIVM

Date: 21 January 1998

For the "Flow rate of the river" and "Effluent discharge of this STP" only one unit is allowed in EUSES. More units should be made available.

31.

Source: P. Gingnagel, RIVM

Date: 21 January 1998

In the screen of "Local STP input and configuration" the default of "number of inhabitants feeding this STP" is often changed to generate a site specific "Effluent discharge of this STP". The site specific data of STP are often submitted as effluent discharge rate of a STP. No data on number of inhabitants are given because the site specific STP mainly concerns the industry. At the moment the input for "number of inhabitants feeding this STP" must be changed to get a site specific effluent discharge of a STP. The input of the number of inhabitants or equivalent must be derived from the default parameter of EUSES (200 l/d per equivalent or inhabitant) and the submitted flow rate of a site specific STP. The input of a site specific effluent discharge rate should be allowed directly in the field "Effluent discharge of this STP".

32.

Source: P. Gingnagel, RIVM

Date: 21 January 1998

The print outputs of EUSES are difficult to read especially when many use patterns and life cycle steps are selected. In EUSES a screen on "use pattern" and "Risk characterisation result table for the environment" are presented. These screens should also be presented in the print output because all selected industry and use categories with the relevant life cycle steps and the risk characterisation results are viewed. These tables could be separately incorporated in the print output of EUSES.

33.

Source: P. Gingnagel, RIVM

Date: 21 January 1998

The maximum number of use patterns in EUSES that can be selected is ten (screen "use patterns"). After inserting a 11th use pattern the message "Add usage failed" will follow. The information that only ten use patterns are allowed is not available in the help function. No restrictions should be made on the number of use patterns or more use patterns should be allowed.

34.

Source: T. Vermeire, RIVM

Date: 18 March, 1998

In the case that only 2 LC50-values are available and 2 NOECs for aquatic organisms, the assessment factor chosen by EUSES is 100. It is assumed that in this case it is unknown whether the lowest NOEC is also for the same taxonomic group with the lowest LC50. The documentation and the help should, however, make this more explicit.

35.

Source: Els Smit, RIVM

Date: 23 March

After choosing "new study" in the main menu the programme should ask immediately to enter "name" and "description" to avoid an error message at saving.

36.

Source: Stefan Schwartz, Universität Osnabrück

Date: 16 June 1998

EUSES should also allow to use separate models: it should be possible to enter only the data needed for a specific model.

37.

Source: Stefan Schwartz, Universität Osnabrück

Date: 16 June 1998

The error messages could be improved with regard to the "solutions" provided. In many case one is referred to the manual and no further advice is given.

38.

Source: Stefan Schwartz, Universität Osnabrück

Date: 16 June 1998

It should be able to adjust the width of the columns in the "Use patterns" table to improve readability and to allow printing.

39.

Source: Stefan Schwartz, Universität Osnabrück

Date: 16 June 1998

In the screen "Emission input data" the phrase "main category" should be added on the relevant position.

40

Source: Stefan Schwartz, Universität Osnabrück

Date: 16 June 1998

Remove the "Load defaults" button on the screen "Defaults". It does not belong there and the function can already be approached via the main menu.

41.

Source: Paul van der Poel, RIVM

Date: 23 August 1998

In some cases it should be possible to specify the regional tonnage of a substance per life cycle step (e.g. Screen "Intermediate results tonnages" per life cycle step for each IC/UC combination). This applies, for instance, to a substance imported to 1 formulating source in a region (100 % of EU-tonnage) with subsequent diffuse industrial or private use (10% rule applies: 10 % of the EU-tonnage in a region). This can now be done by entering two identical IC/UC combinations in the "Use patterns" screen, one for each life cycle step. "Intermediate results tonnages" screens will appear for each IC/UC/life cycle step entry.

III. Inconsistencies

1. (4)

Source: J. de Bruijn, RIVM

Date: 26 March 1997

The officially accepted erratum of Appendix II of chapter 3 does not produce the same results as SimpleTreat in EUSES. The current version of SimpleTreat 3.0 debugged included a different estimation routine for Koc than the TGD and EUSES.

2. (22)

Source: E. van de Plassche, RIVM

Date: 14 October, 1997

In the assessment of secondary poisoning the PEC (concentration in fish or worm) is in $\text{mg.kg}^{-1}_{\text{wwt}}$ whereas the PNEC is in $\text{mg.kg}^{-1}_{\text{dw}}$. The PNEC usually is derived from the NOAEL or NOEC of tests with experimental animals, fed dry laboratory chow. Theoretically a correction is necessary for the conversion from dry weight to fresh weight. In view of the difference in diet (laboratory chow versus worms or fish) such a correction seems difficult to perform.

3.*

Source: S. Bintein, Ministère de l'environnement

Date: 22 October 1997

The parameter Surplus Sludge is a fixed value in the TGD (0.011) and a variable in SimpleTreat 3.0 in EUSES.

4.*

Source: B. Scharenberg, UBS

Date: 22 October 1997

The concentration of suspended matter in the continental system (25 mg.l^{-1}) is different from the regional value (15 mg.l^{-1}). This makes the region an area with net sedimentation. The TGD only reports the regional value.

5.

Source: Tjalling Jager, RIVM

Date: 10 November 1997

EUSES does not consider direct emission of fertilisers and pesticides to agricultural soil (processing, Table A3.1). The TGD-Erratum of 19 February 1997 (Doc. ECB TGD/01/97) specifies to direct these emissions to agricultural soil on the regional and continental scale.

6.

Source: Tjalling Jager, RIVM

Date: 10 November 1997

Page III-39, Table III-12 mentions concentration of biota in water (BIOTAwater) of $0.1 \text{ kg}_{\text{wwt}}.\text{m}^{-3}$. The value in EUSES is 1 mg.l^{-1} , the SimpleBox documentation mentions $1 \text{ mg}_{\text{dwt}}.\text{l}^{-1}$ (this is not correct as it is multiplied with a BCF on wwt basis!).

7.

Source: Theo Vermeire, RIVM

Date: 18 March 1998

According to the TGD the dry weight solids produced per person per day (SOLIDS) is 0.011 kg.eq⁻¹.d⁻¹; in EUSES the value is 0.09 kg.eq⁻¹.d⁻¹.