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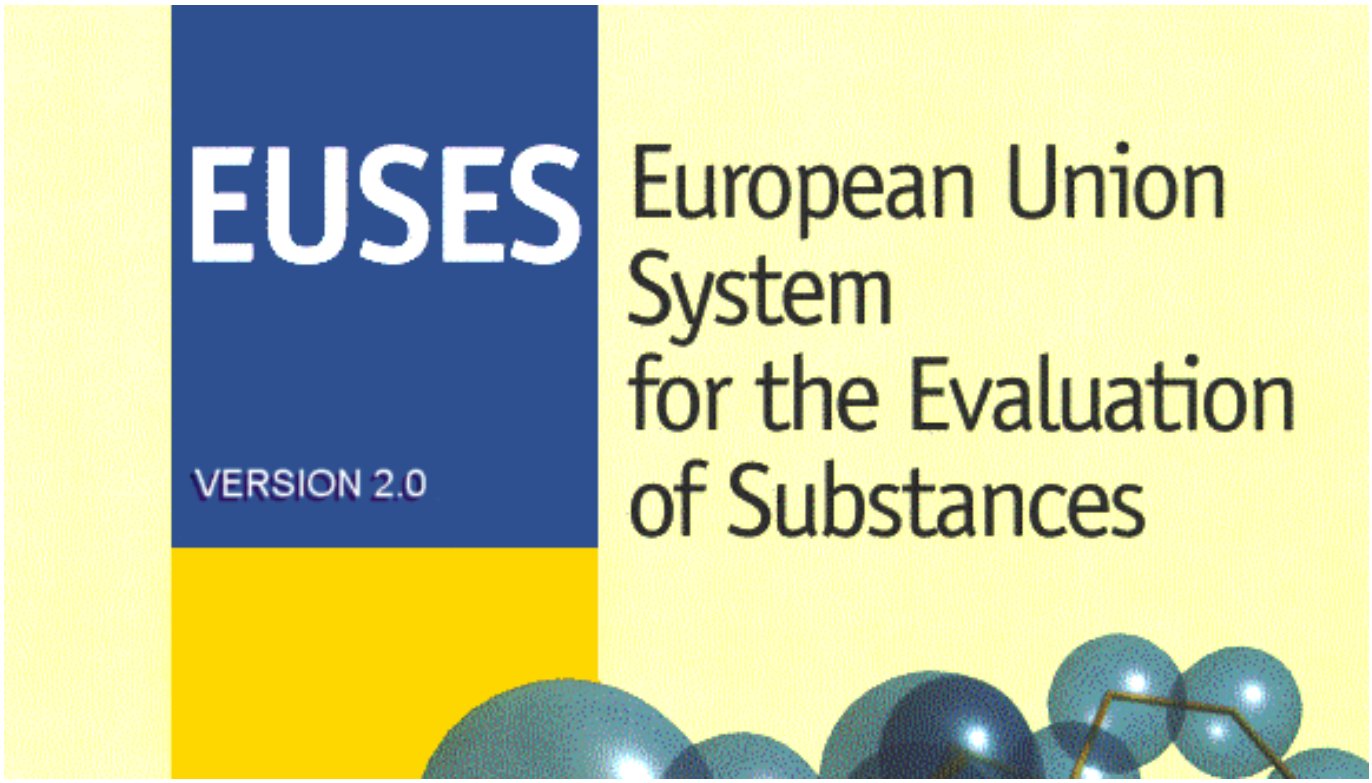

Background report

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PREFACE

This report describes the second version of the PC-program 'European Union System for the Evaluation of Substances', EUSES 2.0. EUSES 2.0 is designed to be a decision-support system for the evaluation of the risks of substances to man and the environment. The system is based on the EU Technical Guidance Documents for risk assessment of new and existing substances and biocides. The documentation and program can be obtained from the European Chemicals Bureau, Ispra, Italy.

The development of EUSES 2.0 was commissioned by the European Commission to the National Institute of Public Health and the Environment (RIVM) of The Netherlands[1]. The work was supervised by an EU working group comprised of representatives of the European Chemicals Bureau, EU Member States and the European chemical industry. TSA Group Delft was responsible for programming the system.

It is recommended that experts in the risk assessment of substances are responsible for the evaluation and selection of data and the application of the system. Adequate interpretation of the results of the system is required as a basis for risk management decisions.

The report has been edited by J.P.A. Lijzen and M.G.J. Rikken of the National Institute of public Health and the Environment. The RIVM project team consisted of the following persons: T.G. Vermeire (project leader), J.P.A. Lijzen, M.G.J. Rikken, J. Bakker, C.E. Delmaar, H. den Hollander, D. van de Meent, P. van der Poel, M. Pronk, J. Struijs and W.H. van der Zon. The subcontractor for the programming was TSA Group Delft.

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[1] RIVM Project M/601900, RIVM Report No. 601900005

CONTENTS

SUMMARY

This report describes the second version of the PC-program 'European Union System for the Evaluation of Substances', EUSES 2.0. EUSES 2.0 is designed to be a decision-support system for the evaluation of the risks of substances to man and the environment. The system is fully based on the EU Technical Guidance Documents for the risk assessment of new and existing substances and biocides. The documentation and program can be obtained from the European Chemicals Bureau, Ispra, Italy.

In the European Union, Directive 92/32/EC, EC Council Regulation (EC) 793/93 and EC Directive 98/8/EC require the risk assessment for new substances, existing substances, and biocides, respectively. Principles for this risk assessment have been laid down supported by a detailed package of Technical Guidance Documents. Against this background the European Union System for the Evaluation of Substances, EUSES, was developed. EUSES is fully in line with the most recent package of Technical Guidance Documents of 2003. EUSES is the result of a co-ordinated effort of EU Member States, the European Commission and the European Chemical Industry.

EUSES facilitates the quantitative assessment of the risks posed by new and existing substances and biocides to man and the environment. This assessment is transparent and easy to perform: EUSES is well documented and available as a user-friendly computer program. Risks to man pertain to consumers, workers and man exposed through the environment. Protection goals in the environment include sewage treatment plant populations of micro-organisms, aquatic, terrestrial and sediment ecosystems and populations of predators. This assessment includes the marine environment. The system can be used to carry out tiered risk assessments of increasing complexity on the basis of increasing data requirements. Virtually all default settings can be changed and all estimated parameter values and intermediate results can be overwritten by measured data.

The risk assessment is carried out in a stepwise procedure starting with data input and estimation and further involving the estimation of emissions, the prediction of environmental distribution, the calculation of human and environmental exposure, the derivation of no-effect levels and the risk characterisation. The exposure assessment in EUSES covers the whole life cycle of substances as well as their fate in all environmental compartments at three spatial scales: the personal scale for consumers and workers, the local scale for man and ecosystems near point sources and the regional scale for man and ecosystems exposed as a result of all releases in a larger region. Both short- and long-term time scales are considered, where appropriate. The exposure assessment aims at 'reasonable worst case' results by applying unfavourable, but not unrealistic, standard exposure scenarios and, as much as possible, mean, median or typical parameter values. Where appropriate, in the effects module no-effect levels are derived for all ecosystems and populations considered. The human effects assessment covers all relevant endpoints for both threshold and non-threshold substances.

The end-point of EUSES is a quantitative comparison per substance of the results of the effects and the exposure assessment. The resulting risk characterisation ratios (RCRs) can be regarded as indicators for the likelihood of adverse effects occurring.

EUSES is designed to facilitate the risk assessment of a broad range of substances in accordance with the EU Technical Guidance Documents. The user needs a sufficient degree of expertise to be able to appreciate the pros and cons of the Technical Guidance Documents and the system, to evaluate the quality of the input data, to make a proper data selection, to understand the assumptions made as well as the inherent limitations of the estimation methods, and, finally, to correctly interpret the results.

ACKNOWLEDGEMENTS

The development of a decision support tool such as EUSES requires the input of a large number of experts in different scientific fields. Scientific experts from EU Member States, the European Chemical Industry and the European Chemicals Bureau have been involved, notably the experts in the RIVM EUSES Working Group and the EU EUSES 2.0 Working Group. Software expertise was provided by TSA Group Delft. The contributions of all persons to the EUSES 2.0 project are gratefully acknowledged.

The development of EUSES was commissioned by the European Chemicals Bureau. Support was provided by the Danish Environmental Protection Agency and the Netherlands' Ministry of Housing, Spatial Planning and the Environment, Directorate-General for Environmental Protection.

READERS GUIDE

This EUSES 2.0 background report describes EUSES, the European Union System for the evaluation of Substances. EUSES has been developed to support the risk assessment of new and existing substances and biocides as laid down in European legislation and the EU Technical Guidance Documents (TGD; EC 2003c). Therefor, the system implements and integrates the models proposed in the TGD into a consistent risk assessment system. This document has some overlap with the TGD. This document gives however a more detailed technical description of the models, which estimate exposure to, and effects of chemical substances as well as the risk characterisation. The TGD gives more guidance on the total risk assessment process, including testing strategy and data evaluation.

For help with the EUSES 2.0 computer program the reader is referred to the EUSES 2.0 user manual and the on-line help of the program itself. The on-line help refers back to this EUSES 2.0 background document. This document is divided in several parts: chapters I to 4 and Appendices I to V. The number of the chapter and page number are shown in the header of each page.

I. INTRODUCTION	This chapter describes the historical and regulatory background of EUSES. The main structure of the system is explained, including considerations of time and spatial scales. Validity and limitations are discussed.
II. MODEL DESCRIPTION	This chapter explains the calculation modules of EUSES. This includes a description (text and figures) of the processes, assumptions, limitations and exposure scenario's. Each module is discussed separately.
III. MODEL CALCULATIONS	This chapter gives the mathematical process descriptions (equations and default values). The amount of background information is strictly limited. Therefor, this chapter is meant for reference purposes only. The modules are discussed in the same order as in Chapter II.
IV. REFERENCES	The final chapter gives the literature references used.
APPENDIX I	This appendix gives further guidance to the reader with a glossary and explanation of the abbreviations used in the text.
APPENDIX II	This appendix describes the data items incorporated in the EEC-OECD HEDSET.
APPENDIX III	This appendix contains the emission factors for different use categories. Furthermore, lists of synonyms for the function of chemicals are given to obtain the best entry to the tables.
APPENDIX IV	Logic diagrams of the model for estimating the exposure at the workplace, EASE

I. INTRODUCTION

Contents

I.1 HISTORICAL BACKGROUND

Quantitative risk assessment as a science and as a basis for regulatory decision-making emerged only about 20 years ago (Paustenbach, 1995; Van Leeuwen and Hermens, 1995). Progress since has been considerable and in 1992, Chapter 19 of Agenda 21 of the United Nations Conference on Environment and Development (UNCED) included as a first recommendation "expanding and accelerating the international assessment of chemical risks" (United Nations, 1992).

In 1967, the European Community adopted Directive 67/548/EEC on the classification, packaging and labelling of dangerous substances – the first of a growing number of Community directives aimed at protecting human health and the environment. In 1973, the first 5-year European Community Environmental Action Programme was adopted (EC, 1973). Since then, the principles of prevention and risk reduction have been firmly established in many regulations of the European Commission (EC) and with them the concepts of risk assessment and risk management of substances. This legislation is also used as a model by countries outside the EU (EC, 1992a).

With regard to new substances, i.e. substances not on the EU market in the 10 years prior to 18 September 1981 and therefore not appearing in the European INventory of Existing Commercial chemical Substances (EINECS), the so-called 'Sixth amendment' to Directive 67/548/EEC introduced a pre-market testing, hazard assessment and notification procedure. The first article of the seventh amendment, Directive 92/32/EEC (EC, 1992b) required an evaluation of the potential hazards and risks of notified substances on the basis of a specified data set. This Directive also required that principles be laid down for carrying out the risk assessment of new substances. On 20 July 1993, Commission Directive 93/67/EEC was adopted, which laid down these principles (EC, 1993a). A detailed package of Technical Guidance Documents (TGD; EC, 1993b) supported this Directive.

EC Council Regulation (EC) 793/93 on the evaluation and control of the environmental risks of existing substances was adopted on 23 March 1993 (EC, 1993c). This Regulation covers the data-gathering, priority-setting, risk assessment process, and proposals for risk reduction strategies where appropriate. The principles for this risk assessment are laid down in Commission Regulation (EC) 1488/94 of 28 June 1994 (EC, 1994a), which was also supported by a package of TGDs (EC, 1994b). In November 1995, one harmonised set of TGDs for both new and existing substances was adopted by the EU Member States (EC, 1996a).

An EC Directive (98/8/EC) on the placing of biocidal products on the market has been adopted in 1998(EC, 1998). It requires that a biocidal product is only authorised if, besides other requirements, the active substances used in the products are listed in specific. Substance may enter these Annexes after the risk assessment, if they fulfil the requirements of the Directive. The guidance supporting the risk assessment of biocides is the same as described above for new and existing substances with regard to the environment and the human health hazards. The human exposure assessment for biocidal products and the human risk characterisation have been elaborated in separate guidance's (EC, 2003a, and EC, 2003b, respectively).

It is against this background that EUSES (the European Union System for the Evaluation of Substances) was developed. Since the early 1980s, along with the implementation of the European legislation on new chemicals, projects were initiated at a national level to develop a more systematic approach towards the hazard and risk assessment of substances. This was in recognition of the fact that risk assessment of the many substances in use nowadays could only be performed if rapid, systematic and transparent approaches based on the latest scientific developments were available. Such a system can also facilitate mutual acceptance of risk assessments. In 1990, the EU Member States adopted a document describing common principles and a stepwise procedure for the environmental risk assessment of new substances (EC, 1990). In the Netherlands, a risk assessment system integrating risk assessment tools for new substances, existing substances, plant protection products and biocides was developed and this finally resulted in USES 1.0 (RIVM *et al.*, 1994; Vermeire *et al.*, 1994; Jager *et al.*, 1994a/b; Van der Poel, 1994; Linders and Luttik, 1995). USES 1.0 was already much in line with the separate packages of TGDs for new and existing substances and also appeared to be useful as a risk assessment tool outside the European Union. As a next step, a EU-project was initiated to develop an update of USES 1.0 which would be fully in line with the package of amalgamated TGDs for new and existing substances; the result of this project is the European Union System for the Evaluation of Substances (EUSES; EC, 1996b; Vermeire *et al.*, 1997). EUSES is a co-ordinated effort of EU Member States, the European Commission and its European Chemicals Bureau, and the European Chemical Industry.

The EU Technical Guidance Documents in support of Commission Directive 93/67/EEC on risk for New Notified Substances and Commission Regulation (EC) No. 1488/94 on Risk Assessment for Existing Substances have been updated recently (EC, 2003c). Based on these updated TGDs and the additional guidance's for biocides, a second version of EUSES had to be developed. The ECB contracted RIVM to develop a user-friendly computer program EUSES 2.0 in cooperation with an EC EUSES 2.0 Working Group, composed out of representatives of the European Chemical Bureau (JRC Institute for Health and Consumer Protection), EU Member States and the European chemical industry.

I.2 OBJECTIVES

The European Union System for the Evaluation of Substances (EUSES 2.0) was developed for quantitative assessment of the risks posed by new and existing chemical substances and biocides to man and the environment. This assessment must be transparent to all users and easy to perform, and EUSES 2.0 is therefore, well-documented and available as a user-friendly computer program. As required, the risk assessment system is attuned to current chemical management policies and in accordance with the principles laid down in the TGDs for new and existing substances and biocides. Risks to man pertain to consumers, workers and man exposed through the environment. Risks to the environment include risks to sewage treatment plant populations of micro-organisms, aquatic, terrestrial and sediment ecosystems and populations of predators.
EUSES 2.0 is designed to support decision-making by risk managers in government agencies, scientific institutes and industry in the evaluation of new and existing chemical substances. On the basis of the results of the risk assessment process, of which EUSES can be an

important element, and taking other factors into account (e.g. political, social, economic and engineering factors), risk managers may take decisions with respect to regulatory actions to be taken.

Table I-1 *Assessment stages according to the OECD (1989). EUSES is particularly suitable for the stages printed in bold typeface.*

Assessment stages	Effects data
Initial (screening) stage	**Acute toxicity**
Intermediate (refined) stage	**Chronic toxicity**
Comprehensive stage	Field toxicity

In line with most assessment procedures EUSES can be used to carry out tiered risk assessments of increasing complexity, requiring additional data. Using OECD terminology, EUSES can specifically be used in the initial, or screening, and intermediate, or refined, stages of assessment (OECD, 1989; Table I-1). With EUSES, substances can be assessed for their potential risks to man and the environment. On the basis of this screening, it can be decided if more data need to be generated and if a more refined (i.e. intermediate) assessment is necessary. When dealing with (large) numbers of chemicals, this screening can be used to set priorities for data gathering or refined assessments. EUSES can also be applied for intermediate or refined assessments by allowing the replacement of default values, estimated parameter values, or intermediate results by more accurately estimated values or by measured data. EUSES is not specifically designed for site-specific assessments, but adjustment of parameters may allow for insight into specific local or regional situations.

I.3 GENERAL PRINCIPLES

Risk assessment in EUSES is carried out in a stepwise procedure encompassing the following stages (Figure I-):

1. Exposure assessment: estimation of the concentrations/doses to which human populations or environmental compartments are or may be exposed.
2. Effects assessment, comprising
   a. hazard identification: identification of the adverse effects which a substance has an inherent capacity to cause; and
   b. dose-response assessment: estimation of the relationship between the level of exposure to a substance (dose, concentration) and the incidence and severity of an effect.
3. Risk characterisation: estimation of the incidence and severity of the adverse effects likely to occur in a human population or environmental compartment due to actual or predicted exposure to a substance.

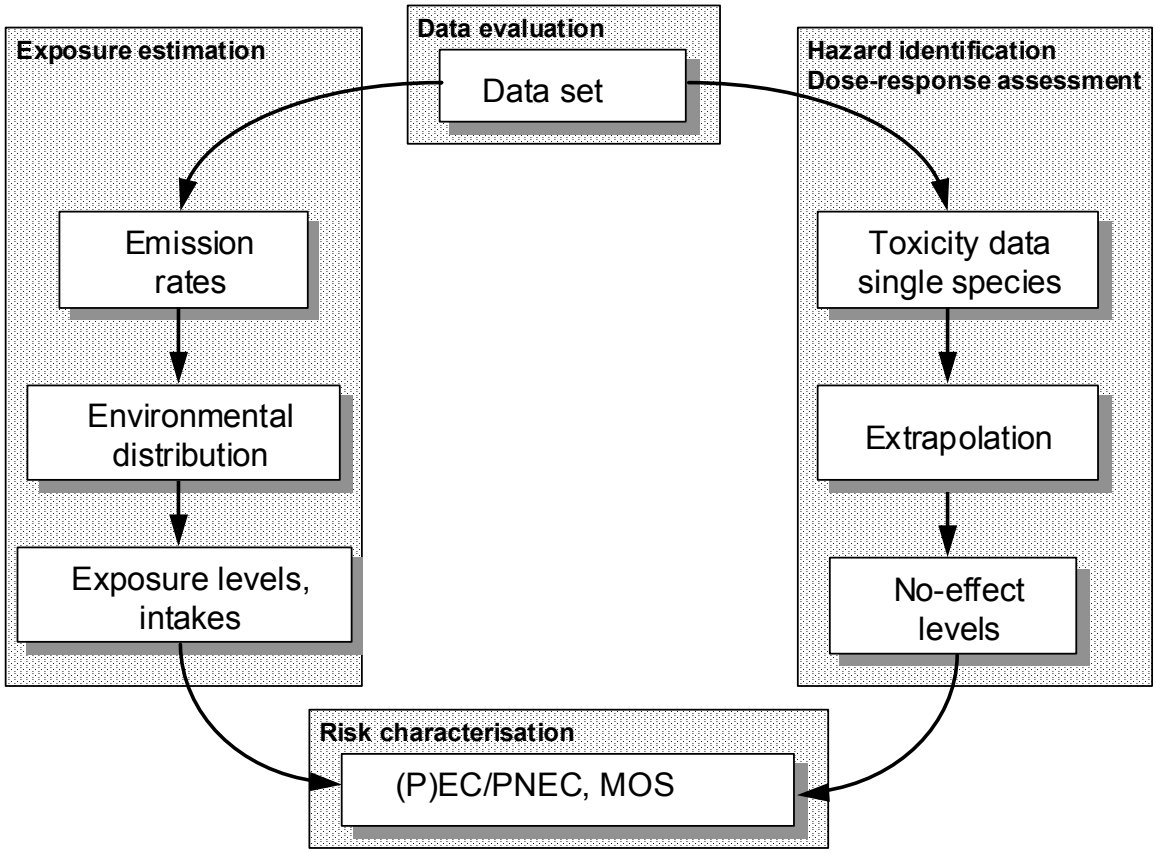

Figure I-1 *Basic steps in EUSES.*

At the risk characterisation stage, this procedure will result in a quantitative comparison per substance of the outcome of the exposure assessment and that of the effects assessment. For new and existing substances this will be a PEC/PNEC, i.e. Predicted Environmental Concentration versus a Predicted No-Effect Concentration for environmental compartments, and a MOS, i.e. Margin of Safety, or the ratio of the estimated no-effect or effect level parameter to the estimated exposure level for human sub-populations. For biocides, the PEC/PNEC-ratio also applies as well as the Margin of Exposure, which is equivalent to the Margin of Safety[1]. In addition the risk characterisation for biocides should be performed by comparing the exposure to the AOEL, the Acceptable Operator Exposure Level, a health based limit value. The generic name for PEC/PNEC, MOS, MOE and AOEL/exposure-ratio in EUSES 2.0 is: Risk Characterisation Ratio (RCR). The RCRs should be seen as surrogate parameters for risk characterisation as they do not quantify the "incidence and severity" of adverse effects. The RCRs are used as indicators for the likelihood of adverse effects occurring, since a better method for a more quantitative risk characterisation with general applicability is not available at the moment.

[1] In EUSES 2.0 the term 'Margin Of Safety (MOS)' will also be used for the 'Margin Of Exposure (MOE)'

The human sub-populations and ecological systems and populations considered to be protection goals in EUSES are shown in Table I-2. The level of protection to be aimed at in the risk assessment can be described as follows:

The risk assessment for man aims at such a level of protection, expressed in the Margin of Safety (new and existing substances) or Margin of Exposure and AOEL/exposure-ratio (biocides), that the likelihood for adverse effects occurring is 'of no concern', taking into account the nature of the potentially exposed population, including sensitive groups, and the nature and severity of the effect(s) and the uncertainties involved (EC, 2003b and c). In the environmental risk assessment it is assumed that ecosystem sensitivity depends on the most sensitive species and that protection of the ecosystem structure also protects community function. The PNEC derived for each ecosystem is regarded as a concentration below which an unacceptable effect will most likely not occur (EC, 2003c).

Risk assessment with EUSES departs from a screening level in which so-called generic exposure scenarios are applied. In the environmental risk assessment, it is assumed then that substances are emitted in a standard environment with predefined environmental characteristics. No measured data are used at this level. The risk assessment covers the whole life cycle of substances (see Figure II-5) as well as their fate in all environmental compartments. As explained in more detail in Section I.5, four spatial scales and two time scales are distinguished. In the risk assessment for workers and consumers, again generic exposure models are applied first of all, covering a wide range of applications. The resulting screening-level risk assessment is in principle valid for all EU countries, as required by the relevant EU regulations.

Table I-2 *Human populations and ecological systems and populations in EUSES.*

Human populations:
• Workers[1]
• Consumers
• Non-professional users of biocides
• Man exposed via the environment
Ecological systems and populations:
• Micro-organisms in sewage treatment systems
• Aquatic ecosystem*
• Terrestrial ecosystem
• Sediment ecosystem*
• (Top) predators*
[1] Professional users of biocides are not considered in EUSES 2.0.[2] Fresh and marine ecosystems

- The exposure assessment in EUSES 2.0 aims at 'reasonable worst-case' results by applying unfavourable, but not unrealistic, standard exposure scenarios and, as much as possible, mean, median or typical parameter values. If the outcome of the reasonable worst case risk characterisation indicates that the substance is "not of concern", the risk assessment for that substance can be stopped with regard to the life cycle stage/effect/population considered. If, in contrast, the outcome is that the substance is "of concern", the assessment must, if possible, be refined by adapting any default parameter value for which this is considered necessary; and
- replacing intermediate results by:
  - the results of other models judged to be more suitable for the substance under investigation; and
  - reliable and representative measured data.

The output of EUSES always shows the result of the standard assessment, in addition to the results of refined assessments made.

EUSES is designed for the risk assessment of a broad range of substances. The user needs a sufficient degree of expertise to be able to appreciate the pros and cons of EUSES, to evaluate the quality of the input data, to make a proper data selection, to understand the assumptions made as well as the inherent limitations of the estimation methods, and, finally, to correctly interpret the results. Indiscriminate use of the system, in particular for 'difficult' substances such as poorly soluble substances, inorganic substances, petroleum substances and ionisable substances, may lead to unacceptable errors. Expert knowledge is essential to identify the problems and adapt the assessment where possible and appropriate. In general, the combined action of several substances together is not considered. However, the so-called Hydrocarbon Block Method, specifically designed for hydrocarbon mixtures, is included in EUSES and is based on the assumption that effects will be concentration-additive.

I.4 SYSTEM STRUCTURE

As outlined in Section I.2, EUSES is, in principle, designed for the initial and intermediate risk assessment of substances to humans and the environment. In the step from initial to intermediate assessment, a certain degree of refinement should take place. Each assessment should involve exposure and effects assessment, resulting in so-called Risk Characterisation Ratios (RCR).

I.4.1 Exposure assessment

For many chemicals information on actual exposure doses or concentrations is limited or even absent and concentrations generally vary significantly in time and space. Doses and environmental concentrations of a chemical are predicted in a two-step procedure. Firstly, releases to environmental compartments or the indoor environment are predicted based on the volume produced, imported or used, the use pattern, and physico-chemical properties of the chemical concerned. Next, environmental concentrations and human daily intake doses are calculated using models, which take into account the transport and fate of the substance.

I.4.2 Effects assessment

Effects assessment concerns the hazard identification and dose-response assessment of toxicological and ecotoxicological data. In ecotoxicological effects assessment, Predicted No-Effect Concentrations (PNECs) are derived from experimental toxicity data using extrapolation factors (in the Netherlands, under specific conditions, also called MPC or MTR). In human toxicological effects assessment, a 'No-Observed-Adverse-Effect' Level (NOAEL), or other no-effect or effect levels, are derived from the available data. EUSES can extrapolate these values to other routes of exposure for which data are lacking.

I.4.3 The EUSES main modules

The main structure of EUSES is presented in ***Figure I-2***. In this section, the function of each module will be discussed. A more detailed description will follow in Chapter II.

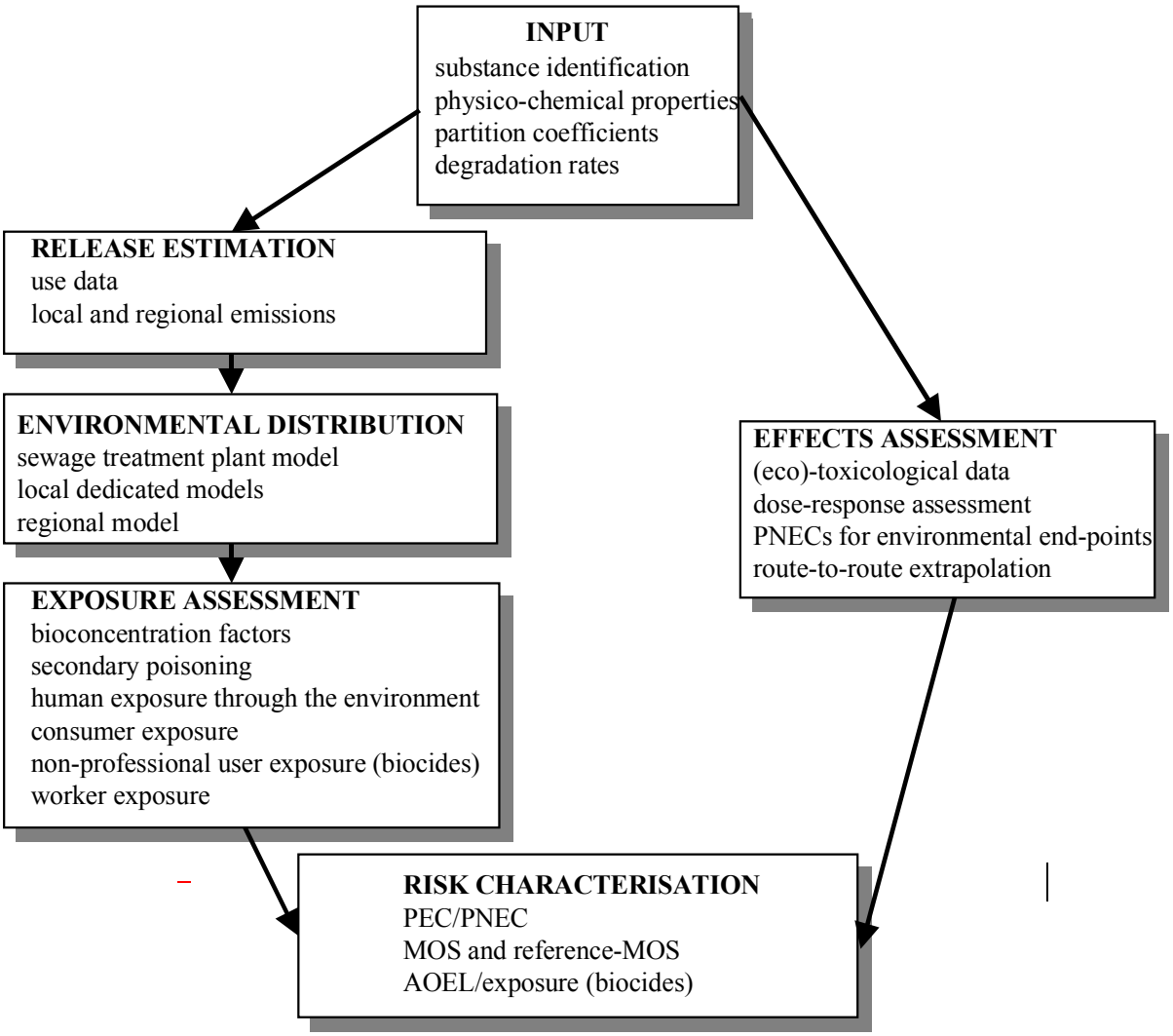

Figure I-2 *The main modules of EUSES.*

Input module

The input module requires the input of substance identification data (name, CAS-number, etc.), the primary data (physicochemical properties) required to run EUSES and essential data either experimentally derived or derived from physicochemical data (partition coefficients, degradation and transformation rates, removal rate constants soil). Since all required information on primary data should be available in the base set, no estimation routines are implemented. For secondary

data the routines recommended in the TGD have been implemented. These secondary data can be overwritten by evaluated, experimental values.

Emission module
Based on the known properties, uses and functions of a substance, emission factors for various life-cycle stages are chosen from a database with default values. Daily emission rates are subsequently calculated using either again default values or specific emission models.

Distribution module
This module contains all the models necessary to estimate the distribution of a substance in the environment at the appropriate spatial scale (see Section I.5). End-points are concentrations in the relevant environmental compartments (air, surface water, marine water, sediment, soil and groundwater).

Exposure module
Based on estimated environmental concentrations, this module calculates the exposure levels for predating birds and mammals (through fish and earthworms) and humans. For humans, exposure through the environment can be estimated as well as exposure through consumer products, including biocides, and exposure at the workplace.

Effect module
No-effect levels for relevant time scales are determined for several end-points: aquatic organisms, terrestrial organisms, micro-organisms in a sewage treatment plant and top predators (fish-eating and worm-eating birds or mammals). This is done on the basis of the evaluated results of single-species tests with experimental organisms. This module also applies route-to-route extrapolation for NOAELs or LOAELs for human populations.

Risk characterisation module
This module compares the results of the exposure assessment of a substance with those of the effect assessment by calculating Risk Characterisation Ratios (RCR) for the various groups to be protected.

Output module (not shown in ***Figure I-2***)
In this module, the input data, defaults changed, intermediate results and final results of the risk assessment are presented in a suitable format. This module will not be discussed in this document.

Most calculated and default values can be replaced by better estimates or measured data. The content of each of these main modules at a more detailed level is shown in ***Table I-3***.

Table I-3 *The structure of EUSES.*

Module	Content
Input module	Data entry in HEDSET format: substance identification and physico-chemical properties Estimation of secondary data (partition coefficients, degradation rates) based om physico-chemical data
Emission module	Estimation of local emissions to wastewater and air for various life-cycle stages Estimation of continental and regional emissions to wastewater, air and soil for various life-cycle stages Emission tables are used, given in Appendix III
Distribution module	Local models: STP model: SimpleTreat Air model: OPS Dilution and sorption in surface and marine waters One-compartment soil model Regional model: Mackay-type level III multi-media model SimpleBox
Exposure module	Secondary poisoning, estimation of exposure levels for predating birds and mammals Exposure of top predators (marine environment only) Exposure of humans through the environment (including food products) Human exposure through use of consumer products, including biocides Human exposure in the workplace
Effects module	Determination of PNECs for the environmental end-points (water, soil, sediment, STP, predators) by applying assessment factors based on available data For soil and sediment, equilibrium partitioning is used when data are lacking
Risk characterisation module	Determination of chronic PEC/PNECs for all ecosystems and for (top) predators at the regional and local scale Determination of Margins of Safety (MOS) for all populations and for each end-point at each relevant spatial and time scale Determination of AOEL/exposure ratios for biocides Estimations of the reference-MOS and reference-AOEL and comparison of these values to the estimated MOS and exposure/AOEL-ratio, respectively

Abbreviations used: STP = Sewage Treatment Plant, OPS = Operational atmospheric transport model for Priority Substances, PEC = Predicted Environmental Concentration, PNEC = Predicted No-Effect Concentration, AOEL = Acceptable Operator Exposure Level

I.5 MODEL DIMENSIONS

Three factors determine the dimensions of EUSES: the spatial scale, the time scale and the *'realism scale'*, the latter being the degree of realism attained in the exposure assessment.

I.5.1 Spatial scales

For the risk assessment system, a distinction can be made between three spatial scales. At the 'personal scale', individual consumers or workers are considered, exposed directly to individual substances and preparations, and to substances embedded in a solid matrix. The local scale considers the protection goals in the vicinity of one large point source of the substance. The regional scale assesses the risks to protection targets due to all releases in a larger region. A fourth spatial scale, the continental scale (defined as the sum of all EU Member States), is added to serve as background for the regional system. EUSES 2.0 furthermore includes three overlying global scales (moderate, tropic and arctic) as option. The concentrations at the continental and global scales are not used for risk characterisation.

Figure I- illustrates the relationships between the spatial scales (personal scale not shown). The local scale receives the background concentration from the regional scale. The regional and continental calculations are carried out with a nested multi-media model. The regional scale receives the inflowing air and water from the continental scale, which in turn is exchanging water and air with the global scales.

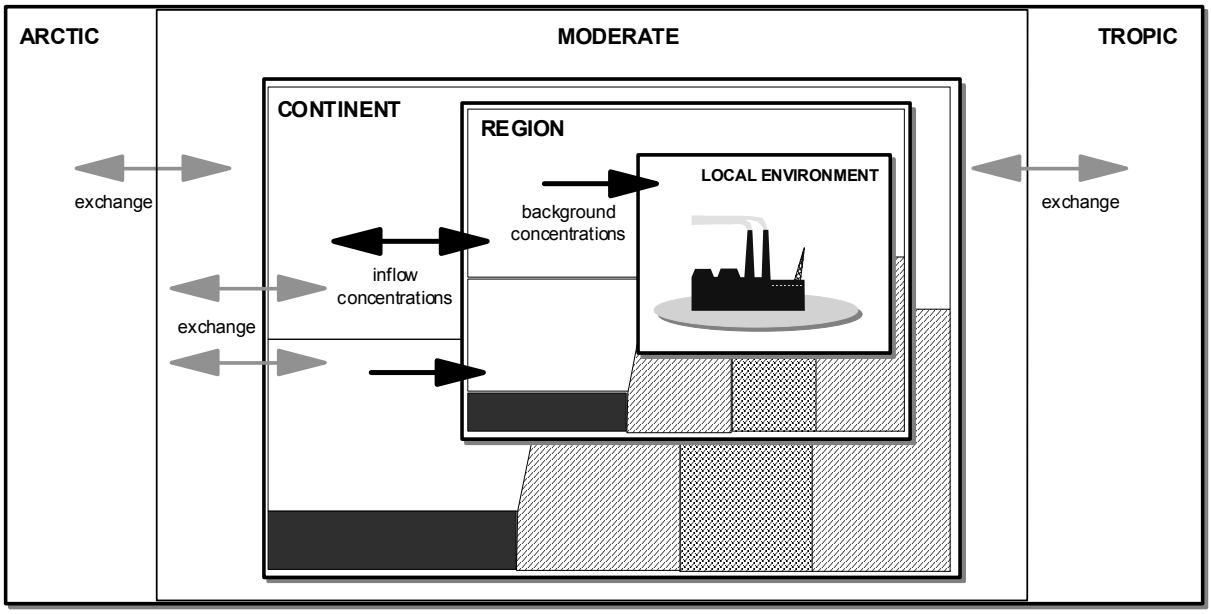

Figure I-3 *The relationships between the exposure assessments at the different spatial scales.*

I.5.1.1 The local scale

The concentrations of substances released from point sources are assessed for a generic local environment. This is not an actual site, but a hypothetical site with predefined, agreed environmental characteristics, the so-called 'standard environment'. These standard environmental conditions can be average values, or reasonable worst-case values, depending on the parameter in question. The exposure targets are assumed to be exposed in, or at the border of the area. In general, concentrations during an emission episode are calculated. This means that local concentrations are calculated on the basis of a daily release rate, regardless of whether the discharge is intermittent or continuous. They represent the concentrations expected at a certain distance from the source on a day when discharge occurs. Only for the soil compartment (being a less dynamic environment than air or surface water) do longer-term averages apply. In principle, degradation and distribution processes are taken into consideration on the local scale. However, because of the relatively small time scale, the ultimate concentration in a compartment is typically governed by only one or two key processes.

I.5.1.2 The regional scale

The concentrations of substances released from point and diffuse sources in a larger area are assessed for a generic regional environment, assuming the same environmental characteristics as the local standard environment. The regional model takes into account the further distribution and fate of the chemical upon release, resulting in steady-state concentrations in the environmental compartments. The regional concentrations are used as background concentrations in the calculation of the local concentrations.

I.5.2 The time scale

Local emissions of industrial chemicals can either be continuous or discontinuous, the latter in the case of batch-processing of substances, for instance. Depending on the emission frequencies and durations, organisms with a relatively short life-span may be exposed locally to toxic concentrations for a considerable amount of time, even if average exposure levels are low. This will be relevant for STP micro-organisms and aquatic organisms. Therefore, for these organisms, the average exposure levels during emission episodes are assumed to be continuous. It follows from this assumption that the estimated environmental concentrations can be considered as estimates of long-term exposure levels, which can be compared to no-effect levels derived from long-term toxicity data. If intermittent release is identified (see Chapter II.3, Release estimation), only short-term effects are considered for the aquatic ecosystem and no-effect levels are derived from short-term toxicity data only. For pesticides, the application regime of the substance is considered.

The exposure of terrestrial organisms is assumed not to be influenced by temporal fluctuations in emission rates, whereas in the case of human beings, these fluctuations are of a rather short-term nature compared to their life span and the time scale on which chronic effects are considered. Humans and terrestrial organisms are therefore assumed to be exposed

to levels averaged over a longer period, and derived from average emission rates.

Exposure of consumers, non-professional users of biocides and workers can be judged as acute, sub-chronic or chronic, depending on the product and its use pattern. The results of the exposure assessment should be compared to experimental animal or human studies of corresponding duration.

Emissions at the regional and continental scale are regarded as diffuse and continuous, leading to steady-state environmental concentrations. These steady-state levels can be considered as estimates of long-term average exposure levels. They can therefore be compared to no-effect levels derived from long-term toxicity data.

I.5.3 The 'realism scale'

A model can never give an exact representation of reality. This is, *inter alia*, due to the complexity of reality, and our limited knowledge of it. Furthermore, the data available for a model are often incomplete and contain measurement errors. In risk assessment, we are typically confronted with this situation, as the available data are limited and mechanisms often poorly understood. The values for nearly all parameters are therefore accompanied by a significant amount of uncertainty, not only resulting from limited scientific understanding (true uncertainty), but also from natural variability in time and space. River flow rates, as an example, can be measured with reasonable accuracy. Nevertheless, variability in time can be a significant source of uncertainty in this parameter. Furthermore, as the standard assessment cannot be performed site-specifically, differences between locations will result in large spatial variability. A model system like EUSES can therefore only give an approximation of the potential risk of a substance.

It is advisable to take this uncertainty into account in the decision-making process. In the EU-frameworks for new and existing substances and biocides, the level of risk is characterised by means of the quotient of exposure and effect parameters: this quotient is a point estimate. To avoid an underestimation of potential risk, a worst-case approach can be followed by choosing a worst-case exposure scenario with the worst possible emission factors, model parameters and environmental conditions. Such an accumulation of worst cases may, however, eventually lead to unrealistically high risk levels which are extremely unlikely to occur. The aim of EUSES is to perform a ‘reasonable worst-case’ risk assessment. The chosen standard exposure scenario represents an unfavourable, but not unrealistic, situation. However, for the model parameters, mean, median or typical values will be used in most cases. As an example, the human indirect exposure scenario on a local scale is a typical worst case since all food products are derived from the vicinity of a point source. In contrast, many model parameters, such as environmental characteristics and bioconcentration factors, are median or typical values.

The degree of conservatism in these assessments is, however, unknown. Quantitative uncertainty analysis is a tool that can be used to tackle the propagation of uncertainties. The scientific aspects of uncertainty analysis with EUSES as well as the pros and cons of this tool in decision making has been investigated and discussed (Jager *et al.*, 1997; Jager, 1998; Jager

et al., 2001a; Bodar *et al.*, 2002). The quantitative uncertainty analysis of the multi-media model Simplebox in EUSES has been investigated separately (Etienne *et al.*, 1997). Several examples have been published as well (Huijbregts *et al.*, 2000; Jager *et al.*, 2001a; Jager *et al.*, 2001b; Vermeire et al, 2001).

I.6 MODEL PARAMETERS

Input

EUSES can be fed automatically or manually with data from the EC Data Set for new substances, or the Harmonised Electronic Data Set (HEDSET) for existing chemicals. Manual input from other sources is also possible.

Data gaps

For the risk assessment of new and existing chemicals, complete data sets will be available, consisting minimally of the so-called EC Base Set data (Directive 67/548/EEC). Data sets will also be available for biocides as specified in Directive 98/8/EC. Secondary chemical-specific data such as partition coefficients and bioconcentration factors will be scarce. These data gaps will be filled by estimated data, using generally agreed procedures like QSARs, or by default values.

Flexibility

As discussed in Section I.2, EUSES first of all provides a baseline risk assessment, i.e. a standard procedure for risk assessment of substances using a defined set of criteria, assumptions, estimation methods, system parameters and default values. A more refined assessment can be achieved by using better estimates or measured data to replace defaults and estimated parameters. Whatever the departure from the standard procedure may be, it should always be clear to the user of (results of) EUSES which parameters have been changed. However, as EUSES will primarily be an instrument in the hands of decision-makers and is designed to give a general evaluation of the risk potential of chemicals at the initial and intermediate level, the increase in flexibility has a limit. Generally agreed exposure scenarios are required for achieving comparability of results obtained by different institutions, and EUSES should not be used for extensive site-specific risk assessments. The system is available to all interested parties, but is not primarily intended to be a research tool for scientists.

I.7 VALIDATION STATUS

EUSES 1.0 became available in April of 1997 and has been extensively used in European risk assessment practice. It is important that the user is aware of the "validity" of this system (see ***Table I-4***, reproduced Jager *et al.*, 1998).

Table I-4 Definitions on model validation

Validation: Proving the reliability, accuracy and usefulness of the model within the specified field of use.

Validation should consist of:

Conceptual validation: Are assumptions, choices and theories correct (or appropriate)? Mainly qualitative and referring.

Algorithm validation/verification: Is the conceptual model translated correctly in mathematical formulations?

Software validation/evaluation: Correctness and efficiency of the software code, quality of interfaces and documentation.

Functional validation: Do model results sufficiently correspond with independent measurements, theoretical analysis, or other models?

It is difficult to specify the degree of certainty that a decision-maker needs when assessing the risks associated with chemicals[2]. 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, 1998). 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).

A strict validation of systems like EUSES is not possible. The result of EUSES is a risk estimate[3]: 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). 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 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.

2 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

3 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.

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

Validation studies of submodules of EUSES 1.0 have been carried out and summarised by Jager *et al.* (1998) in ***Table I-5***. It was noted that validation activities for individual models are seldom directly applicable to EUSES, since this is a generic instrument, using a fixed, standard scenario. Further validation work includes a preliminary validation study of the EASE model for workers, but no definite conclusion was possible due to the limited number of measured data (Bredendiek-Kämper, 2001). The regional model Simplebox has also recently been subject to validation studies (Berding, 2000; Struijs and Peijnenburg, 2002). Berding compared the model results with measurement for a wide range of chemicals and concluded that the model complies with its purpose to calculated regional background concentrations. Struijs and Peijnenburg compared predicted and measured air/water concentrations for two phthalate esters and found that these did not differ more than a factor of 10 if measured partitioning coefficients were used. In both studies, the overall result was greatly affected by uncertainty in emission data.

A detailed 3-year validation study of EUSES 1.0 has been carried out for single submodels on the one hand and the entire system on the other (Schwartz *et al.*, 1998; Schwartz, 2000). Regarding the software, EUSES was found to basically fulfil the postulated quality criteria. However, high complexity, low modularity and incomplete documentation was concluded to result in lack of transparency. The performance of the model was characterised as a good compromise between complexity and practicability. It was noted that, in a strict sense, the method is only applicable for persistent, non-dissociating substances of intermediate lipophilicity.

Table I-5 Summary of the validation status of the EUSES sub-modules (Jager *et al.*, 1998).

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

I.8 SYSTEM LIMITATIONS

Several limitations of EUSES have already been mentioned and are briefly reiterated here:

1. Important boundary conditions for the system are:
   - the chemical-risk policies as laid down by the European Commission;
   - the datasets available for risk assessment purposes;
   - the need for a harmonised, general scheme for rapid and easy-to-perform quantitative hazard and risk assessment at the initial and intermediate level for new and existing substances.
2. EUSES is not specifically designed for use in site-specific assessments.
3. The environmental risk assessment in EUSES is for an environment with standard conditions. To a certain extent, however, these environmental conditions can be adapted.
4. Model analysis, including validation, has been performed to a limited extent and further work is required.
5. It is recognised that certain process formulations are based on limited research and need to be improved; examples are the equations describing the transfer of substances from soil and feed to cattle.
6. Even with a perfect model, unreliable results can still be obtained if quality control of input data is neglected or performed in a very rough manner. EUSES does not present any guidance for this essential step. Nor does the system present any guidance for the derivation of no-effect or effect levels from experimental animal tests or human data.
7. Several hazards are not yet considered in EUSES: examples are global warming, ozone depletion, acidification, eutrophication, depletion of raw materials, effects on materials, calamities and hazardous waste.

I.9 EUSES 2.0 VERSUS EUSES 1.0

The differences in scientific content between EUSES 2.0 and 1.0 mainly stem from the implementation of the updated TGDs (2003) for new and existing substances and biocides, Environmental Emission Scenario Documents for biocides (EUBEES, TGD 2003), and elements of the Technical Notes for Guidance for biocides (EC, 2002a and b). The differences between the TGDs of 1996 and 2003 have been described by Luit *et al.* (2003).

The major differences between EUSES 2.0 and EUSES 1.0 at the scientific level are:

1. Temperature correction is now possible for important physico-chemical and fate properties;
2. All TGD QSARs for the estimation of Koc are now available;
3. Addition of the updated Emission Scenario Documents of the TGD to the emission module;
4. Addition of the environmental emission scenarios for biocides as approved by the EUBEES Working Group to the emission module
5. Introduction of the life cycle stage 'service life' in the emission module;
6. Addition of the risk assessment for biocides for man (non-professional users, humans exposed through the environment) and the environment;
7. The regional model has been updated to Simplebox 3.0 and now includes, next to the regional scale, a global scale.
8. Addition of the marine local and regional risk assessment: among others, this implies an additional sea-compartment in the regional model (Simplebox 3.0);
9. The exposure assessment for predators has been updated: new routines for the estimation of the concentration of substances in worms and introduction of a biomagnification factor in the estimation of the concentration in the diet of top predators in the marine risk assessment.
10. Addition of a link to CONSEXPO 3.0, providing additional consumer exposure scenarios;
11. Replacing EASE 1.0 for worker exposure estimation by EASE 2.0;
12. Introduction of the human risk characterisation for each endpoint (acute toxicity, repeated dose toxicity, fertility, developmental toxicity, maternal toxicity, carcinogenicity).
13. Implementation of the updated human risk characterisation module of the TGD for both threshold and non-threshold substances

Major differences at the technical level are:

1. Adaptation of the program flow: the estimation of fate properties and bioconcentration factors have been moved from the distribution module to the input module;
2. Complete revision of the user interface of the emission module to improve the user friendliness of this complicated part of the risk assessment.
3. Bug fixing and improvements to the user interface based on the prioritised Blacklist of EUSES 1.00 (RIVM/ECB. Blacklist EUSES 1.0. August 1, 2001).
4. EUSES 2.0 has been updated to a 32-bit program to be used under Windows 95, 98, 2000, NT and XP.

II MODEL DESCRIPTION

This chapter describes the risk assessment system and the models that are implemented by means of the backgrounds and scenario choices.

Contents

II.1 INTRODUCTION

In this chapter, the models used in the risk assessment system are described, including their backgrounds and underlying assumptions. The mathematical descriptions of the models are given in Chapter III: Model Calculations. The main modules of the system, as shown in Figure II-1, are discussed separately in Sections II.2-II.7. Sections II.8 and II.9 discuss the assessment of mixtures with the Hydrocarbon Block Method and the specific differences for assessing metals and metal compounds.

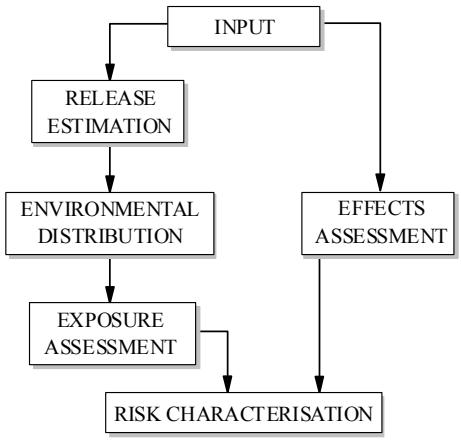

Figure II-1 *System structure.*

It should be noted that this chapter focuses on description of the models applied in the risk assessment system. Data evaluation, testing strategy, as well as the actual process of risk evaluation, are outside the scope of this document. For these items, the reader is referred to the Technical Guidance Document (TGD) on Risk Assessment of New and Existing Substances (EC, 2003).

II.2 INPUT MODULE AND DATASET

The input module requires the input of substance identification data (name, CAS-number, etc.), the primary data (physico-chemical properties) required to run EUSES and essential data either experimentally derived or derived from physico-chemical data (partition coefficients, degradation and transformation rates, removal rate constants soil, bioconcentration factors). This information can be stored in a database. Further information on the substance, such as use pattern and degradation test results, must be entered in the appropriate (sub-)modules.

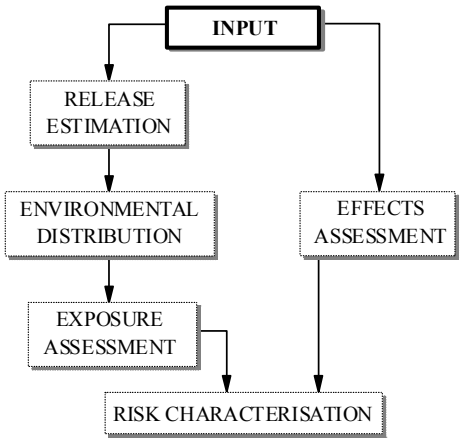

Figure II-2 *System structure.*

Since all required information on primary data should be available in the base set, no estimation routines are implemented. However, QSARs may be used in the evaluation of the measured data (see Chapter 4 of the TGD: EC, 2003). For secondary data the routines recommended in the TGD have been implemented. These secondary data can be overwritten by evaluated, experimental values.

II.2.1 Data set

EUSES is designed to work with limited datasets. The minimum dataset that will be available for risk assessment of new and existing substances is the 'base set' as defined in Annex VIIA of Directive 67/548/EEC. The risk assessment methodology requires many more parameters to be specified, such as partition coefficients and bioconcentration factors. These data will, in most cases, be estimated or set to default values. The data requirements for completing an evaluation may vary for different types of substances. For instance, if an assessment of workplace exposure is required, the user will have to answer additional questions in that specific sub-module to be able to evaluate the risk properly.

The parameters that can be entered, as well as the default values and estimation routines, will be described in detail in Chapter III: Model calculations. In principle, all defaults can be changed by the user to refine the assessment. Sets of changed default values can be saved.

The availability of data will differ, depending on the type of substance one wishes to evaluate. The availability of data for new and existing chemicals and biocides is the subject of the next sections.

II.2.1.1 Data availability for new substances

The risk assessment of new notified substances in the EU is based on the data submitted by the notifiers in accordance with Directive 67/548/EEC (EC, 1967). These data will be supplied in the SNIF format (Substance Notification Interchange Format) and are stored in the New Chemicals Database of the EU at the European Chemicals Bureau in Ispra. EUSES can import

SNIF files directly from this database (check). The Directive lays down a scheme of step-wise, tonnage-related data requirements, with the number of available tests being dependent on the supply level (Figure II-1). At production or import level 0 (between 1 and 100 tonnes/year) the notification must be accompanied by the dataset required under Annex VIIa of Directive 67/548/EEC, the so-called 'base set'. Any gaps in the base set should be filled at this level, unless the notifier can justify not providing the test(s) required. The base set is composed of the following data (see also Figure II-1):

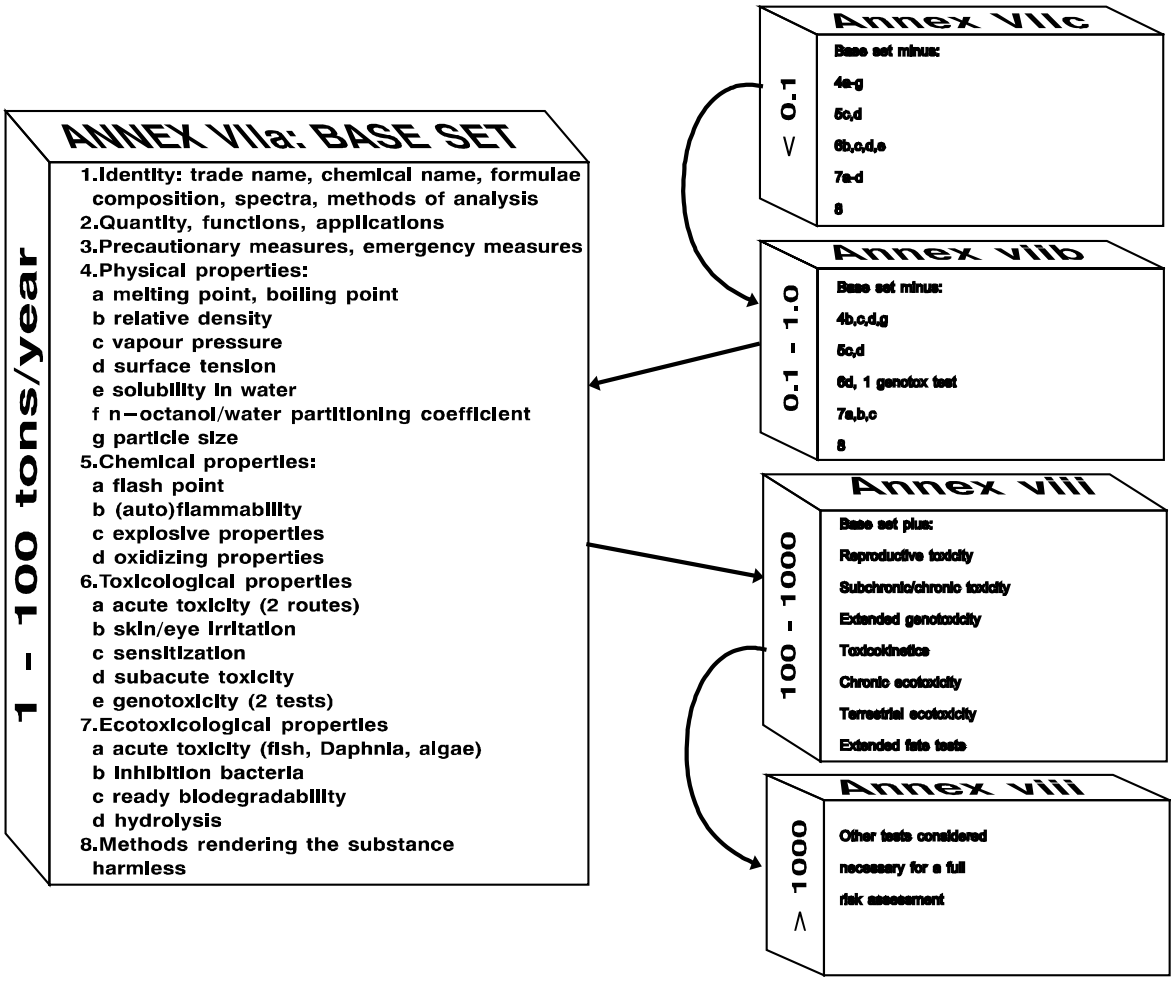

Figure II-3 *Data requirements for new chemicals, depending on the production or import volume.*

- Identity:
  chemical name, trade and other names, CAS number, molecular and structural formula, composition (purity, impurities, additives, spectral data), methods of determination and detection.
- Information on the substance:
  production data, proposed uses, estimated production and/or imports, recommended methods and precautions, emergency measures, packaging.
- Physico-chemical properties:
  physical state, melting point, boiling point, relative density, vapour pressure, surface tension, water solubility, n-octanol/water partition coefficient, flash point, flammability,

explosive properties, self-ignition properties, oxidising properties, granulometry.
- Toxicological studies:
  acute toxicity (2 routes), skin and eye irritation, skin sensitisation, repeated-dose toxicity (28 days), genotoxicity (two *in vitro* tests).
- Ecotoxicological studies:
  acute toxicity for fish and water flea, growth-inhibition test on algae, bacterial inhibition, biodegradation, hydrolysis, adsorption/desorption screening test.

In addition, the base set also includes a screening test for reproductive toxicity in mammals. However, this test is 'for the record' for new substances, as no appropriate screening test is thought to be available.

Measured data on human and environmental exposure levels will almost never be available.

II.2.1.2 Data availability for existing substances

The risk assessment of priority existing substances in the EU is based on the information on the substance submitted by the manufacturers and importers in accordance with Regulation (EEC) No. 793/93. These data will be supplied in the format of the OECD/EC Harmonised Electronic Data SET (HEDSET, see Appendix II) and are stored in the International Uniform ChemicaL Information Data base (IUCLID) of the EU. EUSES can import data directly from HEDSET-files. According to the Regulation, the data to be made available for the risk assessment of priority substances shall at least comprise the base set as defined above for new substances, including the screening test for reproductive toxicity. Any gaps in the base set should be filled, unless the manufacturers or importers can justify not providing the data required.

Information beyond the base set may be available. For the effects assessment there may be several data available on a single end-point and a selection should be made. Exposure results from monitoring studies may also be available and these may be used to overwrite estimated exposure levels.

The chemical-specific data that are required to carry out the computations can be divided into three classes:
- Data provided directly in the HEDSET.
- Data provided indirectly in the HEDSET.
- Data not provided in the HEDSET.

Data provided directly in the HEDSET
Most of the data required are provided directly in the HEDSET. These data are used as such, or with minor manipulation only, as input for one or more computation modules. Examples are: *Quantity produced/imported (HEDSET item 1.5)* and *Partition coefficient (HEDSET item 2.5)*. Missing secondary data can be filled with QSAR estimates or defaults.

Data provided indirectly in the HEDSET
Some of the required data are not provided directly in the HEDSET, i.e. not in the format necessary as input for the computations. For these data, more than minor reworking or

manipulation of the HEDSET information is necessary. Example: rate constants for degradation in the environment. The HEDSET provides information on *Stability (HEDSET item 3.1)*, but the required rate constants need to be extracted or extrapolated from this information. Generic recipes that can be applied to perform these operations are available only for a small number of parameters (e.g. rate constants for microbial degradation). More recipes are in development, but presently not ready for use. This means that in many cases these manipulations can be performed only with minor or major expert assistance.

Data not provided in the HEDSET
Certain additional chemical-specific data are required that are usually not supplied in the HEDSET at all (e.g. emission factors, bioconcentration factors). Derivation of these data from the HEDSET data is an essential part of the risk assessment.

II.2.1.3 Biocides

Data requirements for the active substance are laid down in Annex IIA and IIIA of Directive 98/8/EC. Furthermore 'Technical notes for guidance in support of Directive 98/8/EC of the European Parliament and the Council concerning the placing of biocidal products on the market. Guidance on data requirements for active substances and biocidal products" has been developed and are available on the ECB homepage (http://ecb.jrc.it). The requirements are as follows:

ANNEX IIA
COMMON CORE DATA SET FOR ACTIVE SUBSTANCES

I. APPLICANT
1.1. Name and address, etc.
1.2. Active substance manufacturer (name, address, location of plant)

II. IDENTITY
2.1. Common name proposed or accepted by ISO and synonyms
2.2. Chemical name (IUPAC nomenclature)
2.3. Manufacturer's development code number(s)
2.4. CAS and EC numbers (if available)
2.5. Molecular and structural formula (including full details of any isomeric composition), molecular mass
2.6. Method of manufacture (syntheses pathway in brief terms) of active substance
2.7. Specification of purity of the active substance in g/kg or g/l, as appropriate
2.8. Identity of impurities and additives (e.g. stabilisers), together with the structural formula and the possible range expressed as g/kg or g/l, as appropriate
2.9. The origin of the natural active substance or the precursor(s) of the active substance, e.g. an extract of a flower
2.10. Exposure data in conformity with Annex VIIA to Directive 92/32/EEC (*).

III. PHYSICAL AND CHEMICAL PROPERTIES
3.1. Melting point, boiling point, relative density (1)
3.2. Vapour pressure (in Pa) (1)
3.3. Appearance (physical state, colour) (2)
3.4. Absorption spectra (UV/VIS, IR, NMR), and a mass spectrum, molar extinction at relevant wavelengths, where relevant (1)
3.5. Solubility in water including effect of pH (5 to 9) and temperature on solubility, where relevant (1)
3.6. Partition coefficient n-octanol/water including effect of pH (5 to 9) and temperature

3.7. Thermal stability, identity of relevant breakdown products
3.8. Flammability including auto-flammability and identity of combustion products
3.9. Flash-point
3.10. Surface tension
3.11. Explosive properties
3.12. Oxidising properties
3.13. Reactivity towards container material

IV. ANALYTICAL METHODS FOR DETECTION AND IDENTIFICATION
4.1. Analytical methods for the determination of pure active substance and, where appropriate, for relevant degradation products, isomers and impurities of the active substance and additives (e.g. stabilisers)
4.2. Analytical methods including recovery rates and the limits of determination for the active substance, and for residues thereof, and where relevant in/on the following:
(a) Soil
(b) Air
(c) Water: the applicant should confirm that the substance itself and any of its degradation products which fall within the definition of pesticides given for parameter 55 in Annex I to Council Directive 80/778/EEC of 15 July 1980 relating to the quality of water intended for human consumption(**) can be estimated with adequate reliability at the MAC specified in that Directive for individual pesticides
(d) Animal and human body fluids and tissues

V. EFFECTIVENESS AGAINST TARGET ORGANISMS AND INTENDED USES
5.1. Function, e.g. fungicide, rodenticide, insecticide, bactericide
5.2. Organism(s) to be controlled and products, organisms or objects to be protected
5.3. Effects on target organisms, and likely concentration at which the active substance will be used
5.4. Mode of action (including time delay)
5.5. Field of use envisaged
5.6. User: industrial, professional, general public (non-professional)
5.7. Information on the occurrence or possible occurrence of the development of resistance and appropriate management strategies
5.8. Likely tonnage to be placed on the market per year

VI. TOXICOLOGICAL AND METABOLIC STUDIES
6.1. Acute toxicity
For studies 6.1.1 to 6.1.3, substances other than gases shall be administered via at least two routes, one of which should be the oral route. The choice of the second route will depend on the nature of the substance and the likely route of human exposure. Gases and volatile liquids should be administered by the inhalation route.
6.1.1. Oral
6.1.2. Dermal
6.1.3. Inhalation
6.1.4. Skin and eye irritation (3)
6.1.5. Skin sensitisation
6.2. Metabolism studies in mammals. Basic toxicokinetics, including a dermal absorption study
For the following studies, 6.3 (where necessary), 6.4, 6.5, 6.7 and 6.8, the required route of administration is the oral route unless it can be justified that an alternative route is more appropriate
6.3. Short-term repeated dose toxicity (28 days)
This study is not required when a sub-chronic toxicity study is available in a rodent
6.4. Subchronic toxicity 90-day study, two species, one rodent and one non-rodent
6.5. Chronic toxicity (4)
One rodent and one other mammalian species
6.6. Mutagenicity studies
6.6.1. *In-vitro* gene mutation study in bacteria
6.6.2. *In-vitro* cytogenicity study in mammalian cells

6.6.3. *In-vitro* gene mutation assay in mammalian cells
6.6.4. If positive in 6.6.1, 6.6.2 or 6.6.3, then an *in-vivo* mutagenicity study will be required (bone marrow assay for chromosomal damage or a micronucleus test)
6.6.5. If negative in 6.6.4 but positive *in-vitro* tests then undertake a second *in-vivo* study to examine whether mutagenicity or evidence of DNA damage can be demonstrated in tissue other than bone marrow
6.6.6. If positive in 6.6.4 then a test to assess possible germ cell effects may be required
6.7. Carcinogenicity study (4)
One rodent and one other mammalian species. These studies may be combined with those in 6.5
6.8. Reproductive toxicity (5)
6.8.1. Teratogenicity test — rabbit and one rodent species
6.8.2. Fertility study — at least two generations, one species, male and female
6.9. Medical data in anonymous form
6.9.1. Medical surveillance data on manufacturing plant personnel if available
6.9.2. Direct observation, e.g. clinical cases, poisoning incidents if available
6.9.3. Health records, both from industry and any other available sources
6.9.4. Epidemiological studies on the general population, if available
6.9.5. Diagnosis of poisoning including specific signs of poisoning and clinical tests, if available
6.9.6. Sensitisation/allergenicity observations, if available
6.9.7. Specific treatment in case of an accident or poisoning: first aid measures, antidotes and medical treatment, if known
6.9.8. Prognosis following poisoning
6.10. Summary of mammalian toxicology and conclusions, including no observed adverse effect level (NOAEL), no observed effect level (NOEL), overall evaluation with regard to all toxicological data and any other information concerning the active substances. Where possible any suggested worker protection measures should be included in summary form

VII. ECOTOXICOLOGICAL STUDIES
7.1. Acute toxicity to fish
7.2. Acute toxicity to *Daphnia magna*
7.3. Growth inhibition test on algae
7.4. Inhibition to microbiological activity
7.5. Bioconcentration
Fate and behaviour in the environment
7.6. Degradation
7.6.1. Biotic
7.6.1.1. Ready biodegradability
7.6.1.2. Inherent biodegradability, where appropriate
7.6.2. Abiotic
7.6.2.1. Hydrolysis as a function of pH and identification of breakdown products
7.6.2.2. Phototransformation in water including identity of the products of transformation (1)
7.7. Adsorption/desorption screening test
Where the results of this test indicate the need to do so, the test described in Annex IIIA Part XII.1 paragraph 1.2 shall be required, and/or the test described in Annex IIIA Part XII.2 paragraph 2.2
7.8. Summary of ecotoxicological effects and fate and behaviour in the environment

VIII. MEASURES NECESSARY TO PROTECT MAN, ANIMALS AND THE ENVIRONMENT
8.1. Recommended methods and precautions concerning handling, use, storage, transport or fire
8.2. In case of fire, nature of reaction products, combustion gases, etc.
8.3. Emergency measures in case of an accident
8.4. Possibility of destruction or decontamination following release in or on the following: (a) air (b) water, including drinking water (c) soil
8.5. Procedures for waste management of the active substance for industry or professional users
8.5.1. Possibility of reuse or recycling
8.5.2. Possibility of neutralisation of effects

8.5.3. Conditions for controlled discharge including leachate qualities on disposal
8.5.4. Conditions for controlled incineration
8.6. Observations on undesirable or unintended side-effects, e.g. on beneficial and other non-target organisms

IX. CLASSIFICATION AND LABELLING
Proposals including justification for the proposals for the classification and labelling of the active substance according to Directive 67/548/EEC
Hazard symbol(s)
Indications of danger
Risk phrases
Safety phrases

X. SUMMARY AND EVALUATION OF SECTIONS II TO IX
Notes
(1) These data must be submitted for the purified active substance of stated specification.
(2) These data must be submitted for the active substance of stated specification.
(3) Eye irritation test shall not be necessary where the active substance has been shown to have potential corrosive properties.
(4) The long-term toxicity and carcinogenicity of an active substance may not be required where a full justification demonstrates that these tests are not necessary.
(5) If, in exceptional circumstances, it is claimed that such testing is unnecessary, that claim must be fully justified.

ANNEX IIIA
ADDITIONAL DATA SET FOR ACTIVE SUBSTANCES
III. PHYSICAL AND CHEMICAL PROPERTIES
1. Solubility in organic solvents, including effect of temperature on solubility (1)
2. Stability in organic solvents used in biocidal products and identity of relevant breakdown products(2)

IV. ANALYTICAL METHODS FOR DETECTION AND IDENTIFICATION
1. Analytical methods including recovery rates and the limits of determination for the active substance, and for residues thereof, in/on food or feedstuffs and other products where relevant

VI. TOXICOLOGICAL AND METABOLIC STUDIES
1. Neurotoxicity study
If the active substance is an organophosphorus compound or if there are any other indications that the active substance may have neurotoxic properties then neurotoxicity studies will be required. The test species is the adult hen unless another test species is justified to be more appropriate. If appropriate, delayed neurotoxicity tests will be required. If anticholine esterase activity is detected a test for response to reactivating agents should be considered
2. Toxic effects on livestock and pets
3. Studies related to the exposure of the active substance to humans
4. Food and feedingstuffs
If the active substance is to be used in preparations for use where food for human consumption is prepared, consumed or stored, or where feedingstuff for livestock is prepared, consumed or stored the tests referred to in Section XI, part 1 shall be required
5. If any other tests related to the exposure of the active substance to humans, in its proposed biocidal products, are considered necessary, then the test(s) referred to in Section XI, part 2 shall be required
6. If the active substance is to be used in products for action against plants then tests to assess toxic effects of metabolites from treated plants, if any, where different from those identified in animals shall be required
7. Mechanistic study — any studies necessary to clarify effects reported in toxicity studies

VII. ECOTOXICOLOGICAL STUDIES
1. Acute toxicity test on one other, non-aquatic, non-target organism
2. If the results of the ecotoxicological studies and the intended use(s) of the active substance indicate a danger for the environment then the tests described in Sections XII and XIII shall be required
3. If the result of the test in paragraph 7.6.1.2 of Annex IIA is negative and if the likely route of disposal of the active substance is by sewage treatment then the test described in Section XIII, part 4.1 shall be required
4. Any other biodegradability tests that are relevant from the results in paragraphs 7.6.1.1 and 7.6.1.2 of Annex IIA
5. Phototransformation in air (estimation method), including identification of breakdown products (1)
6. If the results from paragraphs 7.6.1.2 in Annex IIA or from paragraph 4, above, indicate the need to do so, or the active substance has an overall low or absent abiotic degradation, then the tests described in Section XII, part 1.1, part 2.1 and, where appropriate, part 3 shall be required

VIII. MEASURES NECESSARY TO PROTECT HUMANS, ANIMALS AND THE ENVIRONMENT
1. Identification of any substances falling within the scope of List I or List II of the Annex to Directive 80/68/EEC on the protection of groundwater against pollution caused by certain dangerous substances (*)
Notes
(1) These data must be submitted for the purified active substance of stated specification.
(2) These data must be submitted for the active substance of stated specification.

XI. FURTHER HUMAN HEALTH-RELATED STUDIES
1. Food and feedingstuffs studies
    1.1. Identification of degradation and reaction products and of metabolites of the active substance in treated or contaminated foods or feedstuffs
    1.2. Behaviour of the residue of the active substance, its degradation products and, where relevant, its metabolites on the treated or contaminated food or feedstuffs including the kinetics of disappearance
    1.3. Overall material balance for the active substance. Sufficient residue data from supervised trials to demonstrate that residues likely to arise from the proposed use would not be of concern for human or animal health
    1.4. Estimation of potential or actual exposure of the active substance to humans through diet and other means
    1.5. If residues of the active substance remain on feedingstuffs for a significant period of time then feeding and metabolism studies in livestock shall be required to permit evaluation of residues in food of animal origin
    1.6. Effects of industrial processing and/or domestic preparation on the nature and magnitude of residues of the active substance
    1.7. Proposed acceptable residues and the justification of their acceptability
    1.8. Any other available information that is relevant
    1.9. Summary and evaluation of data submitted under 1.1 to 1.8
2. Other test(s) related to the exposure to humans
Suitable test(s) and a reasoned case will be required

XII. FURTHER STUDIES ON FATE AND BEHAVIOUR IN THE ENVIRONMENT
1. Fate and behaviour in soil
    1.1. Rate and route of degradation including identification of the processes involved and identification of any metabolites and degradation products in at least three soil types under appropriate conditions
    1.2. Absorption and desorption in at least three soil types and, where relevant, absorption and desorption of metabolites and degradation products
    1.3. Mobility in at least three soil types and where relevant mobility of metabolites and degradation products
    1.4. Extent and nature of bound residues
2. Fate and behaviour in water
    2.1. Rate and route of degradation in aquatic systems (as far as is not covered by Annex IIA, paragraph 7.6) including identification of metabolites and degradation products

2.2. Absorption and desorption in water (soil sediment systems) and, where relevant, absorption and desorption of metabolites and degradation products
3. Fate and behaviour in air
If the active substance is to be used in preparations for fumigants, if it is to be applied by a spray method, if it is volatile, or if any other information indicates that this is relevant, then the rate and route of degradation in air shall be determined as far as is not covered by Section VII, part 5
4. Summary and evaluation of parts 1, 2 and 3

XIII. FURTHER ECOTOXICOLOGICAL STUDIES
1. Effects on birds
1.1. Acute oral toxicity — this need not be done if an avian species was selected for study in Section VII, part 1
1.2. Short-term toxicity — eight-day dietary study in at least one species (other than chickens)
1.3. Effects on reproduction
2. Effects on aquatic organisms
2.1. Prolonged toxicity to an appropriate species of fish
2.2. Effects on reproduction and growth rate on an appropriate species of fish
2.3. Bioaccumulation in an appropriate species of fish
2.4. *Daphnia magna* reproduction and growth rate
3. Effects on other non-target organisms
3.1. Acute toxicity to honeybees and other beneficial arthropods, e.g. predators. A different test organism shall be chosen from that used in Section VII, part 1
3.2. Toxicity to earthworms and to other soil non-target macro-organisms
3.3. Effects on soil non-target micro-organisms
3.4. Effects on any other specific, non-target organisms (flora and fauna) believed to be at risk
4. Other effects
4.1. Activated sludge respiration inhibition test
5. Summary and evaluation of parts 1, 2, 3 and 4

II.2.2 Data quality

EUSES accepts data as entered by the user. The user is responsible for data selection and the evaluation of data quality. The quality of a test can be considered to be defined by two basic elements: the reliability of the test and its usefulness (IPCS, 1992; see Table II-1 for definitions). Reliability concerns both the methodology and the description of the test. Questions that should be answered are:

- Do the data relate to the correct substance with respect to identity and form?
- Is the method chosen carried out according to existing guidelines?
- Are proper statistical methods used?
- Has Good Laboratory Practice and Quality Assurance been applied?
- Are the data obtained reported accurately and in sufficient detail?

Table II-1 *Definitions on data quality.*

Quality	=	degree of excellence of a test as determined by both its reliability and its usefulness
Reliability	=	inherent quality of a test with respect to methodology and description
Usefulness	=	the extent to which a test is appropriate for a particular hazard or risk assessment *Synonym*: relevance

Usefulness is defined as the extent to which a test is appropriate for risk assessment. In this way usefulness is dependent on the objectives of the reviewer and reflects the merit of the test with regard to a specific hazard/risk assessment. A test which is not completely reliable, e.g. because of the absence of GLP-compliance, may still be useful for a hazard/risk assessment, especially when other data are lacking. On the other hand, a reliable test may not be useful, e.g. because of improper route of exposure or test duration, or the absence of a clear dose-response relationship. When several useful tests on the same end-point are available with varying reliability, a final selection needs to be made on the basis of expert judgement.

II.2.3 Application of (Q)SAR-routines

In Chapter III, the model calculations are given, including the derivation of secondary data from the primary data. As far as possible, internationally recommended methods have been selected. If possible, secondary data will be derived with QSAR (Quantitative Structure- Activity Relationships) estimates. In principle, estimation of parameter values is preferable to use of default values (even though in establishing default values expert judgement should be used). If, however, no estimation methods of an acceptable quality are available, default values and/or assessment factors should be applied. Obviously, the major advantage of the use of estimation methods is that optimum use is made of present knowledge to support the decision-making process, which must necessarily come to a conclusion.

QSARs have been selected that can be easily incorporated in a risk assessment system and do not require routines that analyse certain aspects of the structure of compounds. Thus, the presented QSARs estimate secondary data on the basis of available physico-chemical descriptors of compounds. Because the selected QSARs should be relatively simple and should be applicable for a wide range of substances, estimation of properties on the basis of e.g. geometrical, topological and electronic descriptors has been excluded. Further study on the application of QSARs in risk assessment of chemicals may result in the incorporation of the latter categories of estimation methods into EUSES in the future.

Chapter 4 of the TGD extensively discusses the use of QSARs in risk assessment for new and existing chemicals, and proposes QSARs for several end-points: toxicity for aquatic organisms, *Kow*, *Koc*, BCFs for fish and earthworms, biodegradation, photolysis, hydrolysis and Henry's law constant. Of these, the QSARs for *Koc* and BCFs are included in EUSES.

Missing data for which no acceptable estimation procedure is available can only be substituted by default numbers. In these cases, a mean or reasonable worst-case approach will be followed to set appropriate values for these parameters.

II.3 RELEASE ESTIMATION

II.3.1 Life cycle of substances

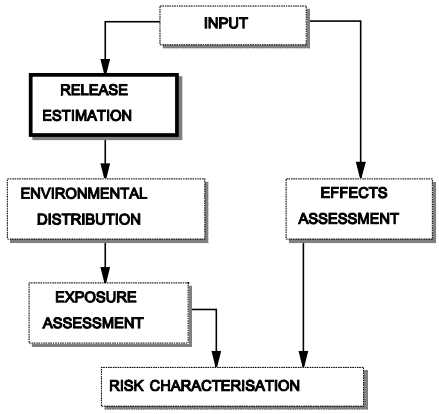

Figure II-4 *System structure.*

Basically the stages of the life cycle of a substance may consist of (see also ***Figure II-5***):

1. **Production**: Chemical synthesis of the substance
2. **Formulation**: Mixing and blending into a preparation or product
3. **Industrial use**: Application of the substance, preparation/product in an industrial process
4. **Private use**: Application of the substance, preparation/product by the public at large
5. **Service life**: Use of articles/products containing the substance over a period > 1 year
6. **Waste treatment**: Final stage where articles/products after their service life are disposed off by incineration or landfilling, or where recovery of the basis material or substance takes place.

Between the various life cycle stages ***transport, storage, and handling*** may occur. This substage has not been indicated in Figure II-5. Emissions due to storage and handling are assumed to be included within the relevant life cycle stage. Transport losses are assumed to occur through accidents only. Such aspects are not considered in risk assessment. The emissions at large depots for chemicals and fuels should be considered as a specific industrial process for which an appropriate emission scenario document might be developed.

The substance of interest may also be released with waste streams originating from all other life cycle stages. This is indicated as WT (waste treatment) with brown arrows to small rectangles. This was done, as it would be very confusing to have so many arrows in the figure going to one and the same part. Red arrows indicate emissions from life cycle stages with dotted lines for air (A). For releases with water (often wastewater) the lines are blue (W). Releases to soil have been omitted, as so far emissions to industrial soil are not addressed in risk assessment.

<u>Production</u>

The life cycle stage production comprises synthesis, isolation and purification (followed by storage and shipment to customers, which is not considered here as explained before). The syntheses has been separated in Figure II-5 as ***Intermediates*** may be converted into another substance (= industrial use) without isolation. In most cases, however, substances will be isolated before conversion (often at another plant). Remains of intermediates – a usually small fraction that is not converted – will go to the next stage in the life cycle of the end product (i.e., the substance produced out of the intermediate considered).
Wastewater waste air streams of chemical industries are often treated with end-of-pipe techniques before release into the environment. Components in off gases may be washed out in scrubbers with water, which means that the substance of interest may be transferred to wastewater. Scrubbing with a solvent other than water will transfer the substance to the solvent and it is likely that the whole amount transferred ends up in waste. The waste of chemical industry is hazardous waste by definition and should be incinerated. On the other

hand, wastewater streams may be stripped with air or nitrogen thus possibly transferring the substance of interest to the air.

Formulation
Formulation is the process of mixing and blending of chemicals yielding a preparation or product. Examples are the formulation of paints. In Figure II-5 two formulation stages are depicted. This is for example the case with many lubricant additives. First a preparation with the additive is composed (so-called performance package). Next this preparation is mixed with the other lubricant components to obtain the finished lubricant.

Industrial use
This stage of the life cycle comprises the application of a chemical or chemical product. Two situations are considered. There may be a situation where the chemical of interest is incorporated in the product produced in the industrial process. An example is the application of a plasticiser, which is incorporated in the polymer matrix of products like flooring. The other situation concerns the application of the chemical of interest as such or in a preparation as a processing aid. An example of a product containing the chemical of interest is an additive in metalworking fluids used for metalworking operations. The application of a chemical as such is, for example, the use of solvents in chemical industry. In principle such solvents may be disposed of after use, e.g. when the solvent is difficult to recover and relatively cheap. In many cases solvents are recovered and recycled after purification. It should be noted that emission factors may be high compared to the input, i.e., the quantity of solvent bought annually; if related to the throughput, however, the emission factors may be very low. Future emission scenario documents, which deal with this aspect, should have a factor "multiplying" the source input to obtain the throughput. Another situation may also occur when the chemical of interest is recovered after use but not recycled in the process itself. Instead, the chemical is reused for another purpose either at the same plant or elsewhere in a different process. An example may be a solvent first used for a chemical reaction or an extraction, which is sold for a second use to a manufacturer of glues after use (second life). This aspect is more difficult to cover in an ESD that is focussed at a specific industry or process. If a situation like this is met in the process of risk assessment the second process should be evaluated with an emission scenario for that specific process/industrial category.

Private use
This life cycle stage is principally about the same as industrial use in respect to the use as a processing aid or use resulting into incorporation in a product. The difference is that private use is concerned with an area source with diffuse releases. In other words we are dealing here with very small point sources connected to relatively large areas (emissions from households in a village or city) or to a line source (traffic emissions along a motorway). It should be noted that use of chemicals/chemical products in the industrial category 6 "Public domain" almost have the same characteristics as private use (industrial category 5). Recycling of chemicals is not likely to occur at all.

Service life
Articles that have the chemical of interest incorporated may have a service life of many years. During this service life the chemical may slowly be released into the environment. For

example, a plasticiser in flooring will gradually evaporate and be removed by cleaning processes. As new flooring is manufactured every year a large quantity of plasticiser present in flooring is built up and the releases will – at a constant application level of plasticiser in flooring – grow to a maximum. If the use of a chemical is stopped the releases from the life cycle stage of service life still may last for quite some time.

Waste treatment

During all relevant life cycle stages the chemical of interest passes through may give a waste stream, which is treated in some way or the other. In Figure II-5 these streams are presented in the same way as the environmental releases with a small rectangle (WT). After the life cycle stage of service life the actual stage of waste treatment is presented. Waste treatment is the final stage where several situations may be distinguished. Waste streams, which are invaluable or not suited for any other use, may be incinerated or disposed off in a landfill. Incineration may result in a release to air if the chemical of interest is not degraded completely and not retained by flue gas cleaning equipment. Releases with wastewater may occur if the chemical of interest is not degraded completely and is transferred to wastewater by scrubbers at flue gas treatment. Unchanged chemical may also end up in bottom ash and go to a landfill. Bottom ash may also be used for application in road construction for example (with possible leaching to soil). For most chemicals these releases are more or less hypothetical. Only chemical compounds like metal oxides may be expected to remain unchanged at incineration. In a landfill it is assumed that provisions have been taken that leaching of substances from the waste into the soil is prevented and that leachate is caught and treated in a wastewater treatment plant. A model of such a landfill – as described in Van der Poel (1999) – has not been implemented in EUSES 2.0.

In quite some cases a waste stream is recovered after service life and made suitable for reuse. A well-known example is the collection of waste paper, which is – often after de-inking – repulped and sold as recycled paper. At the secondary paper production process chemicals used in the original paper or in the ink present on the paper will be released into air or wastewater, or end up in waste (de-inking sludge).

In principle also the chemical of interest may be recovered from a waste stream and reintroduced in the life cycle (broken line). An example is platinum in automotive catalysts. It should be noted that it may take quite some time between collection of the waste and processing.

Furthermore, certain waste streams may be reused directly (without preliminary treatment). Certain plastic articles may be collected and transformed into articles with low requirements in respect to characteristics such as colour. This also presented by a broken line as second life in Figure II-5.

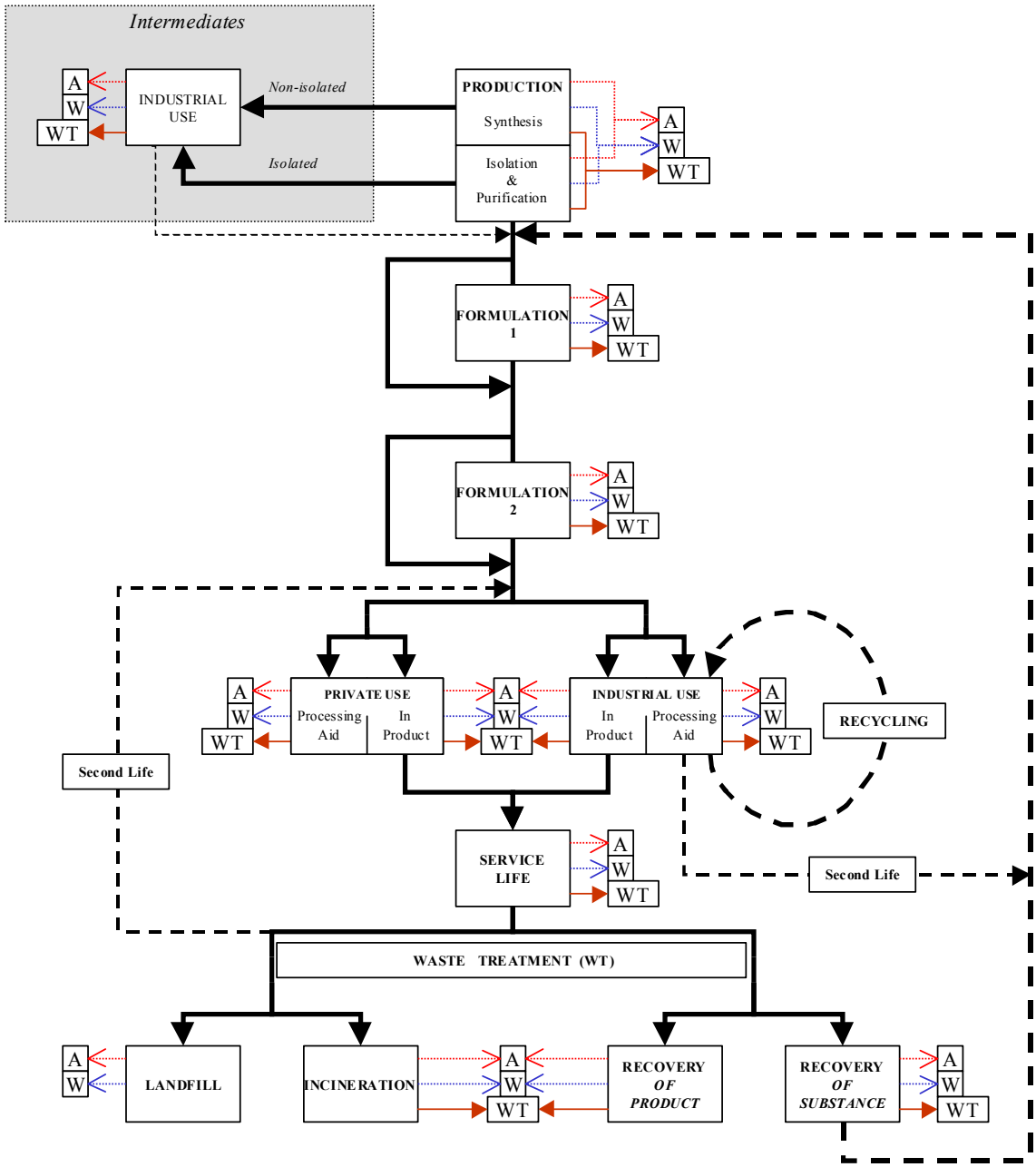

Figure II-5 *Life cycle of a substance with all possible stages, which may occur in all possible applications of the chemical (A = emission to air, W = emission to water, and WT = release with waste going to waste treatment; emission to soil have not been presented).*

II.3.1.1 Life cycle in respect to a specific chemical

In the risk assessment of a substance all relevant stages of the life cycle have to be considered. As an example ***Figure II-6*** presents the relevant life cycle stages for a chemical

with 3 applications, viz., as an intermediate, a solvent for chemical reactions (reaction medium), and a solvent for paints. For transparency of the figure releases and waste streams from the processes have been omitted. For waste only the final stage of the life cycle is presented.

Intermediate
At the industrial use of the chemical of interest A is converted into chemical B (so, for chemical B this is the life cycle stage of production). The situation may occur that a considerable part of chemical A is not reacted and present in chemical B without the necessity to remove chemical A for the use of chemical B. In the example it is assumed that chemical B is applied in articles with a life span exceeding one year (suppose chemical A is an alcohol, which esterified with phthalic acid to the plasticiser – chemical B – applied in PVC flooring). So, chemical A follows from here on the life cycle stages applicable to chemical B. The relevant life cycle stages for chemical B are presented by broken lines.

Reaction medium (solvent)
In the example it is assumed that the solvent is distilled and purified. The purified solvent is recycled in the process with an intermediate storage in a separate tank (fresh solvent purchased from the producer is stored separately). Solvent present in the residue from the purification is sent for waste treatment. If the quality of recycled solvent becomes too poor for reuse it is sold – for a "second life" to paint manufacturers.
The throughput of solvent – the quantity of solvent used in a year – may be *x* times or more the quantity of fresh solvent brought into the process. If the emission factors for the process are known – or derived from an ESD or the A-tables – the quantity for the calculation of a point source should be multiplied by factor *x*. This means, however, that one must know about the specific process or a worst case assumption is made (for example, substances with UC 48 ‘solvents’ have a recycle factor of 5).

Solvent for paints
Paint manufacturers will use as much of "second life" solvent as the price will be lower than for fresh solvent. For the risk assessment the fraction of the tonnage dedicated to "paints" should be raised with the quantity of "second life" solvent before the fraction of the main source is used.
In ***Figure II-6*** both the life cycle stages industrial use and private use (paint application) have been presented as no details might be present on the usage of the paint. The stages of service life and waste treatment have been omitted as it may be assumed that all solvent will have been removed from the coating layer after paint application.

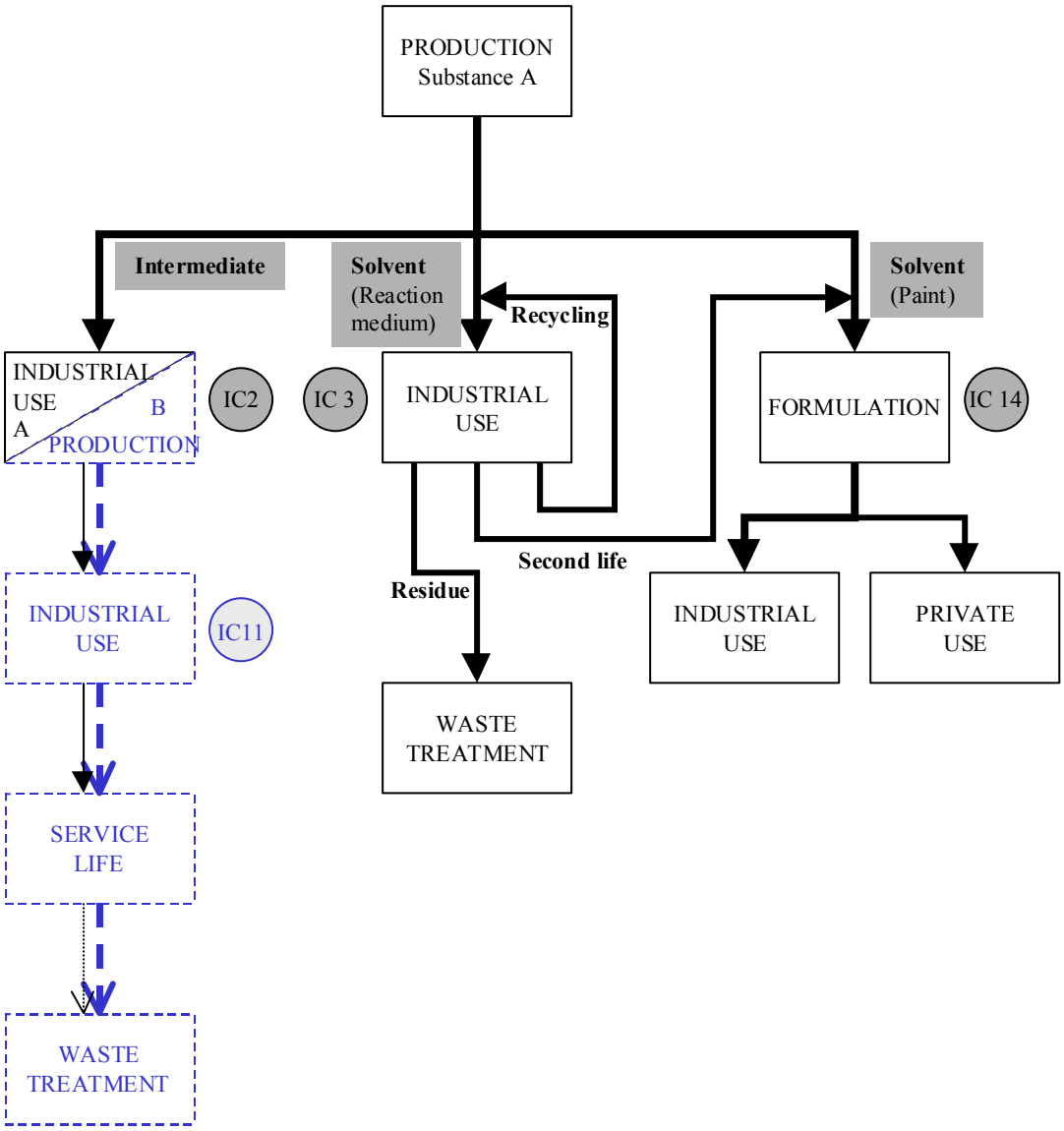

Figure II-6 *Life cycle stages of a chemical applied in three industrial categories (unreacted fraction of application as an intermediate follows the life cycle stages of the end product, which is indicated in blue)*

II.3.1.2 Life cycle in respect to Emission Scenario Document (ESD)

Emission scenario documents may be written to cover emissions in an industrial category, one or several processes within one industrial category, comparable processes within more than one industrial category, and possibly one or more stages of the life cycle. Furthermore, an ESD may be dealing with all relevant use categories or a specific selection of use categories. As a (hypothetical) example an ESD for IC 14 "Paints, lacquers and varnishes industry" is considered. ***Figure II-7*** shows the life cycle stages that are covered in the (hypothetical) ESD. At the left the 6 possible stages are presented and at the right the stages discussed in the ESD.

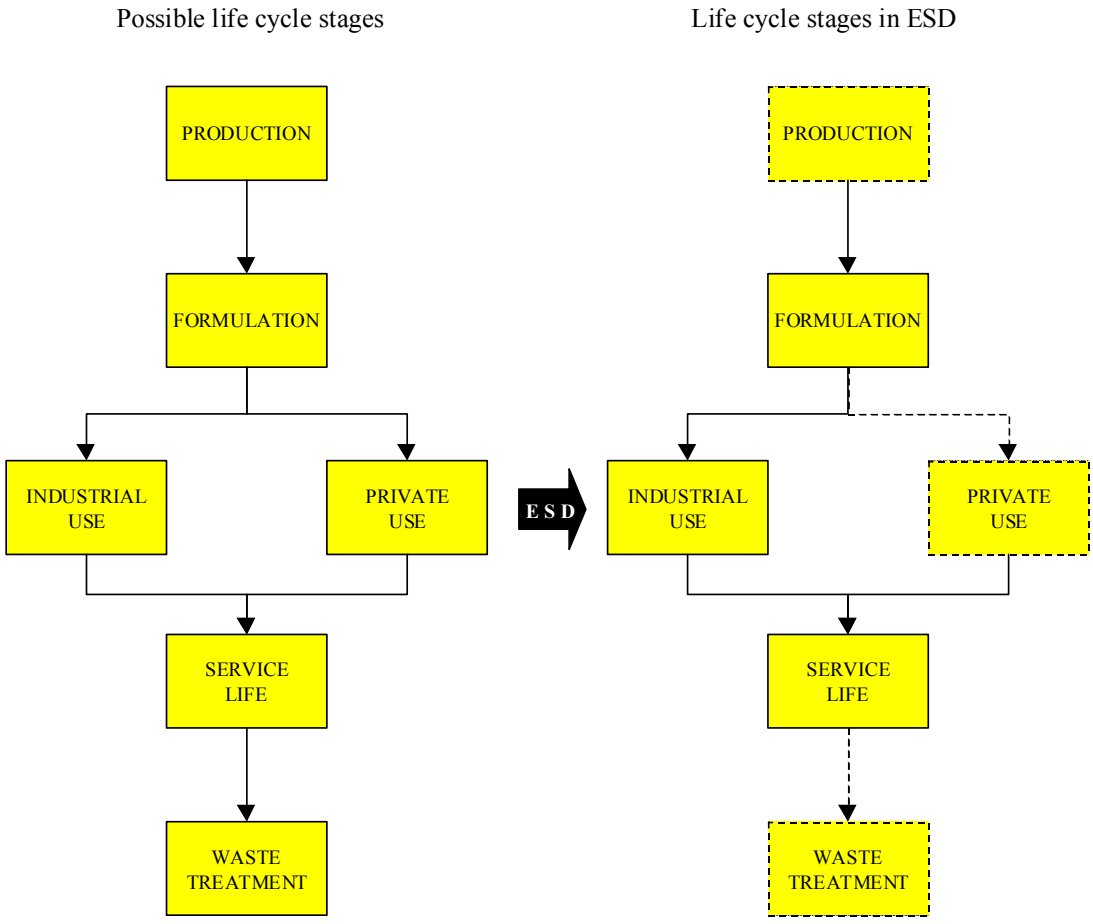

Figure II-7 *The possible life cycle stages (left) and the selected stages for the ESD (right)*

As can be seen in ***Figure II-7*** the first life cycle stage, which is covered in the ESD, is formulation. In this example formulation means the manufacture of paint products. Such products consist of components like binders (UC 2 "Adhesives, binding agents"), solvents (UC 48), pigments (UC 10 "Colourants"), fillers (UC 20), and a variety of additives (many without a specific UC classified as UC 0 "Others").
The application of the paints is considered in the life cycle stage of industrial use.

Professional paint application – at an industrial scale – occurs in many industrial categories. Paints are used in for example IC 4 "Electrical/electronic industry), IC 6 "Public domain" (as far as body repair and paint refinishing shops belong here), and IC 16 "Engineering industries: civil and mechanical" (if automobile manufacture belongs there). The ESD should make very clear which industrial processes with their respective paint application techniques are considered in the document and which not.
The life cycle stage of service life means the period during which the finished paint coatings last before they reach the waste stage. The stage of service life is not of concern for those constituents of paint, which disappear from the coating at drying/curing just after application. This applies to solvents as presented in ***Figure II-8***

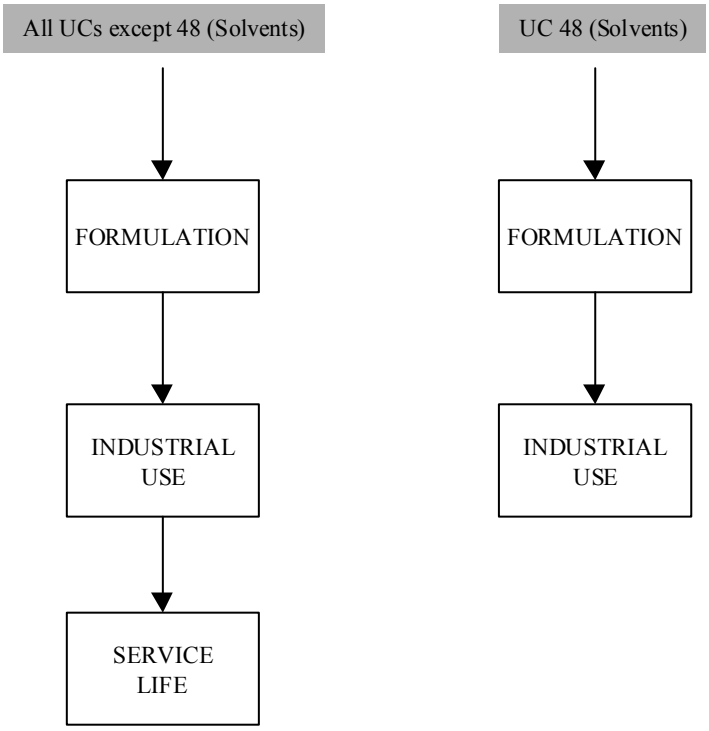

Figure II-8 *Relevant life cycle stages for chemical applied in paints depending upon their function or use category UC (the stage of waste treatment has been omitted)*

It is not necessary, however, to drop the life cycle stage for certain functions. Suppose that the chemical of interest is used as an initiator in a polyester paint. In the curing process almost the whole amount will disintegrate; only a tiny fraction might be present in the matrix of the finished coating. If the chemical of interest is one of the reacting components of the polyester present in a slight excess a relative larger fraction may remain in the finished coating. So, it may be decided to include such components ("functions of UCs") in the stage of service life with emission factors starting from 0 (zero) for solvents. Such defaults should be discussed in the ESD.

II.3.2 Types of emissions and sources

Emission patterns vary widely from well-defined point sources (single or multiple) to diffuse releases from large numbers of small point sources (like households) or line sources (like a motorway with traffic emissions), and from continuous to discontinuous releases. Continuous emissions are characterised by an almost constant emission rate over a prolonged period (e.g. the emission of a substance from a continuous production process such as an oil refinery). Discontinuous emissions can be peak emissions or block emissions. Peak emissions are characterised by a relatively large amount discharged in a short time, whereby the time intervals between peaks and the peak height can vary greatly (e.g. the discharge of spent liquid - reaction mixture - after isolation of the synthesised substance in a batch process). Block emissions are characterised by a flow rate which is reasonably constant over certain time periods, with regular intervals with a low or even zero background emission (e.g. the emissions from traffic during the day; during rush hours emissions are particularly high).

The quantities released during a certain process may vary from 100%, as is the case, with household products like detergents or volatile solvents in paints for example, to below 1% for substances like intermediates produced in closed systems.

II.3.3 Functions and use

It is clear that the releases of a substance are dependent on its use patterns. Three types of category are distinguished: main category, industrial category and function or use category. An overview of these categories is given in ***Table II-2***

Main category (MC)
The main categories (MCs) are intended to provide a general description of the exposure relevance of the use(s) of a substance. In the context of environmental risk assessment they are also used to characterise release scenarios for the estimation of emissions to the environment during specific stages of the life cycle of the substance (production, formulation and processing). They can therefore be allocated to release fractions that are used as default values where specific information is lacking. ‘Use in closed systems’ as such refers to the processing stage when a substance is used in a transformer or the circulation circuit of refrigerator, for example; on the other hand it may also refer to the production stage in the case of a substance like an intermediate that is manufactured in a closed system. ‘Use resulting in inclusion into or onto a matrix’ may refer to the stage of formulation, e.g. when a substance is included in the emulsion layer of a photographic film. It also may refer to the processing stage (industrial use), e.g. when a substance applied as a UV-stabiliser in paint ends up in the finished coating layer. ‘Non-dispersive use’ and ‘wide dispersive use’ are related to the number (and size) of the emission sources.

Although the HEDSET allows for one entry of the MC only for all stages of the life cycle, the approach of MCs is used in many cases for more than one stage of the life cycle. The interpretation often differs for the stage considered and is specified below:

Table II-2 *Categories considered in the HEDSET.*

MAIN CATEGORIES		
I	Use in closed systems	- non-isolated intermediates - isolated intermediates stored on-site - isolated intermediates with controlled transport
II	Use resulting in inclusion into or onto a matrix	
III	Non-dispersive use	
IV	Wide dispersive use	

INDUSTRIAL CATEGORIES	
1	Agricultural industry
2	Chemical industry: basic chemicals
3	Chemical industry: chemicals used in synthesis
4	Electrical/electronic industry
5	Personal/domestic
6	Public domain
7	Leather processing industry
8	Metal extraction, refining and processing industry
9	Mineral oil and fuel industry
10	Photographic industry
11	Polymers industry
12	Pulp, paper and board industry
13	Textile processing industry
14	Paints, lacquers and varnishes industry
16	Engineering industries: civil and mechanical
15/0	Others

USE CATEGORIES	
1	Absorbents and adsorbents
2	Adhesive, binding agents
3	Aerosol propellants
4	Anti-condensation agents
5	Anti-freezing agents
6	Anti-set-off and anti-adhesive agents
7	Anti-static agents
8	Bleaching agents
9	Cleaning/washing agents and additives (detergents; soaps; dry cleaning solvents; optical brighteners in detergents)
10	Colouring agents (dyestuffs; pigments; colour forming agents; fluorescent brighteners)
11	Complexing agents
12	Conductive agents (electrolytes; electrode materials)
13	Construction materials and additives
14	Corrosion inhibitors
15	Cosmetics
16	Dust binding agents
17	Electroplating agents
18	Explosives (blasting agents; detonators; incendiaries)
19	Fertilizers
20	Fillers
21	Fixing agents
22	Flame retardants and fire preventing agents
23	Flotation agents
24	Flux agents for casting
25	Foaming agents (chemical/physical blowing agents; frothers)
26	Food/feedstuff additives
27	Fuels (gasoline; kerosine; gas oil; fuel oil; petroleum gas; non-mineral oil)
28	Fuel additives (anti-fouling agents; anti-knock agents; deposit modifiers; fuel oxidizers)
29	Heat transferring agents (cooling agents; heating agents)
30	Hydraulic fluids and additives
31	Impregnation agents
32	Insulating materials
33	Intermediates (monomers; pre-polymers)
34	Laboratory chemicals
35	Lubricants and additives
36	Odour agents
37	Oxidizing agents
38	Plant protection products, agricultural
39	Biocides, non-agricultural (disinfectants; preservative products; pest control products; specialist biocides)
40	pH-regulating agents
41	Pharmaceuticals (veterinary medicines)
42	Photochemicals (desensitisers; developers; fixing agents; photosensitive agents; sensitisers; anti-fogging agents; light stabilisers; intensifiers)
43	Process regulators (accelerators; activators; catalysts; inhibitors; siccatives; anti-siccatives; cross-linking agents; initiators; photo-initiators; etc.)
44	Reducing agents
45	Reprographic agents (toners for photo-copying machines; toner additives)
46	Semiconductors (photovoltaic agents)
47	Softeners (coalescing agents; bates in leather technology; devulcanizing agents; emollients; swelling agents; water softeners; plasticisers)
48	Solvents
49	Stabilizers
50	Surface-active agents
51	Tanning agents
52	Viscosity adjustors (pour-point depressants; thickeners; thixotropic agents; turbulence supressors; viscosity index improvers)
53	Vulcanizing agents
54	Welding and soldering agents
55/0	Others

MC	Stage	Interpretation
Ia	Production	Non-isolated intermediates (IC=3, UC=33, see ***Table II-2***)
Ib	Production	Isolated intermediates stored on-site, or substances (other than intermediates) produced in a continuous production process
	Formulation	Dedicated equipment and (very) little cleaning operations
Ic	Production	Isolated intermediates stored off-site, or substances (other than intermediates) produced in dedicated equipment
	Formulation	Dedicated equipment and frequent cleaning operations
II	Formulation	Inclusion into or onto a matrix
	Processing	Inclusion into or onto a matrix
III	Production	Multi-purpose equipment
	Formulation	Multi-purpose equipment
	Processing	Non-dispersive use (industrial point sources)
IV	Processing	Wide dispersive use (many small point sources or diffuse releases; normally no emission reduction measures)

Industrial category (IC)

The industrial categories (ICs) specify the branch of industry (including personal and domestic use, and use in the public domain) where considerable emissions occur during application of the substance as such, or during application and use of preparations and products containing the substance. Some important emission sources have not been included specifically in this scheme and must hence be allocated to the category 'Others' (No. 15/0), e.g. emissions of substances (in preparations) other than fuels and fuel additives used in motor vehicles.

It should be noted that considerable emissions may occur under another category than the one to which a substance has been allocated. A substance used in a paintpaint will be allocated to IC 14 'Paints, lacquers and varnishes'. Although local emissions of solvents may be considerable at one point source (the paint factory) during the formulation stage (paint production), most of the solvent will be emitted during paint application. The application could be classified in several industrial categories, depending on the type of paint. In the case of a do-it-yourself paint, it would belong to IC 5 'Personal/domestic', in the case of motor-car repair or professional house painting it would be IC 15/0 'Others' (wide dispersive use, so diffuse releases) and in the case of motor-car production 16 'Engineering industry: civil and mechanical' (non-dispersive use, so few large point sources).

Confusion may arise when the use of a substance, belonging to a certain specific process of an industrial category occurs in another branch of industry. An example is the application of an additive for an epoxy resin applied in the electronics industry for embedding of electronic components. Although the processing takes place in IC 4 'Electrical/electronics engineering industry', the processing of epoxy resins belongs to IC 11 'Polymers industry'. The release estimates of the process will be found in the table for the latter category (see Section II.3.4)

For the chemical industry, two separate industrial categories exist, one for basic chemicals and another for chemicals used in synthesis. Basic chemicals are considered to comprise commonly used chemicals such as solvents and pH-regulating agents such as acids and alkalis. The primary chemicals from the oil-refining process are also considered as basic chemicals. Chemicals used in synthesis fall into two classes, namely intermediates (substances produced from a starting material, to be converted in a subsequent reaction into a downstream substance) and other

substances. These other substances consist mainly of 'process regulators' (e.g. accelerators, inhibitors, indicators).

Industrial category 5 (personal/domestic) covers the use and application of substances (as such or in formulations) at the scale of households. The type of products involved are types of products involved are adhesives, cosmetics, detergents and pharmaceuticals. Some applications have been covered in other industrial categories at the stage of private use. These applications comprise fuels and fuel additives (mineral oil and fuel industry), paint products (paints, lacquers and varnishes industry) and photochemicals (photographic industry). Industrial category 6 (public domain) covers use and application in public buildings, streets, parks, offices, etc.

Use or Function category (UC)
The use or function category specifies the specific function or goal of the substance. These 55 categories have a varying level of detail. For substances used in photography, for example, there is only one category: UC 42 'Photochemicals'. Depending on the specific function of the photochemical, however, emissions can vary to a large extent, e.g. substances used to influence the crystal growth of silver compounds during the production of films are released to an extent of over 50 %, while other substances will hardly be released at all at this stage. There is no general category such as 'Plastics additives' and many other specific categories are also lacking; exceptions are categories like 47 'Softeners' (= plasticisers) and 49 'Stabilisers' (heat- and UV-stabilisers). To obtain the best entry to the tables for emission factors, Appendix IIIa/b contains lists of synonyms for functions of substances. The synonyms and their definitions have been derived from the US-EPA ChemUSES list (US-EPA, 1980). In general, the data supplied by industry should help to find the correct entry to the release tables apart from the classification specified in the HEDSET.

II.3.4 Emission estimation

The releases of a substance at different stages of its life cycle should be estimated by order of preference from:
1) specific information for the substance (e.g. from producers, product registers or open literature);
2) emission scenario documents as far as these have not been implemented already in EUSES (or use category documents);
3) emission factors as included in the release tables of Appendix III.

In many cases, little or no specific information on releases will be available, and the number of processes covered in emission scenario documents is still limited. Therefore, use will have to be made of the emission factors of the release tables of Appendix III, which have been implemented in EUSES. If the calculations used in an emission scenario document of the TGD are similar, the values (defaults) have been incorporated in the A- and B-tables. If specific calculations occur in the emission scenario documents of the TGD these equations and accompanying defaults for the parameters used, are presented in Chapter III Model calculations. In Section II.3.6 reference is made to the sources of data used in the establishment of these tables. For all ICs distinguished in the HEDSET, emission factors have been generated for all

(relevant) stages of the life cycle, i.e. (1) production, (2) formulation, (3) processing, (4) private use and (5) recovery. The estimated emission factors are expressed as the fractions of the mass of the substance which will be released to the air, (waste) water and industrial soil. They are presented in the 'A-tables' of Appendix III.

Unless specific information on use or emission per capita is available, it is assumed that 10% of the European production and use takes place in the standard region. The remainder is assumed to occur in the continental system. Since the regional and continental distribution models are nested (see Section II.4.4), the continental production volume and tonnage are calculated as the total EU production/tonnage minus regional production/tonnage.

The total volume released in the region is averaged over the year and used for the regional PEC calculation. For the local situation the 'B-tables' of Appendix III are used for determining the releases from point sources on the local scale. They provide the fraction of the total volume released that can be assumed to be released through a single point source, and the number of days during which the substance is released, thus allowing the daily release rate at a main point source to be calculated. Local emissions are estimated for every environmental compartment and each relevant stage of the life cycle separately. The emission rate is given averaged per day (24 hours). This implies that, even when an emission only takes place a few hours a day, the emission will be averaged over 24 hours. Emissions to air and water will be presented as release rates during an emission episode.

Any relevant information provided by industry can be used to override the default values of the release tables. Many tables in Appendix III occur more than once and have been recorded only once (at the first occurrence). Further on, reference is made to the number of these tables.

For each stage, the losses in the previous stage are taken into account (see Section III.3, Release estimation). Note that releases during production are *not* taken into account in the other stages, as these releases will generally already be accounted for in the reported production volume. The rapporteur must specify whether or not releases are relevant during each stage. If release is not applicable during a certain life-cycle stage, the release fraction will be set to zero. Application of reasonable worst-case estimates per environmental compartment, as is done in the tables of Appendix III, means that the total emission, summed over the compartments, may exceed 100% of the produced volume. In such cases, the emissions need to be scaled back to a total of 100%.

After losses during the five stages of the life cycle are accounted for, the part of the tonnage remaining is assumed to end up entirely in waste streams. Quantitative methods for estimating emissions at the disposal stage are not currently available. Furthermore, no quantitative methods have for example been developed for estimating emissions of substances during the lifetime of articles in which they are included (main category II), e.g. a flame retardant in plastics used for television sets, radios, etc. However, even though quantitative methodologies are presently lacking for these types of emissions, preliminary quantitative estimations may be performed on a case by case basis.

Emission reduction technologies have not been taken into account in the A-tables of Appendix III, as the kind of technologies applied (with possibly large differences in efficiencies) as well as the degree of penetration may differ among Member States or industry sectors. Only when a

specific abatement measure is common practice for a given process will this will be taken into account. In all other cases, the reasonable worst case is held to apply.

II.3.5 Types of substances and levels of production and use

II.3.5.1 New and existing substances versus biocides

In principle the only difference between new and existing substances and biocides is the fact that biocides are new or existing substance with a specific application (use category 39 "biocides, non-agricultural"). In order to put a biocide on the market a risk assessment for each biocidal application has to be carried out. The risk assessment is carried out for the local scale only so far. The life cycle stages concerned are industrial use and/or private use, and – if applicable – service life and waste treatment. The stages of production and formulation are not considered, as there will be no difference with other chemicals. For the risk assessment the emission scenarios for new and existing substances should be used. In cases where a specific emission scenario (of an emission scenario document of the TGD) exists for the formulation of a product that may contain a biocide, this scenario should be used. This applies, for example, to disinfectants applied in liquid cleaning products. The emission scenario document for industrial categories 5 "Personal/domestic" and 6 "Public domain" should be used here. It should be noted that in EUSES right in the beginning of an assessment a choice has to be made for new and existing substances or biocides. So, the evaluation of a biocide for all relevant stages of the life cycle requires two runs of EUSES. Biocides have been divided in 23 product types according to the Biocidal Products Directive 98/8/EC (EC, 1998), which are presented in ***Table II-3***. As can be seen in this table some product types may be used for various purposes or in various sectors/processes. Furthermore, it has been indicated which life cycle stages are of interest and whether these stages are covered (either in the part for new and existing substances or in the part on biocides) in EUSES. It should be noted that specific emission scenarios for biocides may be used for other use categories as well. For example, the life cycle stage private use for chemicals such as fragrances (UC 36) or colourants (UC 10) notified for liquid cleaners used in the sanitary field can be assessed – for the local scale – better with the biocide emission scenario than with the scenario for new and existing substances. On the other hand, emission scenarios for new and existing substances may be used in some cases if there is no specific emission scenario (yet) for a certain application of a biocidal product type. These cases have been stated in ***Table II-3***. It should be noted that life cycle stages may be "inseparable". For example, human hygiene biocidal products like soap are applied on the skin during bathing (private use) and rinsed off immediately and released with wastewater (waste treatment). The releases in this case are assigned to the life cycle stage private use. For products like creams and deodorants a service life stage (of a very short period) might be recognised as well. In ***Table II-3*** such cases are denoted with a square bracket open ([ ) at the first stage and a square bracket close ( ]) at the last stage concerned.

Table II-3 *Overview of the biocidal product types and the coverage of the appropriate life cycle stages (na = not applicable, NES = scenario for new and existing substances, BPT = specific scenario for application of biocidal product type, and • = not present in this version of EUSES; # refers to a specific emission scenario, i.e. other than the relevant standard scenario of the A- and B-tables. Footnotes at the end of the table.*

Product type	Description of product type	Life cycle stage					
		Production	Formulation	Industrial use	Private use	Service life	Waste treatment
1	Human hygiene biocidal products	NES	NES	na	[•	▪	▪]
	. . . . .	NES	NES	[▪	na	•	▪]
2	Private area and public health area disinfectants and other biocidal products:						
	- Swimming pools	NES	NES	[▪	na	▪	•]
	. . . . .	NES	NES	na	[•	▪	•]
	- Sanitary sector	NES	NES IC 5/6	na	[BPT	na	BPT]
	- Horticulture	NES	NES	[▪	na	•	▪]
	- Tiles and surfaces	NES	NES IC 5/6	[▪	na	na	•]
	. . . . .	NES	NES IC 5/6	na	[•	na	•]
	- Medical sector:						
	-- Disinfection of rooms, furniture and objects	NES	NES	[BPT	na	BPT	BPT]
	-- Disinfection of instruments	NES	NES	[BPT	na	BPT	BPT]
	-- Laundry disinfectants	NES	NES	[BPT	na	BPT]	▪BPT]
	-- Hospital waste disinfectants	NES	NES	[▪	na	•	▪]
	Disinfection of air conditioning systems	NES	NES	[▪	na	•	▪]
	- Disinfection of industrial areas	NES	NES	[▪	na	•	▪]
	- Disinfectants for sewage and wastewater	NES	NES	[▪	na	•	▪]
	- Soil and other disinfectants, …..	NES	NES	[▪	na	•	▪]
	- Disinfection of chemical toilets	NES	NES	[▪	na	•	▪]

Table II.3 (continued) *Overview of the biocidal product types and the coverage of the appropriate life cycle stages (na = not applicable, NES = scenario for new and existing substances, BPT = specific scenario for application of biocidal product type, and • = not present in this version of EUSES; # refers to a specific emission scenario, i.e. other than the relevant standard scenario of the A- and B-tables (continued).*

Product type	Description of product type	Life cycle stage					
		Production	Formulation	Industrial use	Private use	Service life	Waste treatment
3	Veterinary hygiene biocidal products:						
	- Disinfection of animal housing	NES	NES [1)]	[▪	na	•	▪]
	- Disinfection of footwear and animals' feet	NES	NES [1)]	[▪	na	•	▪]
	- Disinfection of milk extraction systems	NES	NES [1)]	[▪	na	•	▪]
	- Disinfection of means of transport	NES	NES [1)]	[▪	na	•	▪]
	- Disinfection of hatcheries	NES	NES [1)]	[▪	na	•	▪]
	- Disinfection of fish farms	NES	NES [1)]	[▪	na	•	▪]
4	Food and feed area disinfectants	NES	NES [1)]	[▪	na	•	▪]
5	Drinking water disinfectants	NES	NES [1)]	[▪	na	•	▪]
6	In-can preservatives:						
	- Washing and cleaning fluids, human	NES	NES IC 5/6 [2,3)]	na▪	[▪	na	▪]
	hygienic products and cosmetics	NES	NES IC 5/6 [2,3)]	[▪	na	•	▪]
	- Detergents	NES	NES IC 5/6 [3)]	[▪	na	•	▪]
	. . . . .	NES	NES IC 5/6 [3)]	[▪	na	•	▪]
	- Paints and coatings	NES	NES IC 14 [3,4)]	NES IC 14	▪	•	▪
	- Fluids used in paper production	NES	NES [3.4)]	BPT	na	▪	BPT
	- Fluids used in textile production	NES	NES [3,4)]	▪	na	▪	▪
	- Fluids used in leather production	NES	NES [3,4)]	▪	na	▪	▪
	- Lubricants: As PT 13						
	- Machine oils: not applicable						
	- Fuels	NES	NES	▪	▪	▪	▪

Table II-3 *(continued) Overview of the biocidal product types and the coverage of the appropriate life cycle stages (na = not applicable, NES = scenario for new and existing substances, BPT = specific scenario for application of biocidal product type, and • = not present in this version of EUSES; # refers to a specific emission scenario, i.e. other than the relevant standard scenario of the A- and B-tables (continued).*

Product type	Description of product type	Life cycle stage					
		Production	Formulation	Industrial use	Private use	Service life	Waste treatment
7	Film preservatives:						
	- Paints and coatings	NES	NES IC 14 [3,4)]	NES IC 14	▪	•	▪
	- Plastics: As PT 9 for polymerised materials						
	- Glues and adhesives	NES	NES IC 14 [3,4)]	▪	•	▪	▪
	- Paper and cardboard	NES	NES [3.4)]	BPT	na	▪	BPT
8	Wood preservatives	NES	NES	▪	na	▪	▪
9	Fibre, leather, rubber and polymerised materials preservatives:						
- Textile and fabrics		NES	NES [3,4,5)]	BPT [5)]	na	BPT	▪
	- Leather and hides	NES	NES [3.4)]	BPT	na	▪	▪
	- Rubber, plastics and other polymerised materials	NES	NES [3.4)]	▪	na	▪	▪
	- Paper and cardboard	NES	NES [3)]	BPT	na	▪	BPT
10	Masonry preservatives	NES	NES	▪	▪	▪	▪
11	Preservatives for liquid-cooling and	NES	NES	[▪	na	▪	▪]
12	Slimicides	NES	NES	[▪	na	▪	▪]
13	Metalworking-fluid preservatives	NES	NES	[NES IC 8	na	NES IC 8	NES IC 8
14	Rodenticides	NES	NES	[▪	na	▪	▪]
	. . . . .	NES	NES	na	[▪	▪	▪]
15	Avicides	NES	NES	[▪	na	▪]	▪
16	Molluscicides	NES	NES	[▪	na	▪]	▪
17	Piscicides	NES	NES	[▪	na	▪]	▪

Table II-3 *(continued) Overview of the biocidal product types and the coverage of the appropriate life cycle stages (na = not applicable, NES = scenario for new and existing substances, BPT = specific scenario for application of biocidal product type, and • = not present in this version of EUSES; # refers to a specific emission scenario, i.e. other than the relevant standard scenario of the A- and B-tables (continued).*

Product type	Description of product type	Life cycle stage					
		Production	Formulation	Industrial use	Private use	Service life	Waste treatment
18	Insecticides, acaricides and products to control other arthropods:						
	- Insecticides for manure	NES	NES	[▪	na	▪	▪]
	- Insecticides for stables	NES	NES	[▪	na	▪	▪]
	- Refuse dumps	NES	NES	[▪	na	▪	▪]
	- Insecticides for empty spaces and spaces with stocks	NES	NES	[▪	na	▪]	▪
	- Aerosols/fumigants used outdoors	NES	NES	[▪	na	▪]	▪
	- Aerosols/fumigants used within fumigation installations	NES	NES	[▪	na	▪]	▪
		NES	NES	[▪	na	▪]	▪
	- Aerosols/fumigants used indoors	NES	NES	[▪	na	▪]	▪
19	Repellents and attractants	NES	NES	[▪	na	▪]	▪
	. . . . .	NES	NES	na	[▪	▪]	▪
20	Preservatives for food or feedstocks	NES	NES [1)]	[▪	na	▪]	▪
21	Antifouling products	NES	NES IC 14	▪	na	▪	▪
22	Embalming and taxidermist fluids	NES	NES [1)]	BPT	na	BPT	BPT

1) If applicable.

2) Only for cleaning fluids the emission scenario for IC 5/6.

3) There may be 2 formulation stages, 1 for a biocidal preparation and the other for the product in which the biocidal preparation is blended.

4) In principle two stages for service life might be distinguished: the shelf life of the product (e.g., paint) and the life span of the finished articles (e.g., painted articles).

5) Including removal of biocides present on imported raw materials.

II.3.5.2 Low and high production volume chemicals

New substances are usually produced in rather low volumes. For existing substances High-Production-Volume Chemicals (HPVCs) will also have to be considered. In 1990 the OECD list of HPVC contained about 1600 chemicals which are either produced in excess of 10,000 tonnes in any one member country or in two or more countries in excess of 1,000 tonnes. For the B-tables, default values have been introduced for every industrial category, above which a chemical is considered to be an HPVC (unless the chemical is considered as an HPVC by the notifier).

In the case of high-production-volume chemicals (HPVC) particularly, the substances often have more than one application, sometimes in different industrial categories. For these substances, the assessment proceeds by breaking down the production volume for every application according to data from industry. For the local situation, in principle all stages of the life cycle need to be considered for each application. Where more than one stage of the life cycle occurs at one location, the local PEC shall be calculated by summing all the relevant emissions from that location. For releases to wastewater, only one point source for the local STP is considered. In the risk assessment of biocides, however, assessments for each individual application are carried out (only for the local scale).For the regional situation, the emissions to each compartment must be summed for each stage of the life cycle and each application.

II.3.6 Remarks on the industrial category

Emission scenario documents have recently been developed and described in the context of the TGD for new and existing substances. These documents cover the industrial categories 3, 5, 7, 8, 10, 12, 13 and 14, but were not yet used for the release estimates in Appendix III.
Emission scenario document have been developed and described in the context of the TGD for new and existing substances. These documents cover the industrial categories 3, 5, 6, 7, 8, 10, 11, 12, 13 and 14 and are available to be used for release estimates. An overview is given in ***Table II-4***.

1. Agricultural industry
There are no use-category documents for this IC. Emissions due to the application (processing stage) of pesticides are beyond the scope of the TGD and EUSES. Several UCs are distinguished, e.g. UC=19 ‘Fertilisers’ and UC=41 ‘Pharmaceuticals’.

2. Chemical industry: basic chemicals
There are no use-category documents for this IC. If a basic chemical is formulated, A- and B-tables are provided. Recovery is not considered as a separate emission stage; emissions of chemicals such as catalysts are included in the emissions at the processing stage. So far, no distinction has been made between UCs, apart from UC=48 ‘Solvents’. Most chemicals will have to be classified as UC=43 ‘Process regulators’ or UC=55/0 ‘Others’.

3. Chemical industry: chemicals used in synthesis
Apart from UC=33 'Intermediates' in this IC too, most chemicals will have to be classified as UC=43 'Process regulators' or UC=55/0 'Others'. Formulation may be feasible for some chemicals, whilst recovery is unlikely. The release tables are based on Ros and Van der Poel (1989) and provided with the relevant data of the emission scenario document for IC 3.

4. Electrical/electronic industry
There are no use category documents for this IC. There are many different applications in this IC, however, e.g. during production of printed circuits and the application of dielectric fluids in transformers and capacitors. The only distinction is between chemicals included into or onto a matrix (MC=II) and others used at point sources (MC=III) in a process.

5. Personal/domestic
Chemicals used in this IC will in many cases be present in formulations, e.g. in cleaners (soaps, detergents, washing powders, etc.) and products for the care of leather, textiles and cars. Emissions will be very diffuse and the only emissions regarded as a point source situation are those of wastewater to an STP (assuming more or less uniform usage by populations and a uniform usage per week and season). For products like fuels and fuel additives the emissions are calculated in IC=9 'Mineral-oil and fuel industry' at the stage of private use. For paint products and photochemicals this is done in IC=14 'Paint, lacquers and varnishes industry' and IC=10 'Photographic industry', respectively. For formulation and private use of soaps, fabric washing, dish cleaning, and surface cleaning substances the emission scenario document for IC 5 of the TGD the relevant data have been incorporated in the A- and B-tables.

6. Public domain
There are no use category documents for this IC. Most chemicals used in this IC will be present in formulations, e.g. in 'cleaners' (UC=9 'Cleaning and washing agents and disinfectants'), non-agricultural pesticides (UC=39 'Pesticides, non-agricultural') and products for the maintenance of roads, buildings, etc. For UC=9, UC=39 and all other UCs, a differentiation in the number of days (B-tables) and the emission factors (A-tables) has been made. . For formulation and industrial use of soaps and surface cleaning substances the emission scenario document for IC 6 of the TGD the relevant data have been incorporated in the A- and B-tables.

7. Leather processing industry
A general For releases to wastewater at the local scale the emission scenario of the emission scenario document for IC 7 of the TGD has been implemented. In all other cases the emission scenarios is presented of the A- and B-tables are used. These have with default values in the tables for common functions of chemicals such as tanning agents (UC=51). For specific UCs (UC=6 'Anti-set-off and anti-adhesive agents', UC=9 'Cleaning/washing agents and disinfectants', UC=10 'Colorants' and UC=31 'Impregnation agents') different values are used.

8. Metal extraction, refining and processing industry
For releases to wastewater at the local scale the emission scenario of the emission scenario document for IC 8 of the TGD has been implemented. In all other cases the emission scenarios of the A- and B-tables are used. The emission scenario also covers biocides. Although these chemicals are used in many different processes, in this IC a use category document is present for metal-working fluids only (processing stage).In all other cases the A- and B-tables are used. The

basis for the tables A- and B-tables is the document of Van der Poel and Ros (1987). The functions of the fluids are cooling and lubrication, so the tables have specific data for UC=29 'Heat transferring agents' and UC=35 'Lubricants and additives'.

9. Mineral oil and fuel industry
There are no use- category or emission scenario documents for this IC.

10. Photographic industry
For releases to wastewater at the local scale the emission scenario of the emission scenario document for IC 10 of the TGD has been implemented. In all other cases the emission scenarios of the A- and B-tables are used. In all other cases the A- and B-tables are used.Several use-category documents are available for this IC. The values in the tables A- and B-tables are based on the document of Ros and Bogte (1985).

11. Polymers industry
Although there is a detailed use-category document on the processing stage of polymers, this has not yet been implemented in the tables. The reactions in which the polymers (and prepolymers such as polyesters) are produced are considered to take place in IC=10 'Polymers industry' at the processing stage (i.e. the substances from the production stage are processed by companies in IC=10). For the processing stage a distinction has been made between 'true' polymerisation reactions (see A-tables) and other reactions (polyadditions, polycondensations, etc.). The processing of polymeric materials (thermoplastics and thermosetting resins) is also considered. In the text accompanying the A-tables a short explanation is given on how to interpret the functions of chemicals and the relevant UCs. Today, many thermoplastics are recycled, but this has not yet been taken into account.
For rubber industry the emission scenario document of the TGD (IC 15 Others: Rubber industry) has been implemented in IC 11 as rubbers are polymers. The emission scenario considers the releases with wastewater at the local scale.

12. Pulp, paper and board industry
For releases to wastewater at the local scale the emission scenario of the emission scenario document for IC 12 of the TGD has been implemented. In all other cases the emission scenarios of the A- and B-tables are used. In all other cases the A- and B-tables are used. The tables A- and B-tables are based on the use-category documents of Cathie *et al.* (1991) and Ros and Berns (1988) on paper production (including dyeing of paper) and recycling. Specific tables have been introduced to cover the printing process, which has been included in this IC.
For UC 39 "Biocides" the specific emission scenario document on the life cycle stages industrial use and waste treatment (paper recycling) has been implemented.

13. Textile processing industry
For releases to wastewater at the local scale the emission scenario of the emission scenario document for IC 13 of the TGD has been implemented. In all other cases the emission scenarios of the A- and B-tables are used. The emission scenario also covers biocides. In all other cases the A- and B-tables are used.
The original scenario derived from the document of Ros (1985) has been used for the emission A- and B-tables.

14. Paints, lacquers and varnishes industry
For releases to wastewater and air at the local scale the emission scenario of the emission scenario document for IC 143 of the TGD has been implemented. In all other cases the emission scenarios of the A- and B-tables are used. In all other cases the A- and B-tables are used. These A- and B-tables distinguish
There are documents available on paint production and paint application, but these have not yet been considered in the emission tables. To obtain better estimates, a distinction has been made between field of application, life cycle stage and substance properties (volatile, "non-volatile - water soluble" and "non-volatile - non water soluble").UCs, water-based and solvent-based types, and application by industries and households (private use). Releases to soil at formulation and application are not considered because local emissions to soil are not part of the risk assessment. Emission to soil during the service life of the paint due to process like leaching are not considered because they were not considered separately from emissions to soil during elimination. Waste treatment is not yet considered in this version of EUSES

16. Engineering industry: civil and mechanical
For this IC no use-category documents exist. Most tables match the ones applied for chemicals classified in IC=55/0 'Others'.

15/0. Others
General tables have been used.

Table II-4 *Overview of the coverage of the appropriate life cycle stages in the emission scenario documents (na = not applicable, NES = scenario for new and existing substances, BPT = specific scenario for application of biocidal product type, and • = not present in this version of EUSES; # refers to a specific emission scenario, i.e. other than the relevant standard scenario of the A- and B-tables.*

Industrial category	Description of product type	Life cycle stage					
		Production	Formulation	Industrial use	Private use	Service life	Waste treatment
5	Personal and domestic production volume > 1000 tonnes/year:	NES	NES	NES	[ESD	na	ESD][1]
6	Public domain production volume > 1000 tonnes/year:	NES	NES	ESD	[ESD	na	ESD][1]
7	Leather processing industry	NES	NES	ESD[2]	na	▪	▪
8	Metal extraction industry	NES	NES	[ESD	na	na	ESD][3]
10	Photographic industry	NES	NES	ESD	NES	na	ESD
11	Polymers industry	NES	[ESD	ESD][4]	na	▪	▪
12	Pulp paper and cardboard	NES	NES	ESD[5]	na	na	ESD[5]
13	Textile processing industry	NES	NES	ESD[6]	NES	ESD[6]	▪
14	Paints, lacquer and varnished industry	NES	NES	ESD[7/8]	NES	▪	▪

1) extension of A-tables

2) emission scenario for biocides is available, see biocides PT 9

3) also applicable to biocides, see PT13

4) the formulation and production steps can often not be viewed separately in the rubber industry.

5) emission scenario for biocides is available, see biocides PT 6, 7 and 9

6) emission scenario for biocides is available, see biocides PT 9

7) emission to air are also considered.

8) emission scenarios for biocides are also available, see PT 6, 7 and 21 (not available in EUSES).

II.3.7 Intermittent releases

Many substances are released to the environment from industrial sources as a result of batch, rather than continuous, processes. In extreme cases, substances may be emitted a few times a year only. Intermittent release needs to be defined, although rapporteurs will have to justify the use of this scenario on a case-by-case basis. Intermittent release can be defined as:

- intermittent but only recurring infrequently, i.e. less than once per month and for no more than 24 hours.

This would correspond to a typical batch process required only for a short period of the year (releases to the environment may be of limited duration only). Thus, for the aquatic compartment, transport processes may ensure that the exposure of aquatic organisms is of short duration only. For intermittent releases to the aquatic compartment a dedicated PNEC is used in the risk characterisation (see Section II.6) and for micro-organisms in the STP, a specific PEC is used. When intermittent release is identified for a substance, this is not necessarily applicable to *all* releases during the life cycle.

II.4 ENVIRONMENTAL DISTRIBUTION

The distribution and fate of a chemical in the environment is in principle assessed on two spatial scales: locally in the vicinity of a point source, and regionally for a larger area which includes all sources, point and diffuse.

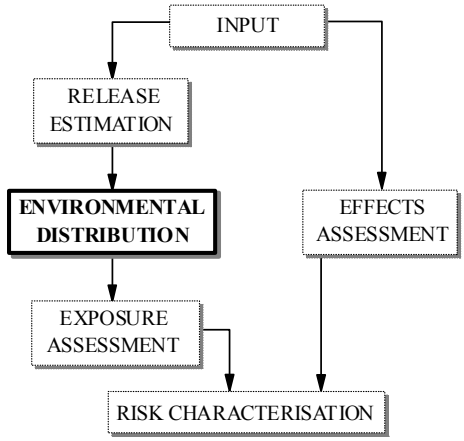

Figure II-9 *System structure.*

In this module, as a first step 'secondary data' are derived from the primary data of the input module. In this context secondary data are partition coefficients and degradation constants in the environment. Estimation routines for these parameters are implemented in the system. Most emissions to wastewater are treated in a Sewage Treatment Plant (STP). The STP model SimpleTreat is discussed in Section II.4.3. The last part of this module contains the actual environmental fate models: a multi-media fate model for the regional calculations and dedicated model approaches for the local environmental compartments. The end result of this module are concentrations (PECs) in the environmental compartments air, surface water, soil, sediment and groundwater. In the following sections, each sub-module is discussed separately.

II.4.1 Partition coefficients

Transport and transformation ('fate') describe the distribution of a substance in the environment, or in organisms, and changes of the substance with time (in concentration, chemical form, etc.). Since measured data on fate processes are not usually available for the various compartments, they must be extrapolated from the primary data of the input module. This section describes the air-aerosol, air-water and solids-water partitioning processes in the various compartments.

II.4.1.1 Gas-aerosol partitioning

The fraction of the chemical associated with aerosol particles is estimated on the basis of the chemical's vapour pressure, according to Junge (1977). In this equation the sub-cooled liquid vapour pressure should be used. This implies that for solid substances, vapour pressure needs to be corrected, which is done according to Mackay (1991).

II.4.1.2 Air-water partitioning

The transfer of a substance from the aqueous phase to the gas phase (e.g. stripping in the aeration tank of an STP, volatilisation from surface water) is estimated by means of its Henry's Law constant. If the value is not available in the input dataset, the required Henry's Law constant and the $K_{air\text{-}water}$ (also known as the 'dimensionless' Henry's Law constant) are estimated from the ratio of the vapour pressure and the water solubility.

II.4.1.3 Solids-water partitioning

Besides volatilisation, adsorption to solid surfaces is the main partitioning process driving distribution in soil, surface waters and sediments. If no measured data are available for a specific adsorbing material, it is assumed that all adsorption can be related to the organic matter in the medium. Due to the different compositions of environmental compartments, there is considerable variation in their sorption capacity. A normalisation to the organic carbon fraction is therefore used to reduce the variance of the sorption coefficients measured in different media. This gives a carbon-normalised partition coefficient (*Koc*). The solids-water partition coefficient (*Kp*) in each compartment (soil, sediment, suspended matter, sewage sludge) can be calculated from the *Koc* value and the fraction of organic carbon in the compartment.

For organic, non-ionic substances, *Koc* can be estimated from *Kow*, as outlined in Chapter 4 of the TGD. The equation given for the class 'predominantly hydrophobics' is implemented as a general default in EUSES. For specific groups of substances, other QSARs are available. These QSARs should be used, if appropriate, and the default estimate will be overwritten in such cases. All estimates are taken from Sabljic *et al.* (1995).

Each compartment is described as consisting of three phases: solids, water and air (only relevant in soil). *Kp* describes the partitioning between solids and water in a compartment, since *Kp* is expressed as the concentration of the chemical adsorbed to solids divided by the concentration dissolved in pore water. The dimensionless form of *Kp*, or the total compartment-water partition coefficient ($K_{comp\text{-}water}$), describes the ratio between the total concentration in the compartment and the pore-water concentration. This parameter is used extensively in the fate models described in Chapter III and is derived from the definition of the compartments in three phases.

II.4.2 Degradation rates in the environment

Transport and transformation ('fate') describe the distribution of a substance in the environment, or in organisms, and changes of the substance with time (in concentration, chemical form, etc.), thus including both biotic and abiotic transformation processes. Since measured data on degradation processes are not usually available for the various compartments, they must be extrapolated from standardised laboratory tests. In this sub-module, degradation rate constants are derived for abiotic degradation (hydrolysis and photolysis) and biotic degradation (in soil, sediment, water and sewage treatment). In general, risk assessment focuses on the parent compound. Nevertheless, if stable degradation products are formed, these should be assessed as well.

Biotic and abiotic degradation in air, surface water and sediment is at this moment only taken into account in the calculations of the regional PEC.

II.4.2.1 Hydrolysis

Values for the half-life (*DT50*) of a hydrolysable substance can be converted to degradation rate constants, which can be used in the fate models. QSAR methods are available for certain groups of substances, but not implemented in EUSES (they are discussed in Chapter 4 of the TGD; EC, 2003). It should be noted that for many substances, the rate of hydrolysis would be highly dependent on the specific environmental pH and temperature. Because of that temperature dependence, EUSES converts the input value of hydrolysis half-lives of standard tests to a value that reflects the average EU outdoor temperature.

II.4.2.2 Photolysis in water

In the vast majority of surface water bodies dissolved organic matter is responsible for intensive light attenuation. Thus photolysis processes are normally restricted to the upper zones of water bodies. Photochemical degradation processes in water may be an important fate process only for those substances that are persistent to other degradation processes (e.g. biodegradation and hydrolysis). The following aspects have to be considered when estimating the photochemical transformation in natural water bodies

- The intensity of the incident light depends on seasonal and geographic conditions and varies within wide ranges. For long-term considerations average values can be used, while for short-term exposure an unfavourable solar radiation(winter season) should be chosen.
- In most natural water bodies, the rate of photoreaction is affected by dissolved and suspended matter. Since the concentration of the chemical under consideration is normally low compared to the concentration of e.g. dissolved humic acids, by far the majority of the sunlight penetrating the water is absorbed by the natural constituents. Using the standard parameters of the regional model (water depth, suspended solids concentration), the reduction may be as large as 98%.

II.4.2.3 Photochemical reactions in the atmosphere

Although for some chemicals direct photolysis may be an important breakdown process, for most substances the most effective elimination process in the troposphere results from reactions with photochemically generated species such as OH-radicals, ozone and nitrate radicals. The specific first-order degradation rate constant of a substance with OH-radicals can either be determined experimentally (OECD, 1992c) or estimated by (Q)SAR-methods (see Chapter 4 of the TGD; EC, 2003).

II.4.2.4 Biodegradation in the sewage treatment plant

The assessment of biodegradability and/or removal in sewage treatment plants should preferably be based on results from tests simulating the conditions in treatment plants. Such a test may be the OECD 303 test or equivalent (EC, 2003). Most of the ready biodegradability tests in use at the moment are aimed at measuring the mineralisation of a chemical. Hence, they give valuable information on the mineralisation of a substance and the possible formation of transformation products. However, they do not give information on the degradation rate of the parent compound, nor do they give a quantitative estimate of the removal percentage in a wastewater treatment plant. Therefore, it is necessary to assign rate constants to the results of the standard tests for use in STP models. These constants are based on a relatively limited number of empirical data. For the purpose of modelling a sewage treatment plant (STP), rate constants were derived from the biodegradation screening tests (rate constants given in Section III.4.2.4). These rate constants have the following prerequisites:

- They are used only for the water-dissolved fraction of the substance. Calculation of partitioning between water and sludge phases is calculated prior to application of the rate constant.
- Sufficiently valid data from internationally standardised tests are preferred.
- For some substances (e.g. certain detergents), higher biodegradation rates may be justified if this can be confirmed by experimental data.

II.4.2.5 Biodegradation in surface water, sediment and soil

The rate of biodegradation in surface water, soil and sediment is related to the structure of chemicals, microbial numbers, organic carbon content and temperature. These properties vary spatially and an accurate estimate of the rate of biodegradation is very difficult, even if laboratory or field data are available. Fate and exposure models normally assume the following simplifications:

- The kinetics of biodegradation are pseudo-first order.
- Only the dissolved portion of the chemical is available for biodegradation.

As mentioned, temperature influences the activity of micro-organisms and thus the biodegradation rate in the environment. When biodegradation rates or half-lives in surface water, sediment and soil have been estimated in simulation tests, EUSES can recalculate these rates obtained to reflect an average EU outdoor temperature. When it is documented for a specific substance that a difference between the temperature employed in the test and the

average outdoor temperature has no influence on the degradation half-life, no correction is needed.

Normally, specific information on biodegradability in sediment or soil is not available. Hence, rate constants for these compartments have to be estimated from the results of standardised tests. It should be noted that the assigned degradation half-lives will only affect the predicted regional concentrations if the residence time of the chemical in that compartment is (much) larger than the assigned half-life (i.e. for inherently biodegradable substances usually only in the soil and sediment compartment).

Since the fate models assume that no degradation takes place in the bound phase, the rate constant for the bulk sediment or soil depends in principle on the sediment-water or soil-water partition coefficient of the chemical. However, for substances with low *Kp*-values, not enough empirical data are presently available to assume any sort of dependence of the soil biodegradation half-life on the solids-water partition coefficient. Nevertheless, for substances with high *Kp*-values there is evidence that some sort of *Kp*-dependence exists. Therefore, degradation half-life classes for (bulk) soil, partly based on *Kp*, have been defined.

The extrapolation of biodegradation test results to rate constants for sediment is problematic, given the fact that sediment generally consists of a relatively thin aerobic top layer and anaerobic deeper layers. For the degradation in the anaerobic layers a rate constant of zero (infinite half-life) is assumed, unless specific information on degradation under anaerobic conditions is available. For the aerobic zone, the same rate constants as those for soil are assumed.

II.4.3 Sewage treatment

Across the European Union, taken as a whole, approximately 80% of the municipal wastewater volume (domestic and industrial loads) is treated in a biological wastewater treatment plant (EC, 2003). Nevertheless, the situation is evolving. The situation with respect to wastewater treatment at industrial plants is less clear. It may be assumed that many of the larger industrial plants are either connected to a municipal wastewater treatment plant or have treatment facilities on site. In many cases, these treatment plants are not biological treatment plants but physico-chemical treatment plants.

In EUSES, the above situation is taken into account as follows:

- On a local scale, it is assumed that wastewater will pass through a STP before being discharged into the environment. For the largest local PEC in surface water, additionally, a concentration assuming no sewage treatment is calculated. This value should be determined in addition to the normal PEC, which assumes sewage treatment, to flag for possible local problems (this PEC/PNEC ratio will not normally be used in risk characterisation).
- On a regional scale, it is assumed that 80% of the wastewater is treated in a biological STP and the remaining 20% released directly into surface waters.

The degree of removal in a wastewater treatment plant is determined by the physico-chemical and biological properties of the substance (biodegradation, adsorption onto sludge, removal due to sludge withdrawal, volatility) and the operating conditions of the plant.

If no measured data are available, the degree of removal can be estimated by means of a wastewater treatment model using log *Kow*, Henry's Law constant and the results of biodegradation tests as input parameters. The model calculates organic carbon normalized partition coefficients, *Koc*, which are estimated as outlined in Chapter 4 of the TGD and according to Sablic *et al*. (1995). If a partition coefficient which is based on Koc is not applicable, a specific partition coefficient can used as direct input. However, it should be remembered that the distribution behaviour of transformation products is not considered in this approach. In the screening phase of exposure assessment, a revised version of the sewage treatment plant model SimpleTreat (Struijs *et al.*, 1991) is implemented: SimpleTreat 3.1 (Struijs, 2003) which differs from SimpleTreat 3.0 (Struijs, 1996) only in the way *Koc* is calculated from *Kow* (Sablic, 1995). Improvement with respect to the version of 1991 has been accomplished in two ways: by incorporating, first, more options in defining the STP environment and, second, improved formulations of the interaction between the chemical and the engineered STP environment. This greater flexibility makes the model suitable for a wide variety of wastewater scenarios in the EU. These may include the absence of primary sedimentation (see Figure II-10a,b), a continuous scale on which the sludge-loading rate can be chosen, and the sewage volume per inhabitant per day. In addition to the aeration technique, these parameters largely define the mode of operation of the plant, which in turn has a significant influence on the fate of the modelled chemical. Process descriptions for air-water exchange and biodegradation have been extended and include a simulation of non-linear Monod kinetics.

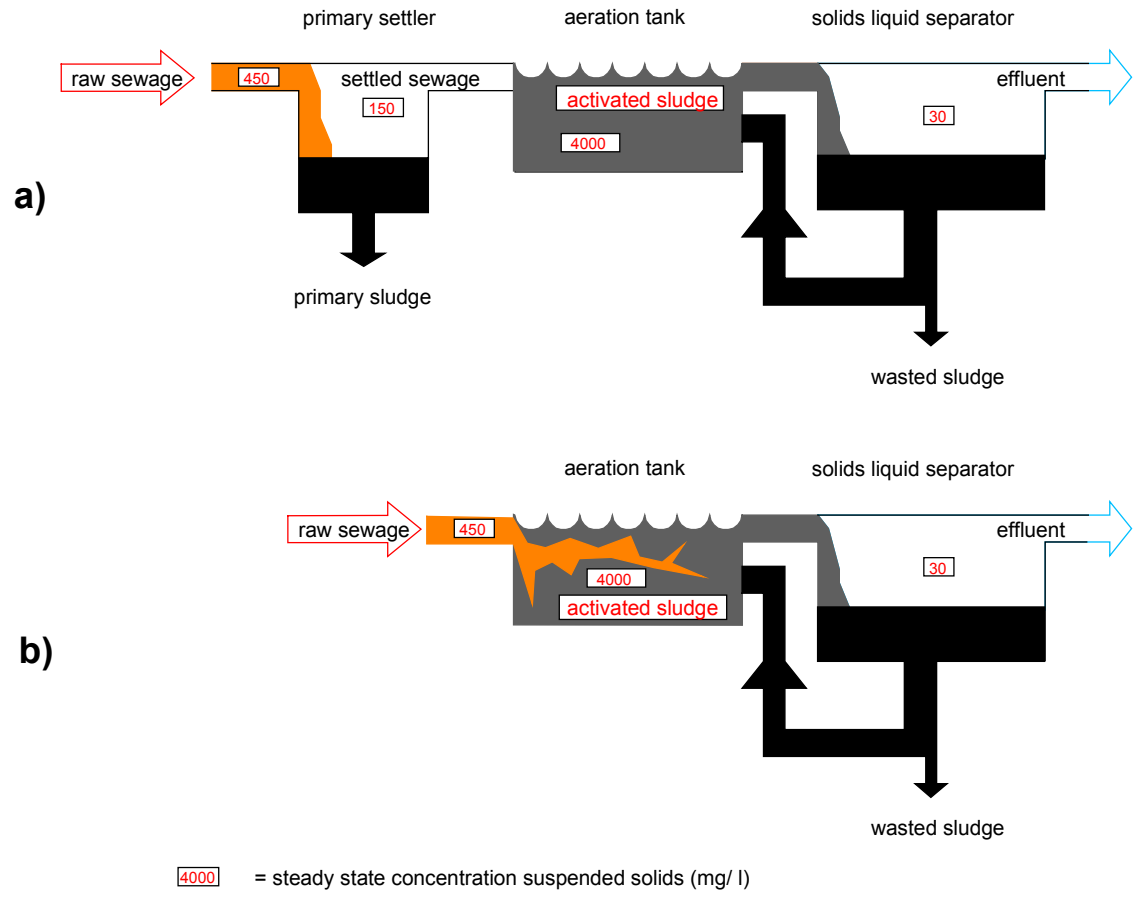

Figure II-10a,b *Schemes of communal biological sewage treatment plants; (a) with and (b) without primary sedimentation.*

The standard sewage treatment plant is modelled as an average-size treatment plant based on aerobic degradation by activated sludge, and consisting of 9 or 6 compartments (see Figure II-11). This model is a multi-media box model of the 'Mackay-type, level III' (see also Section II.4.4). The model calculates steady-state concentrations in a sewage treatment plant consisting of a primary settler (optional), an aeration tank and a solids-liquid separator.

Depending on the test results for ready and/or inherent biodegradability of a substance, specific first-order biodegradation rate constants are assigned to the compound. An improved process formulation for volatilisation from the aeration tank, which is also applicable to semi-volatile substances (Mikkelsen, 1995), has been incorporated in the revised version.

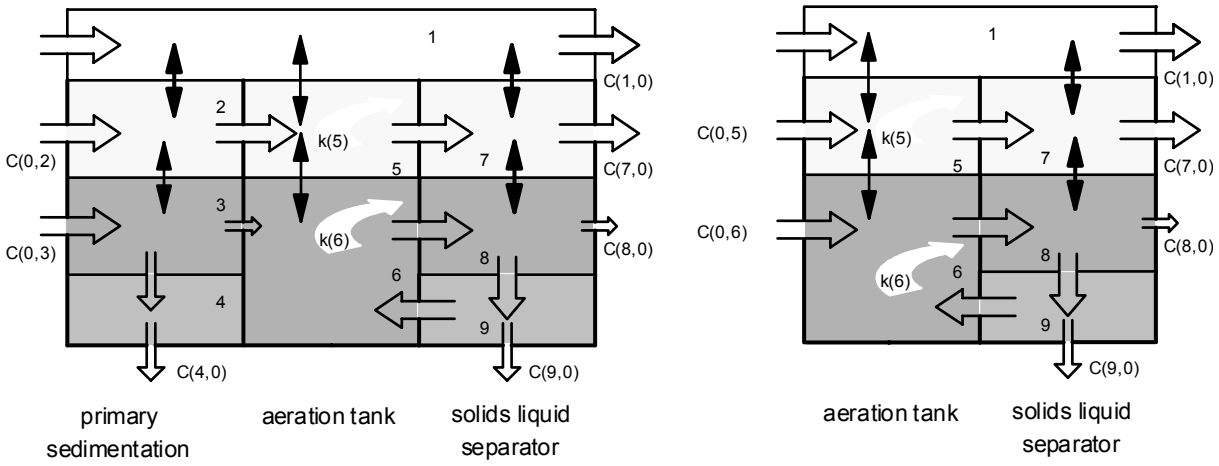

Figure II-11a,b *Box schemes of chemical fate in a communal sewage treatment plant (a) with and (b) without primary sedimentation.*

Typical characteristics of the standard sewage treatment plant are used. At a higher tier in the risk assessment process more specific information on the biodegradation behaviour of a chemical may be available. In order to take this information into account, the following optional scenarios have been implemented:

- temperature dependence of the biodegradation process;
- degradation kinetics according to the Monod equation;
- degradation of the chemical both in the aqueous and in the adsorbed phase;
- variation in the sludge loading rate (and thus in the sludge retention time);
- not considering a primary settler (only for the local spatial scale).

II.4.4 Regional distribution

II.4.4.1 Approach

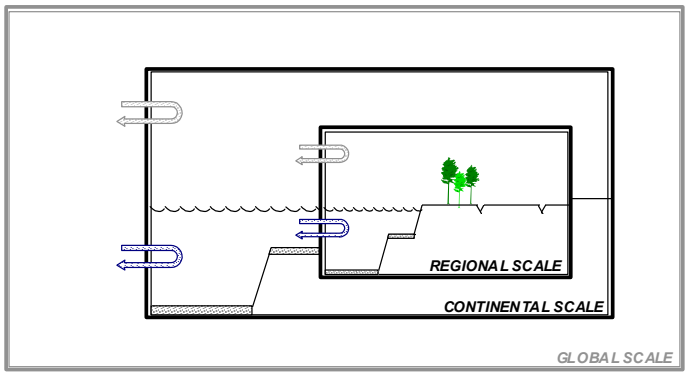

Figure II-12 *Nested multi-media fate model for calculating regional exposure concentrations according to SimpleBox version 3.0.*

The fate of chemicals at regional, continental and global spatial scales differs from the fate at local scales in the sense that more time is available for transport and transformation processes. Concentrations at local spatial scales are almost entirely controlled by mixing (dilution in the background concentrations). The models for calculating the local PEC therefore disregard other removal processes. At longer distances from point sources - or when emissions are diffuse -, i.e. when mixing has progressed, inter-media transport and degradation become relatively more important. For calculating the regional PEC, the multi-media fate-modelling approach is used. The multimedia fate modelling approach is especially useful for the larger spatial scales to consider the non-zero background concentrations of the more persistent chemicals that are transported over long distances with air and water. For this purpose, EUSES 2.0 incorporates a recent version of the SimpleBox model (Version 3.0; Den Hollander and Van de Meent 2004); ***Figure II-12***), in which the fate of chemicals is modelled on different spatial scales simultaneously. Of this model, only two scales (regional and continental) are used; the most inner (local) scale, as well as several other options (substance dependent penetration depth in soil, vegetation compartment, temperature correction), are 'switched off'.

This 'nested' modelling approach recognises that emissions at the regional scale lead to increased concentrations at larger spatial scales, and that emissions at the global and continental scales contribute to increased concentrations at the regional scale. Generally, the contribution of the global background to regional concentrations is expected to be small.

II.4.4.2 Assumptions

The multi-media fate modelling on the regional and continental scales is done as in the original SimpleBox version 1.0 (Van de Meent, 1993). The basic characteristics of this model are shown in ***Figure II-13***. As in all multi-media fate models, a number of simplifying assumptions are made (Cowan *et al.*, 1995; Mackay, 1991; Van de Meent *et al.*, 1995):

- Environmental media (air, water, sediment, 3 soil types) are represented by compartments or 'boxes'. Flows of the chemical into and out of the boxes are modelled by writing mass balances for each of the boxes. Concentrations of chemicals in the boxes are computed by solving the set of mass-balance equations simultaneously.

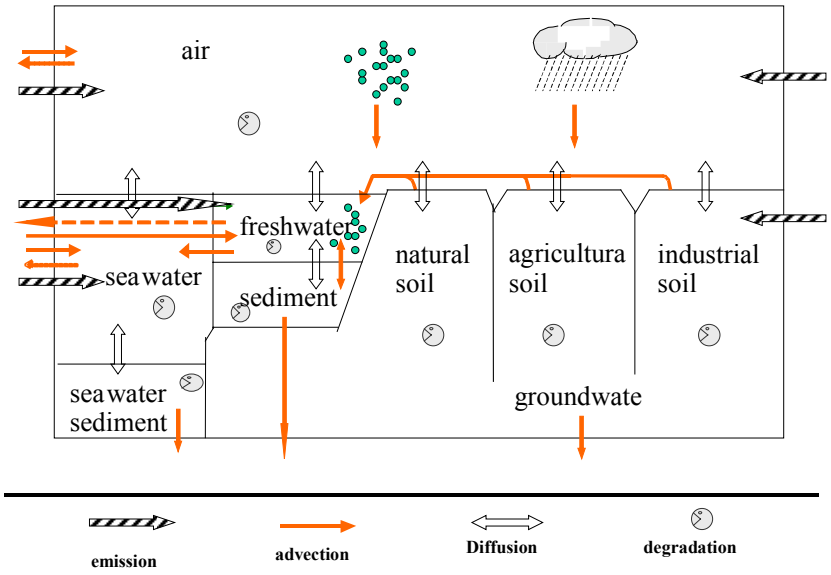

Figure II-13 *Schematic representation of the model for calculating the regional PEC.*

- The environmental media are assumed to be homogeneous and well mixed. Spatial variation in properties of the medium, and spatial differences in concentration are disregarded. Once emitted, chemicals are assumed to be instantaneously spread out through the entire box.
- The properties of the environmental media are assumed to be non-variable. Temporal variation in flow rates, temperatures or partition coefficients are disregarded.
- Emission rates are assumed to be constant in time.
- Removal by (inter-media) transport and degradation are assumed to follow first-order kinetics; the removal rates are proportional to the concentration of the chemical in the box.
- It is assumed that the steady state has been achieved (concentrations have become constant in time). Most multi-media fate models are capable of computing the development of concentrations towards a steady state ('level IV'). For the present purpose, the non-equilibrium steady-state ('level III') solution of the model is used.

II.4.4.3 Compartments

In the multi-media model used, the environmental media are represented by the following homogeneous and well-mixed compartment 'boxes':

Atmosphere

The air compartment consists of gas, rainwater and aerosol particles. The atmospheric sub-phases of air are assumed to be in thermodynamic equilibrium. Aerosol particles and raindrops act as carriers that physically transport chemicals from the atmosphere to the water and soil compartments. The air compartments of the regional and continental scales are modelled as 'open' in the sense that air flows to and from other spatial scales. Along with these air streams, chemicals are imported and exported from and to these scales. Only the lower, well-mixed layer of the atmosphere is considered. The characteristics of the air compartment are set in the model

by the following parameters:
- area; the area of the air compartment is equal to the total area of the system;
- mixing height;
- residence time of air in the system; a value is found from (i) the volume of the air compartment and (ii) the average wind speed;
- aerosol surface area; combined in this model with the specific affinity of chemicals for the aerosol material into the 'Junge-equation constant';
- precipitation rate;
- aerosol-collection efficiency of rainwater;
- deposition velocity of aerosol;
- temperature.

Surface water (freshwater and marine environment)

The water compartment contains the chemical in a truly dissolved state, and associated with particulate matter (colloidal material, suspended sediment particles, aquatic biota). Analogous to the atmosphere, water and particulate phases are assumed to be in thermodynamic equilibrium. Also, sediment particles act as carriers of chemicals across the sediment-water interface. The water compartments of the regional and continental scales are modelled as 'open'. The water boxes have a constant volume, through which water flows from (i) streams from other spatial scales, (ii) run-off from soil, (iii) STP-effluents and (iv) direct rainfall into surface water. The residence time of water in the system is determined by the values of these parameters. The characteristics of the water compartment are set in the model by the following parameters:
- area (set by system area and fraction that is water);
- water depth;
- residence time of water in the system; a value for the residence time follows from the water balance, and is governed by (i) the volume of the water compartment, (ii) run-off from soil, (iii) inflowing water, (iv) STP effluents (set by number of inhabitants, per-capita water use and percentage sewerage) and (v) direct rainfall into surface waters;
- concentration of suspended solids in water;
- deposition velocity of suspended particles.

Sediment (freshwater and marine environment)

The sediment compartment consists of a solid phase and a pore-water phase, which are assumed to be in thermodynamic equilibrium. Only the top few centimetres of the sediment are modelled. If sedimentation is greater than resuspension (positive net sedimentation), this top layer is continuously refreshed by newly deposited material, with the old sediment being buried. The characteristics of the sediment compartment are set in the model by:
- area (set by system area and fraction that is water);
- mixing depth;
- aerobic fraction;
- net sedimentation rate; a value for the net sedimentation follows from the solids balance, and is governed by (i) (biogenic) production of suspended solids, (ii) concentration of suspended particles in the in- and outflowing water, (iii) concentration of suspended solids in STP effluent and (iv) soil erosion rate.

Soil
There are three soil compartments in the model. The different soil compartments reflect typical differences in characteristics (mixing depth, porosity, etc.) and use (emissions): (i) 'natural' soil, which receives input only from the atmosphere by deposition, (ii) 'agricultural' soil, which receives sludge from STPs in addition to atmospheric deposition and (iii) 'industrial' soil, which receives direct emissions. The characteristics of the soil compartments are set in the model by:

- area (set by system area and fraction that is soil);
- mixing depth;
- fraction of rainwater infiltrating into the soil;
- fraction of rainwater running off to surface water;
- soil erosion rate.

II.4.4.4 Processes

In the model, the mass flows of chemical are formulated as functions of the characteristics of the environment and the properties of the chemical. The mechanistic formulations are as in the SimpleBox model (Den Hollander and Van de Meent, 2004). The following processes (mass flows) are accounted for in the model (see ***Figure II-13***):

Emissions
Emissions are modelled as continuous and diffuse. The emission rates are to be specified as input to the model. Both the spatial scale and the environmental compartment to which the emission takes place need to be specified. This is important, because -as a result of the 'level III-character' of the model- the predicted concentrations will, at least in principle, depend on where, and into which compartment the emissions occur. The model accounts for direct non-point emissions to air, water and industrial soil, and indirect emissions with effluent and sludge from sewage treatment plants to water and agricultural soil. The regional and continental models require that the indirect emission to sewage systems is specified; the output of the STP model is used as input (indirect emissions to the water and agricultural soil compartments) for the regional and continental models. Annual averaged STP output is used.

Import and export
Advective transport with air and water between the continental and regional scales ('import' and 'export') are accounted for in the model. The predicted exposure concentrations at the regional scale are the net result of emissions on both spatial scales, and the modelled rates of advection.

Degradation
Degradation in air, water, sediment and soil is accounted for. The overall result of abiotic and biotic transformation processes is considered. The model uses first-order degradation-rate constants (one for each compartment) as input (see also Section).

Inter-media transport
Diffusive and advective inter-media transport mechanisms are accounted for. Diffusive mass transfer is two-way, and the net result flow may be either way, depending on the concentrations of the chemical on either side of the interface. The diffusive inter-media mass-transfer mechanisms modelled are: absorption of the chemical from the gas phase by water or soil,

volatilisation from water or soil, and adsorption and desorption to and from biota and sediment. Advective mass transfer is a one-way phenomenon: the chemical is carried by a physical medium from one compartment into another. The advective inter-media mass-transfer mechanisms modelled are: deposition of the chemical associated with aerosol particles, deposition of the chemical in rainwater, sedimentation/resuspension of the chemical associated with sediment particles, run-off and erosion. To set the inter-media transport rates, the model uses mass-transfer coefficients and partition coefficients (see Section II.4.1) as input.

- Dry deposition of aerosol-bound chemical is controlled by the gas-aerosol partitioning and the aerosol-deposition velocity. The fraction associated with aerosol can be estimated on the basis of the vapour pressure and the amount of aerosol and its specific activity with Junge's equation.
- Wet deposition of gaseous and aerosol-bound chemical is controlled by the chemical's scavenging ratio (the rainwater-air concentration ratio). A default estimate is suggested by the model on the basis of the Henry's Law constant and the aerosol-collection efficiency.
- Sedimentation and resuspension of particle-bound chemical is controlled by the suspended matter-water partition coefficient, the amount of suspended matter present, and the settling/resuspension rates of sediment particles.
- Gas absorption to and volatilisation from water and soil are modelled as diffusive, two-way processes, controlled by Henry's Law constant, solids-water partition coefficients, and a set of partial mass-transfer coefficients.
- Adsorption to and desorption from sediment are modelled similarly. Sorption is controlled by the sediment-water partition coefficient and a set of partial mass transfer coefficients.
- Run-off and erosion. The model assumes equilibrium between the water that runs off and the soil particles. The equilibrium is given by the soil-water partition coefficient. The water running off carries eroded soil particles with it to the surface water.

Leaching

Downward transport of the chemical, from the top layer of the soil to the groundwater, is regarded for this purpose as removal. The receiving groundwater compartment is not part of the system considered here. The model assumes equilibrium between soil and percolating water, given by the soil-water partition coefficient.

Burial

In sedimentation areas, fresh material is added to the well-mixed top layer of the sediment at a constant rate. This leads to an apparent renewal of the top layer of the sediment and, consequently, to an apparent downward transport of chemical from the top layer to the deeper sediment. This transport is regarded as removal, since the deeper sediment layers are not part of the system.

II.4.4.5 Input and output

Input to the model are the aforementioned parameter values for characterising (i) the environment, (ii) the chemical, and (iii) the loadings. Output of the model is a set of steady-state concentrations in air, water, sediment, and in three soil types, at both the regional scale and the

continental scale.

II.4.4.6 Limitations

The limitations of the model are inherent to the model concept itself. It should be emphasised that the main limitation is that the model disregards the spatial and temporal variability in the concentrations that occur in reality. Furthermore, the model largely overgeneralises and oversimplifies the processes of transport and transformation. No thorough validation studies have been reported for this model type so far. The steady-state concentrations computed by the model should be interpreted as the spatially and temporally averaged concentrations of the chemical in the environment, and should be regarded as an approximation only (Cowan *et al.*, 1995).

The model can be applied to all chemicals for which the aforementioned chemical-specific input parameters can be defined. However, the implicit limiting condition needs to be stressed. The estimation procedures for deriving default values for the inter-media transport parameters (specifically the partition coefficients used to derive inter-media mass flows) apply only to non-ionic organic chemicals. This means that, if the model is to be applied to other chemicals (e.g. metals!), values for the partition coefficients need to be specified directly.

II.4.4.7 Parameter values

The standard model parameters for the regional scale are set to mimic a typical densely populated area in the EU of 40 thousand km^2 with 20 million inhabitants. By default, it is assumed that 100 % of European production and use of the chemical takes place within this area. The continental scale is parameterised to mimic 'Western Europe' as the sum of the EU Member States (area 3.56 million km^2). By default, all other parameters are set to the same values as for the regional scale. The standard settings for the parameters are given in Section III.4.4.

II.4.5 Local environmental distribution

Distribution on the local scale is assessed in the vicinity of point sources. Figure II-14 shows the relationship between the local emission routes and the subsequent distribution processes modelled for the different environmental compartments. Each application of the substance and each stage of the life cycle are assumed to occur at different point sources. Therefore, in principle, a local assessment has to be performed for each relevant application and each relevant life-cycle step. A generic standard environment is defined to allow for a risk assessment on the European level. As it is impossible to characterise an 'average European environment', default parameter values are chosen which reflect typical, or reasonable worst-case, settings. Dedicated modelling approaches are used to calculate the concentrations in air, surface water and soil. The sediment and groundwater concentrations are estimated from the surface water and soil concentration respectively.

In defining the standard environments, a number of assumptions have to be made with respect to spatial and time scale. The exposure scenario is summarised below:

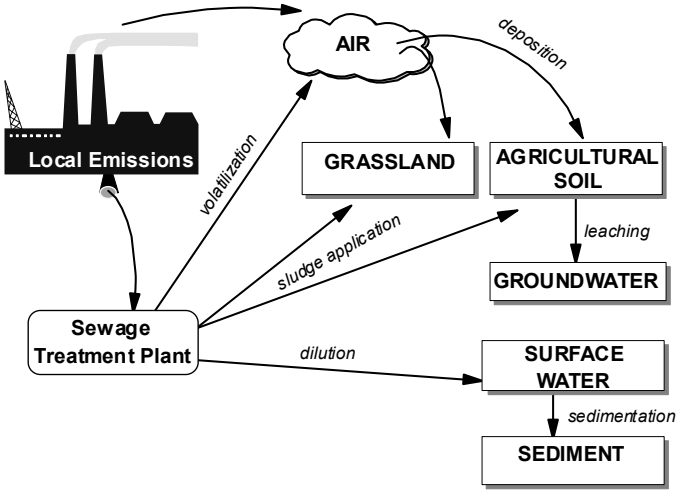

Figure II-14 *Local emission and distribution routes.*

- The concentration in air is calculated as an average concentration 100 meters from the source. This distance is assumed to be representative for the average size of an industrial site. Deposition is calculated as an average for a circle around the source with a radius of 1000 m, which is supposed to represent the local agricultural area. Deposition is used as input for the soil module, using annual average deposition fluxes. The concentration in air is used to calculate human exposure, thus employing an annual average concentration.

- The concentration in surface water is calculated after complete mixing of the effluent outfall. Because of the short time between effluent discharge and exposure, dilution will usually be the dominant 'removal' process. Therefore, degradation in surface water, volatilisation from the water body and sedimentation are not taken into account as removal processes. A standard dilution factor is used and adsorption to suspended matter is accounted for. The resulting dissolved concentration is used for comparison with the PNEC. The concentration in sediment is calculated at the same location, assuming thermodynamic equilibrium. For exposure of aquatic organisms, having a relatively short lifespan, the concentration during an emission episode is calculated. For indirect exposure of humans and predating birds and mammals, annual averages are used, being more appropriate with respect to chronic exposure of these end-points.

- The concentration in soil is calculated as an average concentration over a certain time-

period in agricultural soil, dressed with sludge from an STP and receiving continuous airborne deposition from a nearby point source (production/processing site and STP aeration tank). Two different soil types are distinguished: agricultural soil and grassland, which differ in the amount of sludge applied and the mixing depth. For the terrestrial ecosystem, the concentration is averaged over 30 days, for indirect human exposure over 180 days. The concentration in groundwater is calculated below this agricultural area.

II.4.5.1 Local distribution in air

The air compartment receives its input from direct emission to air, and volatilisation from the sewage treatment plant. The possible fate processes in air are shown schematically in Figure II-15.

The concentration in air is used as input for the calculation of the intake of substances through inhalation in the indirect exposure of humans. Deposition fluxes are used as input for the soil and groundwater model. Therefore, both deposition flux and concentration are calculated as annual average values.

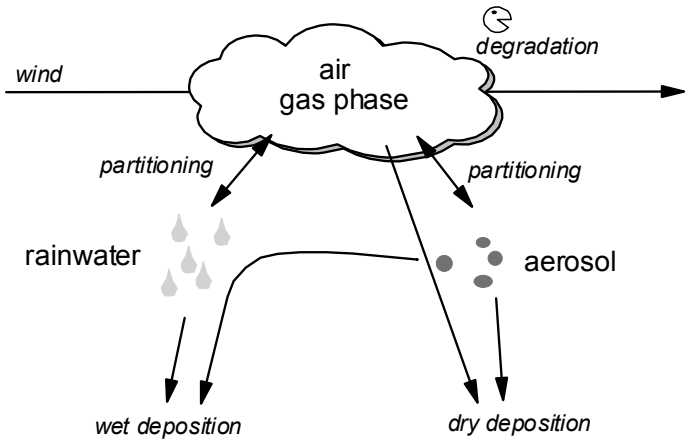

Figure II-15 *Possible fate processes in the air compartment.*

Many air models are available that are highly flexible and can be adjusted to take into account specific information on scale, emission sources, weather conditions, etc. This type of information is not normally available for new chemicals, nor very often for existing chemicals. Hence a standardised exposure assessment is carried out making a number of explicit assumptions and using a number of fixed default parameters. The Gaussian plume model OPS, as described by Van Jaarsveld (1990), is used with the standard parameters as described by Toet and De Leeuw (1992). These authors used the OPS model to carry out a number of default calculations in order to describe a relationship between the basic characteristics of substances (vapour pressure and Henry's Law constant) and the concentration in air and deposition flux to soil near to a point source. The following assumptions/model settings are used:

- Realistic average atmospheric conditions are used, obtained from a 10-year dataset of weather conditions for the Netherlands.
- Transport of vaporised and aerosol-bound chemicals is calculated separately. The partitioning between gas and aerosol is determined by the equation of Junge.
- The atmospheric reaction rate is fixed at a value of 5% per hour. On the spatial scale that is regarded, however, atmospheric reactions do not play any role in the removal of the substance (even at very high reaction rates) (Toet and De Leeuw, 1992).
- Losses due to deposition are neglected for estimation of the concentration and deposition fluxes at this short distance from the source.
- Assumed source characteristics are:

  - source height: 10 metres, representing the height of buildings in which production, processing or use take place;
  - heat content of emitted gases: 0; this assumes there is no extra plume rise caused by excess heat of vapours compared to the outdoor temperature;
  - source area: 0 meter; representing an ideal point source which is obviously not always correct but which is an acceptable choice.
- Calculated concentrations are long-term averages.

The concentration in air at a distance of 100 meters from the point source is estimated. This distance is chosen to represent the average distance between the emission source and the border of the industrial site. The deposition flux of gaseous and aerosol-bound chemicals is estimated analogously to the estimation of atmospheric concentrations, by means of an estimation scheme and with the aid of the OPS model. The deposition flux to soil is averaged over a circular area around the source, with a radius of 1000 m to represent the local agricultural area. Deposition velocities are used for three different categories:
- Dry deposition of gas/vapour: estimated at 0.01 cm/s.
- Wet deposition of gas/vapour: determined with the OPS model.
- Dry and wet deposition of aerosol particles; determined within the OPS model using an average particle-size distribution.

Toet and De Leeuw (1992) have shown that at this small spatial scale physical mixing processes are the dominant fate processes. Therefore, a simple linear relationship between source strength and concentration can be assumed. The applied constant is calculated with the OPS model using the standard settings as described by Toet and De Leeuw (1992). Both the emission from a point source and the emission from a STP are taken into account. The concentration on the regional scale is used as background concentration and therefore summed to the local concentration. The STP is assumed to be a point source and the concentration of the chemical is calculated at 100 m distance from it. The higher of the two concentrations (direct and via STP) is used as the PEC.

II.4.5.2 Local distribution in surface water and sediment (freshwater and marine environment)

Regarding the presence or absence of a sewage treatment plant (STP) a difference is made between the freshwater scenario and marine scenario. By default the inland freshwater scenario uses a municipal STP. Experience with the risk assessment of existing substances has shown that for chemical processing sites located on the coast, the probability that the effluents are treated in a municipal STP is much lower than for inland sites. For a default local marine assessment, industrial effluents (which may have been subject to some treatment on-site) are therefore not treated in a municipal STP. For releases to municipal wastewater of substances that are used for private or public use (substances belonging to IC5 and IC6), however, it is assumed that the degree of treatment in a municipal STP corresponds to the inland freshwater scenario.

For estuaries, which are influenced by currents and tidal movements, it is assumed as a first approach that either the inland or the marine risk assessment covers them. Thus, no specific assessment is proposed. Then, the local concentrations in seawater can be obtained with the

same scenario as presented for the freshwater approach (EC, 2003).

The effluent of the sewage treatment plant is diluted in the surface water.

Figure II-16 shows the possible fate processes in the aquatic compartment. For the calculations, the following assumptions are made:

- Complete mixing of the effluent in the surface water is assumed as a representative exposure situation for the aquatic ecosystem.
- For the initial local assessments, volatilisation, degradation and sedimentation are ignored, because of the short distance between the point of effluent discharge and the exposure location.

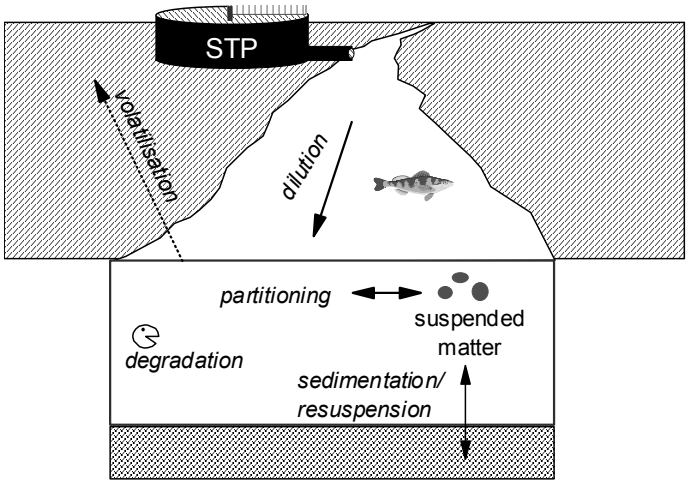

Figure II-16 *Possible fate processes in surface water.*

The distance from the point of discharge where complete mixing may be assumed will vary between different locations. A fixed dilution factor is applied to the effluent concentration. Dilution factors are dependent on flow rates and the industry-specific discharge flow. Owing to the different seasonal, climatic and geographical conditions in the Member States, these dilution factors may vary over wide ranges. They have been reported in a range from 1 (e.g. dry riverbeds in summer) up to 100,000 (De Greef and De Nijs, 1990). The dilution factor is generally linked to the release scenario of the use category. For example, for consumer products an average dilution factor of 10 is recommended for sewage from municipal treatment plants. This is also regarded as a default dilution value for other types of substances, emitted to a freshwater environment, if no specific data are available. A default dilution factor for discharges to a coastal zone (marine environment) of 100 is assumed to be representative for a realistic worst case (EC, 2003).

It must be noted that with the assumption of complete mixing of the effluent in the surface water no account is taken of the fact that in reality in the mixing zone higher concentrations will occur. For situations with relatively low dilution factors this mixing-zone effect can be accepted. For situations with very high dilution factors, however, the mixing zones may be very long and the overall area that is impacted by the effluent before it is completely mixed can be very substantial. Therefore, in case of site-specific assessments the dilution factor that is applied for calculation of the local concentration in surface water should not be greater than 1000 (EC, 2003).

For some substances it is possible that PECs may be calculated in water, which are in excess of the water solubility. These results need to be interpreted carefully on a case-by-case basis. The concentration in surface water will not be corrected, but the results flagged. The PEC has to be interpreted on the basis of the effects found in the aquatic toxicity tests.

The PEC in sediment is compared to the PNEC for sediment-dwelling organisms. The concentration in freshly deposited sediment is taken as the PEC for sediment and the properties of suspended matter are therefore used. The concentration in bulk sediment is derived from the corresponding water-body concentration, assuming a thermodynamic partition equilibrium (see also Di Toro *et al.*, 1991).

II.4.5.3 Local distribution in soil and groundwater

Exposure assessment for the soil compartment is important with respect to exposure of terrestrial organisms. Furthermore, crops for human consumption are grown on agricultural soils and cattle, producing meat and milk, graze on grasslands. Figure II-17 shows the possible fate processes in the soil compartment. The soil compartment receives its input through application of sewage sludge in agriculture, and through dry and wet deposition from the atmosphere.

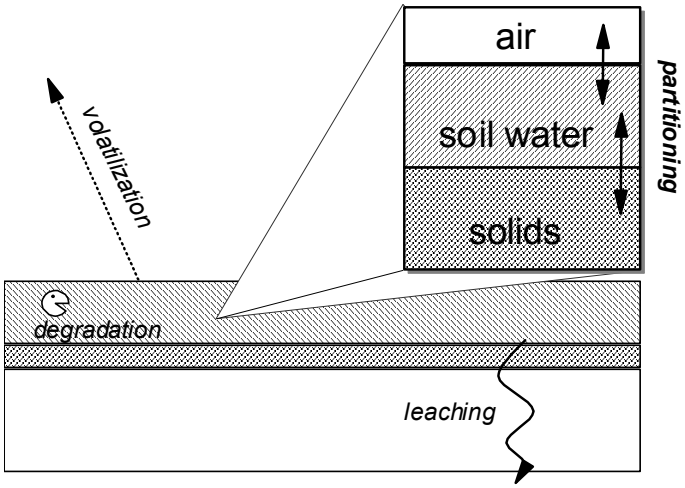

Figure II-17 *Possible fate processes in the soil compartment.*

For sludge application to agricultural soil an application rate of 5000 kg dry weight per hectare per year is assumed while for grassland a rate of 1000 kg/ha/year is used. Sludge application is treated as a single event once a year. Additionally, the soil receives input through wet and dry deposition, as calculated by the air sub-module. Atmospheric deposition is assumed to be a continuous flux throughout the year. It should be noted that the deposition flux is averaged over a year. This is obviously not correct since the deposition flux is linked to the emission episode, but averaging is performed to facilitate calculations. Furthermore, it is impossible to indicate *when* the emission episode takes place in a year.

There are several extensive numerical soil and groundwater models available (mainly for pesticides). These models require a detailed definition of soil and environmental characteristics, however, which makes this type of model less appropriate for a generic risk assessment at EU level. Therefore, a simple, one-compartment soil model is used. The top layer of the soil compartment is described, with influx of airborne deposition and removal from the box by degradation, volatilisation and leaching. Accumulation of a substance may occur when sludge is

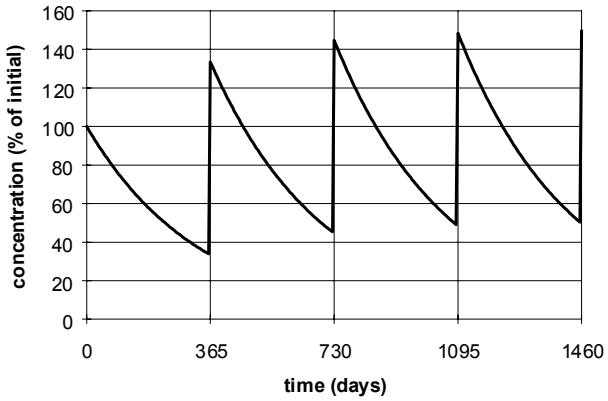

Figure II-18 *Accumulation in soil due to several years of sludge application.*

applied over consecutive years. This is illustrated in **Figure II-18**. As a reasonable worst-case scenario, sludge is assumed to be applied for 10 consecutive years. To provide an indication of the potential persistence of the substance, the percentage of the steady-state situation is calculated.

As shown in **Figure II-18**, the concentration in soil is not constant in time. The concentration will be high just after sludge application (in the beginning of the growing season), and lower at the end of the year due to removal processes. For exposure of the endpoints, the concentration therefore needs to be averaged over a certain time period. Different averaging times are used for these end-points: for the ecosystem a period of 30 days after sludge application is used. In order to determine biomagnification effects and indirect exposure to man, an extended period of 180 days is used. This averaging procedure is illustrated in **Figure II-19** (the average concentration is given by the shaded area, divided by the number of days).

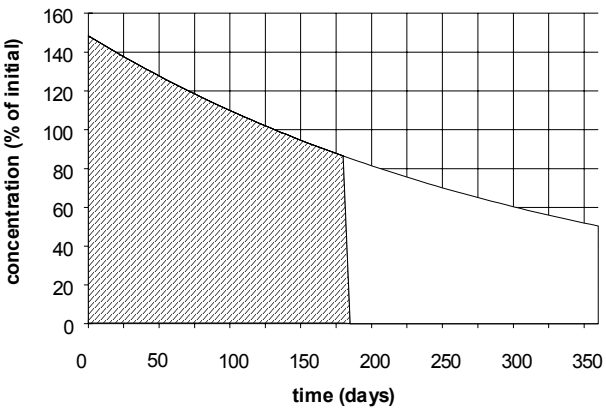

Figure II-19 *The concentration in soil after 10 years. The shaded area is the integrated concentration over a period of 180 days.*

The concentration in groundwater is calculated for indirect exposure of humans through drinking water. Several numerical models are available for calculation of groundwater levels (mainly for pesticides). These models require characterisation of the soil at a high level of detail, however. This makes these models less appropriate for the initial standard assessment. The concentration in the pore water of agricultural soil is therefore taken as an indication of potential groundwater levels. It should be noted that this is a worst-case assumption, neglecting transformation and dilution in deeper soil layers.

II.5 EXPOSURE MODULE

In the exposure module, exposure levels for humans and predating birds and mammals are estimated. The assessment of secondary poisoning of birds and mammals considers exposure through fish and earthworms. For humans, three assessments can be made: indirect exposure through the environment, exposure through consumer products, and exposure at the workplace.

Bioconcentration and bioaccumulation may be of concern for lipophilic organic chemicals and some metal compounds as both direct and indirect toxic effects may be observed after long-term exposure. Some definitions are given in ***Table II-5*** (EC, 2003).

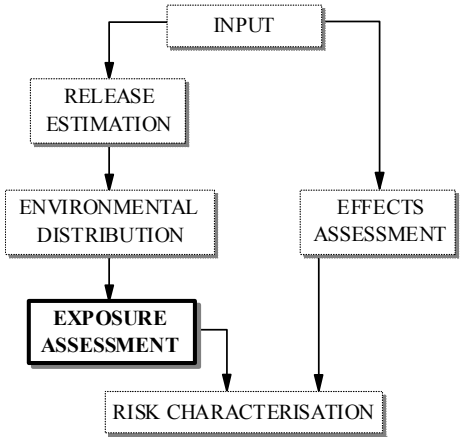

Figure II-20 *System structure.*

Table II-5 *Definitions for exposure assessment.*

Bioconcentration	The net result of the uptake, distribution and elimination of a substance in an organism due to water-borne exposure.
Bioaccumulation	Uptake including all routes, i.e. air, water, soil and food.
Biomagnification	Accumulation and transfer of chemicals via the food chain, resulting in an increase of the internal concentration in organisms at higher levels in the trophic chain.
Secondary poisoning	Toxic effects in the higher members of the food chain, either living in the aquatic or terrestrial environment, which result from ingestion of organisms at the different trophic levels that contain accumulated substances.
BCF	Bioconcentration factor: the ratio between concentration in organism and concentration in environmental compartment.
BAF	Bioaccumulation factor: the ratio between exposure level and concentration in (part of) organism.
BMF	Biomagnification factor: the ratio between the relative concentration in a predatory animal and the concentration in (part of) its prey.

II.5.1 Secondary poisoning

Starting from the concentration in the environment, the resulting concentration in food of higher organisms is estimated. This exposure concentration is compared to the avian or mammalian toxicity of the chemical as an indication of possible effects on birds and mammals in the environment via the food chain. Three example food chains are considered:

- Water (freshwater and marine environment) → fish → fish-eating predator(Romijn *et al.*, 1993).
- Water (marine environment) → fish → fish-eating predator→ top-predator;
- Soil → earthworm → worm-eating predator(Romijn *et al.*,1994).

These three two food chains are examples of secondary poisoning pathways. However, safe levels for fish-eating animals do not exclude the possibility of risks to other birds or mammals

feeding on other aquatic organisms (e.g. mussels and worms). It is therefore emphasised that the proposed methodology merely gives an indication that secondary poisoning is a critical process in the aquatic risk characterisation of a chemical.

The concentrations in food (fish and earthworms) are calculated from the concentration in the environment (surface water and agricultural soil) and the measured or estimated BCFs. For the freshwater and marine environment also a biomagnification factor (BMF) must be applied. The concentrations used to derive and report BMF values should, where possible, be lipid normalised. The BMF should ideally be based on measured data. However, the availability of such data is at present very limited and therefore, the default values given should be used. It is difficult to justify whether the regional or local concentration in water is most appropriate for risk characterisation. Using the local PEC may lead to overestimation of the risk, as birds or mammals also forage from other sites than the area around the point of discharge. However, using regional concentrations may have the opposite effect, as there may be large areas in the region with higher concentrations. Foraging ranges can vary enormously among species, which makes it difficult to decide on the appropriate scale.
For the fish-eating predator (first tier of organisms) it is proposed to use a scenario where 50% of the diet is derived from the local environment and 50% from the regional environment. For the top-predator (second tier of organisms) in marine surface waters it can be assumed that they obtain their prey mainly from the larger-scale regional marine environment that is to a lesser extent influenced by point source discharges. However, since it cannot be ruled out that certain top-predators prey on organisms that receive their food from relatively small areas it is proposed to assume, as a realistic worst case, a 90/10 ratio between regional and local food intake.
This two scenarios are implemented in EUSES. For local surface water, the annual average concentration is used. For the soil compartment, the PEC is used, in which the concentration is averaged over a period of 180 days. Due to the lack of experience with this approach, the assessment is considered provisional.

II.5.1.1 BCF for fish

Fish living in contaminated surface water are able to take up appreciable amounts of (especially lipophilic) substances through the gills or through their food. The concentration in fish may be orders of magnitude greater than the concentration in water. The bioconcentration factor in fish for non-ionic, organic compounds is found to be well correlated with the octanol-water partitioning coefficient (*Kow*), indicating that lipid or fat is the main dissolving medium. The estimation of fish-water bioconcentration is discussed more specifically in Chapter 4 of the TGD (EC, 2003).

When measured BCF-values are not available, the BCF for fish can be predicted from the relationship between *Kow* and BCF. Numerous studies on the estimation of BCFs have been published. The methods that estimate a BCF from log *Kow* are widely used and, in general, most reliable. However, because these methods are based on several assumptions, such as a constant water concentration and no metabolism of the substance by the organism, the resulting values should be considered as a relative measure for the bioaccumulation potential of a substance. Furthermore, these methods may not have the same accuracy for different classes of chemicals. For substances with a log *Kow* of 2-6 a log-linear relationship is used, as developed by Veith *et al.* (1979). For substances with a log *Kow* higher than 6 a parabolic equation is used. Both relationships apply to compounds with a molecular weight of less than 700 g/mol. It should be noted that due to experimental difficulties in determining BCF values for such substances, the parabolic relationship has a higher degree of uncertainty than the linear one. For a discussion of both relationships, see Chapter 4 of the TGD (EC, 2003). For existing substances, experimentally derived BCFs may be available. For new substances, a BCF test is mandatory at level I. In most cases, experimentally determined BCF values are preferred.

II.5.5.2 BCF for earthworms

The concentration in earthworms is thought to be proportional to the concentration in the pore water of soil. For organic chemicals, the main route of uptake into earthworms will be via the interstitial water. Bioconcentration can be described as a hydrophobic partitioning between the pore water and the phases inside the organism and is modelled according to Jager (1998).

Earthworms are also able to take up chemicals from food and it has been hypothesised that this process may affect accumulation at log Kow>5 (Belfroid *et al.,* 1995). The data collected by Jager (1998), however, do not indicate that this exposure route actually leads to higher body residues than expected on the basis of simple partitioning. Care must be taken in situations where the food of earthworms is specifically contaminated (e.g. in case of high concentrations in leaf litter) although reliable models to estimate this route are currently lacking. The model of Jager (1998) was supported by data with neutral organic chemicals in soil within the range log Kow 3-8 and in water-only experiments from 1-6. An application range of 1-8 is advised and it is reasonable to assume that extrapolation to lower Kow values is possible. The model could also be used for chlorophenols when the fraction in the neutral form was at least 5% and when both sorption and BCF are derived from the Kow of the neutral species. The underlying data are however too limited to propose this approach in general for ionised chemicals.

II.5.2 Human exposure through the environment

Indirect exposure of humans via the environment may occur by consumption of food and drinking water, inhalation of air and ingestion of soil. The different routes of exposure that are taken into account in EUSES are shown in Figure II-21. Exposure via soil ingestion and dermal contact is not addressed because these represent significant exposure routes for specific situations of soil pollution only, and are therefore not appropriate for a generic exposure scenario. Assessment of indirect exposure via the environment comprises the following steps:

- Assessing the concentrations in intake media (food, drinking water, air).
- Assessing the intake rate of each medium (using a standard consumption pattern).
- Combining the concentrations in the media with the intake of each medium.

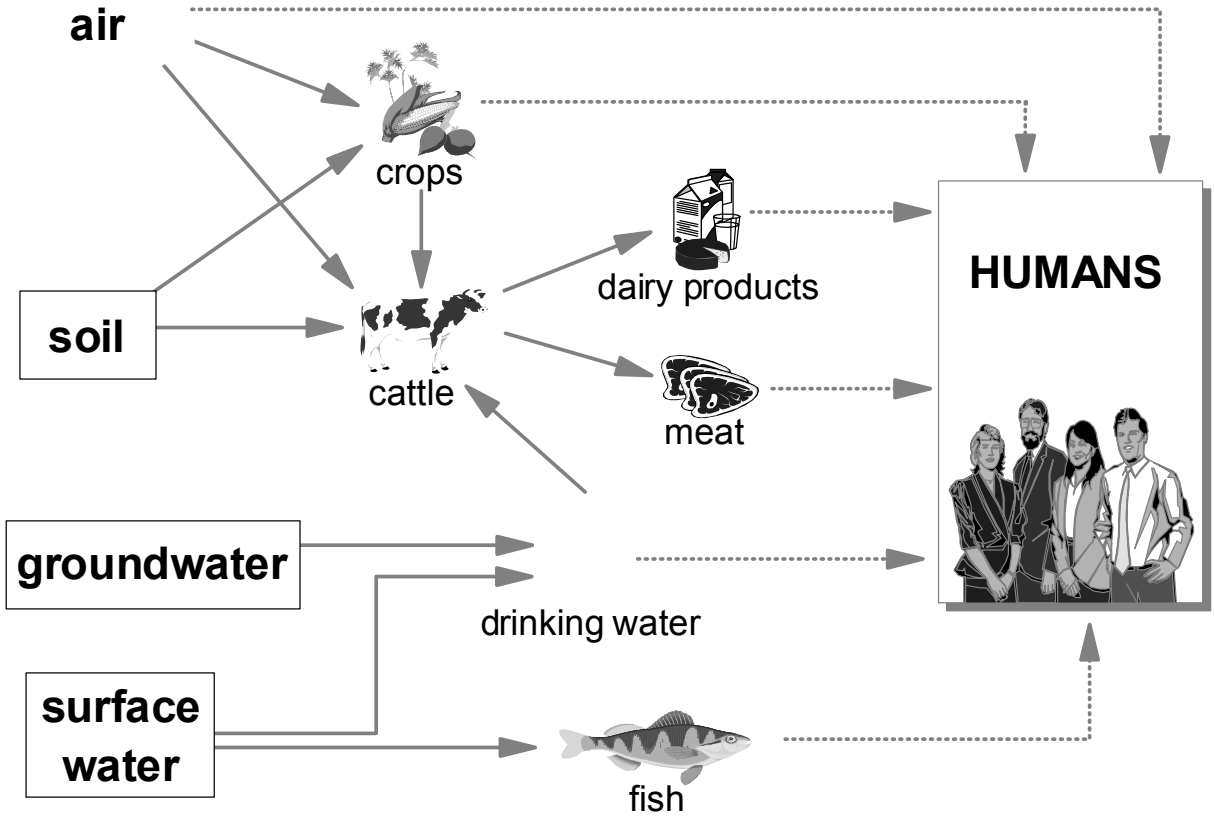

Figure II-21 *Indirect exposure routes for humans through the environment. Solid lines indicate (bio)transfer, broken lines indicate human intake.*

The calculation methods described are simple methods for predicting indirect exposure. Owing to the considerable uncertainties accompanying the methodology, it serves primarily for screening purposes. The concentration of a substance in food is estimated from its concentration in water, soil and air and its bioconcentration or bioaccumulation behaviour. The estimation of most bioconcentration factors (BCF) or bioaccumulation factors (BAF) is highly dependent on *Kow*. These estimations are therefore only valid for organic, non-ionised or non-dissociating chemicals. Other substances can of course be evaluated if experimental BCFs are known. The use of static BCFs or BAFs implies that these factors describe a steady-state situation in which the exposure period is assumed long enough to achieve a steady state. It should be noted that

reliable (and relevant) experimental bioconcentration factors are always preferable to estimated factors.

Table II-6 *Environmental concentrations used as input for indirect exposure calculations.*

Compartment	Local assessment	Regional assessment
surface water	annual average concentration after complete mixing of STP effluent	steady-state concentration in surface water
air	annual average concentration at 100 m from source or STP (maximum)	steady-state concentration in air
agricultural soil	concentration averaged over 180 days after 10 years of sludge application and airborne deposition	steady-state concentration in agricultural soil
pore water	concentration in pore water of agricultural soil as defined above	steady-state concentration in pore water of agricultural soil
groundwater	concentration in pore water of agricultural soil as defined above	steady-state concentration in pore water of agricultural soil

II.5.2.1 Exposure scenario

Human behaviour shows an appreciable amount of variation among the different EU countries, but within countries, too, there may be large deviations among individuals. As a consequence, indirect exposure will vary greatly among the population we seek to protect. The choice for an exposure scenario will have a major influence on the result of the assessment. This choice will always be a compromise, as a scientifically sound solution is extremely difficult to obtain (this would involve elaborate statistical evaluation of human sourcing and mobility behaviour, as well as the distribution and intensity of all local sources).

Indirect exposure is principally assessed on two spatial scales: locally near a point source of the substance, and regionally using averaged concentrations over a larger area. In the local assessment all food products are derived from the vicinity of one point source, while in the regional assessment all food products are taken from the regional model environment. Clearly, the local situation represents a worst case. People do not consume 100% of their food products from the immediate vicinity of a point source. Therefore, the local assessment represents a situation which does not exist in reality. However, one or two routes usually dominate the total exposure and local exposure via these routes may not be unrealistic. In contrast, the regional assessment represents a highly averaged exposure situation which cannot ensure protection of individuals who consume food products from the vicinity of point sources. A regional assessment indicates potential average exposure of the inhabitants of the region. In the light of the above limitations, it is clear that a generic indirect-exposure assessment, as required in this framework, can only be used to indicate potential problems. The assessment should be seen as a helpful tool for decision-making and not as a prediction of human exposure actually occurring at some place or time.

For an indirect-exposure assessment at EU level, a standard consumption pattern is defined. To account for the fact that intake rates vary among countries, for each food product the highest *country-average* consumption rate from the member states will be used. This will of course lead to a total food basket, which is an unrealistic, worst-case scenario. In practice, however, as one or two routes usually dominate indirect exposure, the fact that worst-case intake also occurs via other routes is less important. This makes this scenario appropriate as an initial approximation to indicate possible concern. The outcome of this assessment is comparable to assessing all countries separately (using average intakes), and taking the highest exposure level of all countries. It should be noted that extreme consumers of certain food products are not accounted for, as this would lead to more severe worst-case local assessments.

Table II-7 *Definition of the indirect exposure scenarios.*

Local	The entire food basket is sourced from the vicinity of the local point source as defined in Table II-6. The food basket consists of: fish, root crops, leaf crops, meat, dairy products, drinking water and inhalation of air. For the standard assessment, the highest country-average intake rate of each food product is used.
Regional	The entire food basket is sourced from the region as defined in Table II-6. The food basket consists of: fish, root crops, leaf crops, meat, dairy products, drinking water and inhalation of air. For the standard assessment, the highest country-average intake rate of each food product is used.

II.5.2.2 Exposure via inhalation of air

For volatile compounds, this exposure route can contribute significantly to the total exposure. The concentration in the intake medium (air) is calculated using the distribution models described in Section II.4. The intake scenario chosen has important consequences for exposure via this route; the human individual that is modelled is exposed continuously and chronically to the annual average concentration in air. Exposure through inhalation is summed to exposure through oral routes.

II.5.2.3 Purification of drinking water

Drinking water is prepared from surface water or groundwater. Groundwater can be contaminated through leaching from the soil surface, while surface water can be polluted through direct or indirect emission. Hrubec and Toet (1992) evaluated the predictability of the fate of organic chemicals during drinking-water treatment. One of their conclusions was that groundwater treatment, which is generally not intended to remove organic chemicals, can be ignored. The accuracy of the predicted removal efficiencies for surface-water treatment is rather low. This is due mainly to uncertainties in the most effective treatment processes (such as activated carbon filtration). Purification is modelled as described by Hrubec and Toet (1992). The drinking-water module assumes complete removal of suspended particles from surface water and groundwater. Dependent on the type of storage, two different water-treatment systems for surface water can be distinguished: system 1 includes storage in open reservoirs, while

system 2 includes dune recharge. Removal of the dissolved fraction of a xenobiotic from the surface water is modelled by means of purification factors. For the choice between the two systems and the choice between surface water and groundwater, a worst-case approach will be followed.

II.5.2.4 Bioconcentration in fish

This process has already been discussed in section II.5.1 on secondary poisoning. The same BCF estimation routines are used for human exposure.

II.5.2.5 Biotransfer from soil and air to plants

Plant products form a major fraction of the food products consumed by humans and cattle. Contamination of plants may therefore have a significant influence on human exposure. In endeavouring to predict concentrations in plant tissues, several important conceptual problems will immediately be encountered:

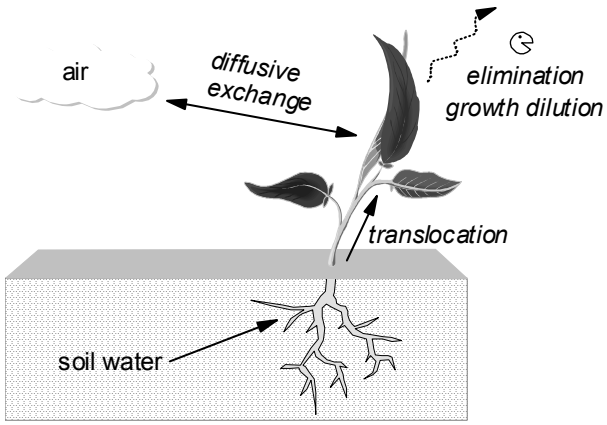

Figure II-22 *Fate processes accounted for in the plant uptake model.*

- There are hundreds of different plant species forming the heterogeneous group of food crops. Furthermore, varietal differences can also account for large differences.
- Different plant tissues are consumed (roots, tubers, fruit, leaves).
- Crops differ in contaminant exposure; many crops are grown in greenhouses, for instance.
- Crops can be exposed through uptake from soil, but also through gas uptake and airborne deposition.

From the above it will be clear that a modelling approach can only roughly approximate concentrations in plants. In the calculations a distinction is made between tuberous plants and leaf crops. The exposure of plants includes uptake from soil as well as uptake from air. Uptake from soil is, in general, a passive process governed by the transpiration stream of the plant (in the case of accumulation in leaves) or physical sorption (in the case of roots). Uptake into the leaves from the gaseous phase can be viewed as a passive process, in which the leaf components (air, water, lipids) equilibrate with the air concentration. K_{ow} and $K_{air\text{-}water}$ (the air-water partition coefficient) are used to assess distribution between the air and the plant. The modelling approach of Trapp and Matthies (1995) is used to estimate levels in leaves and roots. This approach integrates uptake from pore water and air (gas phase) into a one-compartment model. The sink term in the model is formed by diffusive transfer from leaf to air, elimination in the plant tissue and dilution by growth. The source term is formed by uptake and translocation from soil and gaseous uptake from air. Aerosol deposition is not considered in the model. Although this route may be important for some chemicals, it is not yet clear how this route can be satisfactorily quantified and incorporated into the model.

II.5.2.6 Biotransfer to meat and milk

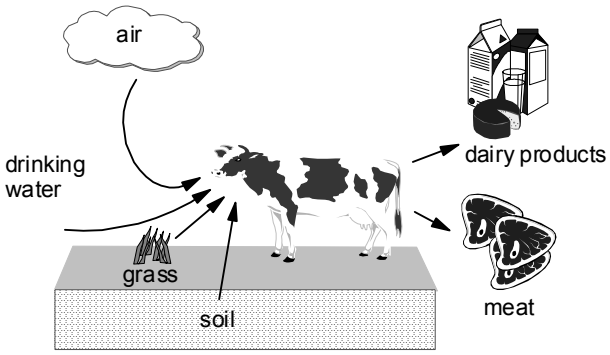

Figure II-23 *Uptake routes for cattle accounted for in the model.*

Lipophilic substances are known to accumulate in meat, and can be subsequently transferred to milk. Cattle can be exposed to substances in grass (or other feed), via adhering soil, drinking water, and through inhalation of air. Bioaccumulation factors can be defined as the steady-state concentration in meat or milk divided by the daily intake of the chemical (through air, grass, soil and drinking water). Travis and Arms (1988) calculated BAFs for the meat and milk of cows by log-linear regression on experimental data for a number of chemicals. Even though the theoretical background is limited, these factors provide a useful tool in risk assessment. Furthermore, the uncertainties in the estimated BAFs are considerable. No distinction is made between different milk products like cheese or yoghurt. For all dairy products, the concentration in milk is used.

II.5.2.7 Total daily intake for humans

After the concentrations in the intake media have been calculated, the total daily intake of humans is estimated by multiplying these concentrations by the daily intake rate of each medium and summing the contribution of each medium. The exposure assessment includes seven pathways: drinking water, fish, root crops, leaf crops, meat, milk and air. Each of these intake media is retrieved exclusively from within the contaminated system.

II.5.3 Human exposure through consumer products

II.5.3.1 Introduction to the consumer exposure models

The consumer, i.e. a member of the general public who may be of any age, either sex, and in any stage of health, may be exposed to a new or existing substance by using consumer products. A consumer product is one that can be purchased from retail outlets by members of the general public and may be the substance itself, or a preparation, or an article containing the substance. The equations for consumer exposure can be used to estimate *external* exposure to substances used as or in consumer products. Absorption or bioavailability is not taken into account by the equations implemented in EUSES, but should be considered during the risk characterisation stage. Suggestions are given as to when each model might appropriately be applied. The equations presented in Chapter III and described here can also be adapted to estimate exposure arising from 'reasonably foreseeable misuse', i.e. when products are not used in accordance with their instructions, but as if they were other, allied products. To adapt the equations, the values for the parameters used in the equations are changed to reflect values foreseen in 'reasonably foreseeable misuse'. For example, the volume of product or the area of application is set to a different value, reflecting reasonable foreseeable misuse.

II.5.3.2 Limitations and uncertainties of the models

The equations described here and presented in Chapter III are derived from work in the context of the OECD (OECD, 1993; Vermeire *et al.*, 1993; Van de Meent *et al.*, 1995). Some changes have been made to the equations, to merge similar equations within the same route of exposure into one general equation for that route. The equations are intended to provide a simple description of consumer exposure, by using first principles only. Most equations give a worst-case estimation of exposure, by assuming that all of the compound in the product is at once available for intake and uptake. Intake and uptake themselves are modelled as simple fractions. If more refined exposure assessments are necessary, the user is referred to programs that contain more complex models, such as CONSEXPO (Van Veen, 2001), or the US-EPA Household models (Versar, 1991; Versar, 1992).

II.5.3.3 Sources of information

Information on product contents and product use can be used in EUSES by changing default values or intermediate results. Information on consumer products is available from a number of sources, but the diversity of consumer products does not allow for a single set of information sources, handbooks or data bases to be consulted. Rather, one has to explore which information sources apply to the product of interest. In the following, an overview is given of possible information sources.
An overview of possible information sources is given in Appendix II of chapter 2 of the Technical Guidance Document (EC, 2003).

The available data have to be assessed with regard to their reliability. The confidence in measured exposure concentrations is determined by the adequacy of techniques, strategies and

quality standards applied for sampling analysis and protocol. In general, exposure concentrations established by using generally accepted techniques and good-quality strategies should be given preference. Subsequently, in a second step, the representativeness of the data has to be established. The type, location, the duration and frequency of sampling should be evaluated. The selected, representative data need to be allocated to specific exposure scenarios to allow meaningful exposure assessment and comparison with compatible results of model calculations.

II.5.3.4 Acute and chronic exposure

Effects related to acute and chronic exposure differ in the sense that acute exposure will cause effects related to the mean or maximum event exposure, while chronic exposure will cause effects related to the lifetime average exposure. Because consumer products are used lifelong, the lifetime average exposure is well approximated by using the annual average exposure, averaging out seasonal usage differences. The equations used for consumer exposure model exposures as resulting from a constant concentration, thereby setting mean and maximum event concentrations equal. For acute exposure, exposure is characterised by the inhalatory, dermal and oral concentrations (C_{inh}, C_{derm} and C_{oral}, respectively). For chronic exposure, the exposure is characterised by the annual average exposure. Both the acute and the chronic characterisation of exposure are given. The former is compared to the LD50, the latter to the chronic NOAEL.

II.5.3.5 Inhalatory consumer exposure

For a substance that is released as a gas, vapour or airborne particulate into a room (e.g. a component of an aerosol insecticide, a carrier/solvent in a cosmetic formulation or a powder detergent) the following holds:

- Release may be the result of the direct release as gas, vapour or particulate, or of evaporation from liquid or solid matrices. In the latter case, the equation represents a worst-case situation by assuming the substance to be directly available as a gas or vapour. The equation applies to both volatile substances and airborne particulates. It is assumed that the substance is released as a vapour, gas or airborne particulates, and that the room is filled immediately and homogeneously with the substance. Ventilation of the room is assumed to be absent. It should be noted that for short-term local exposure the value for the room volume (V_{room}) should be reduced (e.g. to 2 m^3) to represent the volume of air immediately surrounding the user. If a substance is released relatively slowly from a solid or liquid matrix (e.g. solvent in paint, plasticiser or monomer in a polymer, fragrance in furniture polish), the equation (presented in Chapter III) acts as a worst-case estimation, estimating the maximum possible concentration.

ConsExpo implements the EUSES inhalatory model in the “constant concentration”-scenario. The models are entirely equivalent.
In addition, ConsExpo provides more detailed inhalatory models for the following cases:

1. A substance is released into the room air with a constant release rate (“source ventilation” scenario):

- Applies to vapours, particulate matter, aerosols (note, however, that special evaporation

and aerosol scenario's are available also). The scenario can be used if a generation rate or release rate of the substance into air is known or can be estimated. During the entire process the substance is assumed to distributed over the room immediately i.e. the room air is assumed to be homogeneously mixed. This model provides a more detailed description than the "constant concentration" scenario in which it is assumed that all of the chemical is released instantaneously. In addition this model takes the effect of room ventilation into account.

2. A substance is released from a open can filled with a liquid product by evaporation ("evaporation from pure substance", "evaporation from mixture"-scenarios):

- During use of the product the can is open and the substance evaporates into the air, which is supposed to be homogeneously mixed. After use, the can is closed and no additional evaporation takes place. The concentration in the room is removed by ventilation. The release of the chemical is estimated from basic physico-chemical properties of the substance and product composition. The product is assumed to be well-mixed during release of chemical. Use "evaporation from pure substance" in the event that the product is the substance in its pure form, and the "evaporation from mixture" if the active substance is one of the ingredients of the product.

3. A viscous product such as a paint is being applied to a surface with a certain application area ("painting"-scenario):

- From the applied product the active substance evaporates. The product is not assumed to be well mixed: the diffusion of the substance through the product-air interface is simulated by introducing a two-layer description of the applied paint. The upper layer is in direct contact with the air and product evaporates from this layer into the air. From the lower layer the substance diffuses to the upper layer with a certain exchange rate ("layer exchange rate"). Both upper and lower layer are assumed to be well-mixed. After release into the room air, the vaporised substance is removed by ventilation.

4. The substance is released in aerosol-form. This part of the ConsExpo model longer recommended. In a new version of Consexpo a revised model concept will be presented.

To estimate the internal dose ConsExpo offers several uptake models.
However, EUSES works with the concept of potential dose or total intake, and bioavailability or uptake is not estimated explicitly. In order to calculate the potential dose in ConsExpo, the user is advised to use the 'fraction model' to calculate the uptake, with an uptake fraction of 1. This describes the situation in which all of the external exposure is taken up in the system and is therefore equivalent to the potential dose.

For a more detailed description of the models the reader is referred to the ConsExpo manual (Van Veen, 2001).

II.5.3.6 Dermal consumer exposure

For a substance contained in a medium:

- The assumption behind the equations is that all of the substance on the skin is potentially

available for uptake. This is the case when the medium is well mixed or only present as a thin film on the skin. The dermal equations apply to (i) a non-volatile substance in a diluted product, (ii) a non-volatile substance in a medium used without further dilution, and (iii) a non-volatile substance in a volatile medium. In the last case, the dermal exposure concentration (C_{der}) is valid at the very beginning of exposure only. However, this concentration can still be used to calculate the total amount of substance (A_{der}) present on the skin, because the substance is non-volatile and the amount available for uptake does not change when the medium evaporates. The equations can also be used in the case of a volatile substance, but in that case they represent a worst-case situation because volatilisation is not accounted for.

For a non-volatile substance migrating from an article (e.g. dyed clothing, residual fabric conditioner, dyestuff/newsprint from paper):

- The assumption behind the equation is that only part of the substance will migrate from the article and contact the skin. The migration is assumed to be slow enough to be represented by a constant migration rate multiplied by the time of contact. The exposure calculation will involve estimating the amount of substance which will migrate from the area of the article in contact with skin during the time of contact. Dyestuff levels in fabrics and paper are usually given as weight of product per unit area (e.g. mg/m^2). The total amount is then calculated by multiplying by the area of contact ($AREA_{der}$).

ConsExpo implements the EUSES dermal models “dermal a” and “dermal b” in the “fixed product volume”- and the “contact-rate”-scenario resp.
In addition, ConsExpo provides dermal models for the following cases:

1. The substance migrates from the product onto the skin by leaching (“migration to skin”-scenario):

- Migration to the skin is characterised by the fraction of substance that can leach from the product per unit mass of the product (the “leachable fraction”). From this fraction, and the fraction of the product that is in contact with the skin (“skin contact factor”), the total amount loaded to the skin is calculated, assuming that all of the substance that can migrate will migrate immediately, which is in many cases a worst case assumption.

2. The substance diffuses from a product in direct contact with the skin to the skin (“product diffusion”-scenario):

- This scenario is to be used for viscous or solid products in direct contact with the skin. Diffusion of the substance through the product is characterised by a constant diffusion coefficient, for which an estimation has to be made. The model calculates the amount of substance that diffuses to the skin during exposure.

3. The product can be rubbed from surface (“transfer coefficient”-scenario):

- The substance is contained in a product with a certain surface area. When rubbing the product an amount of substance per unit area rubbed will come off (dislodgeable amount). Rubbing is quantified by the surface area rubbed per unit time (“transfer rate”). In addition the model allows for break down of the chemical. This breakdown must be given as a half-life time of the chemical.

ConsExpo offers several uptake models to estimate the internal dose from dermal exposure. As in the case of the inhalatory route, the user of ConsExpo should only use the 'fraction model' with an uptake fraction of 1. This describes the situation in which all of the external exposure is taken up in the system and is therefore equivalent to the potential dose (the output measure in EUSES).

For a more detailed description of the models the reader is referred to the ConsExpo manual (Van Veen, 2001).

II.5.3.7 Oral consumer exposure

For a substance in a product unintentionally swallowed during normal use (e.g. toothpaste):

- The exposure equations may also be used to estimate exposures arising from ingestion of the non-respirable fraction of inhaled airborne particulates.

A substance migrating from an article into food or drink (e.g. plastic film, plastic-coated cups/plates):

- It is assumed that the substance in a layer of thickness (TH_{art}) of article in contact with the food will migrate to the food. The migration rate is assumed to be constant, and the migration rate multiplied by the contact duration is the fraction of substance that has migrated to the food. The equation can be used to give a conservative estimate of substance uptake by a defined volume of food. The value of the migration rate (Fc_{migr}) will be influenced by the type of food (e.g. fatty/dry/moist), the period of exposure and the temperature at which it occurs. Consumer exposure level will be influenced by the proportion of the contaminated food eaten.

The ConsExpo scenarios "single ingestion" and "article-food migration" correspond to the EUSES scenarios of unintentionally swallowing of a substance, and the migration of a substance from an article into food or drink, respectively.

In addition, ConsExpo provides more detailed oral models for the following cases.:

1. Oral exposure due to hand-mouth contact after a substance has been spilled on, or applied to the hands ("hand-mouth contact"-scenario):

- The dermal exposure is supposed to be given as a constant concentration of the substance on the skin. Hand-mouth contact results in an (average) volume-intake rate of the substance, from which the total amount taken in is calculated as the exposure duration times the concentration times the volume-intake rate.

2. Mouthing of a product ("product leaching"-scenario):

- Mouthing of the product leads to migration of the substance from the product into the saliva, which is subsequently swallowed. It is supposed that the fraction of the substance that leaches from the product into the saliva per unit time per unit area of the product is constant. Given the area of the product leached, the initial concentration of the product and the initial leach-rate (amount of substance per unit area per unit time), the amount of substance swallowed is calculated, taking into account that the concentration of the substance in the product decreases in time.

3. The swallowing of the non-respirable substance after inhalatory exposure that deposits in the throat ("non-respirable fraction"-scenario):

- The input needed for this model is an air concentration of the substance together with a specification of the fraction of the inhaled substance that deposits in the respiratory tract (the "non-respirable fraction"). The exposure results from the assumption that the non-respirable fraction is swallowed entirely. To calculate the air concentration of the substance one of the inhalatory scenarios has to be specified.

ConsExpo offers uptake models to calculate the internal dose:
As in the case of the inhalatory and dermal routes, the user of ConsExpo should only use the 'fraction model' with an uptake fraction of 1. This describes the situation in which all of the external exposure is taken up in the system and is therefore equivalent to the potential dose (the output measure in EUSES).

For a more detailed description of the models the reader is referred to the ConsExpo manual (Van Veen, 2001).

II.5.4 Human exposure at the workplace

II.5.4.1 Introduction

Exposure can be considered as a single event or as a series of repeated events or as continuous exposure. The assessment of the exposure of workers to substances in the workplace should be conducted as a distillation and combination of measured and modelled workplace data. The relative importance of these two types of data will vary according to the availability of good-quality data, particularly measured data. The preferential hierarchy is:

1. Measured data;
2. Appropriate analogous/surrogate data, describing similar operations for the same substance or data for the same operation for similar substances;
3. Modelled estimates;

Information needs are described in the TGD, sections 2.2.2.5 and 2.2.3. A handy overview of the steps involved in an occupational exposure assessment is presented in Appendix 1A of the TGD.
Analysis of uncertainty is an essential part of any exposure assessment, because it provides an important insight into the results and may detect weaknesses of both the measured data and the models. This in turn should lead to a more informed interpretation of the results.
Substances in the workplace may enter the body by inhalation, by passing through the skin, or by ingestion. They may also cause local effects following dermal or ocular exposure. Exposure by inhalation is defined as the concentration of substance in the breathing zone atmosphere and is usually expressed as an average concentration over a reference period. By convention this reference period may be either 8 hours to represent long-term (perhaps years) exposure or 15 minutes to represent short-term exposure. With regard to workplace exposure in EUSES, exposure to the skin (dermal exposure) is assessed as the potential dose rate This potential dose rate is an estimate of the amount of contaminant landing on the outside of work wear and on the exposed surfaces of the skin. It is the sum of the exposure estimates for the various body parts,

including hands and feet. In some cases an actual dose rate can be estimated reflecting the mount of contamination actually reaching the skin. Exposure should always be assessed on the first instance for the unprotected worker and, if appropriate, a second assessment should be made taking account of the use of personal protective equipment (PPE), including respiratory protective equipment (RPE). These types of equipment reduce exposure to an extent depending upon the inherent efficiency of the equipment and the skill of the wearer in achieving this efficiency in the circumstances of use. Ingestion exposure is not normally quantified. EUSES estimates external exposure of workers only; in other words, absorption and bioavailability are not taken into account.

The exposure assessment is carried out through an evaluation of different scenarios. An exposure scenario is the set of information and/or assumptions that tell us how the contact between worker and the substance takes place. It is based on the most important characteristics of the substance in the view of occupational exposure e.g. the physical state, the vapour pressure as well as on its uses, processes, tasks (description, duration, frequency) and controls. Similar exposure scenarios may occur for workers and consumers using the same products and technologies. There may, however, be differences e.g. in duration of exposure and quantities used. In addition, in occupational exposure assessments special consideration is usually not given to vulnerable groups
EUSES first of all provides a general-purpose predictive model for exposure assessment in the workplace. If reliable and representative measured data are available these can be used to overwrite the model results before the risk characterisation is carried out. The general-purpose model is called EASE (Estimation and Assessment of Substance Exposure) and will be described below. EASE is not the only possible model. Several other models exist that may be useful, especially for assessing exposure in specific scenarios. Where exposure prediction models have been chosen in preference to those contained in the TGD, then the reasons for the choice, must be stated. Several models for occupational inhalation and dermal exposure have been developed by US-EPA. A TNO model is available for non-volatile substances (De Pater and Marquart, 1999).
EASE cannot be used yet to predict inhalation exposures during:

- Spray painting
- Welding
- Soldering
- Processes which lead to formation of mists
- For substances released as decomposition products.

RIKSKOFDERM is a project, funded by the EU, aiming at the development of better validated predictions of dermal exposure.

II.5.4.2 EASE

Introduction

EASE was specifically developed by the UK Health and Safety Executive for the purpose of modelling inhalation and dermal workplace exposure across a wide range of circumstances. EASE is an analogue model, i.e. it is based on measured data which are assigned to specific scenarios. The user can build scenarios by choosing between several options for each of the

following variables: physical properties during processing (tendency to become airborne, potential for dermal contact), use pattern and pattern of control. Decisions by the assessor on use patterns and patterns of control should be based on information provided by manufacturers and importers and on the experience of the assessor. Numerical ranges have been assigned to these fields using measured data. The logic of deriving scenarios and assigning ranges to the scenarios is described in Appendix IV. Definitions used in EASE have been incorporated into the HELP-function of EUSES.

The data used to assign ranges within the model are all 8-hour time weighted averages and the numbers generated by the model are only valid when the exposures being assessed can be related to such averages. For example, the model will not predict short-term or acute exposures unless these can be related by the assessor to 8-hour time-weighted averages. Such predictions are possible in principle, however, by running the model in a worst-case scenario. Again, except when appropriate information can be related to 8-hour time-weighted averages, the model does not predict exposures resulting from unusual or special circumstances such as heavy workloads or increased inhalation rates. It should be noted that the model does not specifically account for time variables and intensity of use other than as contained in the assumptions. These parameters may have to be considered separately if necessary. Based on evaluations carried out by rapporteurs and others, the model often yields results which are numerically higher than those in apparently analogous situations in workplaces. This may or may not be a reflection of the data on which the model was based or may or may not reflect the fact that these evaluation workplaces were largely associated with manufacturing plant rather than downstream or other uses where, for some industries, exposure levels tend to be higher.

Great care should be taken to ensure that predictive ranges provided by exposure assessments are adequate to enable assessors to make risk assessments with confidence. This is particularly important for substances of high toxicity, which in such cases may consequently need a more comprehensive array of measured data than substances of lower toxicity. As explained previously, occupational exposures by inhalation are expressed as time-weighted average concentrations, usually over eight hours or fifteen minutes. In reality, wide variations in instantaneous or short-term concentrations may occur within these average values, although, clearly, these are more likely to be reflected in fifteen-minute time-weighted averages than in eight-hour averages. Such variations may be an integral part of the process or may arise from reasonably foreseeable accidental releases. They become important in risk assessment when they are high enough and long enough to cause harmful effects in their own right. They are particularly important when these effects are acute and life-threatening or irreversible. The model does not provide direct information on such short-term exposures. A comprehensive array of measured data is preferable and may be essential.

The EASE model was designed to assist exposure assessment for both new and existing substances. It was developed specifically for the purpose of modelling exposure across a wide variety of circumstances encountered in workplaces. It should be noted that the model does not specifically account for time variables and intensity of use other than as contained in the assumptions. The model is concerned with exposures resulting from normal use of substances and does not deal with exposures which result from foreseeable spillages, accidental loss of containment or breakdown of normally reliable control measures. These parameters may have to be considered separately if necessary.

The EASE model for workplace inhalation exposure assessment

Limitations of the inhalation model

The source of inhalation exposure data used to assign ranges within the model was HSE's National Exposure Datebase (NEDB). For the purposes of the model, exposure ranges have been derived by inspection of the interquartile ranges for many substances and processes by means of box and whisker plots. The outputs generated by the model are only valid where the exposures being assessed can be related to continuous exposure at the process under consideration. The model will not directly predict short term or acute exposures but such predictions are possible. Because the inhalation data in EASE are process specific, exposures can be thought of as those experienced for that process either over the whole eight hours or over any shorter period. These shorter periods can be used as an assessment outcome in their own right or they can be time weighted to construct eight hour time weighted averages. Although this device allows short term exposures to be dealt with by EASE, such constructs should be regarded with caution.

The term aerosol in the model is used to describe finely dispersed liquid particulates in air. Finely dispersed solid particulates are assumed to be dusts but this assumption may not hold in all cases and expert judgement may have to be applied to give realistic results.

The basis for the inhalation model

Gases and vapours
The EASE approach to workplace exposure assessment modelling for inhalation exposure to gases and vapours defines logical criteria to describe broadly the types of exposure possible based upon the volatility of substances giving rise to gases and vapours during processing (the tendency to become airborne), use patterns and patterns of control as follows:

A. Volatility (Tendency to become airborne)
Gas
Liquid or Solid, High Vapour Pressure
Liquid or Solid, Moderate to High Vapour Pressure
Liquid or Solid, Moderate Vapour Pressure
Liquid or Solid, Moderate to Low Vapour Pressure
Liquid or Solid, Low Vapour Pressure
Liquid or Solid, Very Low Vapour Pressure
Aerosol
B. Use Pattern
Closed System
Within a Matrix
Non-Dispersive
Wide Dispersive

C. Pattern of Control
Full Containment
Local Exhaust Ventilation (LEV)
Segregation
Direct Handling With Dilution Ventilation
Direct Handling

This treatment leads in principle, to 140 model outcomes equivalent to 140 possible combinations of the criteria in A, B and C. However, whilst the expert system predicts exposures for all possible combinations, the actual ranges are limited to just 59 fields with ranges assigned. This arises because:

Very low vapour pressure liquids or solids have only 3 outcomes in the logic charts.
Closed system pattern of use has only 1 outcome in the logic charts
Full containment pattern of control has only 2 outcomes in the logic charts
Outputs for exposure to aerosols are subsumed into high, medium to high, medium, medium to low and low volatility.
Full containment and LEV patterns of control are not considered appropriate for wide dispersive use.

Dusts

Inhalation exposure to dusts is handled rather differently in EASE to the handling of gases and vapours. The logical criteria are as follows.

D. Particle Size
Granular (Exposure is assumed to be zero)
Respirable or Inhalable
E.Type of Dust
Fibrous
Non-Fibrous

EASE treats fibrous and non-fibrous dusts differently from one another.

Fibrous dusts
For fibrous dusts the criteria are as follows.

F. Tendency to Become Airborne (Inherent Dustiness)
High Inherent Dustiness
Medium Inherent Dustiness
Low Inherent Dustiness
G. Use Pattern (Process Type)
Dry Crushing and Grinding
Dry Manipulation
Low Dust Techniques

H. Pattern of Control
Local Exhaust Ventilation (LEV)
No LEV

This treatment leads, in principle, to 18 model outcomes for fibrous dusts (19 counting zero exposure for granular dust) equivalent to 18 possible combinations of the criteria in F, G and H and all dealt with by EASE. However, the presence of LEV is not considered relevant for "low dust " techniques reducing the fields in the logic charts to 17.

Non fibrous dusts
For non-fibrous dusts the criteria are as follows.

I. Tendency to Become Airborne (Inherent Dustiness) (The expert system and Appendix I consider this aspect last for non fibrous dusts)
Non Fibrous Dust, Non Aggregating
Non Fibrous Dust, Aggregating
J. Use Pattern (Process Type)
Dry Crushing and Grinding
Dry Manipulation
Low Dust Techniques
K. Pattern of Control
Local Exhaust Ventilation (LEV)
No LEV

This treatment leads, in principle, to 12 model outcomes for non fibrous dusts equivalent to 12 possible combinations of the criteria in I, J and K and all dealt with by EASE. However, dustiness is not considered relevant for "low dust " techniques reducing the fields in the logic charts to 10.

Thus the inhalation model is described by a total of 170 fields. Numerical ranges were assigned to these fields using measured data contained within the UK National Exposure

Database (NEDB) (Appendix II). This approach allows upgrading of the numbers in the ranges at a later stage by reference to other databases or as new information becomes available.

The EASE model for dermal exposure assessment

Limitations of the dermal model

Dermal exposure was assumed to be uniform and was assessed as potential exposure rate predominantly to the hands and forearms (approximately 2,000 cm^2). It was assumed that dermal exposure to gases and vapours is very low. It was further assumed that no personal protection of any sort is worn and that exposure depends only upon manual contact. The effect of personal protective equipment (PPE) may need to be considered separately and conclusions drawn on the basis of logic and expertise. The model addresses neither the impact of personal hygiene (such as hand washing) nor evaporation or other types of loss from the skin (for example, through sweating or abrasion).

The basis for the dermal model

The scheme for dermal assessment modelling is similar in construction to that for inhalation. The concept of "potential for dermal contact" forms the basis for the model. It was assumed that only contact with solids and liquids is important and that the only patterns of use and control which lead to important dermal exposure are non-dispersive, wide dispersive use and direct handling, systems within a matrix were assumed to be equivalent to non- dispersive use. The criteria for the development of the inhalation scenarios were combined with contact level criteria as follows.

Contact level criteria

None	No contact
Incidental	1 event per day
Intermittent	2 - 10 events per day
Extensive	> 10 events per day

Exposure ranges are estimates based on data from several sources, principally the United States Environmental Protection Agency (EPA) and the UK Health and Safety Executive (HSE). Ranges for dusts were extrapolated from data for liquids. Units are $mg/cm^2/day$. It should be noted that dermal exposure assessment, in common with the inhalation exposure assessment described above, does not include any form of uptake (such as absorption through the skin in the case of dermal exposure).

Ingestion exposure assessment

Although ingestion exposure may be amenable to the sort of modelling described in this paper, it is considered to be much more dependent on personal factors and upon effective supervision and provision of hygiene facilities than the other two routes. For dusts, the estimation of exposure from ingestion might be better modelled using the level of inhaled

dust as a starting point and estimating the fraction ingested. Using these assumptions, a rough estimation of ingestion exposure may be derived if this is a matter of concern.

The knowledge based system (KBS) for exposure assessment modelling

The logical criteria for both inhalation and dermal exposure predictions were incorporated within a knowledge based (expert) electronic data system (KBS) designed to facilitate the assessment of workplace exposure. The system was developed in an evolutionary way, improving its "expertise" as it grew. It is likely that the model will need to be run several times to take account of different exposure scenarios. The exposure range relevant to each scenario is then shown in the log file.

Mixtures and other special circumstances

The measured data used to derive the ranges in the model were collected in workplaces in which it is unlikely that the substance measured was the only one present. Some substances are in fact always measured as mixtures, for example, oil mist or foundry particulate. Nevertheless, it was assumed for the purposes of the model that measured data could be treated as if the source was the "pure" substance and data which could not be treated in this way was rejected. If a substance is always supplied as or used in a mixture and relevant data on how the mixture might become airborne are not available, a simple approach, would be to reduce the estimated exposure by a factor equivalent to the concentration of the substance in the mixture. Other special circumstances (for example, very long or very short working periods) may require similar adjustments.

II.6 EFFECTS MODULE

In this module, the toxicological data can be entered. For the environmental end-points, extrapolation to Predicted No-Effect Concentrations (PNECs) is performed. For the human risk characterisation, the experimental data are used directly or with minor conversions.

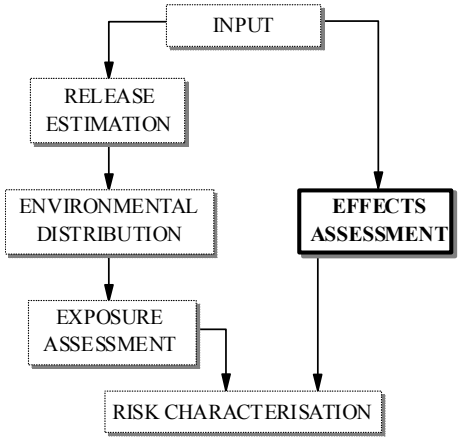

Figure II-24 *System structure.*

II.6.1 Environment

II.6.1.1 Introduction

The protection goals for the environment are the aquatic and terrestrial ecosystem, top predators and microbial activity in an STP. This means that a Predicted No-Effect Concentration (PNEC) has to be derived for each of these goals. A PNEC is regarded as a concentration below which an unacceptable effect will most likely not occur. In principle, the PNEC is calculated by dividing the lowest short-term L(E)C50 or long-term NOEC value by an appropriate assessment factor. The assessment factors reflect the degree of uncertainty in extrapolation from laboratory toxicity-test data for a limited number of species to the 'real' environment. Assessment factors applied for long-term tests are lower, as there is less uncertainty involved in the extrapolation from laboratory data to the natural environment.

II.6.1.2 Quantitative Structure-Activity Relationships

Reliable QSAR estimates for fish, Daphnia and algal toxicity are available for chemicals with a non-specific mode of action. These estimates can be used to assist in data evaluation and/or to contribute to the decision-making process as to whether further testing is necessary. Chapter 4 of the TGD (EC, 2003) gives full details on the use of QSAR estimates for chemicals with a non-specific mode of action and on long-term fish toxicity within the testing strategy. No QSARs for toxicity are implemented in EUSES, but any results can be entered manually.

II.6.1.3 Effects assessment for the aquatic compartment (freshwater and marine environment)

Certain assumptions are made concerning the aquatic environment, which allow an extrapolation to be made from single-species short-term toxicity data to ecosystem effects. It is assumed that:

- Ecosystem sensitivity is determined by its most sensitive components. The sensitivity is estimated using assessment factors on the most sensitive species or statistical extrapolation on the distribution of sensitivities, and
- protecting ecosystem structure protects community function.

These two assumptions have important consequences. By establishing which species is the most

sensitive to the toxic effects of a chemical in the laboratory, extrapolation can subsequently be based on the data for that species. Furthermore, the functioning of any ecosystem in which that species exists is protected, provided the structure is not sufficiently distorted as to cause an imbalance. It is generally accepted that protection of the most sensitive species should protect structure, and hence function. In establishing the size of the assessment factors, a number of uncertainties must be addressed, summarised under the following headings:

- Intra- and inter-laboratory variation of toxicity data.
- Intra- and inter-species variations (biological variance).
- Short-term to long-term toxicity extrapolation.
- Laboratory data to field impact extrapolation.

The size of the assessment factor depends on the confidence with which a PNEC can be derived from the available data. This confidence increases if data are available on the toxicity to organisms at a number of trophic levels, belonging to taxonomic groups and with lifestyles representing various feeding strategies. Thus, lower assessment factors can be used with larger and more relevant datasets than the base-set data. The applied assessment factors are presented in Table II-8.

Table II-8 *Assessment factors to derive a PNEC for the freshwater compartment.*

Information available	Assessment factor
At least one short-term L(E)C50 for each of three trophic levels of the base set (fish, Daphnia and algae)	1000 [(a)]
One long-term NOEC (either fish or Daphnia)	100 [(b)]
Two long-term NOECs for species representing two trophic levels (fish and/or Daphnia and/or algae)	50 [(c)]
Long-term NOECs for at least three species (normally fish, Daphnia and algae) representing three trophic levels	10 [(d)]
At least 10 NOECs for species covering at least 8 taxonomic groups (applying the species sensitivity distribution (SSD) method)	5-1 See section II.6.1.8
Field data, data on model ecosystems	Reviewed on a case-by-case basis[(e]

NOTES:

a The use of a factor of 1000 for short-term toxicity data is a conservative and protective factor and is designed to ensure that substances with the potential to cause adverse effects are identified in the effects assessment. It assumes that each of the uncertainties identified above makes a significant contribution to the overall uncertainty. Under certain circumstances it may be necessary to vary the assessment factor. Except for substances with intermittent release, under no circumstances should a factor lower than 100 be used in deriving a $PNEC_{water}$ from short-term toxicity data.

b An assessment factor of 100 applies to a single long-term NOEC (fish or Daphnia) if this NOEC was generated for the trophic level showing the lowest L(E)C50 in the short-term tests. If the only available long-term NOEC is for a species (standard or non-standard organism) which does not have the lowest L(E)C50 from the short-term tests, it cannot be regarded as protecting other, more sensitive species using the assessment factors available. Thus, the effects assessment is based on the short-term data with an assessment factor of 1000. However, the resulting PNEC based on short-term data may not be higher than the PNEC based on the long-term NOEC available. An assessment factor of 100 also applies to the lowest of two long-term NOECs covering two trophic levels when such NOECs have not been generated from that level showing the lowest

L(E)C50 of the short-term tests. This should, however, not apply in cases where the acutely most sensitive species has an L(E)C50 value lower than the lowest NOEC value. In such cases the PNEC might be derived by using an assessment factor of 100 to the lowest L(E)C50 of the short-term tests.

c An assessment factor of 50 applies to the lowest of two NOECs covering two trophic levels when such NOECs have been generated covering that level showing the lowest L(E)C50 in the short-term tests. It also applies to the lowest of three NOECs covering three trophic levels when such NOECs have not been generated from that level showing the lowest L(E)C50 in the short-term tests.

d An assessment factor of 10 will normally only be applied when long-term toxicity NOECs are available for at least three species across three trophic levels (e.g. fish, Daphnia, and algae or a non-standard organism instead of a standard organism). When examining the results of long-term toxicity studies, the $PNEC_{water}$ should be calculated from the lowest available no-observed-effect concentration (NOEC). Extrapolation to ecosystem effects can be made with much greater confidence, and thus a reduction of the assessment factor to 10 is possible. This is only sufficient, however, if the species tested can be considered to represent one of the more sensitive groups. A factor of 10 cannot be decreased on the basis of laboratory studies.

e The assessment factor to be used for mesocosm studies or (semi-) field data will need to be reviewed on a case-by-case basis.

The greater diversity of taxa in the marine environment, compared to freshwaters, will produce a broader distribution of species sensitivity. In those cases where only data for freshwater or saltwater algae, crustaceans and fish are available a higher assessment factor should be applied than that for the derivation of $PNEC_{water}$ for freshwaters. This higher assessment factor reflects the greater uncertainty in the extrapolation. Where data is available for additional marine taxonomic groups, for example rotifers, echinoderms or molluscs the uncertainties in the extrapolation are reduced and the magnitude of the assessment factor applied to a data set can be lowered.

Table II-9 *Assessment factors to derive a PNEC for the marine aquatic compartment.*

Information available	**Assessment factor**
Lowest short-term L(E)C50 from freshwater or saltwater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels	10000 [a]
Lowest short-term L(E)C50 from freshwater or saltwater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels, + two additional marine taxonomic groups (e.g. echinoderms, molluscs)	1000
One long-term NOEC (from freshwater or saltwater crustacean reproduction or fish growth studies)	1000 [b]
Two long-term NOECs from freshwater or saltwater species representing two trophic levels (algae and/or crustaceans and/or fish)	500 [c]
Lowest long-term NOECs from three freshwater or saltwater species (normally algae and/or crustaceans and/or fish) representing three trophic levels.	100 [d]
Two long-term NOECs from freshwater or saltwater species representing two trophic levels (algae and/or crustaceans and/or fish) + one long-term NOEC from an additional marine taxonomic group (e.g. echinoderms, molluscs)	50
Lowest long-term NOECs from three freshwater or saltwater species (normally algae and/or crustaceans and/or fish) representing three trophic levels + two long-term NOECs from additional marine taxonomic groups (e.g. echinoderms, molluscs)	10
At least 10 NOECs for species covering at least 8 taxonomic groups (Species Sensitivity Distribution)	5-1, See section II.6.1.8

NOTES:

a In specific cases this factor can be varied (see TGD). Except for substances with intermittent release, under no circumstances should a factor lower than 1000 be used in deriving a PNECwater for saltwater from short-term toxicity data.

b A factor of 1000 applies if the NOEC was generated for the taxonomic group showing the lowest L(E)C50 in the short-term algal, crustacean or fish tests. Otherwise, a factor of 10000 should be applied to the short–term data. However, normally the lowest PNEC should prevail.

c A higher assessment factor of 1000 applies to the lowest of the two long-term NOECs when such NOECs have not been generated for the species showing the lowest L(E)C50 of the short-term tests. This should not apply in cases where the acutely most sensitive species has an L(E)C50-value lower than the lowest NOEC value. In such cases the PNEC might be derived by applying an assessment factor of 1000 to the lowest L(E)C50 of the short-term tests.
Additional considerations for lowering the assessment factor of 500 are presented in the TGD.

d Additional considerations for lowering the assessment factor of 100 are presented in the TGD.

For substances for which intermittent release is defined (see Section II.3.7 for the definition of intermittent release), exposure may be of short duration only. For dynamic systems like rivers at least, the likelihood of long-term effects arising from such exposure is low, the principal risk being short-term toxicity effects. In extrapolating to a PNEC, generally only short-term effects

need be considered. Therefore, an assessment factor of 100 is applied to the lowest L(E)C50 of at least three short-term tests from three trophic levels to derive a PNEC for such situations.
In paragraph 0 the statistical extrapolation method is described, that can be used when sufficient toxicity data are available.

II.6.1.4 Effects assessment for micro-organisms in an STP

As chemicals may cause adverse effects on microbial activity in STPs, it is necessary to derive a PNEC. Current test systems for measuring the impact of chemicals on microbial activity have different end-points and sensitivities. A number of internationally accepted test systems exist. Available data (e.g. Umweltbundesamt, 1993, Reynolds *et al.*, 1987) suggest the following order of increasing sensitivities among particular test systems: respiration inhibition test (EC C.11, OECD 209) < inhibition control in base-set tests < growth inhibition test with P. putida < inhibition of nitrification.

Table II-10 provides a complete listing of the test systems, effect concentrations that are determined using them and the corresponding assessment factors.

Table II-10 *Test systems for derivation of the PNEC for micro-organisms.*

Test	Available value	Assessment factor
Activated sludge, respiration inhibition		
Respiration inhibition tests EU Annex V C.11, OECD 209 ISO 8192	NOEC or EC10	10
	EC50	100
Base set biodegradation, inhibition control		
Inhibition control in standardised biodegradation tests: • Ready biodegradability tests EU Annex V C.4 A-F; OECD 301 A-F; ISO-7827, -9439, -10707, -9408 • Inherent biodegradability tests OECD 302 B-C; ISO 9888	Tested conc. at which toxicity to inoculum can be ruled out [a]	10
Activated sludge, other tests		
Activated sludge growth inhibition tests ISO-15522	NOEC or EC10	10
	EC50	100
Pilot scale activated sludge simulation tests OECD 303 A ISO-11733	Expert judgement [b]	Case by case Down to 1
Tests with specific populations of bacteria or protozoa		
Inhibition of nitrification ISO-9509 (1989)	NOEC or EC10	1
	EC50	10
Ciliate growth inhibition tests (preferably with *Tetrahymena*, cf. OECD, 1998)	NOEC or EC10	1
	EC50	10
Growth inhibition test with *Pseudomonas putida* [c] NF EN ISO 10712	NOEC or EC10	1
	EC50	10

a The tested concentration at which toxicity to the inoculum can be ruled out with sufficient reliability (cf. corresponding text section above) could be considered as a NOEC for the toxicity to micro-organisms of a STP;

b Based on case-by-case expert judgement, the tested concentration not impairing proper functioning of the continuous activated sludge unit could be considered as NOEC for micro-organisms in STPs

c Bringmann & Kühn (1980) method to be used only if no other tests are available

II.6.1.5 Effects assessment for sediment (freshwater and marine environment)

No data for sediment-dwelling organisms will be available for new substances. To date, only a few tests on sediment organisms have been conducted in Europe with existing substances. However, research is in progress in this field in various countries. In the absence of any ecotoxicological data for sediment-dwelling organisms, the PNEC may provisionally be calculated using the equilibrium-partitioning method. This method which is regarded as a "screening approach" uses the PNEC for aquatic organisms and the sediment-water partition coefficient (OECD, 1992b; Di Toro *et al.*, 1991). In the partitioning method, it is assumed that:

- Sediment-dwelling organisms and water-column organisms are equally sensitive to the chemical.
- Concentration in sediment, interstitial water and benthic organisms are in thermodynamic equilibrium: the concentration in any of these phases can be predicted using the appropriate partition coefficients.
- Sediment-water partition coefficients can either be measured or derived on the basis of a generic partition method from separately measurable characteristics of the sediment and the properties of the chemical.

Regardless of whether the partition coefficient in sediment is measured or estimated, the following remark should be noted for the calculation of the PNEC using the equilibrium-partitioning method. The approach considers uptake via the water phase only, but uptake may also occur via ingestion of sediment. This may become important, especially for adsorbing chemicals. Thus, for these compounds the total uptake may be underestimated. There is evidence from studies in soil (Belfroid *et al.*, 1995) that the proportion of the total dose remains low for chemicals with a log *Kow* up to 5. Although it is recognised that, in principle, results for the soil compartment may not be extrapolated to the sediment compartment, the possible underestimation of exposure is considered acceptable when using the equilibrium-partitioning method for chemicals with a log *Kow* between 3 and 5. For compounds with a log *Kow* greater than 5 or with a corresponding adsorption or binding behaviour, the equilibrium method is used in a modified form. In order to take uptake via ingestion of sediment into account, the PEC/PNEC ratio in sediment is increased by a factor of 10 in risk characterisation for these compounds. It should be kept in mind that this approach is considered as a screening assessment of the risk to sediment-dwelling organisms.

If no measured data are available for the determination of PEC in sediment nor for the calculation of PNEC, no quantitative risk characterisation for sediment can be performed.

If one or more acute toxicity tests for sediment-dwelling organisms is/are available, the lowest of the PNECs resulting from the equilibrium partitioning and assessment factor approach is used. Depending on the toxicity data available for sediment-dwelling organisms, assessment factors are selected for extrapolating single-species toxicity tests to a PNEC for the sediment compartment.

Finally, when long-term toxicity test data are available for benthic organisms the PNECsed is calculated using assessment factors for long-term tests and this result should prevail in the risk assessment (See section 3.5.4 of the TGD (EC, 2003)).

Assessment factors for deriving a PNEC for the freshwater sediment compartment are presented in ***Table II-11***.

Table II-11 *Assessment factors to derive a PNEC for the freshwater sediment compartment.*

Information available	Assessment factor
None	1[a]
One or more short-term tests (LC50) with benthic organism(s)	1[a] (equilibrium partitioning) or 1000 (based on LC50). Lowest value is used.
One long term test (NOEC or EC10)	100
Two long term tests (NOEC or EC10) with species representing different living and feeding conditions	50
Three long term tests (NOEC or EC10) with species representing different living and feeding conditions	10

a applied to PNEC water using the equilibrium partitioning method

Substances that are potentially capable of depositing on or sorbing to sediments to a significant extent have to be assessed for toxicity to sediment-dwelling organisms. In addition, marine sediment effects assessment is necessary for substances that are known to be persistent in marine waters, and may accumulate in sediments over time. To avoid extensive testing of chemicals a log Koc or log Kow of ≥ 3 can be used as a trigger value for sediment effects assessment.

For the marine effect assessment of sediment-dwelling organisms attention should be paid to the fact that very often contaminants are not analysed in whole sediment but in a certain fraction of the sediment, for example in the sediment fraction of particles < 63 μm. The organic carbon content of this fraction is typically 15-30% for marine sediment while for whole marine sediments it is generally less than 2%. It is important, for reasons of comparability of PEC and PNEC values, that the organic carbon content of sediment used for toxicity tests are comparable with those of actual marine sediments. Results are converted to a standard sediment, which is defined as a sediment with an organic matter content of 8.5% or an organic carbon content of 5.0%.

It is not necessary to apply the equilibrium partitioning method to predicted environmental concentrations obtained from application of an exposure model when such a model will have used the same Koc or log Kow value as that used to predict the PNECsediment. The reason is that the resulting PEC/PNEC ratio for sediment will have the same value as for the water compartment. In this case no quantitative risk characterisation for marine sediment should be performed. Under these circumstances the assessment conducted for the aquatic compartment will also cover the sediment compartment for chemicals with a log Kow up to 5. For substances with a log Kow > 5 (or with a corresponding Koc), however, the PEC for the aquatic compartment is increased by a factor of 10. The increased factor is justified by the fact that the

equilibrium partitioning method considers mainly the exposure via the water phase and does not include that potential additional accumulation via sediment ingestion may occur for certain types of sediment dwelling invertebrates.

A PNEC marine sediment is derived by application of the following assessment factors to the lowest LC50 value from acute tests (***Table II-12***)

Table II-12 *Assessment factors to derive a PNEC for the marine sediment compartment.*

Information available	**Assessment factor** [c]
None	1[a]
One acute freshwater or marine test	10000 and equilibrium partitioning method [b]
Two acute tests including a minimum of one marine test with an organism of a sensitive taxa	1000 and equilibrium partitioning method [b]
One long term freshwater sediment test	1000
Two long term freshwater sediment tests with species representing different living and feeding conditions	500
One long term freshwater and one saltwater sediment test representing different living and feeding conditions	100
Three long term sediment tests with species representing different living and feeding conditions	50
Three long term tests with species representing different living and feeding conditions including a minimum of two tests with marine species	10

a Applied to PNEC water using the equilibrium partitioning method

b Either of which method results in the lowest PNECsediment is used.

c The general principles of notes (c) and (d) as applied to data on aquatic organisms (section II.6.1.3) shall also apply to sediment data. Additionally, where there is convincing evidence that the sensitivity of marine organisms is adequately covered by that available from freshwater species, the assessment factors used for freshwater sediment data may be applied. Such evidence may include data from long-term testing of freshwater and marine aquatic organisms, and must include data on specific marine taxa.

II.6.1.6 Effects assessment for the terrestrial compartment

The terrestrial ecosystem comprises an above-ground community, a soil community and a groundwater community. In this section only effects on soil organisms exposed directly via pore water and/or soil are addressed.

For most chemicals, the number of toxicity data on soil organisms will be limited. At the base-set level for new and existing substances there is no requirement for toxicity tests with soil organisms. For new substances, toxicity tests with plants and earthworms can be requested at level I. For existing substances data will probably be scarce: for most chemicals the dataset will consist of short-term tests for earthworms and plants. Long-term tests exist for micro-organisms, springtails and earthworms, for example, but results from such tests are not commonly found for existing substances. To compensate for this lack of toxicity data, the equilibrium-partitioning

method is therefore used, following the approach used for sediment.

Natural soils used in ecotoxicological tests differ in characteristics such as organic matter and clay content, soil pH and soil moisture content. The bioavailability of the test compound, and therefore the toxicity observed, is influenced by these soil properties. This means that results from different test soils cannot be compared directly. If possible data should be normalised using relationships that describes the bioavailability of chemicals in soils. Results are converted to a standard soil, which is defined as a soil with an organic matter content of 3.4% or an organic carbon content of 2.0% .

Three situations can be distinguished for deriving a PNEC for soil:
- If no toxicity data are available for soil organisms, the equilibrium-partitioning method is applied to identify a potential risk to soil organisms. This method is regarded as a 'screening approach' and has been already explained for sediment.
- If toxicity data are available for a producer, a consumer and/or a decomposer, the PNEC is calculated using assessment factors. The assessment factors are presented in ***Table II-13***.
- If only one test result with soil-dwelling organisms is available, the risk assessment is performed both on the basis of this test, using assessment factors, and on the basis of the equilibrium-partition method. From these two PNECs, the lowest is chosen for risk characterisation.

As with sediment, the equilibrium-partitioning method for soil assumes that the bioavailability and therefore toxicity of chemicals to soil organisms is determined only by the concentration in the pore water of the soil. Further effects that chemicals adsorbed to soil particles may have on soil organisms via ingestion are not considered in this approach. The applicability of the equilibrium-partitioning method has been tested less for soil-dwelling than for sediment-dwelling organisms. Van Gestel and Ma (1993) have demonstrated the validity of the model for the short-term toxicity of several chlorophenols, chlorobenzenes and chloroanilines to earthworms. As with sediment, the equilibrium-partitioning method may not be suitable for lipophilic compounds and species exposed primarily through food (Van Gestel, 1992). Therefore, the same approach is used as for the derivation of the PNEC of sediment: in order to take uptake via ingestion of soil into account, the PEC/PNEC ratio in soil is increased by a factor of 10 for compounds with a log *Kow* > 5 (or for compounds with a corresponding adsorption or binding behaviour, e.g. ionisable substances) in the risk characterisation.

The same assessment factors are used for the terrestrial system (see ***Table II-13***) as for the aquatic system (see ***Table II-8***), depending on the type of study (short-term or long-term toxicity test), the number of trophic levels tested, and the general uncertainties in predicting ecosystem effects from laboratory data. The assessment factors for the soil compartment are not based on comprehensive experience, and as more information on the sensitivity of soil organisms becomes available these factors may have to be adjusted.

Table II-13 *Assessment factors to derive a PNEC for the terrestrial compartment.*

Information available	Assessment factor
L(E)C50 short-term toxicity tests (e.g. plants, earthworms or micro-organisms)	1000
NOEC for one long-term toxicity test (e.g. plants)	100
NOEC for additional long-term toxicity tests for two trophic levels	50
NOEC for additional long-term toxicity tests for three species at three trophic levels	10
At least 10 NOECs for species covering at least 8 taxonomic groups (Species Sensitivity Distribution)	5 – 1 See section II.6.1.8
Field data, data on model ecosystems	Case-by-case

NOTE:
The PNEC for soil is calculated on the basis of the lowest effect value measured. If short-term tests with a producer, a consumer and/or a decomposer are available, the test result is divided by a factor of 1000 to calculate the PNEC. If only one terrestrial test is available (earthworms or plants), the risk assessment should be performed both on the basis of this terrestrial test and on the basis of the equilibrium-partitioning method using aquatic toxicity data as an indication of the risk to soil organisms. As a precaution, the lowest resulting PNEC is used. The other factors listed in Table II-13 are applied, if more tests than the short-term toxicity test have been conducted.

II.6.1.7 Assessment of secondary poisoning

An estimation is made of whether the PEC in water can lead to concentrations in fish that may lead to deleterious effects in higher organisms feeding on fish. If secondary poisoning is to be avoided, the concentration of chemicals in food should be below the No-Observed-Effect Concentration (NOEC) in a (sub)chronic dietary toxicity test with animals representative of fish-eating birds or mammals. The NOEC is considered as a maximum concentration in food which will not lead to adverse effects after ingestion of this food. Only toxicity studies reporting on dietary and oral exposure are relevant, as the pathway for secondary poisoning refers exclusively to uptake through the food chain. The results of these tests may be expressed as a concentration in the food (NOEC in mg/kg) or a dose (NOAEL in mg/kg body weight/day) causing no effect. For the assessment of secondary poisoning, the results must be expressed as the concentration in food (mg/kg food). In the absence of a NOEC, EUSES converts the NOAEL for mammals to a concentration in food. Conversion factors for several experimental mammalian species are given in Section III.6.1.5.

Effects on birds and mammal populations are rarely in the form of mortality following short-term exposure. Therefore, results from (sub-)chronic studies are preferable, such as NOECs for mortality, reproduction or growth. For new substances, the results of mammalian repeated-dose toxicity test(s) are used in the assessment of secondary poisoning effects. For existing substances, toxicity data for birds may be available. Extrapolation from such test results gives a PNEC in food that should be protective of other mammalian and avian species. Assessment factors are used which take into account interspecies variation, subchronic to chronic toxicity extrapolation, and laboratory data to field impact extrapolation.

Acute lethal doses (LD50, rat, bird) are not suitable for extrapolation to chronic toxicity, as these

tests are not dietary tests. Acute-effect concentrations (LC50, 5 day avian dietary studies) are acceptable for extrapolation because these are dietary studies. An assessment factor of 1,000 is applied to the results from such a test. An assessment factor of 100 (10x10) is applied to the NOEC for the 28-day repeated-dose study with mammals to derive the $PNEC_{oral}$. If a 90-day toxicity text is submitted instead of the 28-day test, this assessment factor may be reduced to 30. When chronic studies are available, an assessment factor of 10 may be used. Reproduction-toxic effects are regarded as chronic effects and the same assessment factor may be used. The suggested assessment factors should be seen as default values. When other factors are judged to be more appropriate, they can be entered by the user.

II.6.1.8 Statistical extrapolation method

The effects assessment performed with assessment factors can be supported by a statistical method based on species sensitivity distributions (SSDs). The method can be used for aquatic as well as terrestrial or sediment toxicity data. The results of this method can be entered in EUSES, the statistical method itself is not included. The ETX 4.1 tool of the RIVM could be used for this. The TGD (2003) gives information on the background en gives guidance on the data requirements.

The basic assumption of SSDs is that the sensitivities of a set of species can be described by some distribution, usually a parametric distribution function such as the normal or logistic distribution. The available test data (NOECs in this context) are seen as a sample from this distribution and are used to estimate the parameters of the SSD. Aldenberg and Jaworska (2000) refined the way to estimate the uncertainty of percentiles of the SSD by introducing confidence levels. The difference between the logistic and the normal distribution are small and are mainly noticeable in the tails of the distribution. At small sample size, as is usually the case for deriving PNECs, there is no statistical or theoretical justification for choosing the logistic or normal distribution.

The method work as follows: long-term toxicity data are log-transformed and fitted according to a distribution function and a prescribed percentile of that distribution is used as a criterion that can be divided by an additional assessment factor. The data requirements are a minimum of 10, preferably 15, NOECs available from at least 8 taxonomical groups that are mentioned in the TGD. Specific guidance is given to data pre-processing, especially when several toxicity values are available for the same species.

Whether the sample of toxicity data derives from a normal distribution can be assessed with goodness-of-fit (GOF) tests. Two different types of tests are implemented. The Anderson-Darling goodness-of-fit test highlights differences between the tail of the distribution and the input data, and is generally regarded as a very powerful general test (Aldenberg *et al.*, 2002). The Kolmogorov-Smirnov test focuses on differences in the middle of the distribution and is not very sensitive to discrepancies of fit in the tail of the distribution.
A lack of fit may be caused by very different factors, such as statistical artefacts from the determination of the NOEC or possible bimodality of the SSD. If the data do not fit any distribution, the left tail of the distribution (the lowest effect concentrations) should be analysed more carefully. If a subgroup of species can be identified as particularly sensitive

and if the number of data on this subgroup is sufficient, the distribution can be fit to this subgroup. In case of lack of fit, the SSD method should not be used.

The concentration corresponding with the point in the SSD profile below which 5% of the species sensitivity data occur (the 5th percentile or HC5) should be derived as an intermediate value in the determination of a PNEC. A 90% confidence interval associated with this concentration is also derived, to judge uncertainty associated with the HC5. Additional assessment factors may be used to derive the PNEC.

II.6.1.9 PBT assessment

The PBT assessment has been introduced in the marine risk assessment of the revised TGDs (2003) (section 4.4) to address concern for substances that are considered Persistent as well as Bioaccumulative and Toxic (PBT substances) and substances that are considered very Persistent and very Bioaccumulative (vPvB). The PBT assessment applies to new substances, priority existing substances and biocides. This assessment is not included in EUSES 2.0 program.

The PBT assessment is different from the local and regional assessment approaches since it seeks to protect ecosystems where the risks are more difficult to estimate. The basic concerns are the accumulation of hazardous substances in parts of the marine environment, the effect of which can be unpredictable in the long term, and the difficulty to reverse the accumulation. The PBT-assessment is particularly developed to take into account the unacceptable high uncertainty in predicting reliable exposure and/or effect concentrations hampering quantitative risk assessment for substances with PBT characteristics.

The PBT-assessment basically consists of the identification of PBT substances using specific criteria for the inherent properties (see section 4.4.2 of the TGD) and an evaluation of the sources, emissions and pathways to the marine environment. Since for PBT substances a “safe” concentration in the environment cannot be established cessation of emissions is the ultimate goal and the appropriate way to achieve this goal must be identified.

II.6.2. Effects assessment for humans

II.6.2.1 Introduction

The protection goals for the human species are three distinct sub-populations: workers, consumers and man exposed through the environment. A range of different data, human as well as experimental, acute as well as (sub-)chronic, needs to be considered as possible input from the available datasets (especially for existing substances).

II.6.2.2 Effect parameters

In EUSES, the quantitative risk characterisation for man is carried out by comparing the results

of the effects assessment with those of the exposure assessment. Quantitative risk assessment should address both local and systemic effects, for all endpoints of concern, i.e. acute toxicity, irritation/corrosivity, sensitisation, repeated dose toxicity, mutagenicity, carcinogenicity and reproductive toxicity (addressing a.o. fertility and developmental toxicity). Both spatial and time scales need to be comparable between the effect parameter and the exposure parameter as well as the route of exposure. In the case of workers and consumers, the scenarios can represent an acute situation or a more (sub)chronic type of exposure. Acute exposure is considered to occur infrequently and over a discrete period of time, which is usually significantly less than one day. Foreseeable misuses will often belong to this category. Risk characterisation for acute exposures is carried out on the basis of acute toxicity data. If exposures can be judged to occur repeatedly over a longer period of time, the scenario is qualified as subchronic or chronic. This time scale can apply to workers, consumers and man exposed via the environment. In such cases the risk characterisation is carried out on the basis of subchronic or chronic toxicity data, originating from repeated dose toxicity studies (28 and 90 days duration and longer), carcinogenicity studies and reproductive toxicity studies.

A distinction need to be made between substances with a threshold for toxicity and those without one. The latter situation applies to substances considered genotoxic or (possibly) carcinogenic to man by a genotoxic mechanism of action. The user can flag substances for these properties by entering the appropriate EU classification in the input (**Table II-14**). The dose-response analysis and risk characterisation for non-threshold substances differs from that of threshold substances.

Table II-14 Classification flags in EUSES.

Causes burns (C, R34)
Causes severe burns (C, R35)
Irritating to skin (Xi, R38)
Irritating to eyes (Xi, R36)
Risk of serious damage to eyes (Xi, R41)
Irritating to respiratory system (Xi, R37)
May cause sensitisation by inhalation (Xn, R42)
May cause sensitisation by skin contact (Xi, R43)
Limited evidence of a carcinogenic effect (Xn, R40)
May cause cancer (T, R45)
May cause cancer by inhalation (T, R49)
May cause heritable genetic damage (T, R46)
Possible risk of irreversible effects (Xn, R68)

In some cases no quantitative risk characterisation is possible. This applies, for instance, if an effect parameter for a specific route of exposure is lacking. Such data gaps may be filled by EUSES by conversion from effect parameters for other routes of exposure. This route-to-route extrapolation applies to both threshold and non-threshold effect parameters and will be explained in the next section (II.6.2.3.). Alternatively, effect parameters may be available for analogue substances and considered relevant input for the substance under investigation by the user. Since a threshold for local irritation and sensitisation very often cannot be derived from the toxicological database, EUSES allows the user to flag substances for these properties by entering the appropriate EU classification (EC, 2001) in the input (**Table II-14**).

Threshold substances

In the effects assessment of substances with a threshold for toxicity no-observed adverse effect levels (NOAELs) are derived (where possible) for each relevant endpoint. These NOAELs, which depend on the experimental study design (i.e. selected dose levels and spacing between dose levels) and do not take into account the dose-response curve, form the input for the risk characterisation. A NOAEL is preferred over a lowest-observed adverse effect level (LOAEL).

In parallel to the NOAEL/LOAEL, a benchmark dose may be derived. In the benchmark dose approach (for software see http://cfpub.epa.gov/ncea/cfm/bmds.cfm) a dose-response curve is fitted to the complete experimental data for each effect parameter, and the derived benchmark dose (BMD; EUSES uses the term Critical Effect Dose, CED) is independent of the experimental study design.
For acute toxicity the data usually do not allow the derivation of a NOAEL. If for acute toxicity both an LD50 value and a Discriminating Dose are entered, EUSES chooses the LD50 for the risk characterisation of acute exposure.

If both animal data and human data are available, as a general rule, well-reported relevant human data for any given toxicological end-point and route of exposure are to be given preference. Exemptions from this general rule are human volunteer studies, which are strongly discouraged from an ethical point of view and results of which should only be used in justified cases. The potential differences in sensitivity of human studies and animal studies should be taken into account, on a case-by-case basis.

Exposure of workers and consumers can be by inhalation, via the skin and through ingestion. The ingestion route for workers is the least probable. Relevant routes of exposure of man via the environment are inhalation of contaminated air and oral exposure to the contaminant in food and drinking water.

Based on the above analysis, ***Table II-15*** shows the effect parameters that can be found in the scientific database for substances which constitute relevant input for the risk characterisation for man in EUSES. Effects data need to be entered only as far as is necessary for the risk characterisation, depending on the subpopulation (worker, consumer, man exposed via the environment), time scale (acute, (sub-)chronic) and route of exposure (oral, dermal, inhalatory) for which the assessment is made.

Table II-15 *Effect parameters [a] for human risk characterisation in EUSES.*

Time scale	Effect parameter	Unit	Species	Exposure route
Acute	N(L)OAEL	$mg.kg_{bw}^{-1}.event^{-1}$	man	oral, dermal
	N(L)OAEL	$mg.m^{-3}$	man	inhalatory
	N(L)OEC in medium	$mg.cm_{medium}^{-3}$	man	dermal
	LD50	$mg.kg_{bw}^{-1}.event^{-1}$	mammal	oral, dermal
	LC50	$mg.m^{-3}$	mammal	inhalatory
	Discriminating Dose	$mg.kg_{bw}^{-1}.event^{-1}$	mammal	oral
(Sub-) chronic	N(L)OAEL	$mg.kg_{bw}^{-1}.d^{-1}$	man, mammal	oral, dermal
	N(L)OAEL	$mg.m^{-3}$	man, mammal	inhalatory
	N(L)OEC in medium	$mg.cm_{medium}^{-3}$	man	dermal
	N(L)OEC in food	$mg.kg_{food}^{-1}$	mammal	oral
	CED [b]	$mg/kg_{bw}^{-1}.d^{-1}$	man, mammal	oral, dermal
	CED	$mg.m^{-3}$	mammal	inhalatory

NOTE:

a In principle and where possible, for each endpoint of concern (acute toxicity, irritation/corrosivity, sensitisation, repeated dose toxicity, mutagenicity, carcinogenicity and reproductive toxicity) effect parameters have to be derived.

b Critical Effect Dose (or Benchmark Dose, BMD).

Non-threshold substances

In the effects assessment for carcinogens for which a threshold does not exist or cannot be determined, the T25 is the key effect parameter to be used in the risk characterisation. The T25 is defined in the TGD as the chronic dose that will give tumours in 25% of the animals at a specific tissue site after correction for spontaneous incidence within the standard life time of that species (Dybing *et al.*, 1997). Additionally the BMD05 (EUSES uses the term Critical Effect Dose CED), i.e. the Benchmark-dose representing a 5% response, should be used in certain cases where the dose-response data are adequate for modelling purposes and clearly show the T25 to be less relevant. The data for these effect parameters (TGD: dose-descriptors) should preferentially be derived from lifetime oral studies or inhalation studies according to accepted guidelines. Occasionally, skin painting studies may be used.

The lowest tumorigenic doses showing a significant response on biological or statistical basis are generally used for obtaining the T25. The T25 is calculated from the tumour incidences at the selected tumorigenic dose using linear intrapolation or extrapolation, e.g. in case of a net 15% incidence, the dose is multiplied by 25/15.The T25 may have to be corrected for intercurrent mortality.

The derivation of the CED is already referred to above. The derivation of the T25 or CED, possibly corrected for intercurrent mortality, is not part of EUSES 2.0 and these effect parameters should be entered as such.

II.6.2.3 Route-to-route extrapolation

When data are lacking for a relevant route of human exposure, the possibility of using data derived from another route of exposure may be considered. However, it should be realised that there is no simple, direct and generally applicable way in which toxicity data derived from one route of exposure can be used to assess the risks to man from exposure by another route. Factors to be taken into account are:

a. nature of effect: route-to-route extrapolation should be used only for substances that produce systemic toxicity distant from the site of entry into the body. It should not be used for substances that act directly and locally at the anatomical point of contact.
b. toxicokinetic data: differences among routes of exposure with respect to bioavailability (degree and rate of absorption), metabolism (a.o. first pass effects) and internal exposure pattern (kinetics).

EUSES provides some pragmatic approaches to calculating an approximate effect parameter by route-to-route extrapolation. Application of these methods is optional for the user.
Since the oral route is the route most often used in toxicity studies, the following extrapolations are the most common:

- Dermal effect parameter from an oral value: direct calculation of the dermal effect parameter from the value of the oral effect parameter using the absorption rates via either route.
- Inhalatory effect parameter from an oral value: the TGD (EC, 2003) gives two methods for extrapolation:

1) The ratio of the inhalatory LC50 to the oral LD50 is used to estimate the inhalatory N(L)OAEL from the oral N(L)OAEL.
2) Direct calculation of the inhalatory effect parameter from the value of the oral effect parameter using the absorption rates via either route and the respiration rate for the appropriate test species.

In EUSES only method 2 is implemented.
Other extrapolations (dermal to oral/inhalation, inhalation to oral/dermal) are also implemented.

II.6.2.4 Other conversions

NOEC to NOAEL
If a (sub-)chronic, oral N(L)OAEL or T25 in mg/kg body weight/day for mammals is not available but an N(L)OEC or T25 in mg/kg diet for mammals in food is known, EUSES converts the latter value to the former by taking into account the daily food consumption and the average body weight of the species concerned.

Ppm to $mg.m^{-3}$
In the exposure assessment for vapours, the unit ppm is often preferred by toxicologists since adverse effects are thought to be related to molecules per volume of air, rather than to weight of chemical per unit of volume. Dusts are measured gravimetrically and therefore, their concentration is expressed on a weight-per-volume basis. The sub-model EASE therefore predicts vapour exposure ranges in ppm whereas no-effect levels for inhalation exposure are expressed in $kg.m^{-3}$ (internally) or $mg.m^{-3}$ (on screen). EUSES will convert the output of EASE in ppm to a concentration in $kg.m^{-3}$.

Correction for time scale (duration and frequency) of exposure

EUSES does not recalculate effect parameters which are derived from experiments with an intermittent exposure schedule to yield a continuous effect parameter or vice versa. If required, the user will have to make his or own correction. For instance, the following formula can be used to recalculate the intermittent inhalatory NOAEL to yield a continuous value:

$$NOAEL_{inh,continuous} = NOAEL_{inh,\text{int}ermittent} \cdot \frac{x}{24} \cdot \frac{y}{7} \qquad \left[mg \cdot m^{-3}\right]$$

with x = hours per day of intermittent exposure
y = days per week of intermittent exposure

This formula should be used with caution, since it is certainly not applicable to all substances and all tests. Repeated exposure schedules allow time for recovery, whereas on the other hand threshold doses may be exceeded sooner. Therefore, the underlying assumption that the product of time and concentration is constant will not always be valid.

II.7 RISK CHARACTERISATION

In this module, the Risk Characterisation Ratios (RCR) are derived for all end-points, environmental and human. RCRs are derived by comparing exposure levels to suitable (no)-effect levels. For the environmental end-points, the RCR is the ratio of PEC to PNEC, while for the human end-points this is the so-called Margin Of Safety (MOS).

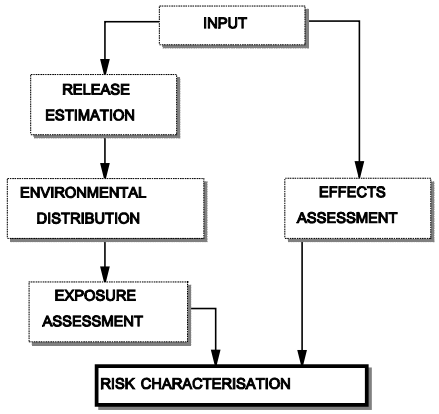

Figure II-25 *System structure.*

II.7.1 Risk characterisation for the environment

Having conducted the exposure assessment and the dose (concentration) - response (effect) assessment for all environmental compartments, the risk characterisation is carried out by comparing the PEC with the PNEC. This is done separately for each of the protection goals:

- aquatic ecosystem (freshwater and marine environment),
- terrestrial ecosystem,
- sediment-dwelling organisms,
- top predators,
- micro-organisms in sewage treatment plants.

A list of the various PEC/PNEC ratios for the inland and marine environment following from the previous chapters is given in ***Table II-16*** and ***Table II-17***. Depending on whether the risk characterisation is performed for a new substance or for an existing substance, different conclusions can be drawn on the basis of the PEC/PNEC ratio for the different end-points and different strategies can be followed when PEC/PNEC ratios greater than one are observed. More guidance is given in the TGD (EC, 2003).

Table II-16 *Overview of possible PEC/PNEC ratio's for the inland environmental risk assessment.**

Protection goal	**Local**	**Regional**
Aquatic organisms	$PEClocal_{water}$ / $PNEC_{water}$	$PECreg_{water}$ / $PNEC_{water}$
Sediment-dwelling organisms	$PEClocal_{sed}$ / $PNEC_{sed}$	$PECreg_{sed}$ / $PNEC_{sed}$
Terrestrial organisms	$PEClocal_{soil}$ / $PNEC_{soil}$	$PECreg_{agric}$ / $PNEC_{soil}$
STP micro-organisms	PEC_{stp} / $PNEC_{micro\text{-}organisms}$	
Fish-eating predators	(0.5 $PEClocal_{oral,fish}$ + 0.5 $PECreg_{oral,fish}$) / $PNEC_{oral}$	
Worm-eating predators	(0.5 $PEClocal_{oral,worm}$ + 0.5 $PECreg_{oral,worm}$) / $PNEC_{oral}$	

* It should be noted that these ratios must be derived for all stages of the life cycle of a compound.

Table II-17 *Overview of possible PEC/PNEC ratio's for the marine environmental risk assessment.**

Protection goal	**Local**	**Regional**
Aquatic organisms	$PEClocal_{water,marine}$ / $PNEC_{water, marine}$	$PECreg_{water, marine}$ / $PNEC_{water, marine}$
Sediment-dwelling organisms	$PEClocal_{sed, marine}$ / $PNEC_{sed, marine}$	$PECreg_{sed, marine}$ / $PNEC_{sed, marine}$
Fish-eating predators	$(0.5\ PEClocal_{water, ann, marine} + 0.5\ PECreg_{water, marine}) \cdot BCF_{fish} \cdot BMF / PNEC_{oral}$	
Top-predators	$(0.1\ PEClocal_{water, ann, marine} + 0.9\ PECreg_{water, marine}) \cdot BCF_{fish} \cdot BMF^2 / PNEC_{oral}$	

* It should be noted that these ratios must be derived for all stages of the life cycle of a compound.

II.7.2 Risk characterisation for humans

II.7.2.1 Introduction

For threshold-based effects, the quantitative risk characterisation is carried out by calculating 'Margins Of Safety' (MOS). The MOS is the ratio of an effect or no-effect parameter value, e.g. an acute, oral LD50, a subchronic, inhalatory NOAEL or CED, or a chronic LOEC in food, and an exposure value of corresponding time scale and route of exposure. For each subpopulation to be protected, the risk characterisation should be performed for each relevant exposure scenario, , for the time scales and route(s) of exposure chosen, and for each relevant endpoint. The following combinations of subpopulation, time scales and routes of exposure can occur:

- Man exposed via the environment:
  - Time scale: chronic.
  - Routes of exposure: inhalatory, oral and inhalatory combined.
  - Relevant endpoints: repeated dose toxicity, mutagenicity/carcinogenicity (unless via a non-threshold mode of action), reproductive toxicity.
- Consumers:
  - Time scales: acute and (sub-)chronic.
  - Routes of exposure: inhalatory, dermal and oral, all routes combined.
  - Relevant endpoints (depending on exposure scenario): acute toxicity, irritation/corrosivity, sensitisation, repeated dose toxicity, mutagenicity/carcinogenicity (unless via a non-threshold mode of action), reproductive toxicity.
- Workers:
  - Time scales: acute and (sub-)chronic.
  - Routes of exposure: inhalatory, dermal, inhalatory and dermal combined.
  - Relevant endpoints (depending on exposure scenario): acute toxicity, irritation/corrosivity, sensitisation, repeated dose toxicity, mutagenicity/carcinogenicity (unless via a non-threshold mode of action), reproductive toxicity.

The MOS should account for the various uncertainties and variabilities in the extrapolation from experimental data to the human situation (interspecies differences, intraspecies differences, differences in duration and in route of exposure, dose-response relationship), for the uncertainties in the available data set (adequacy of and confidence in available data set, nature of effect), and for the uncertainties in the exposure estimate of the exposure scenario under consideration. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOS (RMOS). In judging the acceptability of the MOS, in a second step of the quantitative risk characterisation the MOS is compared to this reference-MOS. Although the interpretation of the ratio MOS versus reference-MOS is outside the scope of EUSES, in general there will be concern if the MOS is well below the reference-MOS; if the MOS is well above the reference-MOS there will usually be no concern. If the MOS is in the range of the reference-MOS, a thorough evaluation of the aspects that can only be dealt with in a qualitative way, as well as the uncertainties in the exposure estimate, is required.

If no quantitative risk characterisation is possible because the available data do not allow the derivation of a threshold, the user can make this visible in the output of EUSES (see section II.6.2. Effects assessment for humans and **Table II-14**).

Next to the MOS approach, for biocides it is necessary to derive Acceptable Operator Exposure Levels (AOELs). The AOEL is a health-based exposure limit for operators and bystanders. It relates to the internal (absorbed) dose available for systemic distribution from any route of absorption and is expressed as internal level ($mg/kg_{bw}/d$). The AOEL is based on the highest level at which no adverse effect is observed in tests in the most sensitive relevant animal species, or, if appropriate data are available, in humans. As default-procedure, the AOEL is based on the NOAEL (or exceptionally, LOAEL) from an oral short-term toxicity study (28- or 90-day study), which is to be converted to an internal dose by correction for systemic bioavailability. To translate this internal N(L)OAEL into an AOEL, assessment factors accounting for uncertainties in the extrapolation from experimental data to the human situation have to be applied: hence, the internal N(L)OAEL is to be divided by the overall assessment factor or reference-MOS (RMOS). For risk characterisation the AOEL is compared to the internal exposure values of corresponding time scale. Although the interpretation of the ratio AOEL versus internal exposure is outside the scope of EUSES, in general there will be concern if the internal exposure is well above the AOEL; if the internal exposure is well below the AOEL there will usually be no concern.

For non-threshold-based effects (e.g. genotoxicity, genotoxic carcinogenicity), the MOS approach is not applicable, and an AOEL generally cannot be set. Two methods of risk characterisation are described in the TGD:

1. Determination of the lifetime cancer risk.
   The T25 derived (see section II.6.2.2), possibly converted to the appropriate route of human exposure, by default is first extrapolated to an equivalent human dose applying allometric scaling factors for the interspecies conversion and, if deemed necessary, a route-to-route assessment factor. The estimated lifetime daily exposure and the resulting HT25 are then used to derive the lifetime cancer risk (LR). This lifetime cancer risk is to be evaluated against existing criteria.
2. MOE-approach
   The Margin of Exposure approach is equivalent to the MOS-approach for threshold substances. The MOE is the ratio of the selected dose descriptor, T25 or CED05 (see section II6.2.2), possibly converted to the appropriate route of human exposure, and the estimated lifetime daily exposure. Next, the MOE should be compared to the reference MOE. Like the MOS, the MOE should account for the various uncertainties and variabilities in the extrapolation from experimental data to the human situation (interspecies differences, intraspecies differences, differences in duration and in route of exposure, dose-response relationship), for the uncertainties in the available data set (adequacy of and confidence in available data set, nature of effect), and for the uncertainties in the exposure estimate of the exposure scenario under consideration. Additionally, a specific assessment factor should be used for low risk extrapolation since, contrary to the risk assessment for threshold effects, for non-threshold effects a dose without effect cannot be derived. Therefore, a target margin between the high risk related to the dose descriptor and a very low risk for the population exposed needs to be set. The magnitude of the low risk extrapolation factor is policy-driven. Without prejudice, EUSES applies by default a low risk extrapolation factor of

250,000. This factor is derived from linear extrapolation of the lifetime cancer risk of 25:100, associated with the T25, to a default low reference risk level of 1:1,000,000.
All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOE (RMOE). In judging the acceptability of the MOE, in a second step of the quantitative risk characterisation the MOE is compared to this reference-MOE. Although the interpretation of the ratio MOE versus reference-MOE is outside the scope of EUSES, in general there will be concern if the MOE is well below the reference-MOE; if the MOE is well above the reference-MOE there will usually be no concern. If the MOE is in the range of the reference-MOE, a thorough evaluation of the aspects that can only be dealt with in a qualitative way, as well as the uncertainties in the exposure estimate, is required.

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II.7.2.2 Man exposed via the environment

The exposure of man via the environment is assessed by estimating the total daily intake of a substance in food, drinking water and air. The total intake via air is converted to an external oral dose and taken together with estimated intakes via food and drinking water. The risk characterisation is performed by calculating the MOS, i.e. the ratio between this total daily intake and the relevant effect parameter, which is the oral N(L)OAEL from repeated dose toxicity studies, carcinogenicity studies (unless carcinogenicity is via a non-threshold mode of action) and/or reproductive toxicity studies. It is assumed that man is exposed throughout his or her lifetime. Additionally, the air concentration to which man is estimated to be exposed can be compared to the inhalatory N(L)OAEL for these endpoints, if available. The comparisons should be made for both the local and the regional scale.
For genotoxic carcinogens the lifetime cancer risk and the MOE will be calculated based on the lifetime total daily intake and the relevant effect parameter, which is the oral T25 or CED05. A lifetime cancer risk and MOE can also be calculated based on the air concentration to which man is estimated to be exposed and the inhalatory T25 or CED05.

II.7.2.3 Consumers

Depending on the exposure scenario, for consumers MOSs can be calculated for both acute and (sub-)chronic endpoints and for all relevant routes of exposure, unless the effect is non-threshold based (see below) or for an endpoint the data do not allow the derivation of a threshold. It is essential to realise that the risk assessment is based on external exposure estimates or measurements only. It may be the case that absorption and bioavailability should be taken into account, e.g. when all exposure scenarios via all routes are combined.
For genotoxic carcinogens the lifetime cancer risk and the MOE will be calculated based on the estimated lifetime daily exposure and the relevant effect parameter, the oral, dermal or inhalatory T25 or CED05.

II.7.2.4 Workers

Depending on the exposure scenario, also for workers MOSs can be calculated for both acute and (sub-)chronic endpoints, unless the effect is non-threshold based (see below) or for an

endpoint the data do not allow the derivation of a threshold. Since the output of the EASE model is based on 8-hour time-weighted averages (see Section II.5.4.2 EASE) and cannot be considered as an estimate for acute exposures, it is to be noted that with the EASE output only MOSs for the (sub-)chronic endpoints can be calculated. For the MOS calculation for acute endpoints acute exposure data have to be introduced in EUSES separately. EASE predicts inhalation exposure ranges for vapours, fibres and non-fibrous dust. Since the model output is expressed as ranges, the result of the risk characterisation will also be a range.
It is essential to realise that the risk assessment is based on external exposure estimates or measurements only. In some cases, absorption and bioavailability should be taken into account, e.g. when for a certain scenario there is combined (dermal and inhalation) exposure.
For genotoxic carcinogens the lifetime cancer risk and the MOE will be calculated based on the estimated lifetime daily exposure and the relevant effect parameter, the dermal or inhalatory T25 or CED05. Since the daily exposure for workers applies to a working life of 40 years and a workday of 8 hours with 5 days per week and 40 weeks per year, it needs to be corrected to a lifetime exposure value by dividing with a factor of 8.4 (24/8 x 7/5 x 52/48 x 75/40)

II.8 HYDROCARBON BLOCK METHOD (HBM)

In this section, the Hydrocarbon Block Method (HBM) is described, which is implemented in EUSES for the environmental risk assessment of petroleum substances. The method was originally devised by CONCAWE (The Oil Companies' European Organisation for Environmental and Health Protection). The approach has been devised only recently and, hence, experience with its application is limited. Although work has been done to validate the general approach, it should be recognised that there are still uncertainties regarding some technical details which should be borne in mind when considering the outcome of the risk characterisation.

II.8.1 Outline of the method

There are many petroleum substances (e.g. refinery streams and solvents) which, although described by a single EINECS number, are hydrocarbon mixtures of varying degrees of complexity. The compositional complexity of many petroleum hydrocarbon substances is compounded by the fact that their composition will vary depending on the source of crude oil and the details of the process used in their production. This compositional complexity poses particular problems when environmental risk assessment is required. Difficulties in carrying out a risk assessment for petroleum substances arise because the individual components have specific and different physico-chemical properties, ecotoxicological properties, and potentials for being degraded in the environment. Each component will be subjected to different distribution and fate processes on release to the environment. Each component will behave independently and reach its own concentration in each environmental compartment. Therefore, a PEC for the whole petroleum substance does not exist. It would in theory be possible to identify each individual component of a petroleum substance and then to determine a PEC for each of them. In practice this approach demands a degree of analytical resolution that is not achievable for most petroleum substances and, even if possible, handling such large quantities of data would be impractical. However, since hydrocarbons of similar structure will have similar physico-chemical properties and environmental-degradation potentials, they will have similar distributions and fates within a given environment. It is therefore possible to group or 'block' such hydrocarbons, so that components having similar properties may be considered together (it should be noted that a 'block' may consist of a single component or a large number of components with similar fate and distribution properties). Once the blocks for a substance have been established, PEC values can be calculated for each block for each environmental compartment.

Since PECs can be obtained for single components, or groups of similar components only, it follows that PNECs must also be estimated for the same individual components or groups of components. Therefore, ecotoxicity data obtained on the whole substance, whether obtained using Water-Accommodated Fractions (WAFs) or dispersions, cannot be used to estimate PNECs. PNECs must be based on the toxicity of the individual blocks. These blocks should show similar modes of action.

From the above it is clear that the PEC/PNEC ratio of the whole substance cannot be derived directly, as neither the PEC nor the PNEC for the whole substance will be available. The

PEC/PNEC ratio is therefore derived from the PEC/PNEC ratios of the blocks of components, based on the proportional contribution of each of the blocks to the composition of the whole substance, and assuming that effects will be concentration-additive:

$$\frac{PEC}{PNEC}\ whole\ substance = \frac{PEC_A}{PNEC_A} + \frac{PEC_B}{PNEC_B} + \frac{PEC_C}{PNEC_C}\ etc.$$

where A,B,C etc. are the blocks.

II.8.2 Definition of blocks

Blocks will primarily be defined on the basis of those physico-chemical and degradation properties that are key in determining the distribution and fate of their components. Care should be taken to ensure that blocks are not so wide as to include components without broadly similar fates and distributions after release. Similarly, blocks should, whenever possible, contain substances with a similar mode of action and a narrow range of toxicity. Both the fate and toxicity criteria for block definition need to be satisfied simultaneously. More guidance on defining blocks is given in Appendix IX of Part II of the TGD (EC, 2003).

II.8.3 Additivity of toxicity

Petroleum substances are composed mainly of hydrocarbons. These act via a similar mode of toxic action: non-polar narcosis. Therefore, it can be assumed that for hydrocarbon components of petroleum substances effects will be simple concentration-additive. The situation is less clear with regard to chemicals with different modes of action. Components of petroleum hydrocarbons with specific modes of action are likely to be blocked together, provided they have the same specific mode of action. In the first instance the PEC/PNEC ratio of this block shall be added to the total PEC/PNEC ratio. From this it will be clear whether the PEC/PNEC ratio for that block influences any potential for environmental risk for the specific petroleum substance. If it does, further investigation on whether or not there is additivity of the modes of action would be required.

Chemicals which may have a specific mode of action that are present in petroleum substances may be metallic constituents (e.g. vanadium and nickel in crude fuel oils and asphalt) and heterocyclic compounds (e.g. carbazole compounds in cracked fuels). However, they are often present in low amounts compared to the components having a non-specific mode of action.

II.8.4 QSARs

Identification of blocks when applying the HBM will frequently be dependent on the use of QSARs for the estimation of physico-chemical properties (e.g. log *Kow*, water solubility, melting point and vapour pressure) and degradation rates (e.g. photodegradation and hydrolysis rates) when measured values are not available. There are reasonably well accepted methods for the generation of these data using readily available databases or QSARs. There are no widely accepted QSARs for biodegradation but it is considered adequate, at least for screening, if experimentally determined rate constants for the blocks of interest are not available, to use QSAR estimates for block identification according the principles laid down in Chapter 4 of the TGD (EC, 2003) on the Use of QSARs.

The use of QSARs is well established for predicting the acute toxicity of simple hydrocarbons, and can be used to supplement the available ecotoxicity data. Whilst the accuracy of QSARs for more complex hydrocarbons and for chronic toxicity may need further consideration, they provide an adequate default when experimental data are not available (in particular where the values are found not to be crucial to the outcome of the risk assessment). For block identification, QSARs for short-term (algae, daphnids and fish) and long-term (daphnids and fish) toxicity are given in Chapter 4 of the TGD (EC, 2003). These QSARs can be used for chemicals with a non-specific mode of action, i.e. for most petroleum substances. Considering the standard assessment factors, a factor of 10 on the QSAR derived long-term NOEC is used.

II.9 ENVIRONMENTAL RISK ASSESSMENT FOR METALS AND METAL COMPOUNDS

The methods for risk assessment of new and existing organic chemicals are used as a starting point for the risk assessment of metals. There are a number of fundamental differences between metals and organic chemicals that must be taken into account when assessing the risks to man and the environment, e.g.:

- Unlike most organic chemicals, metals, and a limited number of organometallo-compounds like methylmercury and methyltin, are a class of chemicals of natural origin. As a consequence, natural background concentrations and the exposure due to these background concentrations should be taken into account during risk assessment.
- The availability of metals for uptake by organisms under field conditions is limited, will vary from site to site and is highly dependent on the speciation of the metal. Hence, it is of the utmost importance that both PEC and PNEC are based on similar levels of availability in both exposure and effect assessment, taking the speciation into account.
- Some of the metals are essential trace elements. Within a certain range of concentrations element requirements are satisfied and ecosystem functioning is maintained. Both in data selection and in setting PNEC values care should be taken that these element requirements are satisfied.
- The same toxic form can originate from a variety of different substances, e.g. Zn^{2+} from $ZnSO_4$, $ZnCl_2$ etc. In general, therefore, it is necessary to take into account all metal species that are emitted to the environment, which in the end lead to concentrations of the toxic form.

Substantial levels of information are available regarding the fate and toxicity of metal ions and this information will be examined to improve the assessment process. However, it is recognised that many of the specific fate and toxicity extrapolations are either not appropriate or need modification. The interaction of metal ions with the media in both the aquatic and soil compartments may result in a high level of uncertainty regarding the true level of bioavailability of the toxic species necessary for a practical assessment.

II.9.1 Exposure assessment

When the metal compound is soluble or can be transformed to a soluble form, the exposure calculations can be based on the relevant soluble metal ion. Since the actual bioavailability of the metal ion will be determined by the properties of the receiving medium, such as the pH and water hardness, the precise physico-chemical characteristics of this receiving medium must be defined. In general, it will be defined in a way which optimises the bioavailability of the toxic species with respect to the ranges for pH, water hardness etc. that are found in the natural environment. This environmental definition will probably differ for each metal assessed.

Transport of metals between the aqueous phase and soil, sediment and suspended matter should be described on the basis of measured solid-water equilibrium partition coefficients in soil, sediment and suspended matter (*Kp*), respectively, instead of using common mathematical relationships based on, for example, octanol-water partition coefficients, as is usually done for organic chemicals (see Section II.4.1). The same applies to the bioconcentration factors

required: only experimentally determined values should be used (see Section II.5.1). For soils, the *Kp*-values to be used should, as far as possible, be derived for the soil type of interest. The soil usage should also be taken into account (for instance cultivated versus non-cultivated soils) since this may be of importance for the most appropriate *Kp*-values.

II.9.2 Equilibrium partitioning/bioavailability

It should be borne in mind that *Kp*-values are both environment- (site) and compound-specific, and depend on the speciation of the metal in both the solid and the liquid (pore water) phase. In a natural soil or sediment system, metals can be distributed over the following fractions:

- dissolved in the pore water,
- reversibly or irreversibly bound to soil or sediment particles,
- reversibly or irreversibly bound to organic ligands,
- encapsulated in secondary clay minerals and metal (hydr)oxides,
- encapsulated in the primary minerals.

It is recognised that for various organisms, only the metal species present in the aqueous phase (pore water) are available for direct uptake by biota and thus mainly responsible for effects on biota. Other uptake routes may also be important, especially for metals with high *Kp*-values, but at the moment little is known on how to treat these processes quantitatively in the risk assessment.

II.9.3 Effects assessment

Toxicity data are available for most metals in sufficient quantity, since there are few compounds, and various toxicity data exist at least for the soluble metal salts. Most data are available for the toxic effects of metals on aquatic organisms, with fewer data available on terrestrial and sediment-dwelling organisms. Most data are based on total concentrations of the metals under investigation. These data can be used for the effects assessment in all compartments following the procedures for organic compounds (see Section II.6). However, some metal-specific criteria must be taken into account:

- Physico-chemical test conditions that define the metal speciation and bioavailability should be relevant for field conditions: water hardness, pH, alkalinity, presence of complexing agents (humic acids and EDTA).
- The content of metal already present in the test medium, especially for soils taken from the field and natural waters. As metals are natural constituents of the biosphere, these background concentrations can influence the test results. However, it should be noted that the bioavailability of the background concentration for soils is probably less than that of the ‘added’ metal.
- With regard to essential metals, organisms of a given habitat are conditioned to the natural concentration range for essential elements. Within this range they can regulate their metal uptake in such a way that their internal concentration is kept relatively stable (homeostasis). This implies that organisms tested should originate and be cultivated within this optimum concentration range.

PNECs can be derived through the application of assessment factors on the basis of the available data assessed according to the criteria given above. However, because of the specific mode of action that metals may have for some species, care should be taken in extrapolating short-term toxicity data to the PNEC using the standard assessment factors. Calculated PNECs derived for essential metals may not be lower than natural background concentrations.

Although some exceptions exist, in general ionic metal species are considered to be the dominant metal species taken up, and are thus considered to be the metal species responsible for the toxic effect.

II.9.4 Risk Characterisation

The risk characterisation of metals basically follows the principles set out in Section II.7 . However, it is of the utmost importance that both PEC and PNEC are based on similar levels of availability. Since sufficient monitoring data are available for most metals, risk assessment will often be based on measured rather than calculated environmental concentrations, especially for a regional assessment. Usually, most monitoring data deal with total concentrations. Especially in the case of aqueous systems, it is often possible to convert measured total concentrations to dissolved concentrations. For terrestrial systems this is possible by applying the appropriate *Kp*-values.

III MODEL CALCULATIONS

In this chapter, the model equations are presented with a short explanation of the modelled processes. For background and discussion on these model approaches, the reader is referred to Chapter II and the TGD (EC, 2003). Chapter III follows the same structure as the previous chapter; the modules and sub-modules described in Chapter II are handled separately.

Contents

III.1 INTRODUCTION

This chapter, the model calculations of the system are specified in detail. As discussed in the previous chapter, the system consists of six main modules: Input, Release Estimation, Environmental Distribution, Exposure Assessment, Effects Assessment and Risk Characterisation. In several modules, sub-modules are distinguished when the calculations describe a specific, well-defined process. As an example, the environmental distribution module has a separate sub-module describing sewage treatment. Each module or sub-module is first described by the parameters that are required for the calculations (input), the intermediate results (which are also shown to the user), and the resulting parameters used in subsequent calculations (output). The parameters are presented in the following manner:

Input

[Symbol] [Description of required parameter] [Unit]

These parameters are the input to the module. They may be derived either from the data set, or from the output of other modules.

Intermediate results

[Symbol] [Description of intermediate parameter] [Unit] ^{c}

These parameters are the results of the calculations in this module, but are not used in other modules. They are output to the screen to give the user the opportunity to modify these results. In some modules, several levels of intermediate results are specified when an intermediate parameter influences another intermediate parameter.

Output

[Symbol] [Description of resulting parameter] [Unit] ^{c}

These parameters are the results of the calculations in this module which are used in other modules. In some modules, several levels of output are specified when an output parameter influences another output parameter.

For the explanation of symbols used in an equation, the same table format is used:

Input

[Symbol] [Description of required parameter] [Unit] S/D/O/P/^{c}/*

Output

[Symbol] [Description of resulting parameter] [Unit] O/^{c}/*

The S, D, O or P classification of a parameter indicates the status:

S Parameter must be present in the input data set for the calculation to be executed (there is no method implemented in the system to estimate this parameter; no default value is set).

D Parameter has a standard default value (most defaults can be changed by the user). Defaults are presented in the sub-module, where they are used in separate tables. Sets of changed default values can be saved.

U This parameter is 'unspecified', no default value is set.

O Parameter is output from another calculation (most output parameters can be overwritten by the user with alternative data).

P Parameter value can be chosen from a 'pick-list' with values.

^{c} Default or output parameter is closed and cannot be changed by the user.

* An asterisk is added when a parameter can be set to a different value on the regional and continental spatial scale.

For the symbols, as far as possible, the following conventions are applied:

- Parameters are mainly denoted in capitals.
- Specification of the *parameter* is in lower case.
- Specification of the *compartment* for which the parameter is specified is shown as a subscript.

The following symbols are frequently used:

E	for emissions (direct and indirect via STP)	[kg.d^{-1}]
F	for 'dimensionless' fractions	[kg.kg^{-1}] or [m^3.m^{-3}]
C	for the concentration of a chemical	[kg$_c$.kg^{-1}] or [kg$_c$.m^{-3}]
RHO	for densities of compartments or phases	[kg.m^{-3}]
K	for inter-media partition coefficients	[-] or [m^3.kg^{-1}]
k	for rate constants (e.g. degradation rates)	[d^{-1}]
DT50	for half-lives	[d]
T	for a fixed period of time (e.g. an exposure period)	[d]
TEMP	for temperature	[K]
DEPTH	for soil or water depth	[m]
PEC	for Predicted Environmental Concentrations	[kg$_c$.kg^{-1}] or [kg$_c$.m^{-3}]
PNEC	for Predicted No-Effect Concentrations	[kg$_c$.kg^{-1}] or [kg$_c$.m^{-3}]
RCR	for Risk Characterisation Ratios	[-]

As an example, the symbol Foc_{soil} means the fraction (*F*) organic carbon (*oc*) in the soil compartment ($_{soil}$). For other parameters, interpretable symbols are chosen. SI units are applied for the sake of consistency in the program. As a consequence, some parameters have an uncommon unit (e.g. *Kp* will internally have the unit m^3.kg^{-1} instead of the more commonly used l.kg^{-1}). Kilograms of chemical are indicated by the unit kg$_c$. Other kilograms will usually be indicated as wet weight or dry weight (kg$_{wwt}$ and kg$_{dwt}$, respectively). It should be noted that for the dimension 'time' the non-SI unit 'days' is used, since this is a more relevant unit in the framework of risk assessment.

The equations in this chapter are numbered. The same equation numbering is also used in the EUSES on-line help and in the code of the program.

III.2 INPUT MODULE

In the input module, the basic scope of the assessment is selected and basic substance information must be entered. This includes substance identification and physico-chemical properties. Other input data such as toxicity data or measured partition coefficients can be entered in the dedicated sub-modules.

III.2.1 Assessment types

The user of EUSES is able to determine the scope of the risk assessment at the start of the program. It is possible to choose between:

Assessment types

Environmental assessment of Biocides (biocides, non-agricultural) on the local scale only

I Environmental assessment (local scale).
II Assessment for predators exposed via the environment (local scale).
III Assessment for humans exposed via the environment (local scale).
IV Assessment for humans exposed to or via consumer products (non-professional user).

New and Existing Substances and Biocides

I Environmental assessment, with two options:
  Ia local scale
  Ib regional scale
II Assessment for predators exposed via the environment (both scales combined)
III Assessment for humans exposed via the environment, with two options:
  IIIa local scale
  IIIb regional scale
IV Assessment for humans exposed to or via consumer products.
V Assessment for humans exposed at the workplace.

Hydrocarbon Block method

- Block method for mixtures, local and regional scale

The calculations for the different assessment types are given in Sections III.3 to III.7. The specific differences in the assessment with the Hydrocarbon Block Method and the additional requirements for assessment of metals and metal compounds are described in Section III.8 and III.9.

III.2.2 Input data

The following data on substance identification and physicochemical data need be entered in this module.

Also data on partition coefficients and bioconcentration factors, on degradation and transformation and on removal rates constants for soil can be entered in this module. Information on these data can be found in the chapter 4.1 (partition coefficients), 4.2 (degradation and transformation rates), 4.4.6 (bioconcentration factor for aquatic biota) 4.5.4 (removal rate constants local soil), 5.1 and 5.2 (bioconcentration factors for secondary poisoning and human exposure). The input data can be related to the Kow (using a QSAR or Koc), have defaults that can be overwritten or are calculated from other parameters and can be overwritten. Besides, information on biodegradation is needed.

Substance identification input

	general name	
	CAS no.	
	EC notification no.	
	EINECS no.	
Physico-chemical properties input		
MOLW	molecular weight	[$kg_c.mol^{-1}$]
Kow	octanol-water partition coefficient	[-]
$VPtemp_{test}$	vapour pressure at the temperature of the data set	[Pa]
$SOLtemp_{test}$	water solubility at the temperature of the data set	[$kg_c.m^{-3}$]
TEMPtest	temperature of the measured physico-chemical data	[K]
TEMPboil	boiling point (used for some release estimations and EASE)	[K]
TEMPmelt	melting point (used for solids only and for EASE)	[K]
Physico-chemical properties output		
$VPtemp_{env}$	vapour pressure at the environmental temperature	[Pa]
$SOLtemp_{env}$	water solubility at the environmental temperature	[$kg_c.m^{-3}$]

Table III-1 Defaults for the physico-chemical properties input

Parameter	Symbol	Unit	Value
Enthalpy of vaporisation	H_{0_VP}	[$J.mol^{-1}$]	5.10^4
Enthalpy of solution	H_{0_SOL}	[$J.mol^{-1}$]	1.10^4
Gas constant	R	[$Pa.m^3.mol^{-1}.K^{-1}$]	8.314 [a]
Environmental temperature	TEMP	[K]	
Freshwater environment (12 °C)			285
Marine environment (12 °C)			285[b]

[a] This default cannot be changed by the user.

[b] Although the TGD (2003) proposed a temperature of 9 °C, due to the small differences it was decided to keep the temperature the same for all compartments on the moderate global scale the same.

Experimentally derived chemical properties will usually be measured at a standard temperature, which is different from the temperature used in the models of EUSES. For most chemicals and most properties, a temperature correction will not be necessary between the standard 20 or 25 degrees and the environmental temperature used in the system (by default 12 °C in the environment and 15 °C in the STP). When experimentally determined physico-chemical data

have been obtained at a temperature which, for the substance under consideration, would significantly change when extrapolated to the relevant temperature of the exposure models employed, then a temperature correction should be considered.

The vapour pressure may for some substances change considerably according to the temperature even within a temperature range of only 10 °C. In this case a general temperature correction should be applied according to the following equation:

$$VPtemp_{env} = VPtemp_{test} \cdot e^{\left(\frac{H_{0\_VP}}{R} \cdot \left(\frac{1}{TEMPtest} - \frac{1}{TEMPenv}\right)\right)} \quad \textbf{(1)}$$

Care must be taken when the melting point is within the extrapolated temperature range. The vapour pressure of the solid phase is always lower than the extrapolated vapour pressure of the liquid phase.

The same approach can be followed for correcting the water solubility:

$$SOLtemp_{env} = SOLtemp_{test} \cdot e^{\left(\frac{H_{0\_SOL}}{R} \cdot \left(\frac{1}{TEMPtest} - \frac{1}{TEMPenv}\right)\right)} \quad \textbf{(2)}$$

Input			
$VPtemp_{test}$	vapour pressure at the temperature of the data set	[Pa]	S
$SOLtemp_{test}$	water solubility at the temperature of the data set	[$kg_c.m^{-3}$]	S
H_{0_VP}	enthalpie of vapourisation	[$J.mol^{-1}$]	D
H_{0_SOL}	enthalpie of solution	[$J.mol^{-1}$]	D
R	gas constant	[$Pa.m^3.mol^{-1}.K^{-1}$]	D
TEMPtest	temperature of the measured physico-chemical data	[K]	S
TEMPenv	environmental temperature	[K]	D
Output			
$VPtemp_{env}$	vapour pressure at the environmental temperature	[Pa]	O
$SOLtemp_{env}$	water solubility at the environmental temperature	[$kg_c.m^{-3}$]	O

III.3 RELEASE ESTIMATION FOR NEW AND EXISTING SUBSTANCES AND BIOCIDES

Releases to all spatial scales are estimated, based on use pattern and substance properties. The tables in Appendix III provide default release estimates for each category of substance. Release estimation applies either the tonnage of the substance as a starting point or representative dimensions (quantities, concentrations, etc.) for the process or the average consumption. In both cases emission factors (fractions released to the relevant environmental compartments) are used. These emission factors have been collected in the A-tables of Appendix III. In the TGD the A-tables the (realistic) worst case estimates are based on expert judgement and in some cases on use category documents. In this version of EUSES the emission factors of specific emission scenario documents of the TGD have been incorporated.
The B-tables of the TGD contain data to determine the estimates for the daily quantity applicable for each relevant stage of the life cycle based on the tonnage. In this version of EUSES specific data on representative source size of the emission scenario documents of the TGD have been incorporated as well.
It should be noted that release estimation using average capacities or consumption concerns the local scale only. For the regional scale an "overall" emission factor should be used.

Input: use pattern of the substance		
PRODVOL	production volume of chemical in EU	[$kg_c.d^{-1}$]
HPVC	high-production volume chemical	[yes/no]
IMPORT	volume of chemical imported to EU	[$kg_c.d^{-1}$]
EXPORT	volume of chemical exported from EU	[$kg_c.d^{-1}$]
INDCAT	industrial category	[-]
USECAT	use category	[-]
MAINCAT	main category (for existing substances)	[-]
$Ftonnage_k$	fraction of tonnage for application *k*	[-]
$Fchem_{form}$	fraction of chemical in formulation	[-]
	relevant steps in life cycle	
	specific information on substance use pattern	
Input: physico-chemical properties		
SOL	water solubility	[$kg_c.m^{-3}$]
VP	vapour pressure	[Pa]
MOLW	molecular weight	[$kg_c.mol^{-1}$]
TEMPboil	boiling point (for some release estimations only)	[K]
Intermediate results 1		
TONNAGE	tonnage in EU	[$kg_c.d^{-1}$]
$TONNAGE_k$	relevant tonnage for application *k* in EU	[$kg_c.d^{-1}$]
PRODVOLreg	production volume of chemical in region	[$kg_c.d^{-1}$]
TONNAGEreg	tonnage in region	[$kg_c.d^{-1}$]
$TONNAGEreg_{form}$	regional tonnage of formulation used	[$kg_c.d^{-1}$] [c]
PRODVOLcont	production volume of chemical in continent	[$kg_c.d^{-1}$] [c]
TONNAGEcont	tonnage in continent	[$kg_c.d^{-1}$] [c]
Intermediate results 2		
$F_{i,j}$	fraction of tonnage released during stage *i* to compartment *j*	[-]
$Fmainsource_i$	fraction of the main local source during life-cycle stage *i*	[-]
$Temission_i$	number of days per year for the emission in stage *i*	[$d.yr^{-1}$]
Intermediate results 3		
$RELEASEreg_{i,j}$	regional release during life-cycle stage *i* to compartment *j*	[$kg_c.d^{-1}$]
$RELEASEcont_{i,j}$	continental release during life-cycle stage *i* to compartment *j*	[$kg_c.d^{-1}$]
Output		
$Elocal_{i,j}$	local emission during episode to comp. *j* during stage *i*	[$kg_c.d^{-1}$]
$Temission_i$	number of days per year for the emission in stage *i*	[$d.yr^{-1}$]
$Ereg_j$	total regional emission to compartment *j* (annual average)	[$kg_c.d^{-1}$]
$Ereg_{direct\text{-}water}$	direct regional emission to surface water (annual average)	[$kg_c.d^{-1}$]
$Econt_j$	total continental emission to compartment *j* (annual average)	[$kg_c.d^{-1}$]
$Econt_{direct\text{-}water}$	direct continental emission to surface water (annual average)	[$kg_c.d^{-1}$]

With:

i	stage of the life cycle	*j*	compartment
1	production	air	air
2	formulation	water	(waste) water
3	industrial use	ind	industrial soil (regional scale only)
4	private use	surf	surface water (regional scale only)
5	service life	agric	agricultural soil (regional only, no estimation
6	waste treatment		

Table III-2 *Defaults for emission calculations.*

Parameter	Symbol	Unit	Value
Fraction of EU production volume of substance produced in the region	$Fprodvol_{reg}$	[-]	1 [a]
Fraction connected to sewer systems	$Fconnect_{stp}$	[-]	0.80

a For life cycle stage Private use the default remains 0.10.

III.3.1 Calculation of the tonnage of substance

The total production volume in the EU is available in the data set and denoted by *PRODVOL*. *TONNAGE* is the volume of substance that is used for subsequent life-cycle stages.

$$TONNAGE = PRODVOL + IMPORT - EXPORT \quad (3)$$

Input			
PRODVOL	production volume of chemical in EU	[$kg_c.d^{-1}$]	S
IMPORT	volume of chemical imported to EU	[$kg_c.d^{-1}$]	S
EXPORT	volume of chemical exported from EU	[$kg_c.d^{-1}$]	S
Output			
TONNAGE	tonnage of substance in EU	[$kg_c.d^{-1}$]	O

When a substance has more than one application, the tonnage must be broken down for the different, relevant applications (indicated by the index *k*). Each application has a different combination of industrial and use category (INDCAT/USECAT).

$$TONNAGE_k = Ftonnage_k \cdot TONNAGE \quad (4)$$

Input			
TONNAGE	total tonnage of substance in EU	[$kg_c.d^{-1}$]	O
$Ftonnage_k$	fraction of total tonnage for application *k*	[-]	S
Output			
$TONNAGE_k$	relevant tonnage for application *k* in EU	[$kg_c.d^{-1}$]	O

This also implies that all parameters depending on the tonnage should also receive a subscript *k* (e.g. releases, environmental concentrations, risk characterisation ratios). This is not shown in this rest of this documentation.

It should be noted that the production volume is *not* broken up according to this fraction since a chemical is usually produced according to one production method (independent of subsequent usages). In the program, production *can* be set to 'relevant' for more than one usage. In that case, each production stage can be calculated with the relevant percentage of the total production volume.

If application *k* concerns a biocide the life cycle stages concerning the application – such as industrial use – have to be evaluated separately (see section III.2.1. Assessment types). This can

only be done for the local scale. The calculations are presented in III.3.6.

A fixed fraction of total EU production and tonnage is assumed for the standard region. The regional and continental fate calculations are done with a nested multimedia model (as explained in Section II.4.4). Therefore, the produced volume and tonnage for the continental box must exclude the values for the regional system.

$$PRODVOLreg = Fprodvol_{reg} \cdot PRODVOL \quad (5)$$

$$PRODVOLcont = (1 - Fprodvol_{reg}) \cdot PRODVOL \quad (6)$$

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \quad (7)$$

$$TONNAGEcont = (1 - Fprodvol_{reg}) \cdot TONNAGE \quad (8)$$

Input			
PRODVOL	production volume of chemical in EU	[$kg_c.d^{-1}$]	S
TONNAGE	tonnage of substance in EU	[$kg_c.d^{-1}$]	O
$Fprodvol_{reg}$	fraction of production volume for region	[-]	D
Output			
PRODVOLreg	regional production volume of substance	[$kg_c.d^{-1}$]	O
TONNAGEreg	regional tonnage of substance	[$kg_c.d^{-1}$]	O
PRODVOLcont	continental production volume of substance	[$kg_c.d^{-1}$]	O^c
TONNAGEcont	continental tonnage of substance	[$kg_c.d^{-1}$]	O^c

III.3.2 Releases during each life-cycle stage

III.3.2.1 Release information from A and B-tables of Appendix III

The fractions released at every relevant stage of the life cycle and to every relevant compartment are derived from the A-tables in Appendix III. These fractions are denoted by $F_{i,j}$, where *i* is the stage in the life cycle and *j* is the compartment. For the local assessments, the B-tables provide the fraction from a main point source and the expected number of emission days per year. In the A and B-tables of Appendix III, the production volume for the region (*PRODVOLreg*) must be used for *T* at the stage of production. *TONNAGEreg* should be used for the subsequent life-cycle stages. It should be noted that in the emission tables, the production volume or tonnage is expressed in tonnes/year. When a chemical is applied in a formulation at a rather low level, the tonnage must be corrected to the tonnage of the total formulation. This tonnage is only used to retrieve the correct fraction of the main source and number of emission days from the B-tables.

$$TONNAGEreg_{form} = \frac{1}{Fchem_{form}} \cdot TONNAGEreg \qquad (9)$$

Input			
TONNAGEreg	regional tonnage of substance	[$kg_c.d^{-1}$]	O
$Fchem_{form}$	fraction of chemical in formulation	[-]	S
Output			
$TONNAGEreg_{form}$	regional tonnage of formulation used	[$kg_c.d^{-1}$]	O[c]
Input for A and B tables in Appendix III			
PRODVOLreg	regional production volume of chemical (stage of production)	[$kg_c.d^{-1}$]	O
TONNAGEreg	regional tonnage of substance (A-tables)	[$kg_c.d^{-1}$]	O
$TONNAGEreg_{form}$	regional tonnage of substance (B-tables)	[$kg_c.d^{-1}$]	O[c]
HPVC	high-production volume chemical	[yes/no]	P
INDCAT	industrial category	[-]	P
USECAT	use category	[-]	P
MAINCAT	main category (for existing substances)	[-]	P
SOL	water solubility	[$kg_c.m^{-3}$]	S
VP	vapour pressure	[Pa]	S
MOLW	molecular weight (only used to estimate log Henry in Table A3.7 for industrial use in IC=8)	[$kg_c.mol^{-1}$]	S
TEMPboil	boiling point (only for some release estimations)	[K]	S
Output from A tables in Appendix III			
$F_{i,j}$	fraction of tonnage released during stage *i* to compartment *j*	[-]	O
Output from B tables in Appendix III			
$Fmainsource_i$	fraction of the main local source during life cycle stage *i*	[-]	O
$Temission_i$	number of days per year for the emission in stage *i*	[$d.yr^{-1}$]	O

In case there is more than one usage of a chemical, the emission tables are accessed with the regional tonnage $TONNAGEreg_k$ derived from Equation (4) and (7). It should be noted that the production volume is *not* broken up. In case the Block Method is used (see Section III.8) the total tonnage/production volume is used to access the tables. The break up for the separate blocks is done in the calculation of the releases to each compartment (Sections III.3.2.2 and III.3.2.3).

III.3.2.2 Continental releases

The annual average release per stage of the life cycle can be calculated with the following series of equations. For each relevant stage, the losses in the previous stage are taken into account. Note that releases during production are *not* taken into account in the other stages, as these releases will generally already be accounted for in the reported production volume.

1. production

$RELEASEcont_{1,j}$:	air	$F_{1, air} \cdot PRODVOLcont$
	water	$F1, water \cdot PRODVOLcont$
	soil	$F_{1, ind} \cdot PRODVOLcont$
	surf	$F_{1, surf} \cdot PRODVOLcont$
	total	$\Sigma F_{1, j} \cdot PRODVOLcont$
	amount used:	$TONNAGEcont$

2. formulation

$RELEASEcont_{2,j}$:	air	$F_{2, air} \cdot TONNAGEcont$
	water	$F_{2, water} \cdot TONNAGEcont$
	soil	$F_{2, ind} \cdot TONNAGEcont$
	surf	$F_{2, surf} \cdot TONNAGEcont$
	total	$\Sigma F_{2, j} \cdot TONNAGEcont$
	rest:	$(1-\Sigma F_{2, j}) \cdot TONNAGEcont$

3. industrial use

$RELEASEcont_{3,j}$:	air	$F_{3, air} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEcont$
	water	$F_{3, water} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEcont$
	soil	$F_{3, ind} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEcont$
	surf	$F_{3, surf} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEcont$
	total	$\Sigma F_{3, j} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEcont$

4. private use

$RELEASEcont_{4,j}$:	air	$F_{4, air} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEcont$
	water	$F_{4, water} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEcont$
	soil	$F_{4, ind} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEcont$
	surf	$F_{4, surf} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEcont$
	total	$\Sigma F_{4, j} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEcont$
	rest:	$(1-\Sigma F_{3, j} - \Sigma F_{4, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$

5. service life

$RELEASEcont_{5,j}$:	air	$F_{5, air} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
	water	$F_{5, water} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
	soil	$F_{5, ind} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
	surf	$F_{5, surf} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
	total	$\Sigma F_{5, j} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$

6. waste treatment

$RELEASEcont_{5,j}$:

air	$F_{6,\,air} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j} - \Sigma F_{5,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
water	$F_{6,\,water} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j} - \Sigma F_{5,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
soil	$F_{6,\,ind} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j} - \Sigma F_{5,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
surf	$F_{6,\,surf} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j} - \Sigma F_{5,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$
total	$\Sigma F_{6,j} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j} - \Sigma F_{5,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEcont$

Input			
$F_{i,j}$	fraction of tonnage released during stage *i* to compartment *j*	[-]	O
PRODVOLcont	production volume of substance in continent	[$kg_c.d^{-1}$]	O
TONNAGEcont	tonnage of substance in continent	[$kg_c.d^{-1}$]	O
Output			
$RELEASEcont_{i,j}$	continental release during life-cycle stage *i* to compartment *j*	[$kg_c.d^{-1}$]	O

III.3.2.3 Regional releases

1. production

$RELEASEreg_{1,j}$:	air	$F_{1, air} \cdot PRODVOLreg$
	water	$F_{1, water} \cdot PRODVOLreg$
	soil	$F_{1, ind} \cdot PRODVOLreg$
	surf	$F_{1, surf} \cdot PRODVOLreg$
	total	$\Sigma F_{1, j} \cdot PRODVOLreg$
	amount used:	$TONNAGEreg$

2. formulation

$RELEASEreg_{2,j}$:	air	$F_{2, air} \cdot TONNAGEreg$
	water	$F_{2, water} \cdot TONNAGEreg$
	soil	$F_{2, ind} \cdot TONNAGEreg$
	surf	$F_{2, surf} \cdot TONNAGEreg$
	total	$\Sigma F_{2, j} \cdot TONNAGEreg$
	rest:	$(1-\Sigma F_{2, j}) \cdot TONNAGEreg$

3. industrial use

$RELEASEreg_{3,j}$:	air	$F_{3, air} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEreg$
	water	$F_{3, water} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEreg$
	soil	$F_{3, ind} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEreg$
	surf	$F_{3, surf} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEreg$
	total	$\Sigma F_{3, j} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEreg$

4. private use

$RELEASEreg_{4,j}$:	air	$F_{4, air} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEreg$
	water	$F_{4, water} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEreg$
	soil	$F_{4, ind} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEreg$
	surf	$F_{4, surf} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEreg$
	total	$\Sigma F_{4, j} \cdot (1-\Sigma F_{2, j}) \cdot TONNAGEreg$
	rest:	$(1-\Sigma F_{3, j} - \Sigma F_{4, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$

5. service life

$RELEASEreg_{5,j}$:	air	$F_{5, air} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
	water	$F_{5, water} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
	soil	$F_{5, ind} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
	surf	$F_{5, surf} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
	total	$\Sigma F_{5, j} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$

6. waste treatment

$RELEASEreg_{6,j}$:	air	$F_{6, air} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j} - \Sigma F_{5, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
	water	$F_{6, water} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j} - \Sigma F_{5, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
	soil	$F_{6, ind} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j} - \Sigma F_{5, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
	surf	$F_{6, surf} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j} - \Sigma F_{5, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$
	total	$\Sigma F_{6, j} \cdot (1-\Sigma F_{3, j} - \Sigma F_{4, j} - \Sigma F_{5, j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGEreg$

Input			
$F_{i,j}$	fraction of tonnage released during stage *i* to compartment *j*	[-]	O
PRODVOLreg	regional production volume of substance	[$kg_c.d^{-1}$]	O
TONNAGEreg	regional tonnage of substance	[$kg_c.d^{-1}$]	O
Output			
$RELEASEreg_{i,j}$	regional release during life-cycle stage *i* to compartment *j*	[$kg_c.d^{-1}$]	O

III.3.3 Local emission rates: new and existing substances

For estimating local releases, point sources (and therefore, presumably, single stages of the life cycle) need to be identified. The main point sources are identified for each stage of the life cycle and each relevant application. Exception are intermediates (IC/UC=3/33) where emissions at production are added to emissions during industrial use (and production is set to zero) unless it is explicitly stated that the chemical is processed elsewhere. Each application and each relevant stage of the life cycle is assessed separately.

The emission rate is given as a release rate during an emission episode, and averaged per day (24 hours). It should be noted that in the emission scenario documents the emissions can be given in tonnes.yr^{-1}. In EUSES the output is calculated in kg d^{-1}.

III.3.3.1 Emissions based on tonnage with general B-tables (possibly updated with emission factors of emission scenario documents of the TGD)

$$Elocal_{i,j} = Fmainsource_i \cdot RELEASEreg_{i,j} \frac{365}{Temission_i} \quad j \in \{air,water\} \qquad (10)$$

III.3.3.1.1 IC 14 Paints, lacquer and varnished industry

Life cycle stage Formulation

$$Elocal_{2,j} = \frac{TONNAGEreg \cdot 10^3 \cdot Fmainsource_2 \cdot F_{2,j}}{Temission_2} \quad j \in \{air,water\} \qquad (11)$$

Input			
TONNAGEreg	relevant tonnage in the region for this application	[tonnes.yr^{-1}]	O
Temission$_i$	number of emission days per year	[d.yr^{-1}]	D
Fmainsource$_i$	fraction of the main local source	[-]	D
$F_{2,j}$	fraction of the tonnage released to compartment *j* during formulation	[-]	D, P
Output			
Elocal$_{2,water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O
Elocal$_{2,air}$	local emission to air	[kg$_c$.d^{-1}]	O

Table III-3 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
number of emission days per year	Temission$_2$	[d.yr^{-1}]	B-table[2)]
fraction of the main local source	Fmainsource$_2$	[-]	B-table[2)]
fraction of the tonnage released to compartment *j*	$F_{2,j}$	[-]	[1)]

[1)] see pick-list ***Table III-4***

[2)] Table B 2.3 for HPVC, Table 2.10 for non-HPVC

Table III-4 Emission factors to air ($F_{2,air}$) and (waste)water ($F_{2,water}$) for formulation of various types of paint and coating products. I= volatile[1)], II = non-volatile & water soluble[2)] and III = non-volatile & non-water soluble.

Type of application/product	**I**		**II**		**III**	
	$F_{2,air}$	$F_{2,water}$	$F_{2,air}$	$F_{2,water}$	$F_{2,air}$	$F_{2,water}$
furniture	0.01	0.01	0	0.01	0	0.01
UV curable wood lacquer	0.02	0	0	0	0	0
water-borne wood lacquer	0.01	0.02	0	0.02	0	0.02
nitrocellulose wood lacquer (spray)	0.02	0	0	0	0	0
coil coating	0.01	0	0	0.01	0	0.01
can coatings (general)	0.03	0	0	0	0	0
solvent based 2 piece can external white enamel	0.018	0	0	0	0	0
water-borne 2 piece can external white enamel	0.015	0	0	0	0	0
epoxy-phenolic food-can lacquer (solvent-based)	0.015	0	0	0	0	0
general line varnish for metal cans (solvent-based)	0.015	0	0	0	0	0
general line white coating for metal cans (solvent-based)	0.02	0	0	0	0	0
solvent-based general purpose size (metal cans)	0.01	0	0	0	0	0
marine coatings	0.03	0	0	0	0	0
container coating	0.04	0	0	0	0	0
OEM car manufacturing	0.03	0	0	0	0	0
car refinish	0.03	0	0	0	0	0
vinyl matt emulsion	0.01	0	0	0.02	0	0
standard alkyd gloss finish	0.02	0	0	0.02	0	0.01
water-borne exterior woodstain	0.02	0.01	0	0.01	0	0.01
solvent-borne exterior/interior woodstain	0.01	0	0	0	0	0.01
Undefined/unknown	0.04	0.02	0	0.02	0	0.02

[1)] volatile substances are defined as having a vapour pressure of > 10 Pa at 23 °C

[2)] a substance is considered to be “water soluble” if its water solubility is > 1 $g.l^{-1}$

Life cycle stage Industrial use (i=3) and Private use (i=4)

$$Elocal_{i,j} = \frac{TONNAGEreg \cdot Fmainsource_i \cdot F_{i,j}}{Temission_i} \quad j \in \{air,water\} \quad \textbf{(12)}$$

Input			
TONNAGEreg	relevant tonnage in the region for this application	[$kg_c.yr^{-1}$]	O
$Temission_i$	number of emission days per year	[$d.yr^{-1}$]	D
$Fmainsource_i$	fraction of the main local source	[-]	D
$F_{i,j}$	fraction of the tonnage released to compartment *j* during life cycle stage i	[-]	D, P
Output			
$Elocal_{i,water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O
$Elocal_{i,air}$	local emission to air	[$kg_c.d^{-1}$]	O

Table III-5 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
number of emission days per year	$Temission_i$	[$d.yr^{-1}$]	B-table[2)]
fraction of the main local source	$Fmainsource_i$	[-]	B-table[2)]
fraction of the tonnage released to compartment *j*	$F_{i,j}$	[-]	[1)]

[1)] see pick-list ***Table III-6***

[2)] *i* = 3: Table B 3.13; *i* = 4: Table B 4.4 (for wastewater only)

Table III-6 Emission factors to air ($F_{i,air}$) and (waste)water ($F_{i,water}$) for industrial use (*i* = 3) and private use (*i* = 4) of various types of paint and coating products. I= volatile[1)], II = non-volatile & water soluble[2)] and III = non-volatile & non-water soluble.

Type of applicate ion / product	*i*	I		II		III	
		$F_{i,air}$	$F_{i,water}$	$F_{i,air}$	$F_{i,water}$	$F_{i,air}$	$F_{2,water}$
furniture	4	0.97	0.01	0	0.03	0	0.03
UV curable wood lacquer	4	0.98	0	0	0	0	0
water-borne wood lacquer	4	0.92	0.05	0	0.05	0	0.05
nitrocellulose wood lacquer (spray)	4	0.98	0	0	0	0	0
coil coating	3	0.01	0.01	0	0.01	0	0.01
can coatings (general)	3	0.94	0	0	0	0	0
solvent based 2 piece can external white enamel	3	0.96	0	0	0	0	0
water-borne 2 piece can external white enamel	3	0.965	0	0	0	0	0
epoxy-phenolic food-can lacquer (solvent-based)	3	0.93	0	0	0	0	0
general line varnish for metal cans (solvent-based)	3	0.934	0	0	0	0	0
general line white coating for metal cans (solvent-based)	3	0.927	0	0	0	0	0
solvent-based general purpose size (metal cans)	3	0.939	0	0	0	0	0

marine coatings	4	0.97	0	0	0	0	0.05
container coating	4	0.96	0	0	0	0	0
OEM car manufacturing	3	0.97	0	0	0	0	0
car refinish	4	0.97	0	0	0	0	0.01
vinyl matt emulsion	4	0.96	0.01	0	0.03	0	0.03
standard alkyd gloss finish	4	0.96	0.01	0	0.03	0	0.03
water-borne exterior woodstain	4	0.96	0.01	0	0.02	0	0.02
solvent-borne exterior/interior woodstain	4	0.98	0.01	0	0	0	0.03
Undefined/unknown (industrial use)	3	0.98	0.05	0	0.05	0	0.05
Undefined/unknown (private use)	4	0.97	0.01	0	0.01	0	0.01

[1)] volatile substances are defined as having a vapour pressure of > 10 Pa at 23 °C

[2)] a substance is considered to be "water soluble" if its water solubility is > 1 $g.l^{-1}$

III.3.3.2 Emissions based on tonnage with specific B-tables (derived from emission scenario documents)

This calculation is performed for:

- IC 5 Personal/domestic and UC 9 and 15 (if production volume > 1000 tonnes/year) for private use ($i = 4$)
- IC 6 Public domain and UC 9 (if production volume > 1000 tonnes/year) for industrial use ($i = 3$)

The emissions in these scenarios are not included in the regional assessment (only local)

$$Elocal_{i,water} = \frac{TONNAGEreg \cdot Nlocal}{N \cdot Temission_i} \qquad \textbf{(13)}$$

Input

TONNAGEreg	regional tonnage of substance	[$kg_c.d^{-1}$]	O
Nlocal	number of inhabitants feeding one STP	[-]	D
N	number of inhabitants feeding regional system	[-]	D
$Temission_i$	number of days per year for emission in stage *i*	[$d.yr^{-1}$]	D

Output

$Elocal_{i,water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

III.3.3.3 Emission based on average capacities and consumptions (derived from emission scenario documents)

This calculation is performed for:

- IC 7 Leather processing industry for UC 10 Colouring agents and UC 51 Tanning agents at industrial use
- IC 8 Metal extraction industry, refining and processing industry and for UC 11 Complexing agents, UC 14 Corrosion inhibitors, UC 29 Heat transfer agents, UC 35 Lubricants and additives, UC 40 pH-regulating agents, UC 49 Stabilisers and UC 50 Surface-active agents at waste treatment
- IC-10 Photographic industry for UC 42 Photochemicals at industrial use and waste treatment (i.e., silver recovery process)
- IC 12 Pulp, paper and board industry and UC 2 adhesives and binding agents, UC 10 colouring agents, UC 31 Impregnation agents, UC 43, Process regulators, UC 47 softeners and UC 55 others
- IC 13 Textile processing industry UC 10 colouring agents
- IC 14 Paint, lacquers and varnished industry and UC 2 adhesives and binding agents, UC 48 solvents, UC 10 colouring agents, UC 20 fillers and UC 52 viscosity adjusters
- IC 11 Polymers industry and UC 53 vulcanising agents, UC 20 fillers, UC 49 stabilisers and UC 22 flame retardants and other UCs

These emissions in these scenarios are not included in the regional assessment (only local)

III.3.3.3.1 IC 7 Leather processing industry

UC 10 Dyes:

$$Elocal_{3,water} = Qleather \cdot Qsubst \cdot Fdye \cdot (1 - Ffix) \quad (14)$$

Input			
Qleather	quantity of treated raw hide per day	[tonnes.d^{-1}]	D
Qsubst	quantity of substance used per tonne of raw hide	[kg$_c$.tonne^{-1}]	D
Ffix	degree of fixation	[-]	D, P
Fdye	fraction of daily production dyed with on dye	[-]	D
Output			
Elocal$_{3, water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O

Table III-7 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
quantity of treated raw hide per day	Qleather	[tonne.d^{-1}]	15
quantity of substance used per tonne of raw hide	Fconc	[kg.tonne^{-1}]	10
degree of fixation for the dye types:	Ffix	[-]	
sulphur			0.70
metal complex			0.94
acid			1.00
unknown/acid groups			0.96
fraction of daily production dyed with one dye	Frel	[-]	0.50

UC 51 Tanning agents:

$$Elocal_{3,water} = Qleather \cdot Qsubst \cdot (1 - Ffix) \quad (15)$$

Input			
Qleather	quantity of treated raw hide per day	[tonnes.d^{-1}]	D
Qsubst	quantity of substance used per tonne of raw hide	[kg$_c$tonne^{-1}]	S
Ffix	degree of fixation	[-]	S
Output			
Elocal$_{3,water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O

Table III-8 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
quantity of treated raw hide per day	Qleather	[tonne.d^{-1}]	15

III.3.3.3.2 IC 8 Metal extraction industry, refining and processing industry

Life cycle stage Waste treatment

A) Water-based cooling lubricants

A.1) Cooling lubricant emulsions:

$$Cconc = Fconc \cdot RHOconc \quad (16)$$

$$Elocal_{6,water} = \frac{Fproc}{Fproc + 1} \cdot \frac{Cconc \cdot Vproc}{1 + Fproc \cdot K_{ow}} \cdot Frel \cdot (1 - Felim) \quad (17)$$

Input			
Cconc	concentration of substance in concentrate	[$kg_c.m^{-3}$]	O
Fconc	fraction of substance in concentrate	[-]	S/P
RHOconc	density of the concentrate	[$kg_c.m^{-3}$]	D
Vproc	volume of processed liquid treated in recovery unit	[$m^3.d^{-1}$]	D
Fproc	fraction of concentrate in processed liquid	[-]	S/P
K_{ow}	octanol-water partition coefficient	[-]	S
Felim	fraction of the substance eliminated during treatment	[-]	D
Frel	factor of relevance	[-]	D
Output			
$Elocal_{6, water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-9 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
Fraction of substance in concentrate	Fconc	[-]	1)
Density of concentrate	RHOconc	[$kg.m^{-3}$]	1000
Volume of processed liquid treated in recovery plant	Vproc	[$m^3.d^{-1}$]	40
Fraction of concentrate in processed liquid	Fproc	[-]	2)
Octanol-water partition coefficient	K_{ow}	[-]	3)
Fraction of the substance eliminated during treatment	Felim	[-]	0.8
Factor of relevance	Frel	[-]	1

1) see pick-list ***Table III-11***

2) see pick-list ***Table III-12***

3) substance specific property

A.2) water-soluble lubricants:

$$Cconc = Fconc \cdot RHOconc \quad (18)$$

$$Elocal_{6,water} = Cconc \cdot Vproc \cdot Fproc \cdot Frel \cdot (1 - Felim) \quad (19)$$

Input			
Cconc	concentration of substance in concentrate	[$kg_c.m^{-3}$]	O
Fconc	fraction of substance in concentrate	[-]	S/P
RHOprod	density of concentrate	[$kg.m^{-3}$]	D
Vproc	volume of processed liquid treated in recovery unit	[$m^3.d^{-1}$]	D
Fproc	fraction of concentrate in processed liquid	[-]	S/P
Felim	fraction of the substance eliminated during treatment	[-]	D
Frel	factor of relevance	[-]	D
Output			
$Elocal_{6,\ water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-10 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
fraction of substance in concentrate	Fconc	[-]	1)
density of concentrate	RHOconc	[$kg.m^{-3}$]	1000
volume of processed liquid treated in recovery plant	Vproc	[$m^3.d^{-1}$]	40
fraction of concentrate in processed liquid	Fproc	[-]	2)
fraction of the substance eliminated during treatment	Felim	[-]	0.8
factor of relevance	Frel	[-]	1

1) see pick-list, ***Table III-11***

2) see pick-list ***Table III-12***

Table III-11 Pick-list for the composition of cooling lubricants, with the fraction of the substance in concentrate, Fconc (-) and the use category (UC) if applicable. The highest concentration is used as a worst case in case of reported ranges (n.a. = not applicable).

Substance group	UC	traditional SEM[1]	synthetic SEM[1]	SES[2]
base oil (lubricants)	35	0.60	0.30	n.a.
anti-wear additives	35	0.05	0.05	0.05
complex builders (complexing agents)	11	0.05	0.05	0.05
corrosion inhibitor (corrosion protection)	14	0.05	0.20-0.25	0.20-0.40
emulsifier: - anionic - not ionic - others/unknown	49	 0.15-0.2 0.20	 0.10-0.15 0.2	n.a.
extreme pressure additives	35	0.5	0.5	0.5
foam inhibitors	35	0.003	0.003	0.003
friction modifier	35	0-0.05	0.05-0.10	0.05-0.10
metal deactivators	35	0.01	0.01	0.01
pH-regulating agents (neutralisation agents)	40	0.03		0.25

solubilisers	35	0.05	0.05	0.10-0.20
surfactants:	50			
- anionic surfactants		0.25	0.25	0.25
- others/unknown		0.25	0.25	0.25

[1] SEM emulsifiable cooling lubricant

[2] SES water soluble cooling lubricant

Table III-12 Pick-list for fraction of cooling lubricant concentrate in processed liquid, Fproc (-) by type of process. The highest concentration is used as a worst case when ranges are reported.

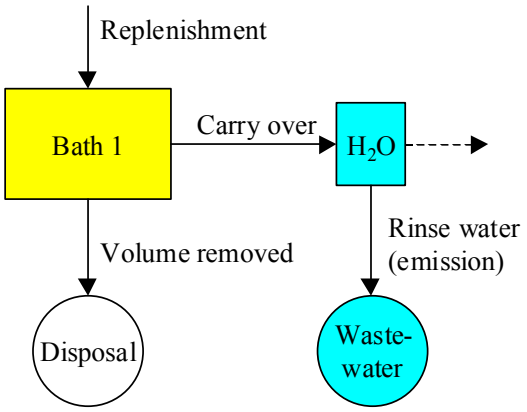
Process	Fproc
broaching	0.10-0.20
thread cutting	0.05-0.10
deep hole drilling	0.10-0.20
parting-off	0.05-0.10
milling, cylindrical milling	0.05-0.10
turning, drilling, automation work	0.03-0.10
sawing	0.05-0.20
tool grinding	0.03-0.06
cylindrical grinding	0.02-0.05
centreless grinding	0.03-0.06
surface grinding	0.02-0.05

III.3.3.3.3 IC-10 Photographic industry and UC 42 Photochemicals

Life cycle stage Industrial use

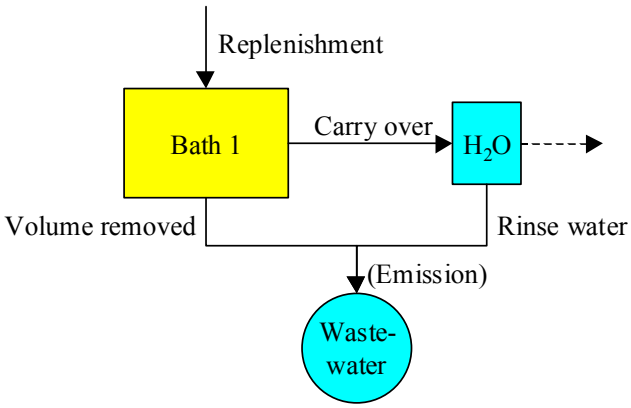
Four typical point sources with photographic processes are considered:
- wholesale finisher
- large X-ray division at a hospital
- large printing office for reprographic activities
- copying facility

In respect to wastewater emissions the following situations are considered:
① Emissions to wastewater resulting from intermediate rinsing between the photochemical process baths where the substance is introduced and the next bath or final rinsing, if the volume removed from the bath is sent for recovery/treatment ("disposal") *(see diagram)*:



$$Elocal_{3,water} = Cform \cdot AREAmaterial \cdot Vcarry\_over \cdot (1 - Fconv) \cdot 10^{-3} \quad \textbf{(20)}$$

②Emissions to wastewater if the volume removed from the bath where the substance is introduced goes also directly to wastewater *(see also diagram)*:



$$Elocal_{3,water} = Cform \cdot AREAmaterial \cdot Vrepl \cdot (1 - Fconv) \cdot 10^{-3} \quad \textbf{(21)}$$

Input			
Cform	concentration of substance in working solution	[$kg_c.m^{-3}$]	S/P
AREAmaterial	surface of processed film or paper	[$m^2.d^{-1}$]	S/P
Vrepl	replenishment rate	[$l.m^{-2}$]	S/P
Vcarry-over	carry-over rate	[$l.m^{-2}$]	S/P
Fconv	fraction of the substance removed or converted during process	[-]	D
Output			
$Elocal_{3,\ water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

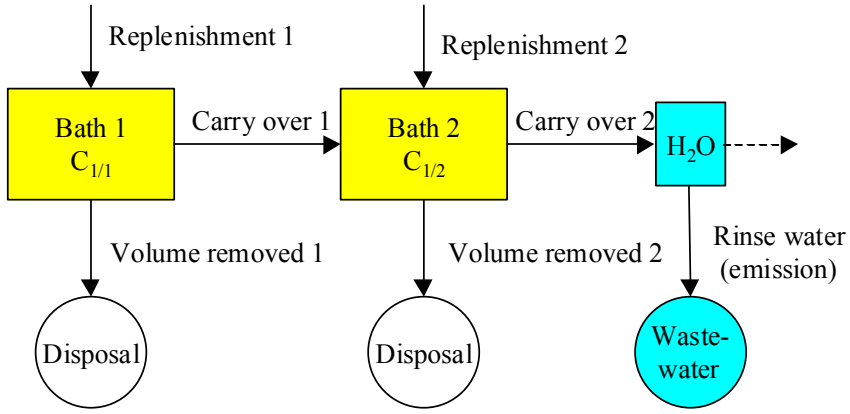
Table III-13 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
concentration of substance in working solution	Cform	[$kg_c.m^{-3}$]	[1)]
surface of processed film or paper	AREAmaterial	[$m^2.d^{-1}$]	[2)]
replenishment rate	Vrepl	[$l.m^{-2}$]	[2)]
carry-over rate	Vcarry-over	[$l.m^{-2}$]	[2)]
fraction of substance removed or converted during process	Fconv	[-]	0

[1)] see pick-list ***Table III-18***

[2)] see pick-list ***Table III-17***

③ Emissions to wastewater when the carry-over of a processing bath, where the substance was entered goes to a next bath, which is followed by a washing step. The volumes removed from the baths are sent for recovery/treatment ("disposal") *(see also diagram)*:



$$Csubst_{1-2} = Cform_{bath\ 1} \cdot \frac{Vcarry\_over}{Vcarry\_over + Vrepl_{bath\ 2}} \qquad (22)$$

$$Elocal_{3,water} = Csubst_{1-2} \cdot AREAmaterial \cdot Vcarry\_over \cdot (1-Fconv) \cdot 10^{-3} \qquad (23)$$

Input			
$Csubst_{1-2}$	concentration of substance from first bath in the second bath	[$kg_c.m^{-3}$]	O
$Cform_{bath\ 1}$	concentration of substance in working solution of bath one	[$kg_c.m^{-3}$]	S/P
AREAmaterial	surface area of processed film or paper	[$m^2.d^{-1}$]	S/P
$Vrepl_{bath\ 2}$	replenishment rate of second bath	[$l.m^{-2}$]	S/P
Vcarry-over	carry-over rate	[$l.m^{-2}$]	S/P
Fconv	fraction of the substance removed or converted during process	[-]	D
Output			
$Elocal_{3,\ water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-14 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
concentration of substance in first bath	$Cform_{bath\ 1}$	[$kg_c.m^{-3}$]	1)
surface of processed film or paper	AREAmaterial	[$m^2.d^{-1}$]	2)
replenishment rate	Vrepl	[$l.m^{-2}$]	2)
carry-over rate	Vcarry-over	[$l.m^{-2}$]	2)
fraction of substance removed or converted during process	Fconv	[-]	0

1) see pick-list ***Table III-18***

2) see pick-list ***Table III-17***

Release of substances from processing photographic materials:

$$\boldsymbol{Elocal_{3,water} = Qsubst \cdot AREAmaterial \cdot Fdiss \cdot (1 - Fconv)} \qquad \textbf{(24)}$$

Input			
Qsubst	quantity of substance in the photographic material	[$kg_c.m^{-2}$]	S/P
AREAmaterial	surface area of processed film or paper	[$m^2.d^{-1}$]	S/P
Fdiss	fraction substance dissolved during processing	[-]	D
Fconv	fraction removed or converted during processing	[-]	D
Output			
$Elocal_{3,\ water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-15 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
quantity of substance in the photographic material	Qsubst	[$kg_c.m^{-2}$]	1)
surface area of processed film or paper	AREAmaterial	[m^2]	2)
fraction of substance removed or converted during process	Fconv	[-]	0
fraction which dissolves during processing	Fdiss	[-]	1

1) see pick-list ***Table III-20***

2) see pick-list ***Table III-17***

Life cycle stage Waste treatment

Release at the disposal company:

$$\boldsymbol{Elocal_{6,water} = Cform \cdot Vtreat \cdot (1 - Fconv) \cdot (1 - Fred)} \qquad \textbf{(25)}$$

Input			
Cform	concentration of substance in the fresh working solution	[$kg_c.m^{-3}$]	P
Vtreat	treated volume of working solution	[$m^3.d^{-1}$]	P
Fconv	fraction of the substance removed or converted during process	[-]	D
Fred	fraction of waste reduction	[-]	D
Output			
$Elocal_{6, water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-16 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
concentration of substance in working solution	Cform	[$kg_c.m^{-3}$]	1)
treated volume of working solution	Vtreat	[m^3]	2)
fraction of substance removed or converted during process	Fconv	[-]	0
fraction of waste reduction	Fred	[-]	0

1) see pick-list ***Table III-18***

2) see pick-list ***Table III-19***

Table III-17 *Pick-list for release estimation parameters replenish rate, Vrepl (l.m-²), carry-over rate, Vcarry-over (l.m-²) and treated area of photographic material, AREAmaterial (m².d-1). When there is no intermediate washing step the replenish rate is set to the lowest value. At direct introduction into wastewater the replenish rate is set to the highest value as worst case.*

Process[a]	Bath	Vrepl[b]	Vcarry-over	AREAmaterial
wholesale finisher				
C-41				
colour negative	developing	0.30–0.60 (0.45)	0.080 / 0.170[c]	680
	bleaching	0.10–0.90 (0.50)		
	fixing	0.40–0.90 (0.65)		
	stabilising	0.90 (0.90)		
RA-4				
colour paper	developing	0.06–0.12 (0.09)	0.040 / 0.070[c]	4950
	bleach fixing	0.07–0.14 (0.10)		
RA-4				
devided bleaching and fixing	developing	0.06–0.12 (0.09)	0.050	
	stopping	0.15–0.20 (0.175)		
	bleaching	0.05–0.10 (0.075)		
	fixing	0.055–0.100 (0.075)		
	stabilising			
E-6				
colour reversal film	primary developing	0.9–1.8 (1.35)	0.080 / 0.170[c]	120
	reversing	1.0–1.1 (1.05)		
	colour developing	1.0–2.0 (1.5)		
	conditioning	0.9–1.1 (1.0)		
	bleaching	0.2 (0.2)		
	fixing	0.4–1.0 (1.2)		
	stabilising	1.0 9(1.0)		
R-3				
colour reversal paper	primary developing	0.17–0.33 (0.25)	0.050	350
	colour developing	0.05–0.50 (0.275)		
	bleach fixing	0.07–0.20 (0.135)		
	stabilising			
R-3				
devided bleaching and fixing	primary developing	0.17–0.33 (0.25)		

Process[a]	Bath	Vrepl[b]	Vcarry-over	AREAmaterial
	colour developing	0.05-0.50 (0.275)		
	bleaching	0.07–0.14 (0.105)		
	fixing	0.055-0.100 (0.775)		
	stabilising			
BW-N				
	developing	0.5-0.6 (0.55)	0.180	40
	fixing	0.4-0.9 (0.65)		
BW-P				
	developing	0.2-0.3 (0.25)	0.070	270
	fixing	0.055-0.30 (0.178)		
x-ray division				
BW-X				
med.	developing	0.35-0.40 (0.375)	0.040	110
	fixing	0.4-0.6 (0.50)		
BW-X				
tech.	developing	0.5-0.6 (0.55)	0.040	
	fixing	0.8-1.2 (0.10)		
printing office				
BW-R				
film	developing	0.2-0.3 (0.25)	0.040	80
	fixing	0.15-0.30 (0.225)		
copy facility				
ECN-2				
cine- and television-film negative	primary bath	0.375	0.180	35
	colour developing	0.845		
	stopping	0.560		
	bleach accelerating	0.180		
	bleaching	0.180		
	fixing	0.560		
	stabilising	0.375		
ECP-2				
cine- and television positive	primary bath	0.374	0.180	350
	colour developing	0.646		
	stopping	0.721		
	primary fixing	0.187		
	bleach accelerating	0.187		
	bleaching	0.187		
	secondary fixing	0.187		
	stabilising	0.374		
VNF-1				
cine- and television-film reversal	primary developing	0.348	0.180	35
	primary stopping	2.254		
	colour developing	1.639		
	secondary stopping	1.332		
	bleach accelerating	0.410		
	bleaching	0.410		
	fixing	1.281		
	stabilising	0.615		

a values of C-41, RA-4, E6, R-3, BW-P and BW-N are related to point source (a) -wholesale finisher
values of BW-X are related to point source (b) –hospital
values of BW-R are related to point source (c) -printing office
values of ECN-2, ECP-2 and VNF-1 are related to point source (d) –copying facility

b recycling processes of bath-solutions for point source (a) –wholesale finisher- are considered

c carry-over rates for professional labs are different from wholesale finishers

Table III-18 *Pick-list for the content of substance in processing solutions for every specific function, Cform ($kg_c.m^{-3}$), and the corresponding equation (Eq = equation, Dev = developer, pH-reg = pH regulator, Antiox = antioxidant, Antifog = antifogging agent, Bleach = bleaching agent, Rehalog = rehalogenating agent, Fix = fixing agent, Stab = stabiliser, Seq = sequestering agent, Rev = reversing agent, Hard = hardening agent, Solv = auxiliary solvent, and Bl Acc = bleaching accelerator*

Process	**Process bath**	**Eq**	**Dev**	**pH-reg**	**Antiox**	**Antifog**	**Bleach**	**Rehalog**	**Fix**	**Stab**	**Seq**	**Rev**	**Hard**	**Solv**	**Bl Acc**
UC			**42**	**40**	**49**	**42**	**8**	**42**	**21**	**49**	**11**	**42**	**55/0**	**48**	**43**
Wholesale finisher															
C-41	developing	3 (n=2)	8	50	6	2					4			19	
	bleaching	1		20			120	120							0.4
	fixing	1		20	8				150						
	stabilising	2								2					
RA-4	developing	1	8	40	8	1.6					4			19	
	stopping	1													
	bleaching	1		10			50	52.5							0.4
	fixing	1			10				90		3				
E-6	primary developing	1	30	35	6.5	2					4			19	
	reversing	3 (n=2)										2			
	colour developing	1	10	50	6	1.6					4			19	
	conditioning	2		20											
	bleaching	3 (n=2)					150	80							0.4
	fixing	1			8				180						
	stabilising	2								2					
R-3	primary developing	1	20	30	2	1.6					4	4		19	
	colour developing	1	7	30	6.5	1.6					4	4		19	
	bleach fixing	1		20	10		60		100						
	stabilising	1								2					
BW-N	developing	1	15	70	20	10					10				
	fixing	1		20	20				150				5		
BW-P	developing	1	15	70	20	10					10				
	fixing	1		20	20				150				5		
Printing office															
BW-R	developing	1	25	20	8	17					10				
	fixing	1		15	15				120						

Process	Process bath	Eq	Dev	PH-reg	Antiox	Antifog	Bleach	Rehalog	Fix	Stab	Seq	Rev	Hard	Solv	Bl Acc
UC			**42**	**40**	**49**	**42**	**8**	**42**	**21**	**49**	**11**	**42**	**55/0**	**48**	**43**
X-ray division															
BW-X	developing	1	20	60	20	17					10				
	fixing	1		20	20				150						
Copying facility															
ECN-2	primary bath	3 (n=3)		0.8	55.6										
	colour developing	3 (n=2)	3	13.5	1.4	0.43					4			19	
	stopping	1				26.3									
	bleach accelerating	1		15.8	6.3										0.4
	bleaching	1		8.5		30.4	80	120							
	secondary fixing	1			12.9				68.2						
	stabilising	1								8					
ECP-2	primary bath	3 (n=3)		0.8									55.6		
	colour developing	3 (n=2)	11.5	9.5	2.4	0.8					4			19	
	stopping	1				26.3									
	primary fixing	1			8.9	0.4			54.8						
	bleach accelerating	1		3.7	2.9										0.4
	bleaching	1					13.7	120							
	secondary fixing	1			8.9	0.4			54.8						
	stabilising	1								1.95					
VNF-1	primary developing	1	0.2	16.1	1.6	0.004			0.8	0.1	4			19	
	primary stopping	1		16.7											
	colour developing	1	6.7	2.6	4.3	0.02				0.06	4			19	
	secondary stopping	1		16.7											
	bleach accelerating	3 (n=3)		4.4	5.6										0.4
	bleaching	3 (n=2)					47.2	120							
	fixing	1			5.2				93.9						
	stabilising	1								2					

N.B. ◘ If a specific bath is not mentioned the worst case default value for the substance with the specified function is used
◘ If the specific process for the photographic point source is not mentioned the worst case situation is used
◘ If the specific point source is not mentioned the worst case situation is used

Table III-19 *Pick-list for treated volume of working solution, Vtreat ($m^3.d^{-1}$) at the disposal company.*

Point source	Photographic process	Treated volume
If specific photographic process in unknown		
	colour process	3.0
	developing	1.0
	bleaching	0.3
	fixing	0.5
	bleach fixing	1.2
	black/white process	5.0
	developing	2.3
	fixing	2.7
If specific photographic process is known		
Whole sale finisher		
C-41	colour negative film	0.2
	developing	0.08
	bleaching	0.08
	fixing	0.04
RA-4	colour positive paper	2.6
	developing	0.78
	bleaching	0.21
	fixing	0.47
	bleach fixing	1.14
E-6	colour reversal film	0.03
	primary developing	0.013
	colour developing	0.013
	bleaching	0.003
	fixing	0.001
R-3	colour reversal paper	0.03
	primary developing	0.019
	colour developing	0.007
	bleach fixing	0.002
	bleaching	0.002
	fixing	0.001
BW-N	black/white negative film	0.06
	developing	0.05
	fixing	0.01
BW-P	black/white positive paper	0.18
	developing	0.16
	fixing	0.02
X-ray division		
BW-X	black/white X-ray	3
	developing	1.2
	fixing	1.8
Printing office		
BW-R	black/white reprographic	1.8
	developing	0.9
	fixing	0.9
	activator	
Copy facility		
Cine	cine- and television film	0.1
	developing	
	bleaching	

Table III-20 *Pick-list for content of substance in photographic material, Qsubst ($kg.m^{-2}$), which is released from the material in processing and cleaning solutions during processing of this material.*

Ingredient	**Paper**	**Film**
sensitizers	$1.0.10^{-6}$	$2.5.10^{-5}$
photographic stabilisers	$5.0.10^{-6}$	$1.0.10^{-4}$
fungicides	$3.0.10^{-5}$	$1.5.10^{-4}$
silver as Ag	$5.0.10^{-4}$	$1.2.10^{-2}$
halides	$3.0.10^{-4}$	$7.0.10^{-3}$
split-off products		
- masking compounds in negative films	$4.0.10^{-5}$	$8.0.10^{-5}$
- remaining groups of colour couplers	$8.0.10^{-5}$	$8.0.10^{-4}$
- stabilisers	0	$8.0.10^{-5}$
wetting agents	$1.0.10^{-5}$	$3.0.10^{-4}$
filter dyestuffs	$5.0.10^{-5}$	$2.5.10^{-4}$

III.3.3.3.4 IC 11 Polymers industry

Manufacture of rubber products (formulation and processing)

$$Elocal_{3,water} = Qrubber \cdot Qsubst \cdot (1 - Ffix) \quad (26)$$

Input			
Qrubber	amount of rubber product produced per day	[kg.d^{-1}]	D
Qsubst	amount of substance per unit of mass of product	[-]	P
Ffix	fraction of the substance remaining in the product	[-]	P
Output			
Elocal$_{3, water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O

Table III-21 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
amount of rubber product produced per day	Qrubber	[kg.d^{-1}]	55 000
amount of substance per unit of mass of product	Qsubst	[-]	1)
fraction of the substance remaining in the product	Ffix	[-]	1)

1) see pick-list ***Table III-22***

Table III-22 Pick-list for contents of rubber additives, Qsubst (-) in tyres and rubber products and the fractions remaining in the product, Ffix (-). When ranges are presented the highest value is chosen to represent the worst case situation.

Parameter	UC	rubber prod.	tires	Ffix
mastication agents/ peptisers	**43**	**0.005 NR** **0.03 SR**	**0.005**	**0.995**
activators	46		0.02	
vulcanising agents		**0.0025 soft** **0.2 hard**	**0.01**	**1.000**
sulphur containing cross-linking agents	53	0.01	0.01	
vulcanising accelerators	43	0.0005-0.01	0.002-0.02	
accelerator activators	43	0.0075-0.025	0.0065	
sulphur-free cross-linking agents	53	0.000005-0.005	.	
co-agents for sulphur-free cross-linking agents	43	0.0025-0.01	0.01	
other cross-linking agents	53	0.000005-0.01	0.000005-0.01	
vulcanising retarders	43	0.0075-0.01	0.0015-0.01	
scorch-inhibitors	43	0.0005-0.005	0.0025	
anti-aging and antiflex-cracking agents/ anti-degradants		**0.004**	**0.004**	**0.98 RP** **0.99 TI**
antioxidants	49	0-0.015	0.0013	
antifatigue agents	49	0.005-0.025	0.001	

Parameter	UC	rubber prod.	tires	Ffix
anti-ozonants	49	0.005-0.035	0.001-0.005	
light protection agent	49	0-0.015	0.001	
anti-hydrolysis agents	49	0.0025-0.015	0.001	
heat protection agents	49	0.0025-0.015	0.005	
agents against metal poisoning	49	0.0025-0.015	0.001	
deactivators	49	0.0025	0.0015	
reversion protection agents	49	0.0025-0.015	.	
anti-cyclisation agents	49	0.0025	.	
quenchers	49	0.0025	.	
other anti-aging agents	49	0.0075-0.015	.	
fillers and pigments		**0.15**	**0.20**	**0.99**
fillers	20	0.05-0.15	0.20	
pigments	10	0.005-0.025	.	
plasticisers		**0.10**	**0.019**	**0.95**
natural plasticisers	47	0.05-0.10	0.012-0.019	
synthetic plasticisers	47	0.05-0.10	0.012-0.019	
processing aids		**0.075**	**0.005-0.025**	**0.995**
lubricants and flow improvers	35	0.025-0.075	.	
tackifiers	2	0.025-0.075	.	
factices		0.025-0.075	.	
filler activator	43	0.025-0.075	.	
blowing agents	25	0.025-0.05	0.015	1
bonding agents	2	0.005-0.02	0.015-0.02	1
stabilisers	49	0.0075-0.015	0.0075-0.015	
other agents		**0.0005-0.015**	**0.0005-0.015**	**0.95**
anti-cyclisation agents	49	.	.	
replastication agents	47	.	.	
emulsifier	49	0.0005-0.0025	.	
flame retardants	22	0.01-0.015	.	
solvents	48	.	.	
surface treatment agents	0/55	0.01-0.0215	0.01	
hardeners	0/55	.	.	
odour agents	36	0.000125-0.0005	.	
anti-static agents	7	0.001-0.003	0.025	
reinforcing agents	13	.	.	

Parameter	UC	rubber prod.	tires	Ffix
homogenisers	49	.	.	
latex-chemicals		**0.025**	**.**	**0.95 RP**
dispersion agents	43	0.005-0.01	.	
emulsifiers	49	0.005-0.025	.	
stabilisers	49	0.005-0.01	.	
wetting and foaming agents	50	0.005-0.01	.	
foam stabilisers	0/55	0.005-0.025	.	
thickeners	52	.	.	
coagulation agents	43	.	.	
vulcanisation agents	53	0.0025-0.01	.	
anti-aging chemicals	49	.	.	
fillers	20	.	.	
plasticisers	47	.	.	
release agents		**0.15**	**0.15**	**0.95**
release agents for unvulcanized rubber	0/55	0.0025-0.025	0.0025-0.025	
mould release agents	0/55	0.025-0.15	0.025-0.15	
mandrel release agents	0/55	0.025-0.15	0.025-0.15	
others		0.025	0.025	0.95
cleaning agents	9	.	.	
other rubber chemicals	0/55	.	.	

NR = natural rubber, SR = synthetic rubber, RP = rubber products, TI = tyres, hard = hard rubber, soft = soft rubber, .=no data

III.3.3.3.5 IC 12 Pulp, paper and board industry

Emissions to surface water of chemicals used in the manufacture of paper (including coating of paper) and recycling of paper.

Life cycle stage Industrial use, Paper production

applied amount per ton of paper:

$$\boldsymbol{Elocal_{3,water} = Qsubst \cdot Qpaper \cdot (1 - Ffix) \cdot (1 - Fclosure)} \qquad \textbf{(27)}$$

Input			
Qsubst	consumption of substance per tonne of paper	[$kg_c.tonne^{-1}$]	S/P
Qpaper	quantity of paper produced on one site per day	[$tonnes.d^{-1}$]	P
Ffix	degree of fixation	[-]	S/P
Fclosure	degree of closure of the water system	[-]	P
Output			
$Elocal_{3,\ water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-23 Defaults for emission calculations

Parameter	Symbol	Unit	Value
consumption of substance per tonne of paper	Qsubst	[$kg_c.tonne^{-1}$]	1)
quantity of paper produced on one site per day	Qpaper	[$tonne.d^{-1}$]	2)
degree of fixation	Ffix	[-]	3)
degree of closure of the water system	Fclosure	[-]	2)

1) see pick-lists ***Table III-26*** and ***Table III-27***

2) see pick-list ***Table III-25***

3) see pick-lists ***Table III-26*** and ***Table III-28***

Estimation if concentration of the substance in process water is used:

$$\boldsymbol{Elocal_{3,water} = Csubst \cdot Qwater \cdot Qpaper \cdot (1 - Ffix)} \qquad \textbf{(28)}$$

Input			
Csubst	concentration of substance in process water	[$kg_c.m^{-3}$]	S/P
Qwater	quantity of water used per tonne of paper	[$m^3.tonne^{-1}$]	P
Qpaper	quantity of paper produced on one site per day	[$tonne.d^{-1}$]	P
Ffix	degree of fixation	[-]	S/P
Output			
$Elocal_{3,water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-24 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
concentration of substance in process water	Csubst	[$kg_c.m^{-3}$]	1)
quantity of water used per tonne of paper	Qwater	[$m^3.tonne^{-1}$]	2)
quantity of paper produced on one site per day	Qpaper	[$tonne.d^{-1}$]	2)
degree of fixation	Ffix	[-]	1)

1) see pick-list ***Table III-26***

2) see pick-list ***Table III-25***

Table III-25 Pick-list for water consumption, Qwater ($m^3.tonne^{-1}$) degree of closure, Fclosure (-) and quantity of paper produced, Qpaper ($tonne.d^{-1}$) for various types of paper. In case of ranges the highest values for water consumption and quantity of paper produced are chosen as worst case. For degree of closure the lowest value is set as worst case.

Type of paper produced	Water consumption	Degree of closure	Quantity of paper produced
printing and writing	40-75	0.40-0.70	100-1000
tissue	57	0.40-0.70	40-200
newsprint	24-35	0.65-0.85	100-1000
packaging and board	2-20	>0.95	100-1000

Table III-26 Pick-list for amount of substance consumed per tonne, Qsubst (kg.tonne^{-1}) and degree of fixation, Ffix (-) for different types of substances used. For a worst case situation the highest value for the quantity of substance used and the lowest fixation rate are used.

Type of substance used	**UC**	**Quantity of substance used, Qsubst [kg.tonne^{-1}]**				**degree of fixation**
		news paper	board	printing writing	tissue	**Ffix [-]**
charge control	43	0.2-1	0.3	0.03	0.03	0.7-0.9
retention aid	43	1-5	1-5			0.7-0.9
retention aid and strenght resin	43		20-30		2-12.5	0.7-0.9
softening	47			2-3		0.60-0.75
sizing agents	31					
natural (e.g. aluminumrosin)		4-10	4-10			0.10-0.30
synthetic						
(AKD =alkylketene dimers)				0.5-3		0.70-0.90
binding agent	2					.
starch		5-15	5-15			
CMC (carboxy methyl cellulose)		5-10				
surface coating (e.g. wax, pur pigmented coating)	55/ 0	1-8	.			.
Concentration in process water [kg.m^{-3}]						
anti-foaming	43	0.0002				.

Table III-27 *Pick-list for applied amount of dye (UC 10) , Qsubst (kg.tonne^{-1}) for various shades and types of paper. The highest value is chosen as a worst case situation.*

degree of shade	news paper	board	printing wrinting	tissue
pale shade			0.1-1	0.1-1
medium shade			1-10	1-10
deep shade			-	10-40

Table III-28 *Pick-list for degree of fixation, Ffix (-) for different types of dyes (UC 10) .The lowest values is chosen as a worst case situation.*

type of dye	substrate	Degree of fixation [-]
anionic direct	bleached and unbleached	0.79-0.90 0.98 with fixing agent
cationic direct	all types	0.90-0.99
basic	bleached pulp mechanical pulp	0.50-0.70 0.60-0.80 0.95 with fixing agent
acid	sized packaging paper	0.40-0.60 0.80-0.90 with fixing agent

Life cycle stage Waste treatment

Release during de-inking process:

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \quad \textbf{(29)}$$

$$Elocal_{6,water} = \frac{TONNAGEreg \cdot Frec \cdot Fmainsource \cdot Fde-ink \cdot (1 - Fremoval) \cdot 10^3}{Temission_6} \quad \textbf{(30)}$$

Input

$Fprodvol_{reg}$	fraction of the region	[-]	D
TONNNAGE	relevant tonnage in the EU for this substance	[tonne.yr^{-1}]	S
TONNAGEreg	relevant tonnage in the region for this substance	[tonne.yr^{-1}]	O
$Temission_6$	number of working days	[d.yr^{-1}]	D
Frec	rate of recycling (recycling fraction)	[-]	D
Fmainsource	fraction of the main source	[-]	D
Fde-ink	fraction released at de-inking	[-]	P
Fremoval	removal rate at on-site primary treatment	[-]	D

Output

$Elocal_{6, water}$	local emission to wastewater	[kg_c.d^{-1}]	O

Table III-29 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
fraction of the region	$Fprodvol_{reg}$	[kg_c.tonne^{-1}]	0.1 [1)]
number of paper production days	$Temission_6$	[d.yr^{-1}]	250
fraction of the main sources	Fmainsource	[-]	0.10
recycling rate	Frec	[-]	0.5

fraction released at de-inking	Fde-ink	[-]	[2)]
removal rate at on-site primary treatment	Fremoval	[-]	
- easily soluble (> 1000 mg.l^{-1})			0.2
- insoluble (≤ 1000 mg.l^{-1})			0.9

[1)] for new substances or existing substances produced at low volumes and which are not used homogeneously throughout the EU, it can be assumed in a first approach that $Fprodvol_{reg} = 1$

[2)] see pick-list ***Table III-30*** or ***Table III-31***

Table III-30 Fraction of ink released at de-inking process, Fde-ink (-) for various types of ink. Highest fraction of de-inking is used as a worst case value.

Type of ink	**Fde-ink [-]**
mineral oil based	0.14-0.28
flexographic	0.30-0.90
non-impact toners	0.06-0.28

Table III-31 Fraction of ink released at de-inking process, Fde-ink (-) for various ink drying processes. Highest fraction released at de-inking is used as a worst case value.

method of ink drying	**Fde-ink [-]**
absorption, penetration, evaporation	0-0.20
oxidation or IR radiation	0.05-0.40
hot polymerisation or UV-fixation	0.10-0.60
ink-jet, laser or xerographic copying	0.40-0.70

III.3.3.3.6 IC 13 Textile processing industry

Life cycle stage Industrial use

Releases during wet processing:

UC 10 dyeing

$$Elocal_{3,water} = Qfibres \cdot Fdye \cdot Qform \cdot Fsubst \cdot (1 - Ffix) \quad (31)$$

Input			
Qfibres	quantity of fibres / fabrics per day	[tonne.d^{-1}]	P
Fdye	fraction of fabric dyed with one dyestuff per day	[-]	D
Qform	quantity of dye-stuff formulation used on fabric	[kg.tonne^{-1}]	D/S
Fsubst	content of dye in the formulation	[kg$_c$.kg^{-1}]	D/S
Ffix	degree of fixation	[-]	P
Output			
Elocal$_{3, water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O

Table III-32 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
quantity of fibres / fabric treated per day	Qfibres	[tonne.d^{-1}]	1)
fraction of fabric dyed with one dye-stuff per day	Fdye	[-]	0.3
quantity of dye-stuff formulation used on fabric	Qform	[kg.tonne^{-1}]	10 2)
content of dye in the dye-stuff formulation	Fsubst	[kg$_c$.kg^{-1}]	1 3)
degree of fixation	Ffix	[-]	4)

1) see pick-list ***Table III-33***

2) if no specific data are available, it should be assumed that the average mass of dye-stuff preparation used is 10 kg per tonne of fabric (1%)

3) if the content of dye-stuff in the preparation is not available, it should be assumed to be 100% (Fsubst = 1)

4) see pick-list ***Table III-34***

Table III-33 Pick-list for daily production volumes, Qfibres (tonne.d^{-1}) at the textile production site.

Textile finishing company	Qfibres
companies total (generic)	12.8
dyeing	14.2
finishing cotton	23.2
finishing natural fibres	18.8
finishing synthetic fibres	5.8
finishing polyester fibres	0.8
using optical brightners	12.2

Table III-34 Pick-list for degree of fixation, Ffix (-) for various types of dyes, dyeing processes and fibres.

Dye	Process	Fibre	Ffix
disperse	continuous	cellulose and polyester	0.95
disperse	printing		0.97
direct	batch	cotton	0.88
reactive	batch	wool	0.95
reactive	batch	cotton	0.70
reactive	batch	general	0.85
vat	continuous	cotton	0.80
vat	printing		0.75
sulphur	continuous	cotton	0.70
sulphur	printing		0.70
acid, one SO_3-group	batch	polyamide and polyacryl	0.90
acid, more than one SO_3-group	batch		0.95
basic	batch	polyacryl, polyester, polyamide and cotton	0.99
azoic (naphtol)	continuous		0.84
azoic (naphtol)	printing		0.87
metal complex	batch		0.94
pigment	continuous		1.00
pigment	printing		1.00
unknown / hardly soluble	continuous		0.97
unknown / acid groups	printing		0.96

Finishing

$$Elocal_{3,water} = Qfibres \cdot Qform \cdot Fsubst \cdot (1 - Ffix) \quad (32)$$

Input			
Qfibres	quantity of fibres / fabrics per day	[tonnes.d^{-1}]	P
Qform	quantity of formulation used on fabric	[kg.tonne^{-1}]	S
Fsubst	content of substance in the applied formulation	[kg_c.kg^{-1}]	D/S
Ffix	degree of fixation	[-]	D/S
Output			
$Elocal_{3,water}$	local emission to wastewater	[kg_c.d^{-1}]	O

Table III-35 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
quantity of fibres / fabric treated per day	Qfibres	[tonne.d^{-1}]	1)
quantity of formulation used on fabric	Qform	[kg.tonne^{-1}]	-
content of substance in the applied formulation	Fsubst	[kg$_c$.kg^{-1}]	1 2)
degree of fixation	Ffix	[-]	0

1) see pick-list ***Table III-33***

2) if the content of the substance in the preparation is not available, it should be assumed to be 100%

Life cycle stage Service life

The release to wastewater (STP) is calculated as:

$$RELEASEreg_{k,5,water} = \frac{Fprodvol_{reg} \cdot F_{5,water} \cdot Qsubst\_tot_k \cdot 10^3 \cdot \sum_{y=1}^{Tservice_k} \left(1 - F_{5,water}\right)^{y-1}}{Temission_5} \quad \textbf{(33)}$$

$$RELEASEreg_{5,water} = \sum_{k=1}^{m} RELEASEreg_{k,5,water} \quad \textbf{(34)}$$

$$Elocal_{5,water} = Fmainsource_5 \cdot RELEASEreg_{5,water} \quad \textbf{(35)}$$

Input			
Qsubst_tot$_k$	annual input of the substance in article *k*	[tonnes.yr^{-1}]	S
Fprodvol$_{reg}$	fraction of EU volume for region	[-]	D
Tservice$_k$	service life of article *k*	[yr]	P
F$_{5,water}$	fraction of the tonnage release over one year during the service to waste water	[-]	S
Temission$_5$	number of emission days per year	[d.yr^{-1}]	D
Fmainsource$_5$	fraction of the main source (STP)	[-]	D
RELEASEreg$_{k,5,water}$	release to waste water for article *k*	[kg$_c$.d^{-1}]	O
RELEASEreg$_{5,water}$	release to waste water for all articles	[kg$_c$.d^{-1}]	O
Output			
Elocal$_{5,\ water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O

Table III-36 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
annual input of the substance in article k	$Qsubst\_tot_k$	[tonnes.yr^{-1}]	
fraction of EU volume for region	$Fprodvol_{reg}$	[-]	0.1
service life of article k	$Tservice_k$	[yr]	[1)]
fraction of the tonnage released over one year during service life	$F_{5,water}$	[-]	
number of emission days per year	$Temission_5$	[d.yr^{-1}]	365
fraction of the main source (STP)	$Fmainsource_5$	[-]	0.002

[1)] see pick-list ***Table III-37***

Table III-37 Service life of some article, $Tservice_k$ (yr). Some values are averages of the ranges presented in the emission scenario document.

Article	Service life
clothes on contact with skin	1.0
other clothes and bed linen	3.5
household linen	7.5
Bedding	5.0
Carpets	14.0
wall-to-wall carpet	17.5
Sunblind	11.5
Tents	12.5
Awning	2.0

III.3.4 Regional emission rates

For the regional-scale assessments, the releases for each relevant application and stage of the life cycle must be summed into one emission for each compartment. The emissions are assumed to be a constant and continuous flux during the year. Of the emissions to water, part is directed to sewage treatment plants (STP).

$$Ereg_j = \sum_{i=1}^{5} RELEASEreg_{i,j} \qquad j \in \{air, ind\} \tag{36}$$

$$Ereg_{water} = Fconnect_{stp} \cdot \sum_{i=1}^{5} RELEASEreg_{i,water} \tag{37}$$

$$Ereg_{direct\text{-}water} = RELEASEreg_{i,surf} + (1 - Fconnect_{stp}) \cdot \sum_{i=1}^{5} RELEASEreg_{i,water} \tag{38}$$

Input			
$RELEASEreg_{i,j}$	regional release during life-cycle stage *i* to compartment *j*	[$kg_c.d^{-1}$]	O
$Fconnect_{stp}$	fraction connected to sewer systems	[-]	D
Output			
$Ereg_{air}$	total regional emission to air (annual average)	[$kg_c.d^{-1}$]	O
$Ereg_{ind}$	total regional emission to industrial soil (annual average)	[$kg_c.d^{-1}$]	O
$Ereg_{water}$	total regional emission to wastewater (annual average)	[$kg_c.d^{-1}$]	O
$Ereg_{direct\text{-}water}$	direct regional emission to surface water (annual average)	[$kg_c.d^{-1}$]	O

III.3.5 Continental emission rates

On the continental scale, all emissions for each compartment are summed over the relevant stages of the life cycle and the various applications, as was done for the regional scale.

$$Econt_j = \sum_{i=1}^{5} RELEASEcont_{i,j} \qquad j \in \{air, ind\} \tag{39}$$

$$Econt_{water} = Fconnect_{stp} \cdot \sum_{i=1}^{5} RELEASEcont_{i,water} \tag{40}$$

$$Econt_{direct-water} = RELEASEcont_{i,surf} + (1 - Fconnect_{stp}) \cdot \sum_{i=1}^{5} RELEASEcont_{i,water} \tag{41}$$

Input			
$RELEASEcont_{i,j}$	continental release during life-cycle stage *i* to compartment *j*	[$kg_c.d^{-1}$]	O
$Fconnect_{stp}$	fraction connected to sewer systems	[-]	D
Output			
$Econt_{air}$	continental emission to air (annual average)	[$kg_c.d^{-1}$]	O
$Econt_{ind}$	continental emission to industrial soil (annual average)	[$kg_c.d^{-1}$]	O
$Econt_{water}$	continental emission to wastewater (annual average)	[$kg_c.d^{-1}$]	O
$Econt_{direct-water}$	direct continental emission to surface water (annual average)	[$kg_c.d^{-1}$]	O

III.3.6 Local emission rates: release estimation for biocides

III.3.6.1 Product-type 2: Private area and public health area disinfectants and other biocidal products

III.3.6.1.1 Sanitary sector

Private use of sanitary disinfectants

This scenario describes the private use of disinfectants for sanitary purposes. Releases take place to an STP, therefore, the STP is viewed as the local main source. The default fraction of 0.002 reflects the fraction of the total wastewater in the region, received by a large STP. In EUSES the standard STP is fed by 10,000 inhabitants with an amount of 0.2 m^3 per day. The emission calculations can be based on A) the annual tonnage or on B) the average consumption per capita.

A) Annual tonnage:

$$TONNAGEreg = TONNAGEreg \cdot Fprodvol_{reg} \quad \textbf{(42)}$$

$$Elocal_{4,water} = TONNAGEreg \cdot Fmainsource_4 \cdot F_{4,water} \cdot \frac{365}{Temission_4} \quad \textbf{(43)}$$

Parameters required for distribution modules	Defaults for this scenario	Unit	Value
Temission	$Temission_4$	[d]	365

Input

TONNAGE	quantity of a.i. used in the European Union	[$kg_c.d^{-1}$]	S
TONNAGEreg	quantity of a.i. used in the Netherlands	[$kg_c.d^{-1}$]	O/S
$Fprodvol_{reg}$	fraction for the region	[-]	D
$Fmainsource_4$	fraction of the local main source	[-]	D
$F_{4.water}$	Fraction released to waste water	[-]	D
$Temission_4$	number of emission days for sanitary proposes at private use	[d]	D

Output

$Elocal_{4,water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O
Temission	number of emission days	[d]	O

Table III-38 Default settings for disinfectants for sanitary purposes at private use.

Parameter	Symbol	Unit	Value
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1
Fraction of the local main source for disinfectant	$Fmainsource_4$	[-]	0.002
Fraction released to waste water	$F_{4,water}$	[-]	1

B) average consumption per capita:

$$Elocal_{4,water} = Nlocal \cdot Vfrom \cdot Cform \cdot Fpenetr \cdot F_{4,water} \quad (44)$$

input			
Nlocal	Number of inhabitants feeding one STP	[-]	D
$F_{4,water}$	Fraction released to waste water	[-]	D
Cform	concentration active substance in biocidal product	[kg.m^{-3}]	S
Fpenetr	Penetration factor of disinfectant	[-]	D
-	type of application	[-]	P
Vform	Consumption per capita	[m^3.cap^{-1}.d^{-1}]	O
output			
$Elocal_{4,water}$	Emission rate to waste water	[kg.d^{-1}]	O

Table III-39 Default settings for calculating concentrations in the STP and surface water of compounds used in human hygiene products

Parameter	Symbol	Unit	Value
Number of inhabitants feeding one STP	Nlocal	[-]	10,000[a]
Fraction released to waste water	$F_{4,water}$	[-]	1
Penetration factor of disinfectant	Fpenetr	[-]	0.5
Consumption per capita	Vform	[m^3.cap^{-1}.d^{-1}]	
- general purpose (tiles floors, sinks)			5.10^{-6}
- lavatory			2.10^{-6}

[a] already defined in the sewage treatment distribution sub module

III.3.6.1.2 Medical sector

Disinfection of rooms, furniture and objects

Two models are used to calculated the release of disinfectants used for sanitary purposes in hospitals, viz. based on A) the annual tonnage and B) based on the applied amount of aqueous solution.

A) annual tonnage:

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \quad (45)$$

$$Elocal_{3,water} = TONNAGEreg \cdot Fhospital \cdot F_{3,water} \cdot \frac{365}{Temission_3} \quad (46)$$

Input			
TONNAGE	relevant tonnage in EU for this application	[kg.d^{-1}]	S
TONNAGEreg	relevant tonnage in the region for this application	[kg.d^{-1}]	S
$Fprodvol_{reg}$	fraction for the region	[-]	D
Fhospital	fraction for the hospital	[-]	D
$F_{3,water}$	fraction released to wastewater	[-]	D
$Temission_3$	number of emission days	[d]	D
Output			
$Elocal_{3,water}$	local emission to waste water during episode	[kg_c.d^{-1}]	O

Table III-40 Default settings for calculating concentrations in the STP and surface water of compounds used in disinfection of rooms, furniture and objects based on the annual tonnage

Parameter	Symbol	Unit	Value
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1
Fraction for the hospital	Fhospital	[-]	0.007
Fraction released to wastewater	$F_{3,water}$	[-]	0.75
Number of emission days	$Temission_3$	[d]	260

B) amount of solution used:

Sanitary purposes

$$Elocal_{3,water} = Vcons_{san} \cdot Cproc_{san} \cdot Fsan \quad (47)$$

Brushes

$$Elocal_{3,water} = Vcons_{obj} \cdot Cproc_{obj} \cdot Fobj \quad (48)$$

Sanitary purposes and brushes

$$Elocal_{3,water} = Vcons_{san} \cdot Cproc_{san} \cdot Fsan + Vcons_{obj} \cdot Cproc_{obj} \cdot Fobj \quad (49)$$

Input			
Fsan	fraction released to waste water for sanitary purposes	[-]	D
Fobj	fraction released to waste water for brushes	[-]	D
$Cproc_{san}$	concentration at which active substance is used, sanitary purposes	[kg.m^{-3}]	S
$Cproc_{obj}$	concentration at which active substance is used, brushes	[kg.m^{-3}]	S
$Vcons_{san}$	amount of water with active substance, sanitary purpose	[m^3.d^{-1}]	D
$Vcons_{obj}$	amount of water with active substance, brushes	[m^{3}d^{-1}]	D
Output			
$Elocal_{3,water}$	emission rate to waste water	[kg.d^{-1}]	O

Table III-41 Default settings for calculating concentrations in the STP and surface water of compounds used in disinfection of room, furniture and objects based on the amount of solution used on a day

Parameter	Symbol	Unit	Value
Fractions release to waste water			
- sanitary purposes	Fsan	[-]	0.55
- brushes	Fobj	[-]	0.95
Amount of water with active substance			
- sanitary purposes	$Vcons_{san}$	[m^3]	0.025
- brushes	$Vcons_{obj}$	[m^3]	0.025

Above a certain tonnage the scenario based on the tonnage should be applied preferably. If the default values are filled out in the formulas for the calculation of the local emissions to wastewater, $Elocal_{water}$, the break-even point can be written in the form:

$$TONNAGEreg = 956 \cdot Cproc_{san}$$ sanitary purposes

$$TONNAGEreg = 1560 \cdot Cproc_{obj}$$ brushes

$$TONNAGEreg = 956 \cdot Cproc_{san} + 1560 \cdot Cproc_{obj}$$ sanitary purposes and brushes

Disinfection of instruments

There are two types of washers: a) washers/disinfectors with replacement of the disinfectant solutions at regular intervals (called "replacement" in the scenario) and b) washers/disinfectors where a fresh disinfectant solution is applied every disinfection operation; the substance is discarded into the sewer after disinfection (called "once-through" in the scenario). Other instruments are disinfected in solutions (or suspensions) of disinfectants to prevent adhesion of blood, pus, etc. These baths are discarded into the sewer after use. If a biocide is notified for both disinfection of scopes and other instruments, the emission for a single point source (one hospital) should be calculated by summing the results of both emission scenarios. It is assumed that in case of more than one washers or disinfectors replacement of all machines occurs on the same day.

Washers or disinfectors, replacement:

Concentration at day of replacement due to carry-over

$$Cproc_{carry\_over} = \frac{Cproc}{(1 + Fcarry\_over)^{Tint_{repl}}} \quad (50)$$

Concentration at day of replacement including conversion

$$Cproc_{repl} = Cproc_{carry\_over} \cdot e^{-kdeg_{disinf} \cdot Tint_{repl}} \quad (51)$$

$$Elocal_{3,water} = Nmax_{mach} \cdot Vproc \cdot Cproc_{repl} \quad (52)$$

Washers or disinfector, once through

$$Elocal_{3,water} = Nmax_{mach} \cdot Vproc \cdot Cproc \quad (53)$$

Input			
Cproc	working concentration of active ingredient	[kg.m^{-3}]	S
$Nmax_{mach}$	number of washers or disinfectors	[-]	D
-	type of washer	[-]	P
Vproc	volume of solution in machine	[m^3]	O
$Tint_{repl}$	Replacement interval	[d]	D
Fcarry_over	Fraction carry-over	[-]	D
$kdeg_{disinf}$	Rate constant for chemical conversion	[d^{-1}]	S/D
Output			
$Elocal_{3,water}$	emission rate to waste water	[kg.d^{-1}]	O

Table III-42 Default settings for calculating concentrations in the STP and surface water of compounds used in disinfection of instruments with washers or disinfectors

Parameter	**Symbol**	**Unit**	**Value**
Maximum number of washers or disinfectors	$Nmax_{mach}$	[-]	3
Volume of solution in machine	Vproc	[m^3]	
- replacement			0.1
- once through			0.01
Replacement interval (replacement)	$Tint_{repl}$	[d]	14
Fraction carry-over (replacement)	Fcarry-over	[-]	0.015
Rate constant for chemical conversion (replacement)	$kdeg_{disinf}$	[d^{-1}]	0

Disinfection of instruments in baths:

$$Tint_{repl} = INT(1/Temission_3 + 0.5) \quad (54)$$

$$Elocal_{3,water} = \frac{Qsubst}{Temission_3} \cdot e^{-kdeg_{disinf} \cdot Tint_{repl}} \quad (55)$$

Input			
$Tint_{repl}$	average time disinfection solution is in use (replacement interval)	[d]	O
Qsubst	amount of active substance used	[kg.d^{-1}]	D
$Temission_3$	emission day, i.e., replacements	[d^{-1}]	D
$kdeg_{disinf}$	rate constant for chemical conversion	[d^{-1}]	S/D
Output			
$Elocal_{3,water}$	emission rate to waste water	[kg.d^{-1}]	O

Table III-43 Default settings for calculating concentrations in the STP and surface water of compounds used in disinfection of instruments with washers or disinfectors

Parameter	Symbol	Unit	Value
Amount of active substance used	Qsubst	[kg.d^{-1}]	0.68
Emission day, i.e., number of replacements	Temission$_3$	[d^{-1}]	0.27
Rate constant for chemical conversion (replacement)	kdeg$_{disinf}$	[d^{-1}]	0

Laundry disinfectants

Two emission scenarios are presented, one for commercial laundries where hospitals send their laundry and one for laundries or hospitals using tumbler washing machines. The size of commercial laundries can vary considerably but large laundries may have three or more washing tubes with a capacity of 8000 kg.day-1 per tube, producing 48 m^3.day^{-1} of waste. It is assumed here that a commercial laundry connected to the standard STP of EUSES/USES (2000 m^3 waste water per day) can have three washing tubes (3 * 48 = 144 m^3 wastewater per day). On the other hand, the situation is considered where a hospital is doing its own laundry or where the contaminated laundry is done at a commercial laundry using a tumbler washing machine. It is estimated that per kg of dirty laundry 6 g of detergent ("soap") is used, 4 g for soaking and 2 g for the washing cycle. In the case of disinfection, it is estimated that about 10% of the amount of soap are disinfectant.

Washing streets

$$Elocal_{3,water} = Nmach \cdot Qmat \cdot Vform_{kg} \cdot Cform \cdot (1 - Fred) \quad (56)$$

Input			
Nmach	number of washing tubes (with disinfectant)	[-]	D
Qmat	capacity of washing tube	[kg.d^{-1}]	D
Vform$_{kg}$	amount of disinfectant for laundry	[m^3.kg^{-1}]	S
Cform	concentration of active substance in disinfectant solution	[kg.m^{-3}]	S
Fred	concentration reduction in washing process	[-]	D
Output			
Elocal$_{3,water}$	emission rate to waste water	[kg.d^{-1}]	O

Table III-44 Default settings for calculating concentrations in the STP and surface water of disinfectants used for doing biologically contaminated laundry from hospitals in washing streets

Parameter	Symbol	Unit	Value
Number of washing tube	Nmach	[-]	3
Capacity of washing tube	Qmat	[kg.d^{-1}]	8,000
Concentration reduction in washing process	Fred	[-]	0

Washing machines

$$Elocal_{3,water} = Nbatch \cdot Qmat \cdot Vform_{kg} \cdot Cform \cdot (1 - Fred) \quad (57)$$

Input			
Nbatch	number of batches	[-]	D
Qmat	capacity of machines	[kg]	D
$Vform_{kg}$	amount of disinfectant for laundry	[$m^3.kg^{-1}$]	S
Cform	concentration of active substance in disinfectant solution	[$kg.m^{-3}$]	S
Fred	concentration reduction in washing process	[-]	D
Output			
$Elocal_{3,water}$	emission rate to waste water	[$kg.d^{-1}$]	O

Table III-45 Default settings for calculating concentrations in the STP and surface water of disinfectants used for doing biologically contaminated laundry from hospitals in tumbler washing machines

Parameter	Symbol	Unit	Value
Number of washing tubes	Nmach	[-]	3
Capacity of washing tube	Qmat	[$kg.d^{-1}$]	8,000
Concentration reduction in washing process	Fred	[-]	0

III.3.6.2 Product type 6: in-can preservatives: Paints and coatings

For emissions of biocides apply emission scenarios from IC 14 Paints, laquers and varnished industry.

III.3.6.3 Product type 6: in-can preservatives,PT 7 film preservatives and PT 9 fibre, leather, rubber and polymerised materials: preservatives used in paper production (IC 12)

The emission scenario document comprises life cycle stages 3 (industrial use) and 6 (paper) recycling. For life cycle stage 3 the emission scenario calculates air releases from the drying sections after size-pressing and releases to wastewater from "broke" in the paper machine at stock preparation. The scenarios presented in this section are the same for in-can preservatives (PT 6), film preservatives (PT 7) and fibre preservatives (PT 9). In some cases other default values have to be applied.

Life cycle stage Industrial use:
Releases from drying sections after size-pressing and coating

$$P_{T2} = P_{T1} \cdot e^{\frac{\Delta H}{R}\left(\frac{1}{T_1}-\frac{1}{T_2}\right)} \quad (58)$$

$$Qsubst = Vform \cdot Cform \quad (59)$$

$$Elocal_{3,air} = Qpaper \cdot Qsubst \cdot Fevap \cdot \left(1 - Fdecomp\right) \quad (60)$$

Input			
Vform	quantity of product with preservative applied per kg of paper	[$m^3.kg^{-1}$]	S
Cform	concentration of active substance in the biocidal product	[$kg_c.m^{-3}$]	S
Qsubst	quantity of active substance applied per kg of paper	[$kg_c.kg^{-1}$]	S/O
-	type of paper produced	[-]	P
Qpaper	quantity of coated paper produced per day	[$kg.d^{-1}$]	O
P_{T1}	vapour pressure at standard temperature	[Pa]	S
P_{T2}	vapour pressure at relevant application temperature	[Pa]	O
ΔH	heat of vaporisation for relevant temperature range	[$kJ.mol^{-1}$]	S
R	universal gas constant	[$kJ.mol^{-1}.K^{-1}$]	D
T_1	standard temperature at which P_{T1} is measured	[K]	S
T_2	relevant application temperature	[K]	S
Fevap	fraction evaporated	[-]	O
Output			
$Elocal_{3,air}$	local emission of active substance to air	[$kg_c.d^{-1}$]	O

Table III-46 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
vapour pressure at standard temperature	P_{T1}	[Pa]	[1)]
heat of vaporisation	ΔH	[$kJ.mol^{-1}$]	[1)]
universal gas constant	R	[$kJ.mol^{-1}.K^{-1}$]	8.314
standard temperature at which P_{T1} is measured	T_1	[K]	298[2)]
relevant application temperature	T_2	[K]	373

[1)] substance specific properties

[2)] when no standard temperature is given a default value of 25 °C is used

Table III-47 Default settings for calculating release to air of biocidal compounds used as in-can preservatives from the drying sections after size-pressing and coating in paper production

Parameter	Symbol	Unit	Value
Quantity of coated paper produced per day	Qpaper	[kg.d^{1}]	
- news print			449,000
- printing and writing paper			66,000
- printing and cardboard for packaging			237,000
- paper for sanitary and domestic use (tissue paper)			222,000
- special and industrial paper (all types)			102,000
Cardboard			
- flat cardboard			329,000
- corrugated cardboard			329,000
Fraction evaporated if volatility (Pa at 100 °C)	Fevap	[-]	
≥ 133			0.0025
13.3-133			0.0005
1.3-13.3			0.0001
<1.3			0
Fixation fraction	Ffix	[-]	
PT 6			0
PT 7			0.8
PT 9			0.8
Fraction decomposed during drying	Fdecomp	[-]	0

Life cycle stage Industrial use: Releases from "broke"

$$Qsubst = Vform \cdot Cform \quad (61)$$

$$Elocal_{3,water} = Qpaper \cdot Qsubst \cdot Fbroke \cdot (1 - Ffix) \cdot (1 - Fclosure) \quad (62)$$

Input			
Vform	quantity of product with preservative applied per kg of paper	[$m^3.kg^{-1}$]	S
Cform	concentration of active substance in the biocidal product	[$kg_c.m^{-3}$]	S
Qsubst	quantity of active substance applied per kg of paper	[$kg_c.kg^{-1}$]	S/O
-	type of paper produced	[-]	P
Qpaper	quantity of coated paper produced per day	[$kg.d^{-1}$]	O
Fbroke	fraction of coated broke produced compared to overall production	[-]	D
Ffix	fixation fraction	[-]	D
Fclosure	degree of closure of the water system	[-]	O
Output			
$Elocal_{3,water}$	local emission of active substance to waste water	[$kg_c.d^{-1}$]	O

Table III-48 Default settings for calculating release to waste water of biocidal compounds used as in-can preservatives from "broke" in paper production

Parameter	Symbol	Unit	Value
Degree of closure of the water system[1)]	Fclosure	[-]	
- news print			0.75[2)]
- printing and writing paper			0.55[3)]
- printing and cardboard for packaging			0.80[4)]
- paper for sanitary and domestic use (tissue paper)			0.75[2)]
- special and industrial paper (all types)			0.55[3)]
Cardboard			
- flat carboard			0.80[4)]
- corrugated cardboard			0.80[4)]
Fraction of coated broke produced compared to overall production	Fbroke	[-]	0.2
Fixation fraction	Ffix	[-]	0

[1)] the degree of closure will not effect the concentration of a substance in the wastewater, it will determine the volume of water and therefore the total amount of substance emitted. The wastewater flow should be adjusted accordingly when the degree of closure is changed.
[2)] a range of 0.65-0.85 was given in the ESD, 0.75 has been chosen as the average value
[3)] a range of 0.4-0.7 was given in the ESD, 0.55 has been chosen as the average value
[4)] a range of 0.65-0.95 and above was given in the ESD, 0.80 has been chosen as the average value

Life cycle stage waste treatment: Paper recycling

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \quad (63)$$

$$Elocal_{6,water} = TONNAGEreg \cdot Frec \cdot Fmainsource_5 \cdot Fdeink \cdot (1 - Fprelim) \cdot (1 - Fdecomp) \cdot \frac{365}{Nwdays} \quad (64)$$

Input

TONNAGE	relevant tonnage in EU for this application	[kg.d^{-1}]	S
TONNAGEreg	relevant tonnage in the region for this application	[kg.d^{-1}]	S/O
$Fprodvol_{reg}$	fraction for the region	[-]	D
$Fmainsource_6$	fraction of the main source (local STP)	[-]	D
-	type of paper recycled	[-]	P
Frec	fraction of paper recycled	[-]	O
Fdeink	fraction of preservatives released at de-inking	[-]	D
Fdecomp	fraction decomposed during de-inking	[-]	D
-	degree of solubility	[-]	P
Fprelim	fraction removed from waste water during preliminary on-site treatment	[-]	O
Nwdays	number of working days	[d]	D

Output

$Elocal_{6,water}$	local emission of active substance to waste water	[kg_c.d^{-1}]	O

Table III-49 Default settings for calculating releases of in-can preservatives from paper recycling

Parameter	Symbol	Unit	Value
Fraction for the region	$Fprovol_{reg}$	[-]	0.1
Fraction of the main source	$Fmainsource_6$	[-]	0.1
Fraction of recycled paper	Frec	[-]	0.54
- news print			0.58
- printing and writing paper			0.11
- paper and cardboard for packaging			0.46
- paper for sanitary and domestic use (tissue paper)			0.54
- special and industrial paper (all types)			0.55
Cardboard			
- flat cardboard			0.92
- corrugated cardboard			0.90
Fraction of preservatives released at de-inking	Fdeink	[-]	1
Fraction decomposed during de-inking	Fdecomp	[-]	0
Fraction removed from wastewater during preliminary on-site treatment	Fprelim	[-]	
- easy soluble[1]			0.1
- poorly soluble			0.7
Number of working days	Nwdays	[d]	340

[1)] Easy soluble substances are defined as having a water solubility >1000 $mg.l^{-1}$. Range of 0-0.2 have been given in the ESD for easy soluble substance and a range of 0.5-0.9 has been reported for poorly soluble substances.

III.3.6.4 Product type 7: Film preservatives applied in the pulp, paper and board industry (IC12)

See section III.3.6.3

III.3.6.5 Product type 9: Fibre, leather, rubber and polymerised materials preservatives: Leather preservatives

Application of biocides at each processing step, curing, pickling, soaking, tanning and finishing:

$$Elocal\_water_i = Qleather \cdot Qsubst_i \cdot (1 - Ffix) \qquad (65)$$

$$Elocal_{water} = \sum_{i=1}^{n} Elocal\_water_i \qquad (66)$$

Input			
Qleather	quantity of treated raw hide per day	[tonnes.d^{-1}]	D
$Qsubst_i$	quantity of substance used per tonne of leather for treatment step *i*	[kg_ctonne^{-1}]	D/P
Ffix	degree of fixation	[-]	S/D
$Elocal\_water_i$	local emission of active substance to water per treatment step	[kg_c.d^{-1}]	O
Output			
$Elocal_{3,water}$	total local emission to wastewater	[kg_c.d^{-1}]	O

Table III-50 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
quantity of treated raw hide per day	Qleather	[tonne.d^{-1}]	15
quantity of substance used per tonne of raw hide	Qsubst	[kg.tonne^{-1}]	5 [1)]
degree of fixation	Ffix	[-]	0.95

see pick-list ***Table III-51***

Table III-51 Pick-list for quantity of substance used per tonne of leather Qsubst (kg.tonne^{-1}).

Parameter	Qsubst
curring	0.1-5 (5)
soaking	0.1-5 (5)
pickling	0.1-5 (5)
tanning	0.1-5 (5)
finishing	0.3

III.3.6.6 Product type 9: Textile processing industry, textile preservatives

Desizing and scouring of imported material, biocides on imported fabrics or biocides applied during sizing.

$$Eimport_{3,water} = Qfibres \cdot Cmat \cdot 10^{-9} \qquad (67)$$

Input			
Qfibres	quantity of fibres / fabrics per day	[kg.d^{-1}]	P
Cmat	estimated content of active substance present in material	[μg_c.kg^{-1}]	D
Output			
$Eimport_{water}$	local emission to wastewater due to imported material	[kg_c.d^{-1}]	O

Table III-52 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
quantity of fibres / fabric treated per day	Qfibres	[kg.d^{-1}]	
cotton spinning			7 000
wool preparation			1 000
wool spinning			2 500
silk, synthetic			1 000
sewing knit			4 000
cotton weaving			2 000
wool weaving			1 000
silk weaving			100
others weaving			1 500
textile enobling			7 000
house and furnish fabric			500
other textile goods			200
cords, filets			3 000
non woven			4 000
mail fabrics			2 000
estimated concentration of active substance present in material	Cmat	[µg.kg^{-1}]	
Default			10
Wool			
Default			0.38
DDE			0.07-0.38
PCB-28/31			0.15-0.34
heptachlor			0.03-0.12
Cotton			
Default			12.4
DDE			0.85-4.5
DDD			0.09-12.8
DDT			0-12.4
heptachlor			0.13-0.45

Application of biocides at each textile processing step *(i),* desizing / scouring, dyeing and finishing (total emissions including emissions due to imported material):

$$Elocal_{3,water} = \sum_{i=1}^{n} Elocal\_water_i + Eimport_{water} \quad \textbf{(68)}$$

Input			
Qfabric	quantity of treated fabric per day	[tonnes.d^{-1}]	D
$Qsubst_i$	quantity of substance used per tonne of fibres/fabric for treatment step *i*	[$kg_c tonne^{-1}$]	S
Ffix	degree of fixation	[-]	S
$Elocal\_water_i$	local emission of active substance to water per treatment step	[$kg_c.d^{-1}$]	O
$Eimport_{water}$	local emission to wastewater due to imported material	[$kg_c.d^{-1}$]	O
Output			
$Elocal_{3,water}$	total local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-53 Defaults for emission calculations. The highest value is chosen for the worst case situation.

Parameter	Symbol	Unit	Value
quantity of treated fabric per day	Qfabric	[tonne.d^{-1}]	1)
quantity of substance used per tonne of fabric	Qsubst	[kg.$tonne^{-1}$]	10
permethrin			0.35-1.81
sulcofuron			8-9.7
permethrin/hexahydropyrimidine			0.55-0.825
degree of fixation	Ffix	[-]	0.7

1) see ***Table III-52***

2) as a worst case, a default value of 10 kg per tonne can be used if no further data is available

Life cycle stage Service life

$$RELEASEreg_{k,5,water} = \frac{Fprodvol_{reg} \cdot F_{5,water} \cdot Qsubst\_tot_k \cdot \sum_{y=1}^{Tservice_k} \left(1 - F_{5,j}\right)^{y-1}}{Temission_5} \quad (69)$$

$$RELEASEreg_{5,water} = 10^3 \cdot \sum_{k=1}^{m} RELEASEreg_{k,5,water} \quad (70)$$

$$Elocal_{5,water} = Fmainsource_5 \cdot RELEASEreg_{5,water} \quad (71)$$

Input			
$Qsubst\_tot_k$	annual input of the substance in article *k*	[tonnes.yr^{-1}]	S
$Fprodvol_{reg}$	fraction of the region	[-]	D
$Tservice_k$	service life of article *k*	[yr]	P
$F_{5,water}$	fraction of the tonnage release over one year during the servie to compartment *j*	[-]	S
$Temission_5$	duration of the emission per year	[d.yr^{-1}]	D
$Fmainsource_5$	fraction of the main source (STP)	[-]	D
$RELEASreg_{k,5,water}$	regional release to wastewater for articles *k*	[kg$_c$.d^{-1}]	O
$RELEASreg_{5,water}$	regional release to wastewater for all articles	[kg$_c$.d^{-1}]	O
Output			
$Elocal_{5,water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O

Table III-54 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
annual input of the substance in article k	$Qsubst\_tot_k$	[tonnes.yr^{-1}]	.
fraction of the region	$Fprodvol_{reg}$	[-]	0.1
service life of article k	$Tservice_k$	[yr]	[1)]
fraction of the tonnage released over one year during service life	$F_{5,water}$	[-]	.
duration of the emission per year	$Temission_5$	[d.yr^{-1}]	365
fraction of the main source (STP)	$Fmainsource_5$	[-]	0.002

[1)] see pick-list ***Table III-55***

Table III-55 Service life of some article, $Tservice_k$ (yr) some values are averages of the ranges presented in the emission scenario document.

Article	Service life
clothes on contact with skin	1.0
other clothes and bed linen	3.5
household linen	7.5
bedding	5.0
carpets	14.0
wall-to-wall carpet	17.5
sunblind	11.5
tents	12.5
awning	2.0

III.3.6.7 Product type 9: Fibre, leather, rubber and polymerised materials preservatives: Rubber industry

For biocides applied in rubber products, use emission scenario document on IC 11 Rubber industry, thought no specific data for biocides is reported.

III.3.6.7 Product type 9: Fibre, leather, rubber and polymerised materials preservatives: Paper industry

See section III.3.6.3

III.3.6.8 Product type 12: Slimicides

Estimation if concentration of the substance in process water is used:

$$Elocal_{3,water} = Csubst \cdot Qwater \cdot Qpaper \cdot (1 - Ffix) \quad (72)$$

Input			
Csubst	concentration of substance in process water	[$kg_c.m^{-3}$]	S/P
Qwater	quantity of water used per tonne of paper	[$m^3.tonne^{-1}$]	P
Qpaper	quantity of paper produced on one site per day	[$tonne.d^{-1}$]	P
Ffix	degree of fixation	[-]	S/P
Output			
$Elocal_{3,water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-56 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
concentration of substance in process water	Csubst	[$kg_c.m^{-3}$]	1)
quantity of water used per tonne of paper	Qwater	[$m^3.tonne^{-1}$]	2)
quantity of paper produced on one site per day	Qpaper	[$tonne.d^{-1}$]	2)
degree of fixation	Ffix	[-]	1)

1) see pick-list ***Table III-58***

2) see pick-list ***Table III-57***

Table III-57 Pick-list for water consumption, Qwater ($m^3.tonne^{-1}$) degree of closure, Fclosure (-) and quantity of paper produced, Qpaper ($tonne.d^{-1}$) for various types of paper. In case of ranges the highest values for water consumption and quantity of paper produced are chosen as worst case. For degree of closure the lowest value is set as worst case.

Type of paper produced	Water consumption	Degree of closure	Quantity of paper produced
printing and writing	40-75	0.40-0.70	100-1000
tissue	57	0.40-0.70	40-200
newsprint	24-35	0.65-0.85	100-1000
packaging and board	2-20	>0.95	100-1000

Table III-58 *Pick-list for amount of substance consumed per tonne, Qsubst (kg.tonne^{-1}) and degree of fixation, Ffix (-) for different types of substances used. For a worst case situation the highest value for the quantity of substance used and the lowest fixation rate are used.*

Type of substance used	**Quantity of substance used, Qsubst [kg.tonne^{-1}]**				**degree of fixation**
	news paper	board	printing writing	tissue	**Ffix [-]**
Concentration in process water [kg.m^{-3}]					
biociden	0.005-0.04	0.005-0.04	0.005-0.04	0.005-0.04	.

III.3.6.9 Product type 13 Metalworking-fluid preservatives

A) water-based cooling lubricants:

A.1) cooling lubricants based on emulsions

$$Elocal_{6,water} = \frac{Fproc}{Fproc+1} \cdot \frac{Cconc \cdot Vproc}{Fproc \cdot K_{ow}+1} \cdot Frel(1-Felim) \qquad \textbf{(73)}$$

$$Cconc = Fconc \cdot RHOconc \qquad \textbf{(74)}$$

Input			
Cconc	concentration of substance in concentrate	[$kg_c.m^{-3}$]	S/O
Fconc	fraction of substance in concentrate	[-]	S/P
RHOconc	density of the concentrate	[$kg.m^{-3}$]	D
Vproc	volume of processed liquid treated in recovery unit	[$m^3.d^{-1}$]	D
Fproc	fraction of concentrate in processed liquid	[-]	S/P
K_{ow}	octanol-water partition coefficient	[-]	S
Felim	fraction of the substance eliminated during treatment	[-]	D
Frel	factor of relevance	[-]	D
Output			
$Elocal_{6,water}$	local emission to wastewater	[$kg_c.d^{-1}$]	O

Table III-59 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
Fraction of substance in concentrate	Fconc	[-]	1)
Density of concentrate	RHOconc	[kg.m^{-3}]	1000
Volume of processed liquid treated in recovery plant	Vproc	[m^3.d^{-1}]	40
Fraction of concentrate in processed liquid	Fproc	[-]	2)
Octanol-water partition coefficient	K_{ow}	[-]	3)
Fraction of the substance eliminated during treatment	Felim	[-]	0.8
Factor of relevance	Frel	[-]	1

1) see pick-list ***Table III-61***

2) see pick-list ***Table III-62***

3) substance specific property

A.2) water-soluble lubricants:

$$Elocal_{6,water} = Cconc \cdot Vproc \cdot Fproc \cdot Frel \cdot (1 - Felim) \quad (75)$$

$$Cconc = Fconc \cdot RHOconc \quad (76)$$

Input

Cconc	concentration of substance in concentrate	[kg$_c$.m^{-3}]	S/O
Fconc	fraction of substance in concentrate	[-]	S/P
RHOprod	density of concentrate	[kg.m^{-3}]	D
Vproc	volume of processed liquid treated in recovery unit	[m^3.d^{-1}]	D
Fproc	fraction of concentrate in processed liquid	[-]	S/P
Felim	fraction of the substance eliminated during treatment	[-]	D
Frel	factor of relevance	[-]	D
Output			
$Elocal_{6,water}$	local emission to wastewater	[kg$_c$.d^{-1}]	O

Table III-60 Defaults for emission calculations.

Parameter	Symbol	Unit	Value
Concentration of substance in concentrate	Cconc	[kg$_c$.m^{-3}]	
Fraction of substance in concentrate	Fconc	[-]	1)
Density of concentrate	RHOconc	[kg.m^{-3}]	1000
Volume of processed liquid treated in recovery plant	Vproc	[m^3.d^{-1}]	40
Fraction of concentrate in processed liquid	Fproc	[-]	2)
Fraction of the substance eliminated during treatment	Felim	[-]	0.8
Factor of relevance	Frel	[-]	1

1) see pick-list ***Table III-61***

2) see pick-list ***Table III-62***

Table III-61 Pick-list for composition of cooling lubricants. Fraction of substance in concentrate, Fconc (-). The highest value is choosen to represent the worst case situation.

Substance group	traditional SEM[1]	synthetic SEM[1]	SES[2]
boric acids (biocide)	-	0-0.03	-
bactericide	0.04	0-0.05	0.03-0.04
fungicide	0-0.01	0-0.01	0-0.01

[1)] SEM emulsifiable cooling lubricant

[2)] SES water soluble cooling lubricant

Table III-62 Pick-list for fraction of cooling lubricant concentrate in processed liquid, Fproc (-) by type of process. In case of a range the highest content is used as the worst case value.

Process	Content [-]
broaching	0.10-0.20
thread cutting	0.05-0.10
deep hole drilling	0.10-0.20
parting-off	0.05-0.10
milling, cylindrical milling	0.05-0.10
turning, drilling, automation work	0.03-0.10
sawing	0.05-0.20
tool grinding	0.03-0.06
cylindrical grinding	0.02-0.05
centreless grinding	0.03-0.06
surface grinding	0.02-0.05

III.3.6.10 Product type 22: Embalming and taxidermist fluids

Taxidermy includes the preservation of animals and concerns as well as large mammals, fishes, birds and reptiles. Embalming consist of three different procedures which involve the use of biocides: surface disinfection (soaps, solutions), arterial injection of fluids and injection of cavity fluids into the torso to substitute body fluids.

Model for calculating release to water for compounds used in taxidermist fluids.

$$Elocal\_water_i = Qskin \cdot Qsubst \cdot (1 - Ffix) \quad (77)$$

$$Elocal_{3,water} = \sum Elocal\_water_i \quad (78)$$

Input			
Qskin	quantity of treated drained skin per day	[kg.d^{-1}]	D
-	type of agent per treatment step	[-]	P
Qsubst	quantity of active substance applied per kg of drained skin	[kg.kg^{-1}]	O
Ffix	fixation fraction	[-]	S/D
Elocal_water$_i$	local emission of active substance to waste water for treatment step *i*	[kg.d^{-1}]	O
Output			
Elocal$_{3,water}$	local emission of active substance to waste water for all treatment steps	[kg$_c$.d^{-1}]	O

Table III-63 Default settings of the model for calculating the release of biocides used in taxidermy.

Parameter	Symbol	Unit	Value
Quantity of treated drained skin per day	Qskin	[kg.d^{-1}]	4
Quantity of active substance applied per kg of drained skin	Qsubst	[kg.kg^{-1}]	0.02
Pickling			
- formaldehyde			0.005
- tanning agent			0.02
Soaking			
- bactericide			0.002
Preservation			
- insecticide			0.02
Fixation fraction	Ffix	[-]	0.95

Model for calculating release to water for compounds used in the embalming process.

$$Elocal_{3,water} = Vform_{arterial} \cdot RHOform \cdot Cform_{arterial} \cdot (1 - Fret_{arterial}) + Vform_{cavity} \cdot RHOform \cdot Cform_{cavity} \cdot (1 - Fret_{cavity}) \quad (79)$$

Input			
-	type of preservation and type of biocide applied	[-]	P
Vform$_{arterial}$	volume of solution applied per embalmed corpse for arterial injection	[m^3]	O/P
Vform$_{cavity}$	volume of solution applied per embalmed corpse for cavity treatment	[m^3]	O/P
RHOform	specific mass of solution	[kg.m^{-3}]	D
Cform$_{arterial}$	content of active substance in solution for arterial injection	[kg.kg^{-1}]	S
Cform$_{cavity}$	content of active substance in solution for cavity treatment	[kg.kg^{-1}]	S
Fret$_{arterial}$	retention rate of arterial fluid	[-]	O/P
Fret$_{cavity}$	retention rate of cavity fluid	[-]	O/P
Output			
Elocal$_{3,water}$	local emission of active substance to waste water	[kg.d^{-1}]	O

Table III-64 Default settings of the model for calculating the release of biocides used in the embalming process .

Parameter	Symbol	Unit	Value
Volume of solution applied per embalmed corpse for both arterial injection and cavity treatment	$Vform_{arterial}$ / $Vform_{cavity}$	[m^3]	
Short-term			
- formaldehyde 4%			0.0060
- formaldehyde 22%			0.0005
Long-term			
- formaldehyde 4%			0.0100
- formaldehyde 22%			0.0005
Retention rate of both arterial injection fluid and cavity treatment fluid	$Fret_{arterial}$ / $Fret_{cavity}$	[-]	
Short-term			
- formaldehyde 4%			0.9
- formaldehyde 22%			0.9
Long-term			
- formaldehyde 4%			0.8
- formaldehyde 22%			0.9
Specific mass of solution	RHOform	[$kg.m^{-3}$]	1,000

Model for calculating release in cemeteries of compounds used in the embalming process.

$$Elocal_{3,soil} = [Vform_{arterial} \cdot RHOform \cdot Cform_{arterial} \cdot (1 - Fret_{arterial}) + Vform_{cavity} \cdot RHOform \cdot Cform_{cavity} \cdot (1 - Fret_{cavity})] \cdot (1 - Freact) \cdot Ncorpse \quad (80)$$

$$Csoil\_av_{cem} = Elocal_{soil} / (LENGTHcem \cdot WIDTHcem \cdot DEPTHmix_{cem-soil} \cdot RHOsoil \cdot krem_{soil}) \quad (81)$$

$$Cporew\_av_{cem} = Csoil\_av_{cem} \cdot RHOsoil / K_{soil-water} \quad (82)$$

Input			
-	type of preservation and type of biocide applied	[-]	P
$Vform_{arterial}$	volume of solution applied per embalmed corpse for arterial injection	[m^3]	O/P
$Vform_{cavity}$	volume of solution applied per embalmed corpse for cavity treatment	[m^3]	O?P
RHOform	specific mass of solution	[$kg.m^{-3}$]	D
$Cform_{arterial}$	content of active substance in solution for arterial injection	[$kg.kg^{-1}$]	S
$Cform_{cavity}$	content of active substance in solution for cavity treatment	[$kg.kg^{-1}$]	S
$Fret_{arterial}$	retention rate of arterial fluid	[-]	O/P
$Fret_{cavity}$	retention rate of cavity fluid	[-]	O/P
Freact	factor for reaction with body	[-]	D
Ncorpse	number of embalmed corpses buried per day	[-]	D
LENGTHcem	length of cemetery	[m]	D
WIDTHcem	width of cemetery	[m]	D
$DEPTHmix_{cem-soil}$	mixing depth of soil	[m]	D
RHOsoil	bulk density of soil	[$kg.m^{-3}$]	D
$K_{soil-water}$	soil-water partition coefficient	[$m^3.m^{-3}$]	O^c
$krem_{soil}$	first order rate constant for removal in soil	[d^{-1}]	O^c
$Elocal_{3,soil}$	daily average input of active substance to the cemetery	[$kg.d^{-1}$]	O
$Csoil\_av_{cem}$	average concentration in soil	[$kg.kg_{wwt}^{-1}$]	O
Output			
$Cporew\_av_{cem}$	average concentration in soil porewater	[$kg.m^{-3}$]	O

Table III-65 Default settings of the model for calculating the release in cemeteries of biocides used in the embalming process.

Parameter	Symbol	Unit	Value
Volume of solution applied per embalmed corpse for both arterial injection and cavity treatment	$Vform_{arterial}$ / $Vform_{cavity}$	[m^3]	
Short-term			
- formaldehyde 4%			0.0060
- formaldehyde 22%			0.0005
Long-term			
- formaldehyde 4%			0.0100
- formaldehyde 22%			0.0005
Retention rate of both arterial injection fluid and cavity treatment fluid	$Fret_{arterial}$ / $Fret_{cavity}$	[-]	
Short-term			
- formaldehyde 4%			0.9
- formaldehyde 22%			0.9
Long-term			
- formaldehyde 4%			0.8
- formaldehyde 22%			0.9
Specific mass of solution	RHOform	[$kg.m^{-3}$]	1,000
Factor for reaction with body	Freact	[-]	0
Daily number of embalmed corpses buried per day	Ncorpse	[-]	0.065
Length of cemetery	LENGTHcem	[m]	100
-Width of cemetery	WIDTHcem	[m]	100
Mixing depth of soil	$DEPTHmix_{cem-soil}$	[m]	0.5
Bulk density of soil	RHOsoil	[$kg.m^{-3}$]	1,700
Specific mass of solution	RHOform	[$kg.m^{-3}$]	1,000

III.4 ENVIRONMENTAL DISTRIBUTION

In the environmental distribution module, five sub-modules are specified:
- Estimation of partition coefficients.
- Estimation of environmental degradation rates.
- Fate in sewage treatment.
- Regional environmental distribution.
- Local environmental distribution.

Environmental distribution is estimated on three spatial scales: local, regional and continental. The environmental characteristics of these scales are (by default) the same.

III.4.1 Partition coefficients

In this section, the characteristics of the environmental compartments are defined. From this definition, the bulk densities of soil, sediment and suspended matter are calculated. The following partitioning processes are quantified in this section:
- Adsorption to aerosol particles.
- Air-water partitioning.
- Adsorption/desorption to solids in soil, sediment, suspended matter and sewage sludge.

The output parameters for bulk densities of compartments and 'dimensionless partition coefficients' are closed for the user. This is done for the sake of internal consistency. For example bulk density of soil is defined by the fractions and densities of the separate phases (solids, water, air). The bulk density should not be changed without changing the fractions or densities of the phases.

Input			
VP	vapour pressure	[Pa]	
MOLW	molecular weight	[$kg_c.mol^{-1}$]	
SOL	solubility	[$kg_c.m^{-3}$]	
Kow	octanol-water partition coefficient	[-]	
TEMPmelt	melting point (only for solids for estimating $Fass_{aer}$)	[K]	
Intermediate results			
VP_L	sub-cooled liquid vapour pressure	[Pa]	
Koc	organic carbon-water partition coefficient	[$m^3.kg^{-1}$]	
Output 1			
RHO_{soil}	wet bulk density of soil	[$kg_{wwt}.m^{-3}$]	c
RHO_{sed}	wet bulk density of sediment	[$kg_{wwt}.m^{-3}$]	c
RHO_{susp}	wet bulk density of suspended matter	[$kg_{wwt}.m^{-3}$]	c
$CONV_{soil}$	conversion factor for soil concentrations: wwt to dwt	[$kg_{wwt}.kg_{dwt}^{-1}$]	c
$CONV_{sed}$	conversion factor for sediment concentrations: wwt to dwt	[$kg_{wwt}.kg_{dwt}^{-1}$]	c
$Fass_{aer}$	fraction of chemical associated with aerosol particles	[-]	
HENRY	Henry's law constant	[$Pa.m^3.mol^{-1}$]	
Kp_{susp}	solids-water partition coefficient in suspended matter	[$m^3.kg^{-1}$]	
Kp_{sed}	solids-water partition coefficient in sediment	[$m^3.kg^{-1}$]	
Kp_{soil}	solids-water partition coefficient in soil	[$m^3.kg^{-1}$]	
Kp_{RS}	solids-water partition coeff. in raw sewage sludge	[$m^3.kg^{-1}$]	
Kp_{PS}	solids-water partition coeff. in settled sewage sludge	[$m^3.kg^{-1}$]	
Kp_A	solids-water partition coeff. in activated sewage sludge	[$m^3.kg^{-1}$]	
Kp_{SLS}	solids-water partition coeff. in effluent sewage sludge	[$m^3.kg^{-1}$]	
Output 2 (internal parameters)			
$K_{air\text{-}water}$	air-water partition coefficient	[$m^3.m^{-3}$]	c
$K_{soil\text{-}water}$	soil-water partition coefficient	[$m^3.m^{-3}$]	c
$K_{susp\text{-}water}$	suspended matter-water partition coefficient	[$m^3.m^{-3}$]	c
$K_{sed\text{-}water}$	sediment-water partition coefficient	[$m^3.m^{-3}$]	c

Table III-66 Default environmental characteristics for local, regional and continental scales

Parameter	Symbol	Unit	Value
General			
Density of solid phase	RHOsolid	[$kg_{solid}.m_{solid}^{-3}$]	2500
Density of water phase	RHOwater	[$kg_{water}.m_{water}^{-3}$]	1000
Density of air	RHOair	[$kg_{air}.m_{air}^{-3}$]	1.3
Environmental temperature Freshwater environment (12 °C) Marine environment (9 °C)	TEMP	[K]	 285 282
Constant of Junge equation	CONjunge	[Pa.m]	[a]
Specific surface area of aerosol particles	$SURF_{aer}$	[$m^2.m^{-3}$]	[a]
Gas constant	R	[$Pa.m^3.mol^{-1}.K^{-1}$]	8.314 [b]
Suspended matter			
Volume fraction of solids in susp. matter	$Fsolid_{susp}$	[$m_{solid}^3.m_{susp}^{-3}$]	0.1
Volume fraction of water in susp. matter	$Fwater_{susp}$	[$m_{water}^3.m_{susp}^{-3}$]	0.9
Weight fraction of organic carbon in susp. solids	Foc_{susp}	[$kg_{oc}.kg_{solid}^{-1}$]	0.1
Sediment			
Volume fraction of solids in sediment	$Fsolid_{sed}$	[$m_{solid}^3.m_{sed}^{-3}$]	0.2
Volume fraction of water in sediment	$Fwater_{sed}$	[$m_{water}^3.m_{sed}^{-3}$]	0.8
Weight fraction of organic carbon sediment solids	Foc_{sed}	[$kg_{oc}.kg_{solid}^{-1}$]	0.05
Soil			
Volume fraction of solids in soil	$Fsolid_{soil}$	[$m_{solid}^3.m_{soil}^{-3}$]	0.6
Volume fraction of water in soil	$Fwater_{soil}$	[$m_{water}^3.m_{soil}^{-3}$]	0.2
Volume fraction of air in soil	$Fair_{soil}$	[$m_{air}^3.m_{soil}^{-3}$]	0.2
Weight fraction of organic carbon in soil solids	Foc_{soil}	[$kg_{oc}.kg_{solid}^{-1}$]	0.02

[a] By default, the product of *CONjunge* and $SURF_{aer}$ is set to 10^{-4} Pa (Van de Meent, 1993); Den Hollander and Van de Meent (2004) uses $2.58.10^{-5}$ Pa.
[b] This default cannot be changed by the user.

III.4.1.1 Bulk densities of compartments

Each of the compartments soil, sediment, and suspended matter is described as consisting of three phases: air (relevant in soil only), solids and water. The bulk density of each compartment is thus defined by the fraction and bulk density of each phase. Both the fractions of solids and water, and the total bulk density are used in subsequent calculations. This implies that the bulk density of a compartment cannot be changed independently of the fractions of the separate phases and vice versa.

$$RHO_{soil} = Fsolid_{soil} \cdot RHOsolid + Fwater_{soil} \cdot RHOwater + Fair_{soil} \cdot RHOair \quad (83)$$

$$RHO_{sed} = Fsolid_{sed} \cdot RHOsolid + Fwater_{sed} \cdot RHOwater \quad (84)$$

$$RHO_{susp} = Fsolid_{susp} \cdot RHOsolid + Fwater_{susp} \cdot RHOwater \quad (85)$$

Input			
$Fwater_{soil}$	volume fraction of water in soil	$[m^3.m^{-3}]$	D
$Fsolid_{soil}$	volume fraction of solids in soil	$[m^3.m^{-3}]$	D
$Fair_{soil}$	volume fraction of air in soil	$[m^3.m^{-3}]$	D
$Fwater_{sed}$	volume fraction of water in sediment	$[m^3.m^{-3}]$	D
$Fsolid_{sed}$	volume fraction of solids in sediment	$[m^3.m^{-3}]$	D
$Fwater_{susp}$	volume fraction of water in suspended matter	$[m^3.m^{-3}]$	D
$Fsolid_{susp}$	volume fraction of solids in suspended matter	$[m^3.m^{-3}]$	D
RHOsolid	density of solid phase	$[kg.m^{-3}]$	D
RHOwater	density of water phase	$[kg.m^{-3}]$	D
RHOair	density of air phase	$[kg.m^{-3}]$	D
Output			
RHO_{soil}	wet bulk density of soil	$[kg_{wwt}.m^{-3}]$	O[c]
RHO_{sed}	wet bulk density of sediment	$[kg_{wwt}.m^{-3}]$	O[c]
RHO_{susp}	wet bulk density of suspended matter	$[kg_{wwt}.m^{-3}]$	O[c]

III.4.1.2 Conversion wet weight-dry weight

In EUSES, concentrations in soil and sediment are total concentrations, and therefore expressed on a wet-weight basis. Optionally, intermediate results can be presented and changed on dry-weight basis. The conversion factors for soil and sediment are derived from the compartment definition in phases. The conversion to dry weight can also be used for entering terrestrial toxicity data.

$$CONV_{soil} = \frac{RHO_{soil}}{Fsolid_{soil} \cdot RHOsolid} \quad (86)$$

$$CONV_{susp} = \frac{RHO_{susp}}{Fsolid_{susp} \cdot RHOsolid} \quad (87)$$

Input			
RHO_{soil}	wet bulk density of soil	$[kg_{wwt}.m^{-3}]$	O[c]
$Fsolid_{soil}$	volume fraction of solids in soil	$[m^3.m^{-3}]$	D
RHO_{susp}	wet bulk density of suspended matter	$[kg_{wwt}.m^{-3}]$	O[c]
$Fsolid_{susp}$	volume fraction of solids in suspended matter	$[m^3.m^{-3}]$	D
RHOsolid	density of solid phase	$[kg.m^{-3}]$	D
Output			
$CONV_{soil}$	conversion factor for soil concentrations: wwt to dwt	$[kg_{wwt}.kg_{dwt}^{-1}]$	O[c]
$CONV_{susp}$	conversion factor for suspended matter conc.: wwt to dwt	$[kg_{wwt}.kg_{dwt}^{-1}]$	O[c]

III.4.1.3 Adsorption to aerosol particles

The fraction of the chemical associated with aerosol particles can be estimated on the basis of the chemical's vapour pressure, according to Junge (1977). In this equation, the sub-cooled liquid vapour pressure should be used. For solids, a correction is applied according to Mackay (1991).

$$Fass_{aer} = \frac{CONjunge \cdot SURF_{aer}}{VP_L + CONjunge \cdot SURF_{aer}} \quad (88)$$

If *TEMPmelt* <= *TEMP* (substance is liquid):

$$VP_L = VP \quad (89)$$

If *TEMPmelt* > *TEMP* (substance is solid):

$$VP_L = \frac{VP}{e^{6.79\left(1 - \frac{TEMPmelt}{TEMP}\right)}} \quad (90)$$

Input			
CONjunge	constant of Junge equation	[Pa.m]	D
$SURF_{aer}$	surface area of aerosol particles	[$m^2.m^{-3}$]	D
VP	vapour pressure	[Pa]	S
TEMP	environmental temperature	[K]	D
TEMPmelt	melting point of substance	[K]	S
Output			
VP_L	sub-cooled liquid vapour pressure	[Pa]	O
$Fass_{aer}$	fraction of chemical associated with aerosol particles	[-]	O

III.4.1.4 Air-water partitioning

The transfer of substances from the aqueous phase to the gas phase (e.g. stripping in the aeration tank of an STP, volatilisation from surface water) is estimated by means of its Henry's Law constant. If the value is not available in the input dataset, the required Henry's Law constant and $K_{air\text{-}water}$ (also known as the 'dimensionless' Henry's Law constant) can be estimated from the ratio of the vapour pressure to the water solubility:

$$HENRY = \frac{VP \cdot MOLW}{SOL} \quad (91)$$

$$K_{air\text{-}water} = \frac{HENRY}{R \cdot TEMP} \quad (92)$$

Input			
VP	vapour pressure	[Pa]	S
MOLW	molecular weight	[$kg_c.mol^{-1}$]	S
SOL	water solubility	[$kg_c.m^{-3}$]	S
R	gas constant	[$Pa.m^3.mol^{-1}.K^{-1}$]	D[c]
TEMP	environmental temperature	[K]	D
Output			
HENRY	Henry's law constant	[$Pa.m^3.mol^{-1}$]	O
$K_{air\text{-}water}$	air-water partition coefficient	[$m^3.m^{-3}$]	O[c]

III.4.1.5 Estimation of Koc

If no *Koc* is available from the dataset, it may be estimated from *Kow*. Several models have been developed for different classes of chemicals. Most relationships are based on *Kow*, since hydrophobic interactions are the most dominant type of interactions between non-polar organic chemicals and the soil organic carbon. Chapter 4 of the TGD discusses these estimation routines in more detail, and proposes the following general defaulte for non-polar, organic compounds (Sabljic *et al.*, 1995). The QSAR was derived from a range of log *Kow* values from 1 - 7.5. For specific groups of substances, other QSARs are available, which are presented in **Table III-67.** Euses will present these formulas to the user. These QSARs should be used, if appropriate, and the estimate of equation **(93)** will be overwritten in such cases (Sabljic *et al.*, 1995).

$$\boldsymbol{Koc = \frac{1.26 \cdot Kow^{0.81}}{1000}} \qquad \textbf{(93)}$$

Input			
Kow	octanol-water partition coefficient	[-]	S
Output			
Koc	organic carbon-water partition coefficient:	[$m^3.kg^{-1}$]	O

Table III-67 QSARS for soil and sediment sorption for different chemical classes (Sabljic et al, 1995).

Chemical class	Equation
Predominantly hydrophobics	$Koc = \frac{1.26 \cdot Kow^{0.81}}{1000}$
Nonhydrophobics	$Koc = \frac{10.47 \cdot Kow^{0.52}}{1000}$
Phenols, anilines, benzonitriles, nitrobenzenes	$Koc = \frac{7.94 \cdot Kow^{0.63}}{1000}$
Acetanilides, carbamates, esters, phenylureas, phosphates, triazines, triazoles, uracils	$Koc = \frac{12.30 \cdot Kow^{0.47}}{1000}$
Alcohols, organic acids	$Koc = \frac{3.16 \cdot Kow^{0.47}}{1000}$
Acetanilides	$Koc = \frac{13.18 \cdot Kow^{0.40}}{1000}$
Alcohols	$Koc = \frac{3.16 \cdot Kow^{0.39}}{1000}$
Amides	$Koc = \frac{17.78 \cdot Kow^{0.33}}{1000}$
Anilines	$Koc = \frac{7.08 \cdot Kow^{0.62}}{1000}$
Carbamates	$Koc = \frac{13.80 \cdot Kow^{0.37}}{1000}$
Dinitroanilines	$Koc = \frac{83.18 \cdot Kow^{0.38}}{1000}$
Esters	$Koc = \frac{11.22 \cdot Kow^{0.49}}{1000}$
Nitrobenzenes	$Koc = \frac{3.55 \cdot Kow^{0.77}}{1000}$
Organic acids	$Koc = \frac{2.09 \cdot Kow^{0.60}}{1000}$
Phenols, benzonitriles	$Koc = \frac{12.02 \cdot Kow^{0.57}}{1000}$
Phenylureas	$Koc = \frac{11.22 \cdot Kow^{0.49}}{1000}$
Phosphates	$Koc = \frac{14.79 \cdot Kow^{0.49}}{1000}$
Triazines	$Koc = \frac{31.62 \cdot Kow^{0.30}}{1000}$
Triazoles	$Koc = \frac{25.70 \cdot Kow^{0.47}}{1000}$

III.4.1.6 Solids-water partitioning in the environment

The solids-water partition coefficient (*Kp*) in each environmental compartment (soil, sediment, suspended matter) can be derived from the normalised partition coefficient, *Koc*, and the fraction of organic carbon in the compartment.

$$Kp_{soil} = Foc_{soil} \cdot Koc \quad (94)$$

$$Kp_{sed} = Foc_{sed} \cdot Koc \quad (95)$$

$$Kp_{susp} = Foc_{susp} \cdot Koc \quad (96)$$

Input			
Foc_{soil}	weight fraction of organic carbon in soil	[kg.kg^{-1}]	D
Foc_{sed}	weight fraction of organic carbon in sediment	[kg.kg^{-1}]	D
Foc_{susp}	weight fraction of organic carbon in suspended matter	[kg.kg^{-1}]	D
Koc	organic carbon-water partition coefficient	[m^3.kg^{-1}]	O
Output			
Kp_{susp}	solids-water partition coefficient in suspended matter	[m^3.kg^{-1}]	O
Kp_{sed}	solids-water partition coefficient in sediment	[m^3.kg^{-1}]	O
Kp_{soil}	solids-water partition coefficient in soil	[m^3.kg^{-1}]	O

III.4.1.7 Solids-water partitioning in sewage treatment plant

Table III-68 Fraction of organic carbon of solids in various STP sludges.

Parameter	Symbol	Unit	Value
Fraction of organic carbon in solids raw sewage	Foc_{RS}	$[kg_{oc}.kg_{solids}^{-1}]$	0.3
Fraction of organic carbon in solids primary settler	Foc_{PS}	$[kg_{oc}.kg_{solids}^{-1}]$	0.3
Fraction of organic carbon in solids activated sludge	Foc_{A}	$[kg_{oc}.kg_{solids}^{-1}]$	0.37
Fraction of organic carbon in solids in solids-liquid separator	Foc_{SLS}	$[kg_{oc}.kg_{solids}^{-1}]$	0.37

The solids-water partition coefficients for various STP sludges are estimated from *Koc*.

$$Kp_i = Foc_i \cdot Koc \qquad i \in \{RS, PS, A, SLS\} \qquad \textbf{(97)}$$

Input			
Koc	organic carbon-water partition coefficient	$[m^3.kg^{-1}]$	O
Foc_{RS}	fraction of organic carbon in raw sewage sludge	$[kg.kg^{-1}]$	D
Foc_{PS}	fraction of organic carbon in settled sewage sludge	$[kg.kg^{-1}]$	D
Foc_{A}	fraction of organic carbon in activated sewage sludge	$[kg.kg^{-1}]$	D
Foc_{SLS}	fraction of organic carbon in effluent sewage sludge	$[kg.kg^{-1}]$	D
Output			
Kp_{RS}	solids-water partition coeff. in raw sewage sludge	$[m^3.kg^{-1}]$	O
Kp_{PS}	solids-water partition coeff. in settled sewage sludge	$[m^3.kg^{-1}]$	O
Kp_{A}	solids-water partition coeff. in activated sewage sludge	$[m^3.kg^{-1}]$	O
Kp_{SLS}	solids-water partition coeff. in effluent sewage sludge	$[m^3.kg^{-1}]$	O

In the absence of better adsorption/ desorption data, the results from the Zahn-Wellens elimination level can be used as an estimate of the extent of adsorption to sludge (the 3^h – value is recommended). Especially for water soluble and highly adsorptive substances this is recommended in the TGD (Part II; EC, 2003).

III.4.1.8 Total compartment-water partitioning

Kp describes the partitioning between solids and water in a compartment. The 'dimensionless' form of *Kp*, or the total compartment-water partition coefficient, is derived from the definition of the compartments in three phases.

$$K_{soil\text{-}water} = Fair_{soil} \cdot K_{air\text{-}water} + Fwater_{soil} + Fsolid_{soil} \cdot Kp_{soil} \cdot RHOsolid \quad (98)$$

$$K_{susp\text{-}water} = Fwater_{susp} + Fsolid_{susp} \cdot Kp_{susp} \cdot RHOsolid \quad (99)$$

$$K_{sed\text{-}water} = Fwater_{sed} + Fsolid_{sed} \cdot Kp_{sed} \cdot RHOsolid \quad (100)$$

Input			
$Fwater_{soil}$	fraction of water in soil	$[m^3.m^{-3}]$	D
$Fsolid_{soil}$	fraction of solids in soil	$[m^3.m^{-3}]$	D
$Fair_{soil}$	fraction of air in soil	$[m^3.m^{-3}]$	D
$Fwater_{sed}$	fraction of water in sediment	$[m^3.m^{-3}]$	D
$Fsolid_{sed}$	fraction of solids in sediment	$[m^3.m^{-3}]$	D
$Fwater_{susp}$	fraction of water in suspended matter	$[m^3.m^{-3}]$	D
$Fsolid_{susp}$	fraction of solids in suspended matter	$[m^3.m^{-3}]$	D
RHOsolid	density of solid phase	$[kg.m^{-3}]$	D
Kp_{soil}	solids-water partition coefficient in soil	$[m^3.kg^{-1}]$	O
Kp_{sed}	solids-water partition coefficient in sediment	$[m^3.kg^{-1}]$	O
Kp_{susp}	solids-water partition coefficient in suspended matter	$[m^3.kg^{-1}]$	O
$K_{air\text{-}water}$	air-water partition coefficient	$[m^3.m^{-3}]$	O[c]
Output			
$K_{soil\text{-}water}$	total soil-water partition coefficient	$[m^3.m^{-3}]$	O[c]
$K_{susp\text{-}water}$	total suspended matter-water partition coefficient	$[m^3.m^{-3}]$	O[c]
$K_{sed\text{-}water}$	total sediment-water partition coefficient	$[m^3.m^{-3}]$	O[c]

III.4.2 Degradation and transformation rates

Since measured data on degradation processes for different compartments are not usually available, they must be extrapolated from standardised laboratory tests. In this section, degradation rate constants are derived for abiotic degradation in surface water (hydrolysis and photolysis) and biotic degradation (in soil, sediment, water and sewage treatment). Abiotic degradation in marine environments should be assessed in a similar manner to abiotic degradation in freshwater environments except that the different physico-chemical conditions in marine environments should be taken into account (for example the generally lower temperature of in average 9°C). Abiotic degradation is not estimated for the compartments soil, sediment and STP. If rate constants are known, their default setting of zero (see table below) may be changed.

Input

	characterisation of biodegradability (ready/inherent/non-biodegradable/specific criteria)	
TEMPtest	temperature of the measured data in standard/simulation test	[K]
$DT50hydr_{water\_temp\ test}$	half-life for hydrolysis in water at the temperature of the data set	[d]
$DT50photo_{water}$	half-life for photolysis in water	[d]
k_{OH}	specific degradation rate constant with OH-radicals	[m^3.$molec^{-1}$.d^{-1}]
$DT50bio_{water\_temp\ test}$	half-life for biodegradation in water at temperature of the data set	[d]
$DT50bio_{soil\_temp\ test}$	half-life for biodegradation in soil at temperature of data set	[d]
$DT50bio\text{-}aer_{sed\_temp\ test}$	half-life for biodeg. in aerobic sediment at temperature of data set	[d]
Intermediate results		
$DT50hydr_{water\_temp\ env}$	half-life for hydrolysis in water at the environmental temperature	[d]
$DT50bio_{stp}$	half-life for biodegradation in STP	[d]
$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]
$DT50bio_{water\_temp\ env}$	half-life for biodegradation in water at the environmental temp.	[d]
$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]
$DT50bio_{soil\_temp\ env}$	half-life for biodegradation in soil at the environmental temp.	[d]
$DT50bio\text{-}aer_{sed}$	half-life for biodegradation in aerobic sediment	[d]
$DT50bio\text{-}aer_{sed\_temp\ env}$	half-life for biodeg. in aerobic sediment at environmental temp.	[d]
Output		
$kdeg_{air}$	total rate constant for degradation in air	[d^{-1}]
$kdeg_{stp}$	total rate constant for degradation in STP	[d^{-1}]
$kdeg_{water}$	total rate constant for degradation in bulk surface water	[d^{-1}]
$kdeg_{soil}$	total rate constant for biodegradation in bulk soil	[d^{-1}]
$kdeg_{sed}$	total rate constant for biodegradation in bulk sediment	[d^{-1}]

Table III-69 Defaults for calculating degradation rates.

Parameter	Symbol	Unit	Value
Concentration of OH-radicals in atmosphere	$OHCONC_{air}$	[molecules.m^{-3}]	5.10^{11}
Fraction of sediment compartment that is aerated	$Faer_{sed}$	[m^3.m^{-3}]	0.10
Rate constant for abiotic degradation in STP	$kabio_{stp}$	[d^{-1}]	0
Rate constant for abiotic degradation in soil	$kabio_{soil}$	[d^{-1}]	0
Rate constant for abiotic degradation in sediment	$kabio_{sed}$	[d^{-1}]	0
Rate constant for anaerobic biodegr. in sediment	$kbio\text{-}anaer_{sed}$	[d^{-1}]	0
Environmental temperature	TEMP	[K]	
Freshwater environment (12 °C)			285
Marine environment (9 °C)			282

III.4.2.1 Hydrolysis in water

Rates of hydrolysis increases with increasing temperature. When hydrolysis half-lives have been determined in standard tests, they should be recalculated to reflect an average EU outdoor temperature by the equation:

$$DT50hydr_{water\_temp\ env} = DT50hydr_{water\_temp\ test} \cdot e^{(0.08 \cdot (TEMPtest - TEMPenv))}$$

Input			
$DT50hydr_{water\_temp\ test}$	half-life for hydrolysis in water at the temperature of the data set	[d]	S
TEMPtest	temperature of the measured data in standard test	[K]	S
TEMP	environmental temperature	[K]	D
Output			
$DT50hydr_{water\_temp\ env}$	half-life for hydrolysis in water at the environmental temperature	[d]	O

Values for the half-life (DT50) of a hydrolysable substance (if known) can be converted to degradation rate constants, which are used in the distribution models.

$$khydr_{water} = \frac{\ln 2}{DT50\,hydr_{water\_temp\ env}} \qquad \textbf{(101)}$$

Input			
$DT50hydr_{water\_temp\ env}$	half-life for hydrolysis in water at the environmental temperature	[d]	O
Output			
$khydr_{water}$	rate constant for hydrolysis in water	[d^{-1}]	O

III.4.2.2 Photolysis in surface water

A value for the half-life for photolysis in water (if known) can be converted to a first-order rate constant.

$$kphoto_{water} = \frac{\ln 2}{DT\,50\,photo_{water}} \qquad \textbf{(102)}$$

Input			
$DT50photo_{water}$	half-life for photolysis in water	[d]	S
Output			
$kphoto_{water}$	rate constant for photolysis in water	[d^{-1}]	O

III.4.2.3 Photochemical reactions in the atmosphere

Although for some chemicals direct photolysis may be an important breakdown process, for most substances, the most effective elimination process in the troposphere is reaction with photochemically generated species like OH-radicals, ozone and nitrate radicals. The specific

degradation rate constant of a substance with OH-radicals can either be determined experimentally (OECD, 1992c) or estimated by (Q)SAR-methods (see Chapter 4 of the TGD). By relating k_{OH} to the OH-radical concentration in the atmosphere, the pseudo-first-order rate constant in air is determined:

$$k\deg_{air} = k_{OH} \cdot OHCONC_{air} \qquad \textbf{(103)}$$

Input			
k_{OH}	specific degradation rate constant with OH-radicals	[m^3.$molec^{-1}$.d^{-1}]	S
$OHCONC_{air}$	concentration of OH-radicals in atmosphere	[molecules.m^{-3}]	D
Output			
$kdeg_{air}$	rate constant for degradation in air	[d^{-1}]	O

III.4.2.4 Biodegradation in the sewage treatment plant

For the purpose of modelling a sewage treatment plant (STP), the rate constants of ***Table III-70*** have been derived to extrapolate from the biodegradation screening tests.

Table III-70 *Elimination in sewage treatment plants: extrapolation from test results to rate constants in the STP model (SimpleTreat).*

Test result	**Rate constant (hr^{-1})**	**Rate constant (d^{-1})**	**Half-life (d)**
		$kbio_{stp}$	$DT50bio_{stp}$
Readily biodegradable	1	24	0.029
Readily biodegradable, but failing 10-d window	0.3	7.2	0.096
Inherently biodegradable, fulfilling specific criteria	0.1	2.4	0.29
Inherently biodegradable, not fulfilling specific criteria	0	0	∞
Not biodegradable	0	0	∞

Specific criteria that the various inherent biodegradation tests must fulfil:

Zahn-Wellens test: Pass level must be reached within 7 days, log-phase (time window) should be no longer than 3 days, percentage removal in the test before biodegradation occurs should be below 15 %.

MITI-II test: Pass level must be reached within 14 days, log-phase (time window) should be no longer than 3 days.

No specific criteria have been developed for positive results in a SCAS test. A rate constant of 0 d^{-1} is assigned to a substance, irrespective of whether it passes this test or not.

Table III-70 gives the following input-output table:

Input			
	results of screening test on biodegradability		P
Output			
$kbio_{stp}$	rate constant for biodegradation in STP	$[d^{-1}]$	O
$DT50bio_{stp}$	half-life for biodegradation in STP	[d]	O

The overall degradation-rate constant is given by:

$$k\,\mathrm{deg}_{stp} = kbio_{stp} + kabio_{stp} \qquad \textbf{(104)}$$

Input			
$kbio_{stp}$	rate constant for biodegradation in STP	$[d^{-1}]$	O
$kabio_{stp}$	rate constant for abiotic degradation in STP	$[d^{-1}]$	D
Output			
$kdeg_{stp}$	rate constant for degradation in STP	$[d^{-1}]$	O

III.4.2.5 Biodegradation in surface water

The table below gives half-lives for biodegradation in bulk surface water (freshwater and marine), based on the results of screening tests for biodegradability.

Table III-71 Half-lives for biodegradation in bulk surface water (freshwater and marine) at the environmental temperature, based on results of screening tests on biodegradability.

Test result	**Half-life for biodegradation in bulk surface water (d)** $DT50bio_{water}$		
	Freshwater	**Estuaries**[a]	**Other marine environments**[b]
Degradable in marine screening test	n.a.	15	50
Readily biodegradable	15	15	50
Readily biodegradable, but failing 10-d window	50	50	150
Inherently biodegradable	150	150	∞
Persistent	∞	∞	∞

n.a. Not applicable
[a] Also including shallow marine water closest to the coastline
[b] The half lives mentioned under this heading are normally to be used in the regional assessement (coastal model)

Input			
	results of screening test on biodegradability		P
Output			
$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]	O

Temperature influences the activity of micro-organisms and thus the biodegradation rate in the environment. When biodegradation rates or half-lives have been determined in simulation tests, it should be considered to recalculate the degradation rates obtained to reflect an

average EU outdoor temperature by the following equation:

$$DT50bio_{water\_temp\ env} = DT50bio_{water\_temp\ test} \cdot e^{(0.08 \cdot (TEMPtest - TEMPenv))} \quad \textbf{(105)}$$

Input			
$DT50bio_{water\_temp\ test}$	half-life for biodegradation in water at temperature of the data set	[d]	S
TEMPtest	temperature of the measured data in simulation test	[K]	S
TEMP	environmental temperature	[K]	D
Output			
$DT50bio_{water\_temp\ env}$	half-life for biodegradation in water at the environmental temp.	[d]	O

Values for the half-life (DT50) for biodegradation can be converted to first order rate constants for biodegradation.

$$kbio_{water} = \frac{\ln 2}{DT50\,bio_{water}} \quad or \quad kbio_{water} = \frac{\ln 2}{DT50\,bio_{water\_temp\ env}} \quad \textbf{(106)}$$

Input			
$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]	O
$DT50bio_{water\_temp\ env}$	half-life for biodegradation in water at the environmental temp.	[d]	O
Output			
$kbio_{water}$	rate constant for biodegradation in bulk surface water	[d^{-1}]	O

III.4.2.6 Overall rate constant for degradation in bulk surface water

The rate constants for the various different transformation processes can be summed into one overall degradation rate constant (used for regional and continental calculations only). It should be noted that different types of degradation (primary and ultimate) are added, which is done for modelling purposes only.

$$k\,\mathrm{deg}_{water} = khydr_{water} + kphoto_{water} + kbio_{water} \quad \textbf{(107)}$$

Input			
$khydr_{water}$	rate constant for hydrolysis in surface water	[d^{-1}]	O
$kphoto_{water}$	rate constant for photolysis in surface water	[d^{-1}]	O
$kbio_{water}$	rate constant for biodegradation in bulk surface water	[d^{-1}]	O
Output			
$kdeg_{water}$	total rate constant for degradation in bulk surface water	[d^{-1}]	O

III.4.2.7 Biodegradation in soil and sediment

In **Table III-72** rate constants are given for degradation in bulk soil. Since it is assumed that no degradation takes place in the bound phase, the rate constant in principle depends on the partition coefficient of the chemical.

Table III-72 *Half-lives for (bulk) soil and aerobic sediment, based on results from standardised biodegradation tests.*

	Half-life for soil and aerobic sediment (d) [a] $DT50bio_{soil}$ / $DT50bio\text{-}aer_{sed}$ [b]		
Kp_{soil} / Kp_{sed} [b] [$m^3.kg^{-1}$]	Readily biodegradable	Readily biodegradable, failing 10-d window	Inherently biodegradable
≤ 0.1	30	90	300
>0.1, ≤ 1.0	300	900	3000
>1.0, ≤ 10	3000	9000	30000
etc.	etc.	etc.	etc.

a In the case of non-biodegradable substances an infinite half-life is assumed.
b For deriving the degradation rate in aerobic sediment, the same half-life as for soil is used, but using the *Kp* for sediment.

Input

	results of screening test on biodegradability		P
Kp_{soil}	solids-water partition coefficient in soil	[$m^3.kg^{-1}$]	O
Output			
$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]	O
$DT50bio\text{-}aer_{sed}$	half-life for biodegradation in aerobic sediment	[d]	O

Temperature influences the activity of micro-organisms and thus the biodegradation rate in the environment. When biodegradation rates or half-lives have been determined in simulation tests, it should be considered to recalculate the degradation rates obtained to reflect an average EU outdoor temperature by the following equations:

$$DT50bio_{soil\_temp\ env} = DT50bio_{soil\_temp\ test} \cdot e^{(0.08 \cdot (TEMPtest - TEMPenv))} \quad \textbf{(108)}$$

$$DT50bio-aer_{sed\_temp\ env} = DT50bio-aer_{sed\_temp\ test} \cdot e^{(0.08 \cdot (TEMPtest - TEMPenv))} \quad \textbf{(109)}$$

Input			
$DT50bio_{soil\_temp\ test}$	half-life for biodegradation in soil at temperature of data set	[d]	S
$DT50bio\text{-}aer_{sed\_temp\ test}$	half-life for biodeg. in aerobic sediment at temperature of data set	[d]	O
TEMPtest	temperature of the measured data in simulation test	[K]	S
TEMP	environmental temperature	[K]	D
Output			
$DT50bio_{soil\_temp\ env}$	half-life for biodegradation in soil at the environmental temp.	[d]	O
$DT50bio\text{-}aer_{sed\_temp\ env}$	half-life for biodeg. in aerobic sediment at environmental temp.	[d]	O

The following equation converts the DT50 to a rate constant for biodegradation in bulk soil. A rate constant for abiotic degradation (if known) is added.

$$kbio_{soil} = \frac{\ln 2}{DT50bio_{soil}} \quad or \quad kbio_{soil} = \frac{\ln 2}{DT50bio_{soil\_temp\ env}} \qquad (110)$$

$$k\deg_{soil} = kbio_{soil} + kabio_{soil} \qquad (111)$$

Input			
$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]	O
$DT50bio_{soil\_temp\ env}$	half-life for biodegradation in soil at the environmental temp.	[d]	O
$kabio_{soil}$	rate constant for abiotic degradation in bulk soil	[d^{-1}]	D
$kbio_{soil}$	rate constant for biodegradation in bulk soil	[d^{-1}]	O
Output			
$kdeg_{soil}$	total rate constant for degradation in bulk soil	[d^{-1}]	O

The extrapolation of test results to rate constants for sediment is problematic, given the fact that sediment generally consists of a relatively thin oxic top layer and anoxic deeper layers. For the degradation in the anoxic layers, a rate constant of zero (infinite half-life) is assumed unless specific information on degradation under anaerobic conditions is available. For the oxic zone, the same rate constant and temperature correction as that for soil is assumed (see **Table III-72**).

$$kbio_{aer\text{-}sed} = \frac{\ln 2}{DT50bio - aer_{sed}} \quad or \quad kbio_{aer\text{-}sed} = \frac{\ln 2}{DT50bio - aer_{sed\_temp\ env}} \qquad (112)$$

$$k\,deg_{sed} = Faer_{sed} \cdot kbio - aer_{sed} + (1 - Faer_{sed}) \cdot kbio - anaer_{sed} + kabio_{sed} \qquad (113)$$

Input			
$DT50bio\text{-}aer_{sed}$	half-life for biodegradation in aerobic sediment	[d]	O
$DT50bio\text{-}aer_{sed\_temp\ env}$	half-life for biodeg. in aerobic sediment at environmental temp.	[d]	O
$Faer_{sed}$	fraction of sediment compartment that is aerated	[$m^3.m^{-3}$]	D
$kabio_{sed}$	rate constant for abiotic degradation in bulk sediment	[d^{-1}]	D
$kbio\text{-}anaer_{sed}$	rate constant for anaerobic biodegradation in sediment	[d^{-1}]	D
Output			
$kbio\text{-}aer_{sed}$	rate constant for biodegradation in aerobic sediment	[d^{-1}]	O
$kdeg_{sed}$	total rate constant for degradation in bulk sediment	[d^{-1}]	O

III.4.3 Sewage treatment

Emissions to wastewater are treated in a sewage treatment plant (STP). For estimation of fate in an STP, the model SimpleTreat 3.1is used, which differs from version 3.0 only with respect to the default calculation of the solids-water partitioning coefficient Kp. This model is not described in detail in this section. For details and the mathematical process descriptions, the reader is referred to the SimpleTreat reference manual (Struijs, 1996). Sewage treatment takes place at the local, regional and continental scale. The definition of STP characteristics is the same at each of these spatial scales. The number of inhabitants is used to scale the size of the STP.

The following options are included in the STP module:
- temperature dependence of biodegradation,
- Monod degradation kinetics,
- not considering a primary settler (this 'six-box option' can only be specified at the local spatial scale).

Input: chemical properties		
HENRY	Henry's law constant	[Pa.m^3.mol^{-1}]
$kdeg_{stp}$	total rate constant for degradation in STP	[d^{-1}]
Kp_{RS}	solids-water partition coeff. in raw sewage sludge	[m^3.kg^{-1}]
Kp_{PS}	solids-water partition coeff. in settled sewage sludge	[m^3.kg^{-1}]
Kp_A	solids-water partition coeff. in activated sewage sludge	[m^3.kg^{-1}]
Kp_{SLS}	solids-water partition coeff. in effluent sewage sludge	[m^3.kg^{-1}]
Input: emissions		
$Elocal_{water}$	local emission rate to wastewater during episode	[kg_c.d^{-1}]
$Ereg_{water}$	regional emission rate to wastewater (annual average)	[kg_c.d^{-1}]
$Econt_{water}$	continental emission rate to wastewater (annual average)	[kg_c.d^{-1}]
Intermediate results		
$EFFLUENTlocal_{stp}$	effluent discharge rate of local STP	[m^3.d^{-1}] [c]
$Fstp_i$	fraction directed to compartment *i* by local STP	[-]
$Fstp\text{-}reg_i$	fraction directed to compartment *i* by regional STP	[-]
$Fstp\text{-}cont_i$	fraction directed to compartment *i* by continental STP $i \in$ {air,water,sludge,degr}	[-]
Output: local		
$Estp_{air}$	local indirect emission to air from STP during episode	[kg_c.d^{-1}]
$Clocal_{eff}$	concentration of chemical (total) in the STP effluent	[kg_c.m^{-3}]
C_{sludge}	concentration in dry sewage sludge	[kg_c.kg^{-1}]
PEC_{stp}	PEC for micro-organisms in STP	[kg_c.m^{-3}]
Output: regional		
$Estp\text{-}reg_{air}$	regional indirect emission to air from STP	[kg_c.d^{-1}]
$Estp\text{-}reg_{water}$	regional indirect emission to surface water from STP	[kg_c.d^{-1}]
$Estp\text{-}reg_{agric}$	regional indirect emission to agricultural soil via sludge	[kg_c.d^{-1}]
Output: continental		
$Estp\text{-}cont_{air}$	continental indirect emission to air from STP	[kg_c.d^{-1}]
$Estp\text{-}cont_{water}$	continental indirect emission to surface water from STP	[kg_c.d^{-1}]
$Estp\text{-}cont_{agric}$	continental indirect emission to agricultural soil via sludge	[kg_c.d^{-1}]

Table III-73 lists the fixed parameters, subdivided into the categories raw sewage, primary sedimentation (9-box only), aerator and solids-liquid separation.

Table III-73 Fixed parameters for raw sewage and the operation of domestic wastewater treatment.

Parameter	Symbol	Unit	Value
raw sewage			
Mass of O_2-binding material per person per day	BOD	[$kg_{O2}.eq^{-1}.d^{-1}$]	0.054
Dry weight of solids produced per person per day	SOLIDS	[$kg_{dwt}.eq.^{-1}\ d^{-1}$]	0.09
Density of solids	RHO_{RS}	[$kg_{dwt}.m^{-3}$]	1500
primary settler (9-box only)			
Depth	$DEPTH_{PS}$	[m]	4
Hydraulic retention time (2 hours)	HRT_{PS}	[d]	0.083
Density of suspended and settled solids	RHO_{PS}	[$kg_{dwt}.m^{-3}$]	1500
activated sludge tank			
Depth	$DEPTH_A$	[m]	3
Density solids of activated sludge	RHO_A	[$kg_{dwt}.m^{-3}$]	1300
Concentration solids of activated sludge	CAS	[$kg_{dwt}.m^{-3}$]	4
Steady-state O_2 concentration in activated sludge	COX	[$kg.m^{-3}$]	0.002
Aeration rate of bubble aeration	G	[$m^3.d^{-1}.eq^{-1}$]	1.13
solids-liquid separator			
Depth	$DEPTH_{SLS}$	[m]	3
Density of suspended and settled solids	RHO_{SLS}	[$kg_{dwt}.m^{-3}$]	1300
Concentration of solids in effluent	$SUSP_{eff}$	[$kg_{dwt}.m^{-3}$]	0.03
Hydraulic retention time (6 hours)	HRT_{SLS}	[d]	0.25

Only four parameters may be specified if the user does not accept the default values (see ***Table III-74***). The sludge loading-rate parameter, k_{SLR} (kg BOD kg_{dwt}^{-1} d^{-1}), is chosen instead of the sludge retention time, SRT (d), to quantify the BOD loading of the installation. In principle, the hydraulic retention time, HRT (hr), could also have been chosen for this purpose. For the operation range relevant for wastewater treatment technology, these three parameters are interdependent according to certain relationships, which in some cases are empirical.

Table III-74 Input parameters characterising size and mode of operation of sewage treatment plant.

Parameter	Symbol	Units	Value
Sewage flow	Q_{stp}	[$m^3.eq^{-1}.d^{-1}$]	0.2
Number of inhabitants feeding system at scale local region EU	Nlocal N *	[eq]	10000 20.10^6 370.10^6
Sludge-loading rate	k_{SLR}	[$kg_{BOD}.kg_{dwt}^{-1}.d^{-1}$]	0.15
Temperature of air above aeration tank (15 °C)	$TEMPstp_{air}$	[K]	288
Temperature of water in aeration tank (15 °C)	$TEMPstp_{water}$	[K]	288
Wind speed (3 m/s)	WINDSPEED	[$m.d^{-1}$]	$2.59.10^5$
Mode of aeration: surface (s) or bubble aeration (b)	M	[-]	s

* Different parameter value possible on regional and continental scale.

III.4.3.1 STP calculations

The SimpleTreat calculations yield the following input-output table:

Input			
HENRY	Henry's law constant	[$Pa.m^3.mol^{-1}$]	O
$kdeg_{stp}$	rate constant for biodegradation in STP	[d^{-1}]	O
$Elocal_{water}$	local emission rate to wastewater during episode	[$kg_c.d^{-1}$]	O
$Ereg_{water}$	regional emission rate to wastewater (annual average)	[$kg_c.d^{-1}$]	O
$Econt_{water}$	continental emission rate to wastewater (annual average)	[$kg_c.d^{-1}$]	O
Kp_{RS}	solids-water partition coeff. in raw sewage sludge	[$m^3.kg^{-1}$]	O
Kp_{PS}	solids-water partition coeff. in settled sewage sludge	[$m^3.kg^{-1}$]	O
Kp_A	solids-water partition coeff. in activated sewage sludge	[$m^3.kg^{-1}$]	O
Kp_{SLS}	solids-water partition coeff. in effluent sewage sludge	[$m^3.kg^{-1}$]	O
Output			
$Clocal_{eff}$	concentration of chemical (total) in STP effluent	[$kg_c.m^{-3}$]	O
C_{sludge}	concentration in dry sewage sludge	[$kg_c.kg_{dwt}^{-1}$]	O
$Fstp_i$	fraction of emission directed to compartment *i* by STP	[-]	O
$Fstp\text{-}reg_i$	fraction directed to compartment *i* by regional STP	[-]	O
$Fstp\text{-}cont_i$	fraction directed to compartment *i* by continental STP $i \in$ {air,water,sludge,degr}	[-]	O

EUSES will perform a check whether the effluent concentration ($Clocal_{eff}$) exceeds the water solubility. If this is the case, the results of this module should be studied in more detail on a case-by-case basis.

III.4.3.2 Calculation of influent concentration

The influent concentration is used for exposure of micro-organisms in the case of intermittent release. For local-scale assessments, it is assumed that one point source is releasing its wastewater to one STP. The concentration in the influent of the STP, i.e. the untreated

wastewater, can be calculated from the local emission to wastewater and the influent discharge of the STP. The influent discharge equals the effluent discharge.

$$Clocal_{inf} = \frac{Elocal_{water}}{EFFLUENTlocal_{stp}} \quad \textbf{(114)}$$

$$Clocal_{eff} = Clocal_{inf} \cdot Fstp_{water} \quad \textbf{(115)}$$

Input			
$Elocal_{water}$	local emission rate to wastewater during episode	[$kg_c.d^{-1}$]	O
$EFFLUENTlocal_{stp}$	effluent discharge rate of local STP	[$m^3.d^{-1}$]	O^c
$Fstp_{water}$	fraction of the emission to wastewater directed to effluent	[-]	O
Output			
$Clocal_{inf}$	concentration in untreated wastewater	[$kg_c.m^{-3}$]	O
$Clocal_{eff}$	concentration of chemical in the STP effluent	[$kg_c.m^{-3}$]	O

For calculating the PEC in surface water (fresh water or marine water) without sewage treatment, the fraction of the emission to wastewater directed to effluent ($Fstp_{water}$) should be set to 1. The fractions to air and sludge ($Fstp_{air}$ and $Fstp_{sludge}$, respectively) should be set to zero. This ($Fstp_{water}$=1) is the default for local emissions to the marine environment.

The effluent discharge of the local STP is given by the following equation. The effluent discharges of the regional and continental STPs are given in Section III.4.4.5 (Equation 127 and 119). It should be noted that measured effluent-discharge rates cannot be entered directly by the user, but have to be derived by adjusting the number of inhabitants and the sewage flow per inhabitant.

$$EFFLUENTlocal_{stp} = Nlocal \cdot Q_{stp} \quad \textbf{(116)}$$

Input			
Nlocal	capacity of the local STP, number of inhabitants	[eq]	D
Q_{stp}	sewage flow per inhabitant	[$m^3.d^{-1}.eq^{-1}$]	D
Output			
$EFFLUENTlocal_{stp}$	effluent discharge rate of local STP	[$m^3.d^{-1}$]	O^c

III.4.3.3 PEC for micro-organisms in STP

For the risk characterisation of a chemical for micro-organisms in the STP, ideally the concentration in the aeration tank should be used. Assuming homogeneous mixing in the aeration tank, the dissolved concentration of a substance there is equal to the effluent concentration:

$$PEC_{stp} = Clocal_{eff} \quad \textbf{(117)}$$

Input			
$Clocal_{eff}$	total concentration of chemical in STP effluent	[$kg_c.m^{-3}$]	O
Output			
PEC_{stp}	PEC for micro-organisms in STP	[$kg_c.m^{-3}$]	O

However, in the case of intermittent release, the concentration in of STP influent is more representative because the highest concentration as a result of shock load is accounted for.

$$PEC_{stp} = Clocal_{inf} \quad \textbf{(118)}$$

Input			
$Clocal_{inf}$	total concentration of chemical in STP influent	[$kg_c.m^{-3}$]	O
Output			
PEC_{stp}	PEC for micro-organisms in STP	[$kg_c.m^{-3}$]	O

III.4.3.4 Calculation of the emission to air from the STP

The (indirect) emission from the STP to air is given by the fraction of the emission to wastewater, directed to air.

$$Estp_{air} = Fstp_{air} \cdot Elocal_{water} \quad \textbf{(119)}$$

Input			
$Fstp_{air}$	fraction of emission to air from STP	[-]	O
$Elocal_{water}$	local emission rate to wastewater during emission episode	[$kg_c.d^{-1}$]	O
Output			
$Estp_{air}$	local emission to air from STP during emission episode	[$kg_c.d^{-1}$]	O

III.4.3.5 Emissions from STP at the regional and continental scale

The indirect emissions via the STP at the regional and continental scale are calculated from the emissions to wastewater and the fate in the STP. The relative fate (expressed as fractions redirected to air, water and sludge) will usually be identical at all three spatial scales. However, when the degradation in the STP is modelled by Monod kinetics, differences in fate are possible.

$$Estp\text{-}reg_i = Fstp\text{-}reg_i \cdot Ereg_{water} \quad \textbf{(120)}$$

$$Estp\text{-}cont_i = Fstp\text{-}cont_i \cdot Econt_{water} \quad \textbf{(121)}$$

$$i \in \{air, water, sludge/agric\}$$

Input			
$Fstp\text{-}reg_i$	fraction directed to compartment *i* by regional STP	[-]	O
$Fstp\text{-}cont_i$	fraction directed to compartment *i* by continental STP	[-]	O
$Ereg_{water}$	regional emission rate to wastewater	$[kg_c.d^{-1}]$	O
$Econt_{water}$	continental emission rate to wastewater	$[kg_c.d^{-1}]$	O
Output			
$Estp\text{-}reg_{air}$	regional emission to air from STP	$[kg_c.d^{-1}]$	O
$Estp\text{-}reg_{water}$	regional emission to water from STP	$[kg_c.d^{-1}]$	O
$Estp\text{-}reg_{agric}$	regional emission to agricultural soil via sludge	$[kg_c.d^{-1}]$	O
$Estp\text{-}cont_{air}$	continental emission to air from STP	$[kg_c.d^{-1}]$	O
$Estp\text{-}cont_{water}$	continental emission to water from STP	$[kg_c.d^{-1}]$	O
$Estp\text{-}cont_{agric}$	continental emission to agricultural soil via sludge	$[kg_c.d^{-1}]$	O

III.4.4 Regional environmental distribution

Steady-state exposure concentrations at the regional and continental scales are calculated for all environmental compartments using a nested version of the multi-media fate model SimpleBox (Van de Meent, 1993; Brandes *et al.*, 1996; see also Section 2.4.4). The version of SimpleBox implemented in EUSES is described in technical detail by. den Hollander, van de Meent and van Eijkeren (2003, in prep.) In this section, the regional model is described by its inputs, outputs and default values. Furthermore, the calculations for the net sedimentation rate and the residence time in air and water are given (these are shown as closed outputs in the defaults section of the EUSES programme).

Input: regional emissions			
$Ereg_j$	direct emission to compartment *j* (annual average flux) $j \in$ {direct-water,ind,agric,air}	$[kg_c.d^{-1}]$	
$Estp\text{-}reg_j$	regional indirect emission to compartment *j* from STP $j \in$ {water,agric,air}	$[kg_c.d^{-1}]$	
Input: continental emissions			
$Econt_j$	direct emission to compartment *j* (annual average flux) $j \in$ {direct-water,ind,agric,air}	$[kg_c.d^{-1}]$	
$Estp\text{-}cont_j$	continental indirect emission to compartment *j* from STP $j \in$ {water,agric,air}	$[kg_c.d^{-1}]$	
Input: chemical properties			
Kow	octanol-water partition coefficient (only for estimation of BCF for aquatic biota)	[S]	
$Fass_{aer}$	fraction of chemical associated with aerosol particles	[-]	
$K_{air\text{-}water}$	air-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{soil\text{-}water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{sed\text{-}water}$	sediment-water partition coefficient	$[m^3.m^{-3}]$	c
Kp_{susp}	solids-water partition coefficient in suspended matter	$[m^3.kg_{solids}^{-1}]$	
RHO_{soil}	wet bulk density of soil	$[kg_{wwt}.m^{-3}]$	c
$kdeg_{air}$	rate constant for degradation in air	$[d^{-1}]$	
$kdeg_{water}$	rate constant for degradation in bulk water	$[d^{-1}]$	
$kdeg_{soil}$	rate constant for degradation in bulk soil	$[d^{-1}]$	
$kdeg_{sed}$	rate constant for degradation in bulk sediment	$[d^{-1}]$	
Output: continental concentrations			
$PECcont_{water,tot}$	continental PEC in surface water (total)	$[kg_c.m^{-3}]$	c
$PECcont_{water}$	continental PEC in surface water (dissolved)	$[kg_c.m^{-3}]$	c
$PECcont_{air}$	continental PEC in air (total)	$[kg_c.m^{-3}]$	c
$PECcont_{agric}$	continental PEC in agricultural soil (total)	$[kg_c.kg_{wwt}^{-1}]$	c
$PECcont_{agric,porew}$	continental PEC in pore water of agricultural soils	$[kg_c.m^{-3}]$	c
$PECcont_{natural}$	continental PEC in natural soil (total)	$[kg_c.kg_{wwt}^{-1}]$	c
$PECcont_{ind}$	continental PEC in industrial soil (total)	$[kg_c.kg_{wwt}^{-1}]$	c
$PECcont_{sed}$	continental PEC in sediment (total)	$[kg_c.kg_{wwt}^{-1}]$	c
Output: regional concentrations			
$PECreg_{water,tot}$	regional PEC in surface water (total)	$[kg_c.m^{-3}]$	
$PECreg_{water}$	regional PEC in surface water (dissolved)	$[kg_c.m^{-3}]$	
$PECreg_{air}$	regional PEC in air (total)	$[kg_c.m^{-3}]$	
$PECreg_{agric}$	regional PEC in agricultural soil (total)	$[kg_c.kg_{wwt}^{-1}]$	
$PECreg_{agric,porew}$	regional PEC in pore water of agricultural soil	$[kg_c.m^{-3}]$	
$PECreg_{natural}$	regional PEC in natural soil (total)	$[kg_c.kg_{wwt}^{-1}]$	
$PECreg_{ind}$	regional PEC in industrial soil (total)	$[kg_c.kg_{wwt}^{-1}]$	
$PECreg_{sed}$	regional PEC in sediment (total)	$[kg_c.kg_{wwt}^{-1}]$	

The following tables give the default settings for the regional and continental systems. Most parameter values are taken from the TGD. It should be noted that several characteristic parameters are given in the tables and the TGD which are actually outputs and not defaults: residence time in air and water, and the net sedimentation rate. Therefore, these parameters may change when default values are changed. To comply with the residence times and sedimentation rate of the TGD, several parameters were set to 'not unreasonable values': the fraction of the continental scale water flow that flows into the regional system and the rate of soil erosion.

Table III-75 General parameter settings for the regional and continental scales.

Parameter	Symbol	Unit	Value
Area of system (land and sea) region EU	AREA(reg) AREA(EU)	[m^2]	$4.04.10^{10}$ $7.04.10^{12}$
Number of inhabitants region EU	N(reg) N(EU)	[eq]	20.10^{6} [a] 370.10^{6} [a]
Fraction connected to sewer systems	$Fconnect_{stp}$	[-]	0.80 [b]
Per-capita water use	Q_{stp}	[$m^3.d^{-1}$]	0.20 [a]

[a] Already defined in STP sub-module.
[b] Already defined in emission module.

Table III-76 Default environmental characteristics for local, regional and continental scales

Parameter	Symbol	Unit	Value
Density of solid phase	RHOsolid	[$kg_{solid}.m_{solid}^{-3}$]	2500 [a]
Volume fraction of solids in sediment (marine and fresh water)	$Fsolid_{sed}$	[$m_{solid}^{3}.m_{sed}^{-3}$]	0.2 [a]
Volume fraction of water in sediment (marine and fresh water)	$Fwater_{sed}$	[$m_{water}^{3}.m_{sed}^{-3}$]	0.8 [a]
Volume fraction of solids in soil	$Fsolid_{soil}$	[$m_{solid}^{3}.m_{soil}^{-3}$]	0.6 [a]
Volume fraction of water in soil	$Fwater_{soil}$	[$m_{water}^{3}.m_{soil}^{-3}$]	0.2 [a]
Volume fraction of air in soil	$Fair_{soil}$	[$m_{air}^{3}.m_{soil}^{-3}$]	0.2 [a]

[a] Already defined in partition coefficients sub-module.

Table III-77 Parameter settings for regional and continental air.

Parameter	Symbol	Unit	Value
Atmospheric mixing height	$HEIGHT_{air}$	[m]	1000
Wind speed of system	WINDSPEED	[$m.d^{-1}$]	$2.59.10^{5}$ [a]
Residence time of air region continent	TAU_{air} *	[d]	0.687 O[c] 9.05 O[c]
Aerosol-deposition velocity	$DEPRATE_{aer}$	[$m.d^{-1}$]	86.4
Aerosol-collection efficiency	$COLLEFF_{aer}$	[-]	2.10^{5}
Average daily precipitation	RAINRATE	[$m.d^{-1}$]	$1.92.10^{-3}$

[a] Already defined in STP sub-module.
* Different parameter value possible on regional and continental scale.

Table III-78 Parameter settings for regional and continental marine and fresh waters.

Parameter	Symbol	Unit	Value
Area fraction of fresh water region (both 3% of land area) continent	F_{water} *	[-]	0.0297 0.015
Area fraction of marine water region continent	$F_{water,marine}$ *	[-]	0.0099 0.5
Water depth fresh water region+cont.	$DEPTH_{water}$ *	[m]	3
Water depth marine region continent	$DEPTH_{water, marine}$ *	[m]	10 200
Fraction of flow from region larger scale continent	$Fflow_{out}$ *	[-]	0.034 0
Residence time of fresh water region continent	TAU_{water} *	[d]	43.3 O[c] 1721 O[c]
Residence time of marine water region continent	$TAU_{water, marine}$ *	[d]	4.04 O[c] 365 O[c]
Suspended-solids conc. region+cont.	$SUSP_{water}$ *	[$kg_{dwt}.m^{-3}$]	0.015 .
Suspended-solids conc. region+cont.	$SUSP_{water, marine}$ *	[$kg_{dwt}.m^{-3}$]	0.005
Concentration of biota (marine and fresh water)	$BIOTA_{water}$	[$kg_{wwt}.m^{-3}$]	0.001
Fraction of rainwater infiltrating in soil	$Finf_{soil}$	[-]	0.25 [a]
Rate of wet precipitation (700 mm/year)	RAINRATE	[$m.d^{-1}$]	$1.92.10^{-3}$ [a]

* Different parameter value possible on regional and continental scale.

Table III-79 Parameter settings for regional and continental marine and fresh water sediments.

Parameter	Symbol	Unit	Value
Sediment mixing depth	$DEPTH_{sed}$	[m]	0.03
Settling velocity of suspended solids	$SETTLRATE_{susp}$	[$m.d^{-1}$]	2.5
(Biogenic) production of suspended solids in fresh water region: $10g.m^{-2}.a^{-1}$ continent: $10g.m^{-2}.a^{-1}$	$SUSPPROD_{water}$ *	[$kg.d^{-1}$]	$3.3.10^{4}$ Oc $2.9.10^{6}$ Oc
(Biogenic) production of suspended solids in marine water region: $10g.m^{-2}.a^{-1}$ continent: $5g.m^{-2}.a^{-1}$	$SUSPPROD_{water, marine}$ *	[$kg.d^{-1}$]	$1.1.10^{4}$ Oc $4.8.10^{7}$ Oc
Suspended solids in STP effluent	$SUSP_{eff}$	[$kg_{dwt}.m^{-3}$]	0.030 [a]
Net sedimentation rate fresh water region continent	NETsedrate *	[$m_{sed}.d^{-1}$]	$7.5.10^{-6}$ O^{c} $7.5.10^{-6}$ O^{c}
Net sedimentation rate marine water region continent	$NETsedrate_{marine}$ *	[$m_{sed}.d^{-1}$]	$4.2.10^{-6}$ O^{c} $1.8.10^{-8}$ O^{c}

[a] Already defined in STP sub-module.
* Different parameter value possible on regional and continental scale.

Table III-80 Parameter settings for regional and continental soils.

Parameter	Symbol	Unit	Value
Area fraction of natural soil (27% of land area) region continent	$F_{natural}$ *	[-]	0.267 0.135
Mixing depth of natural soil	$DEPTH_{natural}$	[m]	0.05
Area fraction of agricultural soil (60% of land area) region continent	F_{agric} *	[-]	0.594 0.30
Mixing depth of agricultural soil	$DEPTH_{agric}$	[m]	0.2
Area fraction of industrial/urban soil (10% of land area) region continent	F_{ind} *	[-]	0.099 0.05
Mixing depth of industrial/urban soil	$DEPTH_{ind}$	[m]	0.05
Fraction of rainwater infiltrating soil	$Finf_{soil}$	[-]	0.25
Fraction of rainwater run-off from soil	$Frunoff_{soil}$	[-]	0.25
Soil-erosion rate	EROSION	$[m.d^{-1}]$	$8.2.10^{-8}$

* Different parameter value possible on regional and continental scale.

Table III-81 Mass-transfer coefficients for regional and continental scales.

Parameter	Symbol	Unit	Value
Partial mass-transfer coefficient air side of air-soil interfaces	$kasl_{air}$	$[m.d^{-1}]$	90,5
Partial mass-transfer coefficient soil side of air-soil interface	$Kasl_{soil}$	$[m.d^{-1}]$	Equation 132
Partial mass-transfer coefficient air side of air-water interface	kaw_{air}	$[m.d^{-1}]$	Equation 139
Partial-mass transfer coefficient water side of air-water interface	kaw_{water}	$[m.d^{-1}]$	Equation 140
Partial mass-transfer coefficient water side sediment-water interface	kws_{water}	$[m.d^{-1}]$	0.24
Partial mass-transfer coefficient sediment side sediment-water interface	kws_{sed}	$[m.d^{-1}]$	$2.4.10^{-3}$

The regional distribution module is handled within this documentation as a 'black-box', only described by it's inputs and outputs. Several parameters, however, must be specified outside the SimpleBox calculation routines. Firstly, since the regional system is nested within the continental system, the values for area and population of the continental system must exclude the regional system.

In the following sections, calculations are given for the parameters that are specified in the TGD (and in the tables above) but are actually intermediate calculation results: residence times in air and water, and net sedimentation rate. These results are closed, to guard the internal consistency

of the model.

Water in SimpleBox is treated as a bulk compartment. The last section shows the derivation of the dissolved concentration from the total concentration.

III.4.4.1 Area and population of the continental system

The area and population of the continental system are derived from the value for the total EU and the regional definition.

$$AREA(cont) = AREA(EU) - AREA(reg) \quad (122)$$

Input			
AREA(EU)	area of EU	[m^2]	D
AREA(reg)	area of regional system	[m^2]	D
Output			
AREA(cont)	area of continental system	[m^2]	O^c

$$N(cont) = N(EU) - N(reg) \quad (123)$$

Input			
N(EU)	number of inhabitants of EU	[eq]	D
N(reg)	number of inhabitants of region	[eq]	D
Output			
N(cont)	number of inhabitants of continental system	[eq]	O^c

III.4.4.2 Residence time in air

The residence time of air in the system is given by the area of the system and the wind speed.

$$TAU_{air} = \frac{\sqrt{AREA \cdot \frac{\pi}{4}}}{WINDSPEED} \qquad (124)$$

Input			
AREA	area of the system	[m^2]	D*
WINDSPEED	wind speed	[$m.d^{-1}$]	D
Output			
TAU_{air}	residence time of air	[d]	O*[c]

III.4.4.3 Residence time in water

The total water flow through the system is caused by inflow from the larger spatial scale, wastewater production, run-off from soil, and direct rainfall into surface waters.

$$FLOW_{water} = Fflow_{out} \cdot FLOW_{water}(*) + WASTEW + RUNOFF + RAINDIRECT \qquad (125)$$

Input			
$FLOW_{water}$(*)	total water flow through system on larger spatial scale	[$m^3.d^{-1}$]	O*[c]
$Fflow_{out}$	fraction of water flow from larger scale to system	[-]	D*
WASTEW	wastewater produced by inhabitants of system	[$m^3.d^{-1}$]	O*[c]
RUNOFF	rainwater run-off from soil	[$m^3.d^{-1}$]	O*[c]
RAINDIRECT	rainfall directly into surface water	[$m^3.d^{-1}$]	O*[c]
Output			
$FLOW_{water}$	total water flow through system	[$m^3.d^{-1}$]	O*[c]

The residence time of water in the system is given by the volume of the water compartment, divided by the total water flow through the system.

$$TAU_{water} = \frac{AREA \cdot F_{water} \cdot DEPTH_{water}}{FLOW_{water}} \qquad (126)$$

Input			
AREA	area of system	[m^2]	D*
F_{water}	area fraction of water	[-]	D*
$DEPTH_{water}$	water depth	[m]	D*
$FLOW_{water}$	total water flow through system	[$m^3.d^{-1}$]	O*[c]
Output			
TAU_{water}	residence time of water	[d]	O*[c]

Water flow through the system due to rainfall directly into surface water:

$$RAINDIRECT = RAINRATE \cdot AREA \cdot F_{water} \quad \textbf{(127)}$$

Input			
RAINRATE	average daily precipitation	[m.d^{-1}]	D
AREA	area of system	[m^2]	D*
F_{water}	area fraction of water	[-]	D*
Output			
RAINDIRECT	rainfall directly into surface water	[m^3.d^{-1}]	O*[c]

Rainwater run-off from soil:

$$RUNOFF = Frunoff_{soil} \cdot (F_{natural} + F_{agric} + F_{ind}) \cdot AREA \cdot RAINRATE \quad \textbf{(128)}$$

Input			
$Frunoff_{soil}$	fraction of rainwater run-off from soil	[-]	D
$F_{natural}$	area fraction of natural soil	[-]	D*
F_{agric}	area fraction of agricultural soil	[-]	D*
F_{ind}	area fraction of industrial/urban soil	[-]	D*
AREA	area of system	[m^2]	D*
RAINRATE	average daily precipitation	[m.d^{-1}]	D
Output			
RUNOFF	rainwater run-off from soil	[m^3.d^{-1}]	O*[c]

Wastewater produced by inhabitants of the system:

$$WASTEW = N \cdot Q_{stp} \quad \textbf{(129)}$$

Input			
N	number of inhabitants of system	[eq]	D*
Q_{stp}	per-capita sewage flow	[m^3.eq^{-1}.d^{-1}]	D
Output			
WASTEW	wastewater produced by inhabitants of system	[m^3.d^{-1}]	O*[c]

III.4.4.4 Net sedimentation rate in region

The suspended matter balance leads to the net sedimentation rate. Suspended matter enters the system through production, inflow from outside, effluent of sewage treatment and erosion of soil surfaces. Suspended matter leaves the system with the outflowing water.

$$NETsedrate =$$

$$[\ SUSPPROD_{water} + SUSP_{water}(*) \cdot Fflow_{out} \cdot FLOW_{water}(*) +$$

$$SUSP_{eff} \cdot EFFLUENT_{stp} + EROSION \cdot (F_{natural} + F_{agric} + F_{ind}) \cdot \qquad (130)$$

$$AREA \cdot Fsolid_{soil} \cdot RHOsolid - SUSP_{water} \cdot FLOW_{water}\ ]$$

$$\cdot \frac{1}{Fsolid_{sed} \cdot RHOsolid} \cdot \frac{1}{AREA \cdot F_{water}}$$

Input			
$SUSPPROD_{water}$	(biogenic) production of suspended solids in water	[$kg_{dwt}.d^{-1}$]	D
$FLOW_{water}$	total water flow through system	[$m^3.d^{-1}$]	O*[c]
$FLOW_{water}$ (*)	total water flow through system on larger spatial scale	[$m^3.d^{-1}$]	O*[c]
$Fflow_{out}$	fraction of water flow from larger scale to system	[-]	D*
$SUSP_{water}$	suspended-solids concentration in water	[$kg_{dwt}.m^{-3}$]	D*
$SUSP_{water}$ (*)	suspended-solids concentration in water on larger scale	[$kg_{dwt}.m^{-3}$]	D*
$SUSP_{eff}$	suspended solids concentration in STP effluent	[$kg_{dwt}.m^{-3}$]	D
$EFFLUENT_{stp}$	effluent of STP	[$m^3.d^{-1}$]	O*[c]
EROSION	soil-erosion rate	[$m.d^{-1}$]	D
$F_{natural}$	area fraction of natural soil	[-]	D*
F_{agric}	area fraction of agricultural soil	[-]	D*
F_{ind}	area fraction of industrial/urban soil	[-]	D*
F_{water}	area fraction of water	[-]	D*
AREA	area of system	[m^2]	D*
$Fsolid_{soil}$	fraction of solids in soil	[$kg.kg^{-1}$]	D
$Fsolid_{sed}$	fraction of solids in sediment	[$kg.kg^{-1}$]	D
RHOsolid	bulk density of solids	[$kg.m^{-3}$]	D
Output			
NETsedrate	net sedimentation rate	[$m.d^{-1}$]	O*[c]

III.4.4.5 Regional and continental effluent discharges

The effluent discharge from regional and continental STPs depends on the fraction connected to treatment plants.

$$EFFLUENT_{stp} = N \cdot Q_{stp} \cdot Fconnect_{stp} \quad \textbf{(131)}$$

Input			
N	number of inhabitants of system	[eq]	D*
Q_{stp}	per-capita sewage flow	[$m^3.eq^{-1}.d^{-1}$]	D
$Fconnect_{stp}$	fraction connected to sewer systems	[-]	D
Output			
$EFFLUENT_{stp}$	effluent of STP	[$m^3.d^{-1}$]	O*[c]

III.4.4.6 Calculation of the dissolved concentration in surface water

In SimpleBox, water is treated as a bulk compartment, including biota and suspended matter. The model calculations therefore yield a total concentration in surface water. In subsequent calculations, and in risk characterisation, the dissolved concentration is required. Therefore, the total concentration is converted as follows. The bioconcentration factor for aquatic biota (BCF_{biota}) used in this equation to calculate the distribution over different phases is calculated from Equation (162/163). This parameter is closed and should be distinguished from BCF_{fish} since measured BCF data for fish cannot be assumed representative for all aquatic biota. It should be noted that when a *Kow* value is not entered (e.g. for a metal), BCF_{biota} is set to zero. If sorption to aquatic biota is relevant for the dissolved concentration in surface water, the *Kp* for suspended matter can be adjusted manually to account for this process.

$$PECreg_{water} = \frac{PECreg_{water,tot}}{1 + Kp_{susp} \cdot SUSP_{water} + BCF_{biota} \cdot BIOTA_{water}} \quad \textbf{(132)}$$

Input			
$PECreg_{water,tot}$	regional concentration in total surface water	[$kg_c.m^{-3}$]	O
Kp_{susp}	solids-water partition coefficient of suspended matter	[$m^3.kg_{solids}^{-1}$]	O
$SUSP_{water}$	concentration of suspended matter in water of region	[$kg_{dwt}.m^{-3}$]	D
BCF_{biota}	BCF for aquatic biota in regional/continental model	[$m^3.kg_{wwt}^{-1}$]	O[c]
$BIOTA_{water}$	concentration of aquatic biota in regional system	[$kg_{wwt}.m^{-3}$]	D
Output			
$PECreg_{water}$	regional PEC in surface water	[$kg_c.m^{-3}$]	O

III.4.4.7 Calculation of porewater concentration in agricultural soil

The concentration in porewater is derived from the total concentration by using the soil-water partition coefficient and the bulk density of the soil. The porewater concentration is used to estimate concentrations in plants and drinking water for indirect human exposure.

$$PECreg_{agric,porew} = \frac{PECreg_{agric,porew} \cdot RHO_{soil}}{K_{soil-water}} \quad \textbf{(133)}$$

Input			
$PECreg_{agric}$	regional PEC in agricultural soil (total)	[$kg_c.kg_{wwt}^{-1}$]	O
RHO_{soil}	wet bulk density of soil	[$kg_{wwt}.m^{-3}$]	O[c]
$K_{soil-water}$	soil-water partition coefficient	[$m^3.m^{-3}$]	O[c]
Output			
$PECreg_{agric,porew}$	regional PEC in porewater of agricultural soil	[$kg_c.m^{-3}$]	O

III.4.4.8 Mass transfer at air-soil and air-water interface on regional and continental scale

Soil–air interface

A substance-dependent soil-side partial mass transfer coefficient (PMTC) at the soil-air interface $kasl_{soil}$ ($m.d^{-1}$) is deduced from the exponential concentration profile in soil:

$$kasl_{soil} = \left(Veff_{soil} + \frac{Deff_{soil}}{d_p} \right) \quad \textbf{(134)}$$

In soil, processes of downward advection (pore water + small particles), diffusion (air, water, solids), and degradation take place simultaneously. These processes are included in Simplebox 3.0 (Hollander *et al.*, 2003). The result is an exponential decrease of the concentration with depth (C_z), characterised by a substance-dependent penetration depth (d_p)

$$C_z = C_0 \cdot e^{-z/d_p}; \qquad d_p = \frac{Veff_{soil} + \sqrt{Veff_{soil}^{\ 2} + Deff_{soil} \cdot k\deg_{soil}}}{2 \cdot k\deg_{soil}} \quad \textbf{(135)}$$

in which:

$$Veff_{soil} = FRw.soil \frac{RAINRATE \cdot F\inf_{soil}}{Fwater_{soil}} + FRs.soil. \frac{SOLIDadv.soil}{Fsolid_{soil}} \quad \textbf{(136)}$$

$$Deff_{soil} = FRa.soil \frac{DIFFgas \cdot Fair_{soil}^{\ 1.5}}{Fair_{soil}} + FRw.soil. \frac{DIFFwater \cdot Fwater_{soil}^{\ 1.5}}{Fwater_{soil}} + FRs.soil \cdot \frac{SOLIDdiff.soil}{Fsolid_{soil}} \quad \textbf{(137)}$$

$$FRw.soil = \frac{Fwater_{soil}}{Fair_{soil} \cdot K_h^{'} + Fwater_{soil} + Fsolid_{soil} \cdot K_p^{'}} \quad \textbf{(138)}$$

$$FRs.soil = \frac{Fsolid_{soil}}{Fair_{soil} \cdot K_h^{'} / K_p^{'} + Fwater_{soil} / K_p^{'} + Fsolid_{soil}} \quad \textbf{(139)}$$

$$FRa.soil = 1 - FRw.soil - FRs.soil \quad \textbf{(140)}$$

Input			
$kdeg_{soil}$	rate constant for degradation in bulk soil	[d^{-1}]	O
RAINRATE	average daily rate of precipitation	[$m.d^{-1}$]	D
$Finf_{soil}$	fraction of precipitation that penetrates into the soil.	[-]	D
d_p	substance-dependent penetration depth	[m]	O[c]
$Veff_{soil}$	effective advection (with penetrating porewater)	[$m.d^{-1}$]	O[c]
$Deff_{soil}$	effective diffusion coefficient	[$m^2.d^{-1}$]	O[c]
FRa.soil	mass fractions of the substance in the air phases of the soil	[-]	O[c]
FRw.soil	mass fractions of the substance in the water phases of the soil	[-]	O[c]
FRs.soil	mass fractions of the substance in the solid phases of the soil	[-]	O[c]
$Fair_{soil}$	volume fractions of air in the soil compartment	[$m_{air}^3.m_{soil}^{-3}$]	D
$Fwater_{soil}$	volume fractions of water in the soil compartment	[$m_{water}^3.m_{soil}^{-3}$]	D
$Fsolid_{soil}$	volume fractions of solids in the soil compartment	[$m_{solid}^3.m_{soil}^{-3}$]	D
Kh'	dimensionless part. coeff. between gas- and water phases of air	[-]	O[c]
Kp'	dimensionless part. coeff. between pore water- and solid phases of soil	[-]	O[c]
DIFFgas	molecular diffusivity of the substance in the gas phases	[$m^2.d^{-1}$]	O[c]
DIFFwater	molecular diffusivity of the substance in the water phases	[$m^2.d^{-1}$]	O[c]
SOLIDadv.soil	rate of advective downward transport of soil particles	[$m.d^{-1}$]	O[c]
SOLIDdiff.soil	solid phase diffusion coefficient in the soil compartment	[$m^2.d^{-1}$]	O[c]
Output			
$kasl_{soil}$	Partial mass-transfer coefficient soil side of air-soil interface	[$m.d^{-1}$]	O

Water-air interface

The partial mass transfer coefficients (PMTC) of the air-water interface depend on the windspeed of the system and the molecular weight of the substance:

$$kaw_{air} = 0.01 \cdot (0.3 + 0.2 \cdot WINDSPEED) \cdot ((0.018 / MOLW)^{(0,67 \cdot 0,5)} \quad \textbf{(141)}$$

$$kaw_{water} = 0.01 \cdot (0.0004 + 0.0004 \cdot WINDSPEED^2) \cdot (0.032 / MOLW)^{(0,5 \cdot 0,5)} \quad \textbf{(142)}$$

Input			
WINDSPEED	wind speed of system	[$m.d^{-1}$]	D
MOLW	molecular weight	[$kg_c.mol^{-1}$]	S
Output			
kaw_{air}	Partial mass-transfer coefficient air side of air-water interface	[$m.d^{-1}$]	O
kaw_{water}	Partial-mass transfer coefficient water side of air-water interface	[$m.d^{-1}$]	O

III.4.5 Local environmental distribution

In this section, the calculation of local environmental concentrations (*PEClocal*) is presented. Dedicated models are used for the compartments air, surface water and soil. Concentrations in sediment and groundwater are derived from the concentrations in surface water and soil, respectively. It should be noted that these calculations are performed for each relevant application and each step of the life cycle.

Several intermediate results of the soil sub-module are closed, since these results are too strictly model-related to allow for changes by the user (e.g. the concentration after 10 years due to deposition only: $Cdep10_i$).

Input: local direct emissions			
$Elocal_{air}$	local direct emission rate to air during episode	$[kg_c.d^{-1}]$	
Temission	number of days per year that emission takes place	$[d.year^{-1}]$	
Input: indirect emissions via STP			
$Estp_{air}$	local indirect emission to air from STP during episode	$[kg_c.d^{-1}]$	
$Clocal_{eff}$	concentration of chemical in STP effluent	$[kg_c.m^{-3}]$	
C_{sludge}	concentration in dry sewage sludge	$[kg_c.kg_{dwt}^{-1}]$	
$EFFLUENTlocal_{stp}$	effluent discharge rate of local STP	$[m^3.d^{-1}]$	c
Input: chemical properties			
$Fass_{aer}$	fraction of chemical bound to aerosol	[-]	
$K_{air\text{-}water}$	air-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{soil\text{-}water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{susp\text{-}water}$	suspended matter-water partition coefficient	$[m^3.m^{-3}]$	c
Kp_{susp}	solids-water partition coefficient of suspended matter	$[m^3.kg^{-1}]$	
$kdeg_{soil}$	rate constant for degradation in soil	$[d^{-1}]$	
Input background concentrations			
$PECreg_{air}$	regional concentration in air	$[kg_c.m^{-3}]$	
$PECreg_{water}$	regional concentration in surface water	$[kg_c.m^{-3}]$	
$PECreg_{water,marine}$	regional concentration in marine surface water	$[kg_c.m^{-3}]$	
$PECreg_{natural}$	regional concentration in natural soil	$[kg_c.kg_{wwt}^{-1}]$	
Intermediate results 1: removal rate constants soil			
$k_{volat\ i}$	rate constant for volatilisation from soil *i*	$[d^{-1}]$	
$k_{leach\ i}$	rate constant for leaching from soil *i* $i \in$ {soil,agric,grassland}	$[d^{-1}]$	
k_i	total rate constant for removal from topsoil *i*	$[d^{-1}]$	
Intermediate results 2			
$Clocal_{air}$	local concentration in air during emission episode	$[kg_c.m^{-3}]$	
$Clocal_{air,ann}$	annual average concentration in air, 100 m from point source	$[kg_c.m^{-3}]$	
DEPtotal	total deposition flux during emission episode	$[kg_c.m^{-2}.d^{-1}]$	
$DEPtotal_{ann}$	annual average total deposition flux	$[kg_c.m^{-2}.d^{-1}]$	
$Clocal_{water}$	local concentration in surface water during emission episode	$[kg_c.m^{-3}]$	
$Clocal_{water,ann}$	annual average local concentration in surface water	$[kg_c.m^{-3}]$	
$Clocal_{water,marine}$	local conc. in marine surface water during emission episode	$[kg_c.m^{-3}]$	
$Clocal_{water,ann,marine}$	annual average local concentration in marine surface water	$[kg_c.m^{-3}]$	
$Clocal_{soil}$	local concentration in agric. soil averaged over 30 days (to assess terrestrial ecosystem)	$[kg_c.kg_{wwt}^{-1}]$	
$Clocal_{agric}$	local concentration in agric. soil averaged over 180 days (to calculate concentration in crops)	$[kg_c.kg_{wwt}^{-1}]$	
$Clocal_{grassland}$	local concentration in grassland averaged over 180 days	$[kg_c.kg_{wwt}^{-1}]$	
$Fst\text{-}st_i$	fraction of steady-state situation achieved in soil *i* $i \in$ {soil,agric,grassland}	[-]	c
Output			
$PEClocal_{air,ann}$	annual average local PEC in air (total)	$[kg_c.m^{-3}]$	

$PEClocal_{water}$	predicted environmental concentration during episode	$[kg_c.m^{-3}]$
$PEClocal_{water,ann}$	annual average local PEC in surface water (dissolved)	$[kg_c.m^{-3}]$
$PEClocal_{water,marine}$	predicted environmental conc. in marine water during episode	$[kg_c.m^{-3}]$
$PEClocal_{water,ann,marine}$	annual average local PEC in marine surface water (dissolved)	$[kg_c.m^{-3}]$
$PEClocal_{sed}$	predicted environmental concentration in sediment	$[kg_c.kg^{-1}]$
$PEClocal_{sed,marine}$	predicted environmental concentration in marine sediment	$[kg_c.kg^{-1}]$
$PEClocal_{soil}$ `	local PEC in agric. soil (total) averaged over 30 days (to assess terrestrial ecosystem)	$[kg_c.kg^{-1}]$
$PEClocal_{agric}$	local PEC in agric. soil (total) averaged over 180 days (to calculate concentration in crops)	$[kg_c.kg^{-1}]$
$PEClocal_{grassland}$	local PEC in grassland (total) averaged over 180 days	$[kg_c.kg^{-1}]$
$PEClocal_{agric,porew}$	local PEC in pore water of agricultural soil	$[kg_c.m^{-3}]$
$PEClocal_{grassland,porew}$	local PEC in pore water of grassland	$[kg_c.m^{-3}]$
$PEClocal_{grw}$	local PEC in groundwater under agricultural soil	$[kg_c.m^{-3}]$

Table III-82 Default settings of the local environmental fate models.

Parameter	Symbol	Unit	Value
Air			
concentration in air at source strength 1 $kg.d^{-1}$	$Cstd_{air}$	$[kg_c.m^{-3}]$	$2.78.10^{-10}$
deposition flux of aerosol-bound chemical at 1 $kg.d^{-1}$	$DEPstd_{aer}$	$[kg_c.m^{-2}.d^{-1}]$	1.10^{-8}
deposition flux of gaseous compounds at 1 $kg.d^{-1}$ $^{10}\log HENRY < -2$ $-2 < {}^{10}\log HENRY < 2$ $^{10}\log HENRY > 2$	$DEPstd_{gas}$	$[kg_c.m^{-2}.d^{-1}]$	 5.10^{-10} 4.10^{-10} 3.10^{-10}
Surface water			
concentration of suspended matter in river water	$SUSP_{water}$	$[kg_{dwt}.m^{-3}]$	0.015 [a]
dilution factor after complete mixing			
Freshwater environment	DILUTION	[-]	10
Marine environment	$DILUTION_{marine}$	[-]	100[b]
Soil			
partial mass transfer coefficient at air side of air-soil interface	$kasl_{air}$	$[m.d^{-1}]$	90,5 [a]
partial mass-transfer coefficient at soil side of air-soil interface	$kasl_{soil}$	$[m.d^{-1}]$	Equation 130 [a]
fraction of rainwater infiltrating in soil	$Finf_{soil}$	[-]	0.25 [a]
rate of wet precipitation (700 mm/year)	RAINRATE	$[m.d^{-1}]$	$1.92.10^{-3}$ [a]

[a] Already defined in regional distribution sub-module.

[b] For discharges to a coastal zone, local dilution will be greater than in a freshwater river. First, initial dilution may occur if the density between the effluent and the saline receiving medium differs. The initial dilution factor is usually around 10. Further dilution due to currents can also be assumed, particularly if the point of release is subject to tidal influences. A dilution factor for discharges to a coastal zone of 100 may then be assumed, which seems to be representative for a realistic worst case. This dilution factor is related to a discharge volume of 2000 m^3/d.

III.4.5.1 Local concentration in air and deposition flux

The air compartment receives its input from direct emissions to air, and volatilisation from the sewage treatment plant. The concentration in air is used as input for indirect exposure of humans via inhalation. Deposition fluxes are used as input for the calculation of local concentrations in soil. Therefore, both deposition flux and concentration in air are calculated as annual average values. The Gaussian plume model OPS, as described by Van Jaarsveld (1990), is applied using the standard parameters given by Toet and de Leeuw (1992). The OPS results are used as the standard concentration and deposition flux at a source strength of 1 kg/d. The concentration of the chemical is calculated at 100 m distance from the point source and the STP, and the higher of these two is used.

$$Clocal_{air} = \max\left(Elocal_{air} , Estp_{air} \right) \cdot Cstd_{air} \qquad \textbf{(143)}$$

$$Clocal_{air,ann} = Clocal_{air} \cdot \frac{Temission}{365} \qquad \textbf{(144)}$$

Input			
$Elocal_{air}$	local direct emission rate to air during episode	[$kg_c.d^{-1}$]	O
$Estp_{air}$	local indirect emission to air from STP during episode	[$kg_c.d^{-1}$]	O
$Cstd_{air}$	concentration in air at source strength of 1 $kg.d^{-1}$	[$kg_c.m^{-3}$]	D
Temission	number of days per year that emission occurs	[$d.year^{-1}$]	O
Output			
$Clocal_{air}$	local concentration in air during episode, 100 m from source	[$kg_c.m^{-3}$]	O
$Clocal_{air,ann}$	annual average concentration in air, 100 m from source	[$kg_c.m^{-3}$]	O

The air concentration on the regional scale is used as the background concentration for the local scale, and is therefore, summed to the local concentration.

$$PEClocal_{air,ann} = Clocal_{air,ann} + PECregional_{air} \qquad \textbf{(145)}$$

Input			
$Clocal_{air,ann}$	annual average local concentration in air	[$kg_c.m^{-3}$]	O
$PECreg_{air}$	regional concentration in air	[$kg_c.m^{-3}$]	O
Output			
$PEClocal_{air,ann}$	annual average predicted environmental conc. in air	[$kg_c.m^{-3}$]	O

In calculating the deposition flux, the emissions from the two sources (direct and STP) are summed.

$$DEPtotal = \left(Elocal_{air} + Estp_{air} \right) \cdot \left(Fass_{aer} \cdot DEPstd_{aer} + (1 - Fass_{aer}) \cdot DEPstd_{gas} \right) \quad (146)$$

$$DEPtotal_{ann} = DEPtotal \cdot \frac{Temission}{365} \quad (147)$$

Input			
$Elocal_{air}$	local direct emission rate to air during emission episode	[$kg_c.d^{-1}$]	O
$Estp_{air}$	local indirect emission to air from STP during episode	[$kg_c.d^{-1}$]	O
$Fass_{aer}$	fraction of chemical bound to aerosol	[-]	O
$DEPstd_{aer}$	standard deposition flux of aerosol-bound compounds at source strength of 1 $kg.d^{-1}$	[$kg_c.m^{-2}.d^{-1}$]	D
$DEPstd_{gas}$	deposition flux of gaseous compounds as function of Henry's Law coefficient, at source strength of 1 $kg.d^{-1}$	[$kg_c.m^{-2}.d^{-1}$]	D
Temission	number of days per year that emission occurs	[$d.yr^{-1}$]	O
Output			
DEPtotal	total deposition flux during emission episode	[$kg_c.m^{-2}.d^{-1}$]	O
$DEPtotal_{ann}$	annual average total deposition flux	[$kg_c.m^{-2}.d^{-1}$]	O

III.4.5.2 Local concentration in surface water (freshwater and marine environment)

The effluent of the sewage treatment plant is discharged into surface water. Dilution in the receiving surface water and sorption to suspended solids are taken into account. The fixed dilution factor represents the dilution at the point of complete mixing of effluent and receiving water. EUSES will perform a check whether the concentration exceeds the water solubility. If this is the case, the results of this module should be studied in more detail on a case-by-case basis. The concentration during an emission episode is calculated for exposure of aquatic organisms. An annual average concentration is calculated for assessing indirect human exposure and secondary poisoning.

For estuaries, which are influenced by currents and tidal movements, it is assumed as a first approach that either the inland or the marine risk assessment covers them. Thus, no specific assessment is proposed. Then, the local concentrations in seawater can be obtained with the same equations as presented for the freshwater approach.

$$Clocal_{water} = \frac{Clocal_{eff}}{(1 + Kp_{susp} \cdot SUSP_{water}) \cdot DILUTION} \quad (148)$$

$$Clocal_{water,marine} = \frac{Clocal_{eff}}{(1 + Kp_{susp} \cdot SUSP_{water}) \cdot DILUTION_{marine}} \quad (149)$$

$$Clocal_{water,ann} = Clocal_{water} \cdot \frac{Temission}{365} \quad (150)$$

$$Clocal_{water,ann,marine} = Clocal_{water,marine} \cdot \frac{Temission}{365} \quad (151)$$

Input			
$Clocal_{eff}$	concentration of chemical in the STP effluent	[$kg_c.m^{-3}$]	O
Kp_{susp}	solids-water partition coefficient of suspended matter	[$m^3.kg^{-1}$]	O
$SUSP_{water}$	concentration of suspended matter in river water	[$kg_{dwt}.m^{-3}$]	D
DILUTION	dilution factor (freshwater environment)	[-]	D/O[c]
$DILUTION_{marine}$	dilution factor (marine environment)	[-]	D
Temission	number of days per year that emission occurs	[$d.yr^{-1}$]	O
Output			
$Clocal_{water}$	local concentration in surface water during emission episode	[$kg_c.m^{-3}$]	O
$Clocal_{water,ann}$	annual average local concentration in surface water	[$kg_c.m^{-3}$]	O
$Clocal_{water,marine}$	local conc. in marine surface water during emission episode	[$kg_c.m^{-3}$]	O
$Clocal_{water,ann,marine}$	annual average local concentration in marine surface water	[$kg_c.m^{-3}$]	O

When a more site-specific assessment is appropriate, account should be taken of the fluctuating flow-rates of typical receiving waters. The low-flow rate (or 10th-percentile) should always be used. Where only average flows are available, the flow for dilution purposes should be estimated as one third of this average. The actual dilution factor after complete mixing can be calculated from the flow rate of the river and the effluent discharge rate. This approach should be used for rivers only and not for estuaries or lakes. A default dilution factor for discharges to a coastal zone of 100 is assumed to be representative for a realistic worst case. In case of site-specific assessment the dilution factor applied for the local concentration in surface water should not be greater than 1000.

$$DILUTION = \frac{EFFLUENTlocal_{stp} + FLOW}{EFFLUENTlocal_{stp}} \quad (152)$$

Input			
$EFFLUENTlocal_{stp}$	effluent discharge rate of local STP	[$m^3.d^{-1}$]	O[c]
FLOW	flow rate of the river	[$m^3.d^{-1}$]	D
Output			
DILUTION	dilution factor (freshwater environment)	[-]	D/O[c]

The concentration on the regional scale is used as background concentration for the local scale. Therefore, these concentrations are summed.

$$PEClocal_{water} = Clocal_{water} + PECreg_{water} \quad (153)$$

$$PEClocal_{water,marine} = Clocal_{water,marine} + PECreg_{water,marine} \quad (154)$$

$$PEClocal_{water,ann} = Clocal_{water,ann} + PECreg_{water} \quad (155)$$

$$PEClocal_{water,ann,marine} = Clocal_{water,ann,marine} + PECreg_{water,marine} \quad (156)$$

Input			
$Clocal_{water}$	local concentration in surface water during episode	[$kg_c.m^{-3}$]	O
$Clocal_{water,ann}$	annual average concentration in surface water	[$kg_c.m^{-3}$]	O
$PECreg_{water}$	regional concentration in surface water	[$kg_c.m^{-3}$]	O
$Clocal_{water,marine}$	local conc. in marine water during emission episode	[$kg_c.m^{-3}$]	O
$Clocal_{water,ann,marine}$	annual average local concentration in marine surface water	[$kg_c.m^{-3}$]	O
$PECreg_{water,marine}$	regional concentration in marine water	[$kg_c.m^{-3}$]	O
Output			
$PEClocal_{water}$	predicted environmental concentration during episode	[$kg_c.m^{-3}$]	O
$PEClocal_{water,ann}$	annual average local PEC in surface water	[$kg_c.m^{-3}$]	O
$PEClocal_{water,marine}$	predicted environmental conc. in marine water during episode	[$kg_c.m^{-3}$]	O
$PEClocal_{water,ann,marine}$	annual average local PEC in marine water	[$kg_c.m^{-3}$]	O

III.4.5.3 Local concentration in sediment (freshwater and marine environment)

The concentration in freshly deposited sediment is taken as the PEC for sediment and the properties of suspended matter are therefore used. The concentration in bulk sediment is derived from the corresponding water-body concentration, assuming a thermodynamic partition equilibrium (see also Di Toro *et al.*, 1991). The local concentration in marine sediment can be obtained with the same approach as presented for freshwater sediment.

$$PEClocal_{sed} = \frac{K_{susp\text{-}water}}{RHO_{susp}} \cdot PEClocal_{water} \quad (157)$$

$$PEClocal_{sed,marine} = \frac{K_{susp\text{-}water}}{RHO_{susp}} \cdot PEClocal_{water,marine} \quad (158)$$

Input			
$PEClocal_{water}$	predicted environmental conc. in surface water during episode	[$kg_c.m^{-3}$]	O
$PEClocal_{water,marine}$	predicted environmental conc. in marine water during episode	[$kg_c.m^{-3}$]	O
$K_{susp\text{-}water}$	suspended matter-water partition coefficient	[$m^3.m^{-3}$]	O[c]
RHO_{susp}	bulk density of suspended matter	[$kg_{wwt}.m^{-3}$]	O[c]
Output			
$PEClocal_{sed}$	predicted environmental concentration in sediment	[$kg_c.kg_{wwt}^{-1}$]	O
$PEClocal_{sed,marine}$	predicted environmental concentration in marine sediment	[$kg_c.kg_{wwt}^{-1}$]	O

III.4.5.4 Local concentration in soil

Concentrations in soil are used as exposure concentrations for terrestrial organisms and for indirect exposure of humans (through crops, meat and dairy products). The topsoil layer is modelled as a single compartment, receiving input through application of sludge dressing and continuous airborne deposition, and with output via leaching, volatilisation and biodegradation. As the concentration is not constant during the year, the exposure concentration is averaged over a certain time period. Ten years of accumulation is accounted for. Three different PECs are calculated in soil, for different end-points (***Table III-83***).

Table III-83 Characteristics of soil and soil-use for the three different endpoints.

Type of soil	**Depth of soil compartment [m]**	**Averaging time [days]**	**Rate of sludge application [$kg_{dwt}.m^{-2}.year^{-1}$]**	**End-point**
	$DEPTH_i$	T_i	$APPLsludge_i$	
Agricult. soil i = soil	0.20	30	0.5	terrestrial ecosystem
Agricult. soil i = agric	0.20 [a]	180	0.5	crops for human consumption and predators
Grassland i = grassland	0.10	180	0.1	grass for cattle

[a] Already defined in regional distribution sub-module

Derivation of the removal-rate constant

For removal from the topsoil, the following processes are quantified:

- biodegradation in soil;
- volatilisation of substance from soil;
- leaching to deeper soil layers.

The diffusive transfer from soil to air is estimated using the classical two-film resistance model. Given a substance-independent air-side partial mass transfer coefficient, $kasl_{air}$, the soil-referenced overall mass transfer coefficient, used for calculating the rate constant for volatilization, $k_{volat\ i}$, becomes:

$$\frac{1}{k_{volat\ i}} = \left(\frac{1}{kasl_{air} \cdot K_{air-water} / K_{soil-water}} + \frac{1}{kasl_{soil}} \right) \cdot DEPTH_i \qquad (159)$$

in which $K_{air\text{-}soil}$, $K_{air\text{-}water}$ and $K_{soil\text{-}water}$ are the dimensionless equilibrium constants between bulk air and bulk soil, bulk air and bulk water, and between bulk soil and bulk water, respectively, and *DEPTHi* (m) is the mixing depth of the soil compartment.

Input			
$kasl_{air}$	partial mass-transfer coeff. at air side of air-soil interface	[$m.d^{-1}$]	D
$kasl_{soil}$	partial mass-transfer coeff. at soil side of air-soil interface	[$m.d^{-1}$]	O
$K_{air-water}$	air-water partition coefficient	[$m^3.m^{-3}$]	O[c]
$K_{soil-water}$	soil-water partition coefficient	[$m^3.m^{-3}$]	O[c]
$DEPTH_i$	mixing depth of soil type *i*	[m]	D
Output			
$k_{volat\ i}$	rate constant for volatilisation from soil *i*	[d^{-1}]	O

A first-order rate constant for leaching can be calculated from the amount of rain flushing the liquid phase of the soil compartment.

$$k_{leach\,i} = \frac{Finf_{soil} \cdot RAINRATE}{K_{soil\text{-}water} \cdot DEPTH_i} \qquad \textbf{(160)}$$

Input			
$Finf_{soil}$	fraction of rainwater that infiltrates into soil	[-]	D
RAINRATE	rate of wet precipitation	[$m.d^{-1}$]	D
$K_{soil-water}$	soil-water partition coefficient	[$m^3.m^{-3}$]	O[c]
$DEPTH_i$	mixing depth of soil type *i*	[m]	D
Output			
$k_{leach\ i}$	rate constant for leaching from soil *i*	[d^{-1}]	O

The overall removal-rate constant is given by the sum of all relevant-removal rate constants.

$$k_i = k_{volat\,i} + k_{leach\,i} + kdeg_{soil} \qquad \textbf{(161)}$$

Input			
$k_{volat\ i}$	rate constant for volatilisation from soil *i*	[d^{-1}]	O
$k_{leach\ i}$	rate constant for leaching from topsoil *i*	[d^{-1}]	O
$kdeg_{soil}$	rate constant for degradation in soil	[d^{-1}]	O
Output			
k_i	rate constant for removal from topsoil *i*	[d^{-1}]	O

Referencing deposition flux to kg soil

To simplify the calculations, the airborne deposition flux (Section III.4.5.1) is referenced to kg substance per kg of soil per day. The total deposition flux is converted as follows:

$$D_{air\,i} = \frac{DEPtotal_{ann}}{DEPTH_i \cdot RHO_{soil}} \qquad (162)$$

Input			
$DEPtotal_{ann}$	annual average total deposition flux	[$kg_c.m^{-2}.d^{-1}$]	O
$DEPTH_i$	mixing depth of soil type *i*	[m]	D
RHO_{soil}	bulk density of soil	[$kg_{wwt}.m^{-3}$]	O[c]
Output			
$D_{air\,i}$	airborne deposition flux per kg of soil *i*	[$kg_c.kg_{wwt}^{-1}.d^{-1}$]	O[c]

Initial concentration after 10 years of sludge application

To take accumulation in soil into account, sludge application is assessed for 10 consecutive years. The PEC in soil is the concentration in the 10th year, averaged over a time period *T*. As a first step, the initial concentration in this year needs to be derived. The contributions of deposition and sludge applications are considered separately. The concentration due to 10 years of continuous deposition only is given by:

$$Cdep10_i = \frac{D_{air\,i}}{k_i} - \frac{D_{air\,i}}{k_i} \cdot e^{-365 \cdot 10 \cdot k_i} \qquad (163)$$

Input			
$D_{air\,i}$	airborne deposition flux per kg of soil *i*	[$kg_c.kg_{wwt}^{-1}.d^{-1}$]	O
k_i	rate constant for removal from top-soil *i*	[d^{-1}]	O
Output			
$Cdep10_i$	concentration in soil *i* due to deposition in 10th year at t=0	[$kg_c.kg_{wwt}^{-1}$]	O[c]

Sludge application is not a continuous process, but is assumed to take place once a year at the beginning of each year. The concentration just after the first year of sludge application is given by:

$$Csludge1_i = \frac{C_{sludge} \cdot APPLsludge_i}{DEPTH_i \cdot RHO_{soil}} \qquad (164)$$

Input			
C_{sludge}	concentration in dry sewage sludge	[$kg_c.kg_{dwt}^{-1}$]	O
$APPLsludge_i$	dry sludge application rate on soil *i*	[$kg_{dwt}.m^{-2}.yr^{-1}$]	D
$DEPTH_i$	mixing depth of soil type *i*	[m]	D
RHO_{soil}	bulk density of soil	[$kg_{wwt}.m^{-3}$]	O[c]
Output			
$Csludge1_i$	concentration in soil due to sludge in first year at t=0	[$kg_c.kg_{wwt}^{-1}$]	O[c]

At the end of each year, a fraction *Facc* of the initial concentration remains in the topsoil layer. Using this fraction, the initial concentration after 10 applications of sludge can be assessed.

$$Facc_i = e^{-365 k_i} \quad \textbf{(165)}$$

$$Csludge10_i = Csludge1_i \cdot \left[1 + \sum_{n=1}^{9} Facc_i^{\,n} \right] \quad \textbf{(166)}$$

Input			
k_i	rate constant for removal from top soil *i*	[d^{-1}]	O
$Facc_i$	fraction accumulating in one year in soil *i*	[-]	O[c]
$Csludge1_i$	concentration in soil *i* due to sludge in first year at t=0	[$kg_c.kg_{wwt}^{-1}$]	O[c]
Output			
$Csludge10_i$	concentration in soil *i* due to sludge in 10th year at t=0	[$kg_c.kg_{wwt}^{-1}$]	O[c]

The sum of the concentrations due to deposition and to sludge is the initial concentration in year 10.

$$Clocal10_i = Cdep10_i + Csludge10_i \quad \textbf{(167)}$$

Input			
$Csludge10_i$	concentration in soil *i* due to sludge in 10th year at t=0	[$kg_c.kg_{wwt}^{-1}$]	O[c]
$Cdep10_i$	concentration in soil *i* due to deposition in 10th year at t=0	[$kg_c.kg_{wwt}^{-1}$]	O[c]
Output			
$Clocal10_i$	initial concentration in soil *i* (in 10th year at t=0)	[$kg_c.kg_{wwt}^{-1}$]	O[c]

Local concentration in soil

The fate of the chemical in soil is modelled with a one-compartment model with a continuous input from airborne deposition and continuous elimination from the topsoil layer. The initial condition is given by $Clocal10_i$. The differential equation describing the one-compartment model can be solved analytically to give the concentration in soil as a function of time. The exposure concentration in soil was defined as the average concentration over a certain time period *T*, and is thus defined by the integral of the concentration in soil *i* from 0 to *T* days:

$$Clocal_i = \frac{1}{T_i} \cdot \int_0^{T_i} Clocal_i(t)\, dt \quad \textbf{(168)}$$

The analytical solution of this integral is then given by:

$$Clocal_i = \frac{D_{air\ i}}{k_i} + \frac{1}{k_i T_i}\left[Clocal\ 10_i - \frac{D_{air\ i}}{k_i} \right] \cdot \left[1 - e^{-k_i T_i}\right] \qquad \textbf{(169)}$$

Input			
$D_{air\ i}$	airborne deposition flux per kg of soil *i*	[$kg_c.kg_{wwt}^{-1}.d^{-1}$]	O[c]
T_i	averaging time for soil *i*	[d]	D
k_i	rate constant for removal from topsoil *i*	[d^{-1}]	O
$Clocal10_i$	initial concentration in soil *i* (in 10th year at t=0)	[$kg_c.kg_{wwt}^{-1}$]	O[c]
Output			
$Clocal_i$	average concentration in soil *i* over *T* days	[$kg_c.kg_{wwt}^{-1}$]	O

The concentration on the regional scale is used as the background concentration for the local scale. For this purpose, the concentration in natural soil is used (input through deposition only), for otherwise sludge application would be taken into account twice.

$$PEClocal_i = Clocal_i + PECreg_{natural} \qquad \textbf{(170)}$$

Input			
$Clocal_i$	local concentration in soil *i*	[$kg_c.kg_{wwt}^{-1}$]	O
$PECreg_{natural}$	regional concentration in natural soil	[$kg_c.kg_{wwt}^{-1}$]	O
Output			
$PEClocal_i$	predicted environmental concentration in soil *i*	[$kg_c.kg_{wwt}^{-1}$]	O

Local concentration in pore water of soil

The concentration in the pore water of soil is calculated by applying the soil-water partition coefficient.

$$PEClocal_{i,porew} = \frac{PEClocal_i \cdot RHO_{soil}}{K_{soil-water}} \qquad \textbf{(171)}$$

Input			
$PEClocal_i$	predicted environmental concentration in soil *i*	[$kg_c.kg_{wwt}^{-1}$]	O
$K_{soil-water}$	soil-water partition coefficient	[$m^3.m^{-3}$]	O[c]
RHO_{soil}	bulk density of wet soil	[$kg_{wwt}.m^{-3}$]	O[c]
Output			
$PEClocal_{i,porew}$	predicted environmental conc. in pore water of soil *i*	[$kg_c.m^{-3}$]	O

Persistence of the substance in soil

Ten consecutive years of accumulation may not be sufficient for some substances to reach a steady-state situation. These substance may accumulate for hundreds of years. To indicate the potential persistence in soil, the fraction of the steady-state concentration is calculated.

$$Fst - st_i = \frac{Clocal\ 10_i}{Cinf_i} \quad \textbf{(172)}$$

Input			
$Clocal10_i$	initial concentration in soil *i* after 10 years	$[kg_c.kg_{wwt}^{-1}]$	O[c]
$Cinf_i$	initial concentration in soil *i* in steady-state situation	$[kg_c.kg_{wwt}^{-1}]$	O[c]
Output			
$Fst\text{-}st_i$	fraction of steady-state situation achieved in soil *i*	[-]	O[c]

The initial concentration in the steady-state year is given by:

$$C\ inf_i = \frac{D_{air\ i}}{k_i} + Csludge1_i \cdot \frac{1}{1 - Facc_i} \quad \textbf{(173)}$$

Input			
$D_{air\ i}$	airborne deposition flux per kg of soil *i*	$[kg_c.kg_{wwt}^{-1}.d^{-1}]$	O[c]
k_i	rate constant for removal from topsoil *i*	$[d^{-1}]$	O
$Facc_i$	fraction accumulating in soil *i* in one year	[-]	O[c]
$Csludge1_i$	concentration in soil *i* due to sludge in first year at t=0	$[kg_c.kg_{wwt}^{-1}]$	O[c]
Output			
$Cinf_i$	initial concentration in soil *i* in steady-state situation	$[kg_c.kg_{wwt}^{-1}]$	O[c]

III.4.5.5 Calculation of concentration in groundwater

The concentration in groundwater is calculated for indirect exposure of humans via drinking water. As an indication for potential groundwater levels, the concentration in pore water is taken after 10 years of sludge application to agricultural soil, averaged over 180 days. Transformation and dilution in deeper soil layers are not accounted for.

$$PEClocal_{grw} = PEClocal_{agric,porew} \quad \textbf{(174)}$$

Input			
$PEClocal_{agric,porew}$	predicted environmental conc. in pore water of agric. soil	$[kg_c.m^{-3}]$	O
Output			
$PEClocal_{grw}$	predicted environmental conc. in groundwater	$[kg_c.m^{-3}]$	O

III.5 EXPOSURE MODULE

In the exposure module, exposure levels for humans and predating birds and mammals are estimated. This module is divided into four specific sub-modules, which will be handled separately:

- Secondary poisoning.
- Indirect human exposure.
- Consumer exposure.
- Workplace exposure.

III.5.1 Secondary poisoning

For the assessment of secondary poisoning, three example food chains are modelled:

1. water (freshwater and marine environment)→fish→predator
2. water (marine environment)→fish→predator→toppredator
3. soil→worm→predator.

Exposure levels are calculated, assuming a scenario whereby 50% of the food is sourced from the local environment and 50% from the regional environment.

Input: chemical properties		
Kow	octanol-water partition coefficient	[-]
Input: environmental properties		
RHO_{soil}	bulk density of soil	$[kg_{wwt}.m^{-3}]$ [c]
$CONV_{soil}$	conversion factor for soil concentrations: wwt to dwt	$[kg_{wwt}.kg_{dwt}^{-1}]$ [c]
$PEClocal_{water,ann}$	annual average local PEC in surface water (dissolved)	$[kg_c.m^{-3}]$
$PEClocal_{water,ann,marine}$	annual average local PEC in marine surface water (dissolved)	$[kg_c.m^{-3}]$
$PEClocal_{agric}$	local PEC in agricultural soil	$[kg_c.\ kg_{wwt}^{-1}]$
$PEClocal_{agric,porew}$	local PEC in pore water of agricultural soil	$[kg_c.m^{-3}]$
$PECreg_{water}$	regional PEC in surface water (dissolved)	$[kg_c.m^{-3}]$
$PECreg_{water,marine}$	regional PEC in marine surface water (dissolved)	$[kg_c.m^{-3}]$
$PECreg_{agric}$	regional PEC in agricultural soil	$[kg_c.kg_{wwt}^{-1}]$
$PECreg_{agric,porew}$	regional PEC in pore water of agricultural soil	$[kg_c.m^{-3}]$
Intermediate results		
BCF_{worm}	bioconcentration factor for earthworms	$[kg_{soil\ wwt}.kg_{worm\ wwt}^{-1}]$
BCF_{fish}	bioconcentration factor for fish	$[m^3.kg_{wwt}^{-1}]$
Output		
BCF_{fish}	bioconcentration factor for fish	$[m^3.kg_{wwt}^{-1}]$
$PEC_{oral,fish}$	concentration in fish from surface water for predators	$[kg_c.kg_{wwt}^{-1}]$
$PEC_{oral,fish,marine}$	concentration in fish from marine surface water for predators	$[kg_c.kg_{wwt}^{-1}]$
$PEC_{oral,fish\ predator,marine}$	concentration in fish-eating predator for marine toppredators	$[kg_c.kg_{wwt}^{-1}]$
$PEC_{oral,worm}$	concentration in earthworms from agricultural soil	$[kg_c.kg_{wwt}^{-1}]$

III.5.1.1 Bioconcentration factor for fish

The methods that estimate a BCF for fish from log *Kow* are widely used and, in general, the most reliable. The following combination of QSARs is advised in Chapter 4 of the TGD. For substances with a log *Kow*, from 1 to 6, the relation by Veith *et al.* (1979) is used, while for substances in the log *Kow* range between 6 and 10 a parabolic equation is applied. Domain of physico-chemical properties: log *Kow* 1 to 10 (outside this range the minimum or maximum *Kow* is used), molecular weight less than 700 g/mol. For chemicals with a molecular weight of more than 700 g/mol, the BCF tends to decrease but in lack of experimental data, the QSAR can be used as an initial worst-case estimate.

if log *Kow* ≤ 6 then:

$$\log BCF_{fish} = 0.85 \cdot \log Kow - 0.70 - 3 \qquad (175)$$

if log *Kow* > 6 then:

$$\log BCF_{fish} = -0.20 \cdot (\log Kow)^2 + 2.74 \cdot \log Kow - 4.72 - 3 \qquad (176)$$

Input			
Kow	octanol-water partition coefficient	[$m^3.m^{-3}$]	S
Output			
BCF_{fish}	bioconcentration factor for fish	[$m^3.kg_{wwt}^{-1}$]	O

III.5.1.2 Exposure concentration for predators in freshwater and marine environment

The biomagnification factor (BMF) is defined as the relative concentration in a predatory animal compared to the concentration in its prey (BMF = Cpredator/Cprey). The BMF should ideally be based on measured data. However, the availability of such data is at present very limited and therefore, the default values given in **Table III-84**should be used. By establishing these factors it is assumed that a relationship exists between the BMF, the BCF and the log Kow. If a BCF for fish is available, it is possible to use that as a trigger instead of log Kow. The BCF triggers recommended are less conservative than the log Kow triggers because they more realistically take the potential for metabolism in biota (i.e. fish) into account. Due to this increased relevance, the use of a measured BCF would take precedence over a trigger based on log Kow.

Table III-84 *Default BMF values for organic substances.*

Log Kow [$m^3.m^{-3}$]	**BCF (fish)** [$m^3.kg_{wwt}^{-1}$]	**BMF_1** [-]	**BMF_2** [-]
< 4.5	< 2	1	1
4.5 - <5	2 – 5	2	2
5 - 8	> 5	10	10
>8 – 9	5 – 2	3	3
> 9	< 2	1	1

Input			
Kow	octanol-water partition coefficient	[$m^3.m^{-3}$]	P
BCF_{fish}	bioconcentration factor for fish	[$m^3.kg_{wwt}^{-1}$]	P
Output			
BMF	biomagnification factor in fish/predator	[-]	O

The exposure level for the first tier of organisms, the fish-eating predators, in freshwater and marine water ($PEC_{oral,fish}$) is calculated from the average of the local and regional PEC for surface water, the measured or estimated BCF for fish and the biomagnification factor (BMF_1).

Input

$$PEC_{oral,fish} = 0.5 \cdot (PEClocal_{water,ann} + PECreg_{water}) \cdot BCF_{fish} \cdot BMF_1 \quad (177)$$

$$PEC_{oral,fish,marine} = 0.5 \cdot (PEClocal_{water,ann,marine} + PECreg_{water,marine}) \cdot BCF_{fish} \cdot BMF_1 \quad (178)$$

BCF_{fish}	bioconcentration factor for fish	[$m^3.kg_{wwt}^{-1}$]	O
$PEClocal_{water,ann}$	annual average local PEC in surface water (dissolved)	[$kg_c.m^{-3}$]	O
$PECreg_{water}$	regional PEC in surface water (dissolved)	[$kg_c.m^{-3}$]	O
$PEClocal_{water,ann,marine}$	annual average local PEC in marine surface water (dissolved)	[$kg_c.m^{-3}$]	O
$PECreg_{water,marine}$	regional PEC in marine surface water (dissolved)	[$kg_c.m^{-3}$]	O
BMF_1	biomagnification factor in fish	[-]	P
Output			
$PEC_{oral,fish}$	conc. in fish for secondary poisoning in freshwater environment	[$kg_c.kg_{wwt}^{-1}$]	O
$PEC_{oral,fish,marine}$	conc. in fish for secondary poisoning in marine environment	[$kg_c.kg_{wwt}^{-1}$]	O

The food chain of the marine environment is, besides a fish-eating predator, also modelled with a toppredator. Toppredators pray on organisms that are in direct contact with the marine aqueous phase and receive the substances from this source (fish-eating predator). For the second tier of organisms, the top-predators, it can be assumed that they obtain their prey mainly from the larger-scale regional marine environment that is to a lesser extent influenced by point source discharges. However, since it cannot be ruled out that certain top-predators prey on organisms that receive their food from relatively small areas it is proposed to assume, as a realistic worst case, a 90/10 ratio between regional and local food intake.

$$PEC_{oral,fish\ predator,marine} = (0.1 \cdot PEClocal_{water,ann,marine} + 0.9 \cdot PECreg_{water,marine}) \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2 \quad (179)$$

Input			
$PEClocal_{water,ann,marine}$	annual average local PEC in marine surface water (dissolved)	[$kg_c.m^{-3}$]	O
$PECreg_{water,marine}$	regional PEC in marine surface water (dissolved)	[$kg_c.m^{-3}$]	O
BCF_{fish}	bioconcentration factor for fish	[$m^3.kg_{wwt}^{-1}$]	O
BMF_1	biomagnification factor in fish	[-]	O
BMF_2	biomagnification factor in predator	[-]	O
Output			
$PEC_{oral,fish\ predator,marine}$	concentration in fish-eating predator for marine toppredators	[$kg_c.kg_{wwt}^{-1}$]	O

III.5.1.3 Bioconcentration factor for earthworms

For organic chemicals, the main route of uptake into earthworms will be via the interstitial water. Bioconcentration can be described as a hydrophobic partitioning between the pore water and the phases inside the organism and is modelled according to the equation as described by Jager (1998). The model was supported by data with neutral organic chemicals in soil within the range log Kow 3-8 and in water-only experiments from log Kow 1-6. An application range of log Kow 1-8 is advised and it is reasonable to assume that extrapolation to lower Kow values is possible.

Table III-85 Default settings for earthworm specific parameters.

Parameter	Symbol	Unit	Value
Fraction of water inside the worm (volume fraction)	$Fwater_{worm}$	[-]	0.84
Fraction of lipids inside the worm (volume fraction)	$Flipid_{worm}$	[-]	0.012
Density of earthworms	RHO_{worm}	$[kg_{wwt}.m^{-3}]$	1000
Fraction of gut loading in worm	$Fgut_{worm}$	$[kg_{dwt}.kg_{wwt}^{-1}]$	0.1

$$BCF_{worm} = \frac{Fwater_{worm} + Flipid_{worm} \cdot Kow}{RHO_{worm}} \qquad \textbf{(180)}$$

Input			
$Fwater_{worm}$	fraction of water inside the worm (volume fraction)	[-]	D
$Flipid_{worm}$	fraction of lipids inside the worm (volume fraction)	[-]	D
Kow	octanol-water partition coefficient	$[m^3.m^{-3}]$	S
RHO_{worm}	density of earthworms	$[kg_{wwt}.m^{-3}]$	D
Output			
BCF_{worm}	bioconcentration factor for earthworms	$[kg_{soil\ wwt}.kg_{wwt}^{-1}]$	O

III.5.1.4 Exposure concentration for worm-eating predators

The concentration in earthworms for secondary poisoning is estimated from the BCF, the gut loading of earthworms and the average of regional and local concentrations in agricultural soil and porewater. The gut loading of earthworms depends heavily on soil conditions and available food. Reported values range from 2-20 % (kg_{dwt} gut/kg_{wwt} voided worm), 10% can therefore be taken as a reasonable value.

$$PEC_{oral,worm} = \frac{0.5 \cdot (PEClocal_{agric,porew} + PECreg_{agric,porew}) \cdot BCF_{worm} + 0.5 \cdot (PEClocal_{agric} + PECreg_{agric}) \cdot Fgut_{worm} \cdot CONV_{soil}}{1 + Fgut_{worm} \cdot CONV_{soil}} \quad \textbf{(181)}$$

Input

$PEClocal_{agric,porew}$	local PEC in pore water of agricultural soil	$[kg_c.m^{-3}]$	O
$PECreg_{agric,porew}$	regional PEC in pore water of agricultural soil	$[kg_c.m^{-3}]$	O
BCF_{worm}	bioconcentration factor for earthworms	$[kg_{wwt}.kg_{wwt}^{-1}]$	O
$PEClocal_{agric}$	local PEC in agricultural soil (averaged over 180 days)	$[kg_c.kg^{-1}]$	O
$PECreg_{agric}$	regional PEC in agricultural soil	$[kg_c.kg^{-1}]$	O
$Fgut_{worm}$	fraction of gut loading in worm	$[kg_{dwt}.kg_{wwt}^{-1}]$	D
$CONV_{soil}$	conversion factor for soil concentrations: wwt to dwt	$[kg_{wwt}.kg_{dwt}^{-1}]$	O^C

Output

$PEC_{oral,worm}$	concentration in earthworms for secondary poisoning	$[kg_c.kg_{wwt}^{-1}]$	O

III.5.2 Indirect exposure of humans via the environment

Human indirect exposure is assessed by estimating the concentrations and intake of drinking water and food products (root crops, leaf crops, meat, milk and fish). Exposure is estimated on both the local and regional scale. Bioconcentration and biotransfer behaviour is estimated from physico-chemical properties using (Q)SAR approaches. It should be noted that reliable and relevant measured data are always preferable, considering the large uncertainties in the (Q)SARs.

Input: chemical properties			
Kow	octanol-water partition coefficient	[-]	
HENRY	Henry's law constant	[Pa.m^3.mol^{-1}]	
$K_{air\text{-}water}$	air-water partition coefficient	[m^3.m^{-3}]	c
$Fass_{aer}$	fraction of chemical associated with aerosol particles	[-]	
$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]	
BCF_{fish}	bioconcentration factor for fish on wet-weight basis	[m^3.kg_{wwt}^{-1}]	
Input: local concentrations			
$CONV_{soil}$	conversion factor soil from dry weight to wet weight	[kg_{wwt}.kg_{dwt}^{-1}]	c
$PEClocal_{water,ann}$	annual average local PEC in surface water (dissolved)	[kg_c.m^{-3}]	
$PEClocal_{air,ann}$	annual average local PEC in air (total)	[kg_c.m^{-3}]	
$PEClocal_{grassland}$	local PEC in grassland (total), averaged over 180 days	[kg_c.kg_{wwt}^{-1}]	
$PEClocal_{agric,porew}$	local PEC in pore water of agricultural soil	[kg_c.m^{-3}]	
$PEClocal_{grassland,porew}$	local PEC in pore water of grassland	[kg_c.m^{-3}]	
$PEClocal_{grw}$	local PEC in groundwater under agricultural soil	[kg_c.m^{-3}]	
Input: regional concentrations			
$PECreg_{water}$	regional PEC in surface water (dissolved)	[kg_c.m^{-3}]	
$PECreg_{air}$	regional PEC in air (total)	[kg_c.m^{-3}]	
$PECreg_{agric}$	regional PEC in agricultural soil (total)	[kg_c.kg_{wwt}^{-1}]	
$PECreg_{agric,porew}$	regional PEC in pore water of agricultural soils	[kg_c.m^{-3}]	

In the regional model, no distinction is made between grassland and other agricultural soils. $PECreg_{agric}$ is also used for the regional grassland concentration. $PECreg_{agric,porew}$ is used for the concentration in groundwater. The indirect exposure calculations are identical for the local and regional scales. Therefore, the indirect exposure equations are described using the following generalised symbols:

Input			
C_{water}	concentration in surface water	$[kg_c.m^{-3}]$	
C_{air}	concentration in air	$[kg_c.m^{-3}]$	
$C_{grassland}$	concentration in grassland soil	$[kg_c.kg^{-1}]$	
$C_{agric,porew}$	concentration in pore water of agricultural soil	$[kg_c.m^{-3}]$	
$C_{grassland,porew}$	concentration in pore water of grassland soil	$[kg_c.m^{-3}]$	
C_{grw}	concentration in groundwater	$[kg_c.m^{-3}]$	
Intermediate results 1			
$K_{leaf-air}$	partition coeff. between leaves and air	$[m^3.m^{-3}]$	
$K_{plant-water}$	partition coeff. between plant tissue and water	$[m^3.m^{-3}]$	
TSCF	transpiration stream concentration factor	[-]	
BAF_{meat}	bioaccumulation factor for meat	$[d.kg_{food}^{-1}]$	
BAF_{milk}	bioaccumulation factor for milk	$[d.kg_{food}^{-1}]$	
F_{pur}	purification factor for surface water	[-]	
Intermediate results 2			
C_{fish}	concentration in wet fish	$[kg_c.kg_{wwt}^{-1}]$	
$Croot_{plant}$	concentration in root tissue of plant	$[kg_c.kg_{wwt}^{-1}]$	
C_{leaf}	concentration in leaves of plant	$[kg_c.kg_{wwt}^{-1}]$	
C_{grass}	concentration in grass (wet weight)	$[kg_c.kg_{wwt}^{-1}]$	
$Fleaf_{porew}$	fraction of total uptake by crops from pore water	[-]	c
$Fleaf_{air}$	fraction of total uptake by crops from air	[-]	c
$Fgrass_{porew}$	fraction of total uptake by grass from pore water	[-]	c
$Fgrass_{air}$	fraction of total uptake by grass from air	[-]	c
C_{drw}	concentration in drinking water	$[kg_c.m^{-3}]$	
Intermediate results 3			
C_{meat}	concentration in meat (wet weight)	$[kg_c.kg_{wwt}^{-1}]$	
C_{milk}	concentration in milk (wet weight)	$[kg_c.kg_{wwt}^{-1}]$	
$Fcattle_i$	fraction of total intake by cattle through medium *i* $i \in$ {grass,drw,air,soil}	[-]	c
Intermediate results 4			
$DOSE_i$	daily dose through intake of *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	
$Fdose_i$	fraction of total dose through intake of medium *i* $i \in$ {drw,fish,leaf,root,meat,milk,air}	[-]	c
Output			
$DOSE_{tot}$	total daily intake for humans	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	

The following table gives the 'temporary' symbols defined in the indirect exposure calculations, and the corresponding specific local and regional symbols.

Temporary symbol	Local concentration	Regional concentration
C_{water}	$PEClocal_{water,ann}$	$PECreg_{water}$
C_{air}	$PEClocal_{air,ann}$	$PECreg_{air}$
$C_{grassland}$	$PEClocal_{grassland}$	$PECreg_{agric}$
$C_{agric,porew}$	$PEClocal_{agric,porew}$	$PECreg_{agric,porew}$
$C_{grassland,porew}$	$PEClocal_{grassland,porew}$	$PECreg_{agric,porew}$
C_{grw}	$PEClocal_{grw}$	$PECreg_{agric,porew}$

Temporary symbol	Local concentration	Regional concentration
C_{fish}	$Clocal_{fish}$	$Creg_{fish}$
C_{leaf}	$Clocal_{leaf}$	$Creg_{leaf}$
C_{grass}	$Clocal_{grass}$	$Creg_{grass}$
$Fleaf_{porew}$	$Flocal\text{-}leaf_{porew}$	$Freg\text{-}leaf_{porew}$
$Fleaf_{air}$	$Flocal\text{-}leaf_{air}$	$Freg\text{-}leaf_{air}$
$Fgrass_{porew}$	$Flocal\text{-}grass_{porew}$	$Freg\text{-}grass_{porew}$
$Fgrass_{air}$	$Flocal\text{-}grass_{air}$	$Freg\text{-}grass_{air}$
C_{root}	$Clocal_{root}$	$Creg_{root}$
C_{meat}	$Clocal_{meat}$	$Creg_{meat}$
C_{milk}	$Clocal_{milk}$	$Creg_{milk}$
C_{drw}	$Clocal_{drw}$	$Creg_{drw}$
$DOSE_i$	$DOSElocal_i$	$DOSEreg_i$
$Fdose_i$	$Fdose\text{-}local_i$	$Fdose\text{-}reg_i$
$DOSE_{tot}$	$DOSElocal_{tot}$	$DOSEreg_{tot}$

III.5.2.1 Concentration in fish

The BCF for fish is estimated in Section III.5.1.1 on secondary poisoning. The concentration in fish for human indirect exposure is given by:

$$C_{fish} = BCF_{fish} \cdot C_{water} \quad \textbf{(182)}$$

Input			
BCF_{fish}	bioconcentration factor for fish on wet-weight basis	$[m^3.kg_{wwt}^{-1}]$	O
C_{water}	concentration in surface water	$[kg_c.m^{-3}]$	O
Output			
C_{fish}	concentration in wet fish	$[kg_c.kg_{wwt}^{-1}]$	O

III.5.2.2 Concentration in crops

The modelling approach proposed by Trapp and Matthies (1995) is used to estimate levels in plants due to uptake from pore water and air (gas phase). This approach integrates uptake from

pore water and air into a consistent, one-compartment model. The sink term in the model is formed by diffusive transfer from leaf to air, elimination in the plant tissue, and dilution by growth; the source term is formed by the uptake and translocation from soil and gaseous uptake from air. Aerosol deposition is not considered in the model. Several plant-specific defaults are required, which are summarised in Table III-86.

Table III-86 Default settings for plant-specific parameters.

Plant properties, taken from Riederer (1990), values for *Brassica oleracea* (rounded)			
Parameter	**Symbol**	**Unit**	**Value**
Volume fraction of water in plant tissue	$Fwater_{plant}$	$[m^3.m^{-3}]$	0.65
Volume fraction of lipids in plant tissue	$Flipid_{plant}$	$[m^3.m^{-3}]$	0.01
Volume fraction of air in plant tissue	$Fair_{plant}$	$[m^3.m^{-3}]$	0.30
Bulk density of plant tissue	RHO_{plant}	$[kg_{wwt}.m^{-3}]$	700
Plant properties, taken from Trapp and Matthies (1995), values referenced to 1 m^2			
Parameter	**Symbol**	**Unit**	**Value**
Leaf surface area	$AREA_{plant}$	$[m^2]$	5
Conductance (0.001 $m.s^{-1}$)	g_{plant}	$[m.d^{-1}]$	86.4
Shoot volume	V_{leaf}	$[m^3]$	0.002
Transpiration stream (1 $l.d^{-1}$)	Qtransp	$[m^3.d^{-1}]$	1.10^{-3}
Correction exponent for differences between plant lipids and octanol	B	[-]	0.95
Growth-rate constant for dilution by growth	$Kgrowth_{plant}$	$[d^{-1}]$	0.035
Pseudo-first-order rate constant for metabolism	$Kmetab_{plant}$	$[d^{-1}]$	0
Pseudo-first-order rate constant for photodegradation	$Kphoto_{plant}$	$[d^{-1}]$	0

The general partitioning between water and plant tissue is assumed to be based on hydrophobic sorption to plant lipids. *Kow* is corrected slightly for the differences between plant lipids and octanol.

$$K_{plant-water} = Fwater_{plant} + Flipid_{plant} \cdot Kow^{b} \quad \textbf{(183)}$$

Input			
$Fwater_{plant}$	volume fraction of water in plant tissue	[$m^3.m^{-3}$]	D
$Flipid_{plant}$	volume fraction of lipids in plant tissue	[$m^3.m^{-3}$]	D
Kow	octanol-water partition coefficient	[$m^3.m^{-3}$]	S
b	correction for differences between plant lipids and octanol	[-]	D
Output			
$K_{plant-water}$	partition coeff. between plant tissue and water	[$m^3.m^{-3}$]	O

The concentration in root tissue is governed mainly by physical sorption, and is given by:

$$C_{root} = \frac{K_{plant-water} \cdot C_{agric,porew}}{RHO_{plant}} \quad \textbf{(184)}$$

Input			
$K_{plant-water}$	partition coeff. between plant tissue and water	[$m^3.m^{-3}$]	O
$C_{agric,porew}$	concentration in pore water of agricultural soil	[$kg_c.m^{-3}$]	O
RHOplant	bulk density of plant tissue (wet weight)	[$kg_{wwt}.m^{-3}$]	D
Output			
C_{root}	concentration in root tissue of plant	[$kg_c.kg_{wwt}^{-1}$]	O

The transpiration-stream concentration factor (*TSCF*) is the ratio between the concentration in the transpiration stream and the concentration in pore water. *TSCF* is given by (Briggs *et al.*, 1982). This estimation of *TSCF* was derived for a small group of pesticides in one plant species (Barley). Domain of physico-chemical properties: log *Kow* -0.5 to 4.5 (outside this range the minimum or maximum *Kow* is used).

$$TSCF = 0.784 \cdot \exp\left[\frac{-(\log Kow - 1.78)^2}{2.44}\right] \quad \textbf{(185)}$$

Input			
Kow	octanol-water partition coefficient	[-]	S
Output			
TSCF	transpiration-stream concentration factor	[-]	O

Gaseous exchange between leaves and air can be described by a leaf-air partition coefficient. $K_{leaf\text{-}air}$ is given by:

$$K_{leaf\text{-}air} = Fair_{plant} + \frac{K_{plant\text{-}water}}{K_{air\text{-}water}} \quad \textbf{(186)}$$

Input			
$K_{plant\text{-}water}$	partition coefficient between plant tissue and water	$[m^3.m^{-3}]$	O
$K_{air\text{-}water}$	air-water partition coefficient	$[m^3.m^{-3}]$	O[c]
$Fair_{plant}$	volume fraction of air in plant tissue	$[m^3.m^{-3}]$	D
Output			
$K_{leaf\text{-}air}$	partition coeff. between leaves and air	$[m^3.m^{-3}]$	O

Elimination of the substance may take place in the leaf tissue by metabolism or photolysis. If rate constants are known for these processes, they may be added:

$$kelim_{plant} = kmetab_{plant} + kphoto_{plant} \quad \textbf{(187)}$$

Input			
$kmetab_{plant}$	rate constant for metabolism in plants	$[d^{-1}]$	D
$kphoto_{plant}$	rate constant for photolysis in plants	$[d^{-1}]$	D
Output			
$kelim_{plant}$	rate constant for total elimination in plants	$[d^{-1}]$	O[c]

The actual one-compartment model for calculating the concentration in the leaf can be described with a simple differential equation. The sink term is formed by diffusive transfer from leaf to air, elimination in the plant tissue and dilution by growth:

$$ALPHA = \frac{AREA_{plant} \cdot g_{plant}}{K_{leaf\text{-}air} \cdot V_{leaf}} + kelim_{plant} + kgrowth_{plant} \quad \textbf{(188)}$$

Input			
$AREA_{plant}$	leaf surface area	$[m^2]$	D
g_{plant}	conductance	$[m.d^{-1}]$	D
$K_{leaf\text{-}air}$	partition coeff. between leaves and air	[-]	O
V_{leaf}	shoot volume	$[m^3]$	D
$kelim_{plant}$	rate constant for elimination in plants	$[d^{-1}]$	O[c]
$kgrowth_{plant}$	rate constant for dilution by growth	$[d^{-1}]$	D
Output			
ALPHA	sink term of differential equation	$[d^{-1}]$	O[c]

The source term is formed by the uptake and translocation from soil and gaseous uptake from air. Since we have two pore-water concentrations, for agricultural soil and grassland, two separate source terms must be estimated. At the moment, the same default plant characteristics are used for grass as for crops.

$$BETA_{agric} = C_{agric,porew} \cdot TSCF \cdot \frac{Qtransp}{V_{leaf}} + (1 - Fass_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}} \quad (189)$$

$$BETA_{grass} = C_{grassland,porew} \cdot TSCF \cdot \frac{Qtransp}{V_{leaf}} + (1 - Fass_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}} \quad (190)$$

Input			
Qtransp	transpiration stream	[$m^3.d^{-1}$]	D
$C_{agric,porew}$	concentration in pore water of agricultural soil	[$kg_c.m^{-3}$]	O
$C_{grassland,porew}$	concentration in pore water of grassland	[$kg_c.m^{-3}$]	O
C_{air}	concentration in air	[$kg_c.m^{-3}$]	O
g_{plant}	leaf conductance	[$m.d^{-1}$]	D
TSCF	transpiration-stream concentration factor	[-]	O
V_{leaf}	shoot volume	[m^3]	D
$Fass_{aer}$	fraction of substance adsorbed to aerosol	[-]	O
Output			
$BETA_{agric}$	source term of differential equation for crops	[$kg_c.m^{-3}.d^{-1}$]	O[c]
$BETA_{grass}$	source term of differential equation for grass	[$kg_c.m^{-3}.d^{-1}$]	O[c]

The steady-state concentration is calculated as the source term divided by the sink term. The default growth-dilution rate constant ensures that a steady state will always be reached within the relevant period of time (assuming constant exposure levels).

$$C_{leaf} = \frac{BETA_{agric}}{ALPHA} \cdot \frac{1}{RHO_{plant}} \quad (191)$$

$$C_{grass} = \frac{BETA_{grass}}{ALPHA} \cdot \frac{1}{RHO_{plant}} \quad (192)$$

Input			
ALPHA	sink term of differential equation	[d^{-1}]	O[c]
$BETA_{agric}$	source term of differential equation, agricultural soil	[$kg_c.m^{-3}.d^{-1}$]	O[c]
$BETA_{grass}$	source term of differential equation, grassland	[$kg_c.m^{-3}.d^{-1}$]	O[c]
RHO_{plant}	bulk density of plant tissue (wet weight)	[$kg_{wwt}.m^{-3}$]	D
Output			
C_{leaf}	concentration in leaves of plant	[$kg_c.kg_{wwt}^{-1}$]	O
C_{grass}	concentration in grass	[$kg_c.kg_{wwt}^{-1}$]	O

As additional information, the contribution of uptake from pore water and air to the total uptake is calculated.

$$Fleaf_{porew} = \frac{C_{agric,porew} \cdot TSCF \cdot \frac{Qtransp}{V_{leaf}}}{BETA_{agric}} \quad (193)$$

$$Fleaf_{air} = \frac{(1 - Fass_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}}{BETA_{agric}} \quad (194)$$

$$Fgrass_{porew} = \frac{C_{grassland,porew} \cdot TSCF \cdot \frac{Qtransp}{V_{leaf}}}{BETA_{grass}} \quad (195)$$

$$Fgrass_{air} = \frac{(1 - Fass_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}}{BETA_{grass}} \quad (196)$$

Input			
Qtransp	transpiration stream	[$m^3.d^{-1}$]	D
$C_{agric,porew}$	concentration in pore water of agricultural soil	[$kg_c.m^{-3}$]	O
$C_{grassland,porew}$	concentration in pore water of grassland	[$kg_c.m^{-3}$]	O
C_{air}	concentration in air	[$kg_c.m^{-3}$]	O
TSCF	transpiration-stream concentration factor	[-]	O
V_{leaf}	shoot volume	[m^3]	D
$Fass_{aer}$	fraction of substance adsorbed to aerosol	[-]	O
$BETA_{agric}$	source term of differential equation for crops	[$kg_c.m^{-3}.d^{-1}$]	O[c]
$BETA_{grass}$	source term of differential equation for grass	[$kg_c.m^{-3}.d^{-1}$]	O[c]
Output			
$Fleaf_{porew}$	fraction of total uptake by crops from pore water	[-]	O[c]
$Fleaf_{air}$	fraction of total uptake by crops from air	[-]	O[c]
$Fgrass_{porew}$	fraction of total uptake by grass from pore water	[-]	O[c]
$Fgrass_{air}$	fraction of total uptake by grass from air	[-]	O[c]

III.5.2.3 Concentration in meat and milk products

Travis and Arms (1988) performed a log-linear regression analysis on experimentally derived bioaccumulation factors and the octanol-water partition coefficient. It should be noted that the uncertainty in these estimates is considerable. The concentrations in meat and milk are calculated by applying the bioaccumulation factors and summing the contributions from air, soil, grass and drinking water. The BAF for meat is derived from data on 36 organic compounds, with a log *Kow* range of 1.5 - 6.5. The BAF for milk was derived from data on 28 organic compounds, with a log *Kow* range of 3 - 6.5. Outside these ranges, the minimum or maximum *Kow* is used.

Table III-87 Default intake rates for cattle.

Parameter	Symbol	Unit	Value
Daily intake for cattle of grass (dry weight)	$ICdwt_{grass}$	$[kg_{dwt}.d^{-1}]$	16.9 [a]
Daily intake for cattle of soil (dry weight)	$ICdwt_{soil}$	$[kg_{dwt}.d^{-1}]$	0.41 [a]
Daily inhalation rate for cattle	IC_{air}	$[m^3.d^{-1}]$	122 [a]
Daily intake for cattle of drinking water	IC_{drw}	$[m^3.d^{-1}]$	0.055 [b]
Conversion dry weight to wet weight grass	$CONV_{grass}$	$[kg_{wwt}.kg_{dwt}^{-1}]$	4 [a]

[a] Source: McKone and Ryan (1989).
[b] Source: ECETOC (1990).

$$BAF_{meat} = 10^{-7.6 + \log Kow} \quad \textbf{(197)}$$

$$BAF_{milk} = 10^{-8.1 + \log Kow} \quad \textbf{(198)}$$

Input			
Kow	octanol-water partition coefficient	[-]	S
Output			
BAF_{meat}	bioaccumulation factor for meat	$[d.kg_{meat}^{-1}]$	O
BAF_{milk}	bioaccumulation factor for milk	$[d.kg_{milk}^{-1}]$	O

The default intake rates for soil and grass are expressed as dry weights. These are converted to wet weights as follows:

$$IC_{grass} = ICdwt_{grass} \cdot CONV_{grass} \quad \textbf{(199)}$$

$$IC_{soil} = ICdwt_{soil} \cdot CONV_{soil} \quad \textbf{(200)}$$

Input			
$ICdwt_{grass}$	daily intake for cattle of grass (dry weight)	$[kg_{wwt}.d^{-1}]$	D
$CONV_{grass}$	conversion factor grass from dry weight to wet weight	$[kg_{wwt}.kg_{dwt}^{-1}]$	D
$ICdwt_{soil}$	daily intake of soil (dry weight)	$[kg_{wwt}.d^{-1}]$	D
$CONV_{soil}$	conversion factor soil from dry weight to wet weight	$[kg_{wwt}.kg_{dwt}^{-1}]$	O[c]
Output			
IC_{grass}	daily intake of grass (wet weight)	$[kg_{wwt}.d^{-1}]$	O[c]
IC_{soil}	daily intake of soil (wet weight)	$[kg_{wwt}.d^{-1}]$	O[c]

The concentrations in meat and milk are calculated as:

$$C_{milk} = BAF_{milk} \cdot \sum C_i \cdot IC_i \quad i \in \{grass, grassland \setminus soil, air, drw\} \quad \textbf{(201)}$$

$$C_{meat} = BAF_{meat} \cdot \sum C_i \cdot IC_i \quad i \in \{grass, grassland \setminus soil, air, drw\} \quad \textbf{(202)}$$

The contribution of each exposure medium to the intake of cattle can be calculated as:

$$Fcattle_i = \frac{C_i \cdot IC_i}{\sum C_i \cdot IC_i} \quad i \in \{grass, grassland \setminus soil, air, drw\} \qquad (203)$$

Input			
C_{grass}	concentration in grass (wet weight)	[$kg_c.kg_{wwt}^{-1}$]	O
IC_{grass}	daily intake of grass (wet weight)	[$kg_{wwt}.d^{-1}$]	O^c
$C_{grassland}$	total concentration in grassland soil (wet weight)	[$kg_c.kg_{wwt}^{-1}$]	O
IC_{soil}	daily intake of soil (wet weight)	[$kg_{wwt}.d^{-1}$]	O^c
C_{air}	total concentration in air	[$kg_c.m_{air}^{-3}$]	O
IC_{air}	daily inhalation rate of cattle	[$m_{air}^3.d^{-1}$]	D
C_{drw}	concentration in drinking water	[$kg_c.m_{drw}^{-3}$]	O
IC_{drw}	daily intake of drinking water	[$m_{drw}^3.d^{-1}$]	D
Output			
C_{meat}	concentration in meat (wet weight)	[$kg_c.kg_{wwt}^{-1}$]	O
C_{milk}	concentration in milk (wet weight)	[$kg_c.kg_{wwt}^{-1}$]	O
$Fcattle_i$	fraction of total intake by cattle through *i* $i \in$ {grass,soil,air,drw}	[-]	O^c

III.5.2.4 Purification of drinking water

Drinking water is produced from surface water or groundwater. Complete removal of suspended particles from surface water and groundwater is assumed. The effects of the treatment processes used for purification of groundwater, which are generally not intended for the removal of organic pollutants, can be neglected. Surface-water treatment is estimated according to Hrubec and Toet (1992). Dependent on the type of storage, two different water-treatment systems for surface water can be distinguished: system 1 includes storage in open reservoirs, while system 2 includes dune recharge. Removal of the dissolved fraction of a xenobiotic from the surface water is modelled by means of purification factors. For the choice between the two systems and the choice between surface water or groundwater, a worst-case approach is followed.

Purification factors for both systems can be taken from the table below. The factors from each relevant column should be multiplied to give the resulting purification factor for each system ($Fsys1_{pur}$ and $Fsys2_{pur}$).

Table III-88 Purification factors, based on Henry's law constant and biodegradation rate.

Treatment process	**log *Kow***			**Henry's law constant** *HENRY* ($Pa \cdot m^3 \cdot mol^{-1}$)		**Aerobic biodegradation rate** $DT50bio_{water}$ (days)	
	≤4	4-5	>5	≤100	>100	>10	≤10
System 1	1	1/4	1/16	1	1/2	1	1
System 2	1	1/2	1/4	1	1/2	1	1/4

Source: Hrubec and Toet (1992).

$$F_{pur} = max\ (Fsys1_{pur}\ ,\ Fsys2_{pur}\ ) \qquad \textbf{(204)}$$

Input			
Kow	octanol-water partition coefficient	[-]	S
HENRY	Henry's law constant	[Pa.m^3.mol^{-1}]	O
DT50bio$_{water}$	half-life for biodegradation in bulk surface water	[d]	O
Fsys1$_{pur}$	purification factor for system 1	[-]	O^c
Fsys2$_{pur}$	purification factor for system 2	[-]	O^c
Output			
F$_{pur}$	purification factor for surface water	[-]	O

$$C_{drw} = \max\ (\ C_{water} \cdot F_{pur}\ ,\ C_{grw}\ ) \qquad \textbf{(205)}$$

Input			
F$_{pur}$	purification factor for surface water	[-]	O
C$_{water}$	dissolved concentration in surface water	[kg$_c$.m^{-3}]	O
C$_{grw}$	groundwater concentration	[kg$_c$.m^{-3}]	O
Output			
C$_{drw}$	concentration in drinking water	[kg$_c$.m^{-3}]	O

III.5.2.5 Total daily intake for humans

The indirect exposure of humans to chemicals originates from several sources. The exposure assessment includes six pathways: drinking water, fish, crops, meat, milk and air. The daily dose for humans is calculated by means of the concentrations in these media and the daily intake values. This approach implies an exposure scenario whereby each of these intake media is retrieved exclusively from within the contaminated system.

$$DOSE_j = \frac{C_j \cdot IH_j}{BW} \qquad j \in \{drw, fish, leaf, root, meat, milk\} \qquad \textbf{(206)}$$

$$DOSE_{air} = \frac{F_{resp} \cdot C_{air} \cdot IH_{air}}{BW} \cdot \frac{BIO_{inh,2}}{BIO_{oral,2}} \qquad \textbf{(207)}$$

The total dose can now be calculated as the sum of the dose for each medium:

$$DOSE_{tot} = \sum_i DOSE_i \qquad \textbf{(208)}$$

$$i \in \{air, drw, fish, leaf, root, meat, milk\}$$

The contribution of each intake medium to the total dose is calculated as:

$$Fdose_i = \frac{DOSE_i}{\sum_i DOSE_i} \quad \textbf{(209)}$$

Input			
C_{drw}	concentration in drinking water	[$kg_c.m^{-3}$]	O
C_{fish}	concentration in fish	[$kg_c.kg_{wwt}^{-1}$]	O
C_{leaf}	concentration in leaves of crops	[$kg_c.kg_{wwt}^{-1}$]	O
C_{root}	concentration in roots of crops	[$kg_c.kg_{wwt}^{-1}$]	O
C_{meat}	concentration in meat	[$kg_c.kg_{wwt}^{-1}$]	O
C_{milk}	concentration in milk	[$kg_c.kg_{wwt}^{-1}$]	O
C_{air}	concentration in air	[$kg_c.m_{air}^{-3}$]	O
F_{resp}	respirable fraction of inhaled substance	[-]	D
IH_i	daily intake of medium *i*	[$kg.d^{-1}$ or $m^3.d^{-1}$]	D
$BIO_{oral,2}$	bioavailability for oral intake	[-]	D
$BIO_{inh,2}$	bioavailability for inhalation	[-]	D
BW	body weight of (adult) human considered	[kg]	D
Output			
$DOSE_i$	daily dose via intake of *i*	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O[c]
$DOSE_{tot}$	total daily intake for humans	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$Fdose_i$	fraction of total dose via intake of medium *i*	[-]	O[c]

In ***Table III-89***, the default consumption rates for each food product are given (taken from ECETOC, 1994). These values represent the highest country-average intake across all EU Member States for each food product.

Table III-89 Standard defaults for indirect exposure of humans.

Parameter	Symbol	Value	Unit	Source
Daily intake of drinking water	IH_{drw}	0.002	[$m^3.d^{-1}$]	(b)
Daily intake of fish	IH_{fish}	0.115	[$kg_{wwt}.d^{-1}$]	(a)
Daily intake of leaf crops (incl. fruit and cereals)	IH_{leaf}	1.20	[$kg_{wwt}.d^{-1}$]	(a)
Daily intake of root crops	IH_{root}	0.384	[$kg_{wwt}.d^{-1}$]	(a)
Daily intake of meat	IH_{meat}	0.301	[$kg_{wwt}.d^{-1}$]	(a)
Daily intake of dairy products	IH_{milk}	0.561	[$kg_{wwt}.d^{-1}$]	(a)
Daily inhalation rate	IH_{air}	20	[$m^3.d^{-1}$]	(b)
Respirable fraction of the inhaled substance	F_{resp}	1	[-]	
Bioavailability for inhalation	BIO_{inh}	0.75	[-]	(c)
Bioavailability for oral uptake	BIO_{oral}	1.0	[-]	(c)
Body weight of adult	BW	70	[kg]	

[a] Source: Euromonitor (1992) as reported by ECETOC (1994).
[b] Source: US-EPA (1989).
[c] Source: Vermeire *et al.* (1993b).

III.5.3 Consumer exposure

Five different consumer exposure scenarios are implemented in EUSES:

- Inhalation: a substance that is released as a gas, vapour or airborne particulate into a room (e.g. a component of an aerosol insecticide, a carrier/solvent in a cosmetic formulation, a powder detergent). Release may be the result of direct release as a gas, vapour or particulate, or by evaporation from liquid or solid matrices. In the latter case, the equation represent a worst-case situation by assuming that the substance is directly available as a gas or vapour.
- Dermal a: a substance contained in a medium. This dermal scenario also applies to i) a non-volatile substance in a medium used without further dilution (set dilution D=1), and ii) a non-volatile substance in a volatile medium.
- Dermal b: a non-volatile substance migrating from an article (e.g. dyed clothing, residual fabric conditioner, dyestuff/newsprint from paper).
- Oral a: a substance in a product unintentionally swallowed during normal use (e.g. toothpaste).
- Oral b: a substance migrating from an article into food or drink (e.g. plastic film, plastic-coated cups/plates).

Input: inhalation		
Q_{prod}	amount of product released	[kg]
Fc_{prod}	weight fraction of substance in product	[-]
V_{room}	room size	[m^3]
$T_{contact}$	duration of contact per event	[d]
n	mean number of events per day	[d^{-1}]
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]
Output: inhalation		
I_{inh}	inhalatory intake of substance	[$kg_c.kg_{bw}^{-1}.d^{-1}$]
C_{inh}	concentration in air of room	[$kg_c.m^{-3}$]
Input: dermal a		
n	mean number of events per day	[d^{-1}]
C_{prod}	concentration of substance in product before dilution	[$kg_c.m^{-3}$]
D	dilution factor	[-]
RHO_{prod}	density of product before dilution	[$kg_c.m\text{-}^{3}$]
Fc_{prod}	weight fraction of substance in product before dilution	[-]
Q_{prod}	amount of product used	[kg]
V_{prod}	volume of product used before dilution	[m^3]
V_{appl}	volume of diluted product actually contacting skin	[m^3]
TH_{der}	thickness of product layer on skin	[m]
$AREA_{der}$	area of contact between product and skin	[m^2]
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]
Output: dermal a		
C_{der}	dermal concentration of substance on skin	[$kg_c.m^{-3}$]
A_{der}	amount of substance on skin per event	[kg_c]
$U_{der,pot}$	amount of substance that can potentially be taken up	[$kg_c.kg_{bw}^{-1}.d^{-1}$]
Input: dermal b		
C_{prod}	concentration of substance in product before dilution	[$kg_c.m^{-3}$]
RHO_{prod}	density of product before dilution	[$kg.m^{-3}$]
Fc_{prod}	weight fraction of substance in product before dilution	[-]
Q_{prod}	amount of product used	[kg]
V_{prod}	volume of product used before dilution	[m^3]
Fc_{migr}	fraction of substance migrating per unit time	[$kg_c.kg^{-1}.d^{-1}$]

$T_{contact}$	duration of contact per event	[d]
TH_{der}	thickness of product	[m]
W_{der}	weight of substance on skin per event	[$kg_c.m^{-2}$]
$AREA_{der}$	area of contact between product and skin	[m^2]
n	mean number of events per day	[d^{-1}]
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]
Output: dermal b		
A_{der}	total amount of compound to which skin is pot. exposed	[kg_c]
$A_{migr,der}$	amount of substance to which skin is expected to be exposed due to migration	[kg_c]
$U_{der,pot}$	potential uptake	[$kg_c.kg_{bw}^{-1}.d^{-1}$]
Input: oral a		
C_{prod}	concentration of substance in product before dilution	[$kg_c.m^{-3}$]
D	dilution factor	[-]
RHO_{prod}	density of product before dilution	[$kg.m^{-3}$]
Q_{prod}	amount of product before dilution	[kg]
Fc_{prod}	weight fraction of substance in product before dilution	[-]
V_{prod}	volume of product before dilution	[m^3]
V_{appl}	volume of diluted product in contact with mouth per event	[m^3]
F_{oral}	fraction of V_{appl} that is ingested	[-]
n	mean number of events per day	[d^{-1}]
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]
Output: oral a		
C_{oral}	concentration in ingested product	[$kg_c.m^{-3}$]
I_{oral}	intake	[$kg_c.kg_{bw}^{-1}.d^{-1}$]
Input: oral b		
$AREA_{art}$	surface area of article in contact with food	[m^2]
TH_{art}	thickness of article in contact with food	[m]
C_{art}	concentration of substance in article	[$kg_c.m^{-3}$]
Fc_{migr}	fraction migrating per time	[$kg_c.d^{-1}$]
V_{prod}	volume of food	[m^3]
$T_{contact}$	duration of contact between article and food	[d]
n	mean number of events per day	[d^{-1}]
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]
Output: oral b		
C_{oral}	concentration in ingested product	[$kg_c.m^{-3}$]
I_{oral}	intake	[$kg_c.kg_{bw}^{-1}.d^{-1}$]
Output: chronic exposure		
$C_{inh,ann}$	annual average inhalation exposure concentration	[$kg_c.m^{-3}$]
$C_{der,ann}$	annual average dermal exposure concentration	[$kg_c.m^{-3}$]
$C_{oral,ann}$	annual average oral exposure concentration	[$kg_c.m^{-3}$]
Output: total exposure		
U_{tot}	total uptake via different routes	[$kg_c.kg_{bw}^{-1}.d^{-1}$]

Table III-90 Defaults for consumer exposure calculations.

Parameter	Symbol	Unit	Value
Respirable fraction of the inhaled substance	F_{resp}	[-]	1 [a]
thickness of product	TH_{der}	[m]	1.10^{-4}
Bioavailability for oral intake	BIO_{oral}	[-]	1 [a]
Bioavailability for inhalation	BIO_{inh}	[-]	0.75 [a]
Bioavailability for dermal uptake	BIO_{der}	[-]	1
Ventilation rate of person	IH_{air}	[$m^3.d^{-1}$]	20 [a]
Human body weight	BW	[kg]	70 [a]

[a] Already defined in section on human indirect exposure.

III.5.3.1 Inhalatory Consumer Exposure

A substance that is released as a gas, vapour or airborne particulate into a room (e.g. a component of an aerosol insecticide, a carrier/solvent in a cosmetic formulation, a powder detergent). For a description of the ConsExpo inhalatory models see Van Veen (2001).

Release may be the result of direct release as gas, vapour or particulate, or by evaporation from liquid or solid matrices. In the last case, the equation represent a worst-case situation by assuming that the substance is directly available as a gas or vapour. The equation applies to both volatile substances and airborne particulates. The concentration in air after using an amount Q_{prod} of the product becomes:

$$C_{inh} = \frac{Q_{prod} \cdot Fc_{prod}}{V_{room}} \qquad \textbf{(210)}$$

The air concentration C_{inh} results in an inhalatory intake of:

$$I_{inh} = \frac{F_{resp} \cdot C_{inh} \cdot IH_{air} \cdot T_{contact}}{BW} \cdot n \qquad \textbf{(211)}$$

Input			
Q_{prod}	amount of product released	[kg]	S
Fc_{prod}	weight fraction of substance in product	[$kg_c.kg_{prod}$]	S
V_{room}	room size	[m^3]	S
F_{resp}	respirable fraction of inhaled substance	[-]	D
IH_{air}	ventilation rate of person	[$m^3.d^{-1}$]	D
$T_{contact}$	duration of contact per event	[d]	S
BW	body weight	[kg]	D
n	mean number of events per day	[d^{-1}]	S
Output			
I_{inh}	inhalatory intake of substance	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
C_{inh}	concentration in air of room	[$kg_c.m^{-3}$]	O

III.5.3.2 Dermal Consumer Exposure

Table III-91 Mean surface area by body part for the adult male (US-EPA, 1989).

Body part	**Mean surface area (m^2)**
Head (face)	0.1180
Trunk	0.5690
Upper extremities	0.3190
Arms	0.2280
upper arms	0.1430
Forearms	0.1140
hands (fronts and backs)	0.0840
Lower extremities	0.6360
Legs	0.5060
Thighs	0.1980
lower legs	0.2070
Feet	0.1120
Total	1.9400

A substance contained in a medium.
The concentration in the product as used can be calculated using the following equation. Depending on how the parameters are provided, three analogous calculations are used:

$$C_{der} = \frac{C_{prod}}{D} = \frac{RHO_{prod} \cdot Fc_{prod}}{D} = \frac{Q_{prod} \cdot Fc_{prod}}{V_{prod} \cdot D} \qquad \textbf{(212)}$$

The total amount to which the skin is exposed is then given by (two options, depending on format of available data):

$$A_{der} = C_{der} \cdot V_{appl} = C_{der} \cdot TH_{der} \cdot AREA_{der} \qquad \textbf{(213)}$$

The potential uptake per kilogram body weight per day is derived as:

$$U_{der,pot} = \frac{A_{der} \cdot n}{BW} \qquad \textbf{(214)}$$

The above dermal equations apply also to i) a non-volatile substance in a medium used without

further dilution (set dilution D=1), and ii) a non-volatile substance in a volatile medium. In the latter case, the concentration C_{der} is valid at the very beginning of exposure only. However, this concentration can still be used to calculate A_{der}, because the substance is non-volatile. The above dermal equations can also be used in the case of a volatile substance, but in that case they represent a worst-case situation. If the duration of contact is specified, a chronic exposure can be calculated by EUSES (equation 221). For a description of the ConsExpo inhalatory models see Van Veen (2001).

Input			
C_{prod}	concentration of substance in product before dilution	[$kg_c.m^{-3}$]	S
D	dilution factor	[-]	S
RHO_{prod}	density of product before dilution	[$kg.m^{-3}$]	S
Q_{prod}	amount of product used	[kg]	S
Fc_{prod}	weight fraction of substance in product before dilution	[-]	S
V_{prod}	volume of product used before dilution	[m^3]	S
V_{appl}	volume of diluted product actually contacting the skin	[m^3]	S
TH_{der}	thickness of product layer on skin	[m]	D
$AREA_{der}$	area of contact between product and skin	[m^2]	P/S
BW	body weight	[kg]	D
n	mean number of events per day	[d^{-1}]	S
Output			
C_{der}	dermal concentration of substance on skin	[$kg_c.m^{-3}$]	O
A_{der}	amount of substance on skin per event	[kg_c]	O
$U_{der,pot}$	amount of substance that can potentially be taken up	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O

A non-volatile substance migrating from an article (e.g. dyed clothing, residual fabric conditioner, dyestuff/newsprint from paper).

The exposure calculation will involve estimating the amount of substance which will migrate from the area of the article in contact with skin during the time of contact. The concentration in the product as used can be calculated according to Equation (209) in case the density of the product and the fraction of substance in the product are known. Dyestuff levels in fabrics and paper are usually given as weight of product per unit area (e.g. mg/m^2). The total amount is then calculated by multiplying by $AREA_{der}$. The amount to which the skin is exposed is given by

$$\boldsymbol{A_{der} = W_{der} \cdot AREA_{der} = C_{der} \cdot TH_{der} \cdot AREA_{der}} \quad \textbf{(215)}$$

where $C_{der} \cdot TH_{der}$ is equal to weight per unit of area:

$$\boldsymbol{W_{der} = C_{der} \cdot TH_{der}} \quad \textbf{(216)}$$

Extractability in simulated body fluids for several classes of dyestuffs and different fabric types has been evaluated by ETAD (1983). For migrating substances, only part of the total amount A_{der} is able to reach the skin. The amount to be used is:

$$\boldsymbol{A_{migr,der} = A_{der} \cdot Fc_{migr} \cdot T_{contact}} \quad \textbf{(217)}$$

where $Fc_{migr} \cdot T_{contact}$ must be much smaller than 1. The potential uptake per kilogram body

weight per day is then derived as:

$$U_{der,pot} = \frac{A_{migr,der} \cdot n}{BW} \quad \textbf{(218)}$$

It should be noted that EUSES does not check whether the estimated daily uptake exceeds the theoretical maximum. This maximum can be derived from the amount of product used (kg), the concentration of the substance ($kg_c.kg^{-1}$) in the product, the use frequency (d^{-1}) and the bodyweight (kg_{bw}).
EUSES also asks to specify the duraction of contact per event to be able to calculate a chronic dermal exposure.

Input			
Fc_{migr}	fraction of substance migrating per unit time	$[kg_c.kg^{-1}.d^{-1}]$	S
$T_{contact}$	duration of contact per event	[d]	S
TH_{der}	thickness of product	[m]	D
W_{der}	weight of substance on skin per event	$[kg_c.m^{-2}]$	S
$AREA_{der}$	area of contact between product and skin	$[m^2]$	P/S
C_{der}	concentration of substance	$[kg_c.m^{-3}]$	O
BW	body weight	[kg]	D
n	mean number of events per day	$[d^{-1}]$	S
Output			
A_{der}	total amount of comp. to which skin is pot. exposed	$[kg_c]$	O
$A_{migr,der}$	amount of substance to which skin is expected to be exposed due to migration	$[kg_c]$	O
$U_{der,pot}$	potential uptake	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

III.5.3.3 Oral consumer exposure

A substance in a product unintentionally swallowed during normal use (e.g. toothpaste).
These equations may also be used to estimate exposures arising from ingestion of the non-respirable fraction of inhaled airborne particulates. The concentration in the product as swallowed is calculated from

$$C_{oral} = \frac{C_{prod}}{D} = \frac{RHO_{prod} \cdot Fc_{prod}}{D} = \frac{Q_{prod} \cdot Fc_{prod}}{V_{prod} \cdot D} \quad \textbf{(219)}$$

and the intake is then given by

$$I_{oral} = \frac{F_{oral} \cdot V_{appl} \cdot C_{oral} \cdot n}{BW} \quad \textbf{(220)}$$

If an undiluted product is swallowed, $D = 1$.
For a description of the ConsExpo inhalatory models see Van Veen (2001).

Input			
C_{prod}	concentration of substance in product before dilution	[$kg_c.m^{-3}$]	S
D	dilution factor	[-]	S
RHO_{prod}	density of product before dilution	[$kg.m^{-3}$]	S
Q_{prod}	amount of product before dilution	[kg_c]	S
Fc_{prod}	weight fraction of substance in product before dilution	[-]	S
V_{prod}	volume of product before dilution	[m^3]	S
V_{appl}	volume of diluted product per event in contact with mouth	[m^3]	S
F_{oral}	fraction of V_{appl} that is ingested	[-]	S
BW	body weight	[kg]	D
n	mean number of events per day	[d^{-1}]	S
Output			
C_{oral}	concentration in ingested product	[$kg_c.m^{-3}$]	O
I_{oral}	intake	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O

A substance migrating from an article into food or drink (e.g. plastic film, plastic-coated cups/plates).

The following equation can be used to obtain a conservative estimate of substance uptake from a defined volume of food. The value of Fc_{migr} will be influenced by the type of food (e.g. fatty/dry/moist), the period of exposure and the temperature at which migration occurs. The consumer exposure level will be influenced by the proportion of the contaminated food eaten. The concentration in the food as a result of migration from an article is given by:

$$C_{oral} = \frac{AREA_{art} \cdot TH_{art} \cdot C_{art} \cdot Fc_{migr} \cdot T_{contact}}{V_{prod}} \quad \textbf{(221)}$$

Oral intake is given by:

$$I_{oral} = \frac{V_{appl} \cdot C_{oral} \cdot n}{BW} \quad \textbf{(222)}$$

Input			
$AREA_{art}$	surface area of article in contact with food	[m^2]	S
TH_{art}	thickness of article in contact with food	[m]	S
C_{art}	concentration of substance in article	[$kg_c.m^{-3}$]	S
Fc_{migr}	fraction migrating per time	[$kg_c.d^{-1}$]	S
V_{prod}	volume of food	[m^3]	S
V_{appl}	volume of diluted product actually ingested	[m^3]	S
$T_{contact}$	contact duration between article and food	[d]	S
BW	body weight	[kg]	D
n	mean number of events per day	[d^{-1}]	S
Output			
C_{oral}	concentration in ingested product	[$kg_c.m^{-3}$]	O
I_{oral}	intake	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O

III.5.3.4 Acute versus chronic consumer exposure

Consumer exposure may be acute or chronic. Because consumer products are used lifelong, the lifetime average exposure is well approximated by using the annual average exposure, averaging out seasonal usage differences. With regard to acute exposures, the equations used for consumer exposure model exposures as resulting from a constant concentration, thereby setting mean and maximum event concentrations equal. Therefore, acute exposure is characterized by the inhalatory, dermal, and oral concentrations, C_{inh}, C_{der}, and C_{oral} respectively, which are given in the model descriptions. For chronic exposures, the intake and potential uptake rates I_{inh}, $U_{der,pot}$ and I_{oral} represent annual average measures of exposure. Where chronic exposure is measured with reference to concentration, the annual average exposure concentrations are to be used:

$$C_{route,ann} = \frac{\int_0^{365} C_{route}(t)\,dt}{365} \qquad route \in \{inh, der, oral\} \qquad (223)$$

where C_{route} represents the exposure concentration via the inhalatory, dermal or oral route. Both the acute and the chronic characterisation of exposure are given. The former is compared to the LD50, the latter to the chronic NOAEL. Because the equations model exposure with reference to constant concentration, the equation can be written as:

$$C_{route,ann} = C_{route} \cdot n \cdot T_{contact} \qquad route \in \{inh, der, oral\} \qquad (224)$$

Input			
C_{route}	exposure concentration through route *route*	[$kg_c.m^{-3}$]	O
$T_{contact}$	event duration	[d]	S
n	mean number of events per day	[d^{-1}]	S
Output			
$C_{inh,ann}$	annual average inhalation exposure concentration	[$kg_c.m^{-3}$]	O
$C_{der,ann}$	annual average dermal exposure concentration	[$kg_c.m^{-3}$]	O
$C_{oral,ann}$	annual average oral exposure concentration	[$kg_c.m^{-3}$]	O

Both the acute and the chronic characterisations are given per route. The acute concentrations are compared to the appropriate acute toxicity value, the chronic intakes or concentrations to the appropriate N(L)OAEL.

III.5.3.5 Total consumer exposure

If a consumer is exposed to a substance in a particular consumer product via different routes, the contribution of each route to the total uptake can be summed. The summation is done for each time scale separately (acute and -sub-chronic).

Differences in bioavailability for the various routes are accounted for by multiplying the intakes (or potential uptakes) with absolute absorption factors.

$$U_{tot} = I_{inh} \cdot BIO_{inh,2} + U_{der,pot} \cdot BIO_{der,2} + I_{oral} \cdot BIO_{oral,2} \quad \textbf{(225)}$$

Input			
I_{inh}	inhalatory intake of substance	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$U_{der,pot}$	potential uptake	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
I_{oral}	intake	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$BIO_{oral,2}$	bioavailability for oral intake (end route)	[-]	D
$BIO_{inh,2}$	bioavailability for inhalation (end route)	[-]	D
$BIO_{der,2}$	bioavailability for dermal uptake (end route)	[-]	D
Output			
U_{tot}	total uptake for one product via different routes	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O

III.5.3.6 ConsExpo

ConsExpo 3.0 (Van Veen, 2001) can be started (or circumvented) from EUSES. When started the selected output of Consexpo is exported to EUSES and used in the further calculation

General input data

With the ConsExpo implements several exposure models for the *inhalatory*, *dermal* and *oral* routes of exposure resp. For all these scenarios the contact of the exposed person with the substance and the physico-chemical properties of the substance have to be defined:

Input: contact	
use frequency	[$year^{-1}$]
use duration	[min]
total duration	[min]
Input: chemical	
molecular weight	[$g.mol^{-1}$]
octanol/water partition coefficient	[number]
vapour pressure	[Pa]
water solubility	[$g.liter^{-1}$]

ConsExpo: inhalatory models

ConsExpo implements the EUSES inhalatory model as the “constant concentration”-scenario. In addition ConsExpo implements five more advanced inhalatory scenarios.

- source-ventilation : a substance is released into the (ventilated) room air with a constant release rate.
- evaporation from pure substance: a substance is released from a open can filled with the (liquid) substance in it’s pure form by evaporation.
- evaporation from mixture: a substance is released by evaporation from a open can filled with a liquid mixture of which the substance is an ingredient.
- painting: a viscous product such as paint is being applied to a surface with a certain application area. The substance, which is part of the paint, diffuses to the surface of the applied product and evaporates.
- spray: PM

Input: source and ventilation	
generation (/release) rate of the substance	[$kg_c.s^{-1}$]
break down rate of the substance	[s^{-1}]

room volume	[m^3]
ventilation rate	[h^{-1}]
ambient air concentration	[$kg_c.m^{-3}$]
Input: evaporation from pure substance model	
release area	[m^2]
temperature	[^oC]
room volume	[m^3]
ventilation rate	[$m^3.h^{-1}$]
Input: evaporation from mixture model	
release area	[m^2]
temperature	[^oC]
room volume	[m^3]
ventilation rate	[h^{-1}]
molecular weight matrix product	[$kg.mol^{-1}$]
weight fraction of the substance in the product	[fraction]

Input: painting model	
release area	[m^2]
product amount	[g]
weight fraction of the substance in the product	[fraction]
density product	[$kg.m^{-3}$]
layer exchange rate	[min^{-1}]
fraction upper layer	[fraction]
room volume	[m^3]
ventilation rate	[h^{-1}]
temperature	[^oC]
molecular weight matrix product	[$kg.mol^{-1}$]

Input: spray model
PM <currently being revised>

ConsExpo offers three uptake models to calculate the internal dose for the inhalatory route:

- Fraction model: a (user-)specified fraction of the exposure enters the body
- Diffusion model:
- Flow model

Input: fraction model	
inhalation rate	[m3.min-1]
absorbed fraction	[fraction] (should be 1 to calculate potential dose)
respirable fraction	[fraction]
Input: diffusion model	
air/blood partition coefficient	[ratio]
blood flow	[$cm^3.min^{-1}$]
volume lung blood	[cm^3]
lung wall permeability	[$cm.min^{-1}$]
lung volume	[liter]
dead space	[fraction]
inhalation rate	[$liter.min^{-1}$]
respirable fraction	[fraction]
Input: flow model	
air/blood partition coefficient	[fraction]
blood flow	[$cm^3.s^{-1}$]
inhalation rate	[$liter.min^{-1}$]
respirable fraction	[fraction]

ConsExpo: dermal models

In addition to the EUSES dermal a and dermal b models (termed "fixed volume" and "contact rate" model resp.) ConsExpo implements three more detailed dermal scenarios.

- Migration to skin
- Product diffusion
- Transfer coefficient

Input: migration to skin model

fraction of chemical that is leachable	[kg/kg]
product amount	[kg]
fraction of the product that is in direct contact with the skin	[fraction]

Input: product diffusion model

concentration compound	[$g.cm^{-3}$]
diffusion coefficient of the substance in product	[$m^2.min^{-1}$]
evaporation rate of the substance from the product	[$cm.min^{-1}$]
thickness product	[cm]

Input: transfer coefficient model

transfer coefficient (area rubbed per unit time)	[$cm^2.min^{-1}$]
dislodgeable amount	[$g.\ cm^{-2}$]
weight fraction of the substance	[fraction]
half life chemical	[min]
contaminated surface	[m^2]

ConsExpo offers three uptake models to calculate the internal dose for the dermal route:

- Fraction model
- Diffusion model
- SKINPERM model

Input: fraction model

absorped fraction	[fraction] (should be 1 to calculate potential dose)

ConsExpo: oral models

In addition to the EUSES oral a and oral b models (termed "single ingestion" and "article-food migration" model resp.) ConsExpo implements three specific oral scenarios:

- Hand-mouth conact scenario
- Product leaching scenario
- Non-respirable fraction scenario

Input: hand-mouth contact model

concentration of compound in the product on the hands	[$g.cm^{-3}$]
intake rate of the product	[$cm^3.min^{-1}$]

Input: product leaching model

concentration compound	[$g.cm^{-3}$]
product volume	[cm^3]
leach rate	[$g.cm^{-2}.min^{-1}$]
area in contact with the mouth	[cm^2]

Input: non-respirable fraction model

non-respirable fraction	[fraction]
inhalation rate	[$liter.min^{-1}$]

In addition to this fraction, a concentration of the substance in air has to be calculated using

one of the inhalatory scenarios.

ConsExpo offers two uptake models to calculate the internal dose for the oral route:
- Fraction model
- Diffusion model

Input: fraction model
absorped fraction [fraction] (should be 1 to calculate potential dose)

ConsExpo output

Existing EUSES output parameter	ConsExpo output	Unit Consexpo	Unit EUSES
Per route			
C_{inh} I_{inh} (if fraction is set to 1 in CONSEXPO)	• Inhalatory exposure as the mean event air concentration of the substance • Inhalatory uptake as the total amount of substance taken up yearly by inhalation (in 'uptake-model' fraction = 1)	$[mg.m^{-3}]$ $[mg.kg_{bw}^{-1}.d^{-1}]$	$[kg_c.m^{-3}]$ $[kg_c.kg_{bw}^{-1}.d^{-1}]$
C_{der} $U_{der,pot}$ (if fraction is set to 1 in CONSEXPO)	• Dermal exposure as the concentration of substance in contact withe skin • Dermal uptake as total amount of substance taken up yearly through the skin (in 'uptake-model' fraction = 1)	$[mg.cm^{-3}]$ $[mg.\ kg_{bw}^{-1}.d^{-1}]$	$[kg_c.m^{-3}]$ $[kg_c.kg_{bw}^{-1}.d^{-1}]$
C_{oral} I_{oral} (if fraction is set to 1 in CONSEXPO)	• Oral exposure as the concentration of substance that is swallowed • Oral exposure as the total amount of substance taken up yearly (in 'uptake-model' fraction = 1)	$[mg.cm^{-3}]$ $[mg.\ kg_{bw}^{-1}.d^{-1}]$	$[kg_c.m^{-3}]$ $[kg_c.kg_{bw}^{-1}.d^{-1}]$

III.5.4 Workplace exposure

(Sub)chronic exposure of workers is estimated by means of the model EASE, implemented in EUSES. In addition acute exposure values can be entered by the user. Different scenarios can be assessed for the inhalatory and dermal route and for each scenario a total exposure is calculated. The user needs to provide answers on the questions presented by this model (see decision trees in Appendix IV). Based on the answers, exposure ranges are estimated for inhalatory exposure to vapours, fibers and dust and for dermal exposure. EASE also produces a log file showing a summary of the choices made.

Input		
-	specific questions on exposure (see decision trees in Appendix IV)	
$C_{inh,worker,acute}$	acute inhalation exposure of workers	[kg.m^{-3}]
$W_{der,worker,acute}$	acute dermal weight of substance on skin of workers	[kg.m^{-1}.d^{-1}]
$U_{der,pot,worker,acute}$	acute potential dermal uptake for workers	[kg.kg$_{bw}^{-1}$.d^{-1}]
Intermediate results		
$W_{der,worker}$	dermal weight of substance on skin of workers	[kg.m^{-2}.d^{-1}]
Output		
$C_{inh,worker,vapour}$	vapour concentration in air for workers	[kg$_c$.m^{-3}]
$C_{inh,worker,fibre}$	fibre concentration in air for workers	[fibers.m^{-3}]
$C_{inh,worker,dust}$	dust concentration in air for workers	[kg.m^{-3}]
$U_{der,pot,worker}$	potential dermal uptake for workers	[kg.kg$_{bw}^{-1}$.d^{-1}]
-	log file of EASE	

III.5.4.1 Inhalatory worker exposure

Input			
-	specific questions on exposure (see decision trees in Appendix IV)		S
$C_{inh,worker,acute}$	acute inhalation exposure of workers	[kg.m^{-3}]	S
Output			
$C1_{inh,worker,vapour}$	vapour concentration in air for workers (in ppm)	[ppm]	O
$C_{inh,worker,fibre}$	fibre concentration in air for workers	[fibers.m^{-3}]	O
$C_{inh,worker,dust}$	dust concentration in air for workers	[kg.m^{-3}]	O
-	log file of EASE		

Table III-92 Default for workplace exposure.

Parameter	Symbol	Unit	Value
average temperature at the workplace	TEMPwork	[K]	293
thickness of product layer on skin	$TH_{der,worker}$	[m]	1.10^{-4}
body weight	BW	[kg]	70[a]
respirable fraction of inhaled substance	F_{resp}	[-]	1[a]
ventilation rate of worker	$IH_{air,worker}$	[m^3.d^{-1}]	10[b]

[a] Already defined in section on human indirect exposure.
[b] Also used in the section on human effect assessment.

The output of EASE for inhalation exposure of workers to vapour is a range with the unit parts per million (ppm). This formula corrects for the average temperature at the workplace during working hours and applies at a standard pressure of 101.3 kPa. The default temperature is assumed to be 293 K.

$$C_{inh,worker,vapour} = \frac{273}{TEMPwork} \cdot MOLW \cdot 10^{-6} \cdot C1_{inh,worker,vapour} \cdot \frac{1000}{22.4} \quad \textbf{(226)}$$

Input			
TEMPwork	average temperature on the workplace	[K]	D
MOLW	molecular weight	[$kg_c.mol^{-1}$]	S
$C1_{inh,worker,vapour}$	vapour concentration in air for workers (in ppm)	[ppm]	O
Output			
$C_{inh,worker,vapour}$	vapour concentration in air for workers	[$kg.m^{-3}$]	O

III.5.4.2 Dermal worker exposure

Input			
-	specific questions on exposure (see decision trees in Appendix IV)		S
$W_{der,worker,acute}$	acute dermal weight of substance on skin of workers	[$kg.m^{-1}.d^{-1}$]	S
$U_{der,pot,worker,acute}$	acute potential dermal uptake for workers	[$kg.kg_{bw}^{-1}.d^{-1}$]	S
Output			
$W_{der,worker}$	dermal weight of substance on skin of workers	[$kg.m^{-2}.d^{-1}$]	O
-	log file of EASE		O

Dermal exposure of workers can be estimated as an external weight (kg_c) per unit skin surface area (m^2) per unit of time (d). For the risk characterisation this exposure has to be recalculated to a potential uptake per kg body weight per day:

$$U_{der,worker,pot,acute} = W_{der,worker,acute} \cdot \frac{AREA_{der,worker}}{BW} \quad \textbf{(227)}$$

$$U_{der,worker,pot} = W_{der,worker} \cdot \frac{AREA_{der,worker}}{BW} \quad \textbf{(228)}$$

Input			
$AREA_{der,worker}$	area of contact between substance and skin	[m^2]	D
BW	body weight	[kg]	D
$W_{der,worker,acute}$	acute dermal weight of substance on skin of workers	[$kg.m^{-1}.d^{-1}$]	S
$W_{der,worker}$	dermal weight of substance on skin of workers	[$kg.m^{-2}.d^{-1}$]	O
Output			
$U_{der,pot,worker,acute}$	acute potential dermal uptake for workers	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$U_{der,pot,worker}$	potential dermal uptake for workers	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O

III.5.4.3 Total worker exposure

If a worker is exposed to a substance via different routes, the contribution of each route to the total uptake can be summed. The summation is done for each time scale separately (acute and – sub-chronic).

Differences in bioavailability for the inhalatory and dermal routes are accounted for by multiplying the intakes (or potential uptakes) with absolute absorption factors.

The vapour exposure concentrations for workers are recalculated to intakes:

$$I_{inh,wor\,ker,acute} = \frac{F_{resp} \cdot C_{inh,wor\,ker,acute} \cdot IH_{air,wor\,ker} \cdot T_{contact,wor\,ker}}{BW} \cdot n \qquad \textbf{(229)}$$

$$I_{inh,wor\,ker,vapour} = \frac{F_{resp} \cdot C_{inh,wor\,ker,vapour} \cdot IH_{air,wor\,ker} \cdot T_{contact,wor\,ker}}{BW} \cdot n \qquad \textbf{(230)}$$

Input

F_{resp}	respirable fraction of inhaled substance	[-]	D
$IH_{air,worker}$	ventilation rate of worker	[$m^3.d^{-1}$]	D
$T_{contact,worker}$	duration of contact with skin of worker per event	[d]	S
BW	body weight	[kg]	D
n	mean number of events per day	[d^{-1}]	S
$C_{inh,worker,acute}$	acute inhalation exposure of workers	[$kg.m^{-3}$]	S
$C_{inh,worker,vapour}$	vapour concentration in air for workers	[$kg.m^{-3}$]	O

Output

$I_{inh,worker,acute}$	acute inhalatory intake of substance for worker	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$I_{inh,worker,\,vapour}$	inhalatory intake of substance for worker	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O

$$U_{tot-v/d,wor\,ker} = I_{inh,wor\,ker,vapour} \cdot BIO_{inh} + U_{der,pot,wor\,ker} \cdot BIO_{der} \qquad \textbf{(231)}$$

$$U_{tot,wor\,ker,acute} = I_{inh,wor\,ker,acute} \cdot BIO_{inh} + U_{der,pot,wor\,ker,acute} \cdot BIO_{der} \qquad \textbf{(232)}$$

Input

$I_{inh,worker,acute}$	acute inhalatory intake of substance for worker	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$I_{inh,worker,\ vapour}$	inhalatory intake of substance for worker	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
BIO_{inh}	bioavailability for inhalation	[-]	D
BIO_{der}	bioavailability for dermal uptake	[-]	D
$U_{der,pot,worker,acute}$	acute potential dermal uptake for workers	$[kg.kg_{bw}^{-1}.d^{-1}]$	O
$U_{der,pot,worker}$	potential dermal uptake for workers	$[kg.kg_{bw}^{-1}.d^{-1}]$	O

Output

$U_{tot,worker,acute}$	total uptake for one scenario via different routes, for acute effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$U_{tot\text{-}v/d,worker}$	total uptake (vapour + dermal) for one scenario via different routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

III.6 EFFECTS ASSESSMENT

III.6.1 Effects assessment for the environment

For the environmental end-points, Predicted No-Effect Concentrations (PNECs) are assessed. For the extrapolation from single-species toxicity tests to the population or ecosystem level, assessment factors are used. A statistical method may be used to support the assessment.

Input: micro-organism effects data			
$EC50_{micro}$	EC50 for STP micro-organisms	$[kg_c.m^{-3}]$	
$EC10_{micro}$	EC10 for STP micro-organisms	$[kg_c.m^{-3}]$	
$NOEC_{micro}$	NOEC for STP micro-organisms	$[kg_c.m^{-3}]$	
Input: aquatic effects data			
$LC50aqua_i$	LC50 for aquatic organisms, trophic level *i*	$[kg_c.m^{-3}]$	
$NOECaqua_i$	NOEC for aquatic organisms, trophic level *i*	$[kg_c.m^{-3}]$	
$LC50aqua_{i,marine}$	LC50 for marine aquatic organisms, trophic level *i*	$[kg_c.m^{-3}]$	
$NOECaqua_{i,marine}$	NOEC for marine aquatic organisms, trophic level *i*	$[kg_c.m^{-3}]$	
Input: terrestrial effects data			
$LC50terr_i$	LC50 for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$	
$NOECterr_i$	NOEC for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$	
$K_{soil\text{-}water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{sed\text{-}water}$	sediment-water partition coefficient	$[m^3.m^{-3}]$	c
RHO_{soil}	bulk density of soil	$[kg_{wwt}.m^{-3}]$	c
Input: bird / mammalian effects data			
$LC50_{bird}$	LC50 in avian dietary study (5 days)	$[kg_c.kg_{food}^{-1}]$	
$NOEC_{bird}$	NOEC for birds	$[kg_c.kg_{food}^{-1}]$	
$NOEC_{mammal,food,chr}$	NOEC for mammals	$[kg_c.kg_{food}^{-1}]$	
$NOAEL_{bird}$	NOAEL for birds	$[kg_c.kg_{bw}.d^{-1}]$	
$NOAEL_{mammal,oral,chr}$	NOAEL for mammals	$[kg_c.kg_{bw}.d^{-1}]$	
T_{bird}	duration of (sub-)chronic test with birds	[d]	
T_{mammal}	duration of (sub-)chronic test with mammals	[d]	
$CONV_{bird}$	conversion factor for NOAEL to NOEC	$[kg_{bw}.d.kg_{food}^{-1}]$	
$CONV_{mammal}$	conversion factor for NOAEL to NOEC	$[kg_{bw}.d.kg_{food}^{-1}]$	

Intermediate results 1			
TOXaqua	toxicological data used for extrapolation of PNEC	[$kg_c.m^{-3}$]	
AFaqua	assessment factor applied in extrapolation of aquatic PNEC	[-]	
$AFaqua_{marine}$	assessment factor applied in extrapolation of marine PNEC	[-]	
TOXmicro	toxicological data used for extrapolation of PNEC	[$kg_c.m^{-3}$]	
AFmicro	assessment factor applied in extrapolation of PNEC	[-]	
TOXoral	toxicological data used for extrapolation of PNEC	[$kg_c.kg_{food}^{-1}$]	
AForal	assessment factor applied in extrapolation of PNEC	[-]	
Intermediate results 2			
TOXterr	toxicological data used for extrapolation of PNEC	[$kg_c.kg_{wwt}^{-1}$]	
AFterr	assessment factor applied in extrapolation of PNEC	[-]	
EPterr	equilibrium partitioning used for PNEC in soil?	[yes/no]	c
EPsed	equilibrium partitioning used for PNEC in sediment?	[yes/no]	c
Output 1			
$PNEC_{water}$	PNEC for aquatic organisms	[$kg_c.m^{-3}$]	c
$PNEC_{water,marine}$	PNEC for marine aquatic organisms	[$kg_c.m^{-3}$]	c
$PNEC_{micro\text{-}organisms}$	PNEC for STP micro-organisms	[$kg_c.m^{-3}$]	c
$PNEC_{oral}$	PNEC for secondary poisoning of birds and mammals	[$kg_c.kg_{food}^{-1}$]	c
$PNECstat_{water}$	PNEC for aquatic organisms with statistical method	[$kg_c.m^{-3}$]	c
$PNECstat_{water,\ marine}$	PNEC for marine aquatic organisms with statistical method	[$kg_c.m^{-3}$]	c
$PNECstat_{soil}$	PNEC for terrestrial organisms with statistical method	[$kg_c.m^{-3}$]	c
Output 2			
$PNEC_{soil}$	PNEC for terrestrial organisms	[$kg_c.kg_{wwt}^{-1}$]	c
$PNEC_{sed}$	PNEC for sediment-dwelling organisms	[$kg_c.kg_{wwt}^{-1}$]	

Table III-93 Default environmental characteristics soil and sediment in all scales

Sediment			
Weight fraction of organic carbon soil solids	Foc_{soil}	[$kg_{oc}.kg_{solid}$-1]	0.02
Weight fraction of organic matter soil solids	Fom_{soil}	[$kg_{om}.kg_{solid}$-1]	0.02
Weight fraction of organic carbon in fresh water and marine sediment	Foc_{sed}	[$kg_{oc}.kg_{solid}$-1]	0.05
Weight fraction of organic matter in fresh water and marine sediment	Fom_{sed}	[$kg_{om}.kg_{solid}$-1]	0.05

III.6.1.1 Aquatic compartment (freshwater and marine environment)

Depending on the available toxicity data for aquatic organisms, assessment factors are selected for extrapolating single-species toxicity tests to a PNEC for the water compartment. If intermittent release is identified for a stage of the life cycle, only short-term effects need to be considered for risk characterisation of that stage (only for the aquatic compartment). The following trophic levels are distinguished for the freshwater and marine environment:

- algae (primary producers);
- crustaceans / *Daphnia* (primary consumers);
- fish (secondary consumers);
- other species (e.g. decomposers).

$$LC50\,aqua_{min} = \min\left(LC50\,aqua_i\right) \quad \textbf{(233)}$$

$$NOECaqua_{min} = \min\left(NOECaqua_i\right) \quad \textbf{(234)}$$

Table III-94 *Assessment factors for deriving the $PNEC_{water}$ for freshwater.*

Available data	**Additional criteria**	**TOXaqua**	**AFaqua**
3 LC50s		$LC50aqua_{min}$	1000
3 LC50s (independent of avail. NOECs)	If intermittent release is identified for a stage of the life cycle	$LC50aqua_{min}$	100
1 NOEC additional (not algae!)	**Same taxonomic group as $LC50aqua_{min}$?** yes no $LC50aqua_{min}/1000 < NOECaqua_{min}/100$ no $LC50aqua_{min}/1000 \geq NOECaqua_{min}/100$	 $NOECaqua_{min}$ $LC50aqua_{min}$ $NOECaqua_{min}$	 100 1000 100
2 NOEC additional	**Same taxonomic group as $LC50aqua_{min}$?** yes no $LC50aqua_{min} < NOECaqua_{min}$ no $LC50aqua_{min} \geq NOECaqua_{min}$	 $NOECaqua_{min}$ $LC50aqua_{min}$ $NOECaqua_{min}$	 50 100 100
3 NOEC algae, *Daphnia* and fish		$NOECaqua_{min}$	10
3 NOEC *not* algae, *Daphnia* and fish	**Same taxonomic group as $LC50aqua_{min}$?** yes No	 $NOECaqua_{min}$ $NOECaqua_{min}$	 10 50
Species Sensitivity Distribution	At least 10 NOECs for species covering at least 8 taxonomic groups	See section III.6.1.6	

The greater diversity of taxa in the marine environment, compared to freshwaters, will produce a broader distribution of species sensitivity. In those cases where only data for freshwater or saltwater algae, crustaceans and fish are available a higher assessment factor should be applied than that for the derivation of $PNEC_{water}$ for freshwaters. This higher assessment factor reflects the greater uncertainty in the extrapolation. Where data is available for additional marine taxonomic groups, for example rotifers, echinoderms or molluscs the uncertainties in the extrapolation are reduced and the magnitude of the assessment factor applied to a data set can be lowered.

Table III-95 Assessment factors for deriving the $PNEC_{water}$ for the marine environment.

Available data	Additional criteria	TOXaqua	AFaqua marine
3 LC50s (algae, *Daphnia* or crustaceans, and fish)		$LC50aqua_{min}$	10000 [a]
3 LC50s (algae, *Daphnia* or crustaceans, and fish) and additional 2 LC50s marine (e.g. echinoderms, molluscs)		$LC50aqua_{min}$	1000
1 NOEC additional (not algae!)	**Same taxonomic group as $LC50aqua_{min}$, based on 3 LC50s?** Yes no $LC50aqua_{min}/10000 < NOECaqua_{min}/1000$ no $LC50aqua_{min}/10000 \geq NOECaqua_{min}/1000$	 $NOECaqua_{min}$ $LC50aqua_{min}$ $NOECaqua_{min}$	 1000 10000 1000
2 NOEC additional	**Same taxonomic group as $LC50aqua_{min}$, based on 3 LC50s?** yes and 2 LC50 marine available [b] yes and 1 LC50s marine available [b] yes and most sensitive species examined [c] yes no $LC50aqua_{min} < NOECaqua_{min}$ no $LC50aqua_{min} \geq NOECaqua_{min}$	 $NOECaqua_{min}$ $NOECaqua_{min}$ $NOECaqua_{min}$ $NOECaqua_{min}$ $LC50aqua_{min}$ $NOECaqua_{min}$	 50 100 100 500 1000 1000
3 NOEC algae, *Daphnia* or crustaceans, and fish	**Same taxonomic group as $LC50aqua_{min}$, based on 3 LC50s?** Yes no $LC50aqua_{min} \geq NOECaqua_{min}$ no $LC50aqua_{min} < NOECaqua_{min}$	 $NOECaqua_{min}$ $NOECaqua_{min}$ $LC50aqua_{min}$	 100 [d] 500 1000
2 NOEC (algae, *Daphnia* or fish) and additional 1 NOEC marine (e.g. echinoderms, molluscs)		$NOECaqua_{min}$	50
3 NOEC (algae, *Daphnia* or fish) and additional 2 NOEC marine (e.g. echinoderms, molluscs)		$NOECaqua_{min}$	10
Species Sensitivity Distribution	At least 10 NOECs for species covering at least 8 taxonomic groups	See section III.6.1.6	

[a] In specific cases this factor can be varied (see TGD). Under no circumstances the AF should be lower than 1000 except if intermittent release is identified for a stage of the life cycle;

[b] A reduced assessment factor of 100 and 50 may be appropriate, when one or two short-term test on marine species *of additional taxonomic groups* (e.g. echinoderms, molluscs) are available, respectively. The short-term marine tests must indicate that they are not from the most sensitive group and it must been determined with a high probability that long-term NOECs generated for these groups would not be lower than already obtained

c It may sometimes be possible to determine with a high probability that, from the two available NOECs, the most sensitive species covering fish, crustacea and algae has been examined. So, a further longer-term NOEC from a third taxonomic group would not be lower than the data already available;
Under specific circumstances this factor may be reduced to a minimum of 10 (see TGD).

$$PNEC_{water} = \frac{TOXaqua}{AFaqua} \quad (235)$$

$$PNEC_{water,marine} = \frac{TOXaqua}{AFaqua_{marine}} \quad (236)$$

Input			
$LC50aqua_i$	LC50 for aquatic organisms, trophic level *i*	[$kg_c.m^{-3}$]	S
$NOECaqua_i$	NOEC for aquatic organisms, trophic level *i*	[$kg_c.m^{-3}$]	S
$LC50aqua_{i,marine}$	LC50 for marine aquatic organisms, trophic level *i*	[$kg_c.m^{-3}$]	S
$NOECaqua_{i,marine}$	NOEC for marine aquatic organisms, trophic level *i*	[$kg_c.m^{-3}$]	S
Output			
$LC50aqua_{min}$	lowest LC50 for aquatic organisms	[$kg_c.m^{-3}$]	O
$NOECaqua_{min}$	lowest NOEC for aquatic organisms	[$kg_c.m^{-3}$]	O
TOXaqua	toxicological data used for extrapolation of PNEC	[$kg_c.m^{-3}$]	O
AFaqua	assessment factor applied in extrapolation of aquatic PNEC	[-]	O
$AFaqua_{marine}$	assessment factor applied in extrapolation of marine PNEC	[-]	O
$PNEC_{water}$	PNEC for aquatic organisms	[$kg_c.m^{-3}$]	O^c
$PNEC_{water,marine}$	PNEC for marine aquatic organisms	[$kg_c.m^{-3}$]	O^c

III.6.1.2 Terrestrial compartment

For most chemicals, the number of toxicity data on soil organisms will be limited. At base-set level, there is no requirement for toxicity tests with soil organisms, except for some Product Types in the Biocides Directive. When no toxicity data are available, equilibrium partitioning will be applied. It should be noted that in case of intermittent release, the equilibrium partitioning method must depart from the PNEC based on chronic effects and not the PNEC derived from LC50s.

If only one test result for soil organisms is available, the lowest of the PNECs resulting from the equilibrium partitioning and assessment factor approach is used. Depending on the toxicity data available for terrestrial organisms, assessment factors are selected for extrapolating single-species toxicity tests to a PNEC for the soil compartment. The following trophic levels are distinguished:

- plants (primary producers);
- earthworms (consumers);
- micro-organisms (decomposers);
- others.

Natural soils used in ecotoxicological tests differ in characteristics such as organic matter and clay content, soil pH and soil moisture content. The bioavailability of the test compound, and therefore the toxicity observed, is influenced by these soil properties. This means that results from different test soils cannot be compared directly. If possible data should be normalised using relationships that describes the bioavailability of chemicals in soils. Results are converted to a standard soil, which is defined as a soil with an organic matter content of 3.4% or an organic carbon content of 2.0% (see section III.4.1).

$$Foc_{soil} = Fom_{soil} / 1.7 \quad \textbf{(237)}$$

$$LC50terr_{standard,i} = LC50terr_i \cdot \frac{Foc_{soil}}{Foc_{soil,exp}} \quad \textbf{(238)}$$

$$NOECterr_{standard,i} = NOECterr_i \cdot \frac{Foc_{soil}}{Foc_{soil,exp}} \quad \textbf{(239)}$$

$$LC50\,terr_{min} = \min\left(LC50\,terr_{standard,i} \right) \quad \textbf{(240)}$$

$$NOECterr_{min} = \min\left(NOECterr_{standard,i} \right) \quad \textbf{(241)}$$

$$PNEC_{soil,ep} = \frac{K_{soil\text{-}water}}{RHO_{soil}} \cdot PNEC_{water} \quad \textbf{(242)}$$

Table III-96 Assessment factors for deriving the $PNEC_{soil}$ for the terrestrial environment.

Available ecotox. data	**Additional criteria**	**TOXterr**	**AFterr**
none		$PNEC_{soil,ep}$	1
1 LC50	$PNEC_{soil,ep} < LC50terr_{min}/1000$ $PNEC_{soil,ep} \geq LC50terr_{min}/1000$	$PNEC_{soil,ep}$ $LC50terr_{min}$	1 1000
>1 LC50		$LC50terr_{min}$	1000
1 NOEC no LC50s	$PNEC_{soil,ep} < NOECterr_{min}/100$ $PNEC_{soil,ep} \geq NOECterr_{min}/100$	$PNEC_{soil,ep}$ $NOECterr_{min}$	1 100
1 NOEC and >0 LC50s	$LC50terr_{min}/1000 < NOECterr_{min}/100$ $LC50terr_{min}/1000 \geq NOECterr_{min}/100$	$LC50terr_{min}$ $NOECterr_{min}$	1000 100
2 NOEC	**NOEC's of two taxonomic groups?** Yes No	 $NOECterr_{min}$ $NOECterr_{min}$	 50 100
3 NOEC	**NOEC's of three taxonomic groups?** Yes No	 $NOECterr_{min}$ $NOECterr_{min}$	 10 50
Species Sensitivity Distribution	At least 10 NOECs for species covering at least 8 taxonomic groups	See section III.6.1.6	

$$PNEC_{soil} = \frac{TOXterr}{AFterr} \qquad (243)$$

If $TOXterr = PNEC_{soil,ep}$ then *EPterr* = 'yes'

Input

Foc_{soil}	weight fraction of organic carbon in soil	$[kg.kg^{-1}]$	D
Fom_{soil}	weight fraction of organic matter in soil	$[kg.kg^{-1}]$	D/O
$Foc_{soil,exp}$	weight fraction of organic carbon in tested soil	$[kg.kg^{-1}]$	S
$LC50terr_i$	LC50 for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$	S
$NOECterr_i$	NOEC for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$	S
$LC50terr_{standard,i}$	Standardised LC50 for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$	S/O
$NOECterr_{standard,i}$	Standardised NOEC for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$	S/O
$PNEC_{water}$	PNEC for aquatic organisms	$[kg_c.m^{-3}]$	O[c]
$K_{soil-water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	O[c]
RHO_{soil}	bulk density of soil	$[kg_{wwt}.m^{-3}]$	O[c]
$PNEC_{soil,ep}$	PNEC for terrestrial organisms derived by eq. part.	$[kg_c.kg_{wwt}^{-1}]$	O[c]

Output

TOXterr	toxicological data used for extrapolation of PNEC	$[kg_c.kg_{wwt}^{-1}]$	O
AFterr	assessment factor applied in extrapolation of PNEC	[-]	O
EPterr	equilibrium partitioning used for PNEC?	[yes/no]	O[c]
$PNEC_{soil}$	PNEC for terrestrial organisms	$[kg_c.kg_{wwt}^{-1}]$	O[c]

III.6.1.3 Sediment compartment (freshwater and marine environment)

For most chemicals the number of toxicity data on sediment-dwelling organisms will be limited. For the initial risk assessment, normally no effect data from tests with sediment-dwelling organisms will be available. Therefore, the equilibrium-partitioning approach is implemented in EUSES. It should be noted that in case of intermittent release, the equilibrium partitioning method must depart from the PNEC based on chronic effects and not the PNEC derived from LC50s.

If one or more acute toxicity tests for sediment-dwelling organisms is/are available, the lowest of the PNECs resulting from the equilibrium partitioning and assessment factor approach is used. Depending on the toxicity data available for sediment-dwelling organisms, assessment factors are selected for extrapolating single-species toxicity tests to a PNEC for the sediment compartment.

In contrast with the other PNECs, the PNEC for sediment is an open parameter to allow for expert estimation from available data outside EUSES.

$$LC50sed_{min} = \min\left(LC50sed_i \right) \quad \textbf{(244)}$$

$$NOECsed_{min} \ or \ EC10sed_{min} = \min\left(NOECsed_i \ or \ EC10sed_i \right) \quad \textbf{(245)}$$

$$PNEC_{sed,ep} = \frac{K_{susp\text{-}water}}{RHO_{susp}} \cdot PNEC_{water} \quad \textbf{(246)}$$

Table III-97 *Assessment factors for deriving the $PNEC_{sediment}$ for freshwater environment.*

Available ecotox. Data	**Additional criteria**	**TOXterr**	**AFterr**
None		$PNEC_{sed,ep}$	1
≥1 LC50	$PNEC_{sed,ep} < LC50sed_{min}/10000$ $PNEC_{sed,ep} \geq LC50sed_{min}/10000$	$PNEC_{sed,ep}$ $LC50sed_{min}$	1 1000
1 NOEC/EC10		$NOECsed_{min}$/ $EC10sed_{min}$	100
2 NOEC/EC10	With species representing different living and feeding conditions	$NOECsed_{min}$/ $EC10sed_{min}$	50
3 NOEC/EC10	With species representing different living and feeding conditions	$NOECsed_{min}$/ $EC10sed_{min}$	10

For the marine effect assessment of sediment-dwelling organisms attention should be paid to the fact that very often contaminants are not analysed in whole sediment but in a certain fraction of the sediment, for example in the sediment fraction of particles < 63 μm. The organic carbon content of this fraction is typically 15-30% for marine sediment while for whole marine sediments it is generally less than 2%. It is important, for reasons of comparability of PEC and PNEC values, that the organic carbon content of sediment used for toxicity tests are comparable with those of actual marine sediments. Results for marine and freshwater sediments should be converted to a standard sediment, which is defined as a sediment with an organic matter content of 8.5% or an organic carbon content of 5.0% (see section III.4.1).

$$LC50sed_{standard,i} = LC50sed_i \cdot \frac{Foc_{sed}}{Foc_{sed,exp}} \quad \textbf{(247)}$$

$$NOECsed_{standard,i} = NOECsed_i \cdot \frac{Foc_{sed}}{Foc_{sed,exp}} \quad \textbf{(248)}$$

$$PNEC_{sed,marine,ep} = \frac{K_{susp-water}}{RHO_{susp}} \cdot PNEC_{water,marine} \quad \textbf{(249)}$$

Table III-98 Assessment factors for deriving the $PNEC_{sediment}$ for marine environment.

Available ecotox. Data	**Additional criteria**	**TOXterr**	**AFterr**[a]
None		$PNEC_{sed,marine,ep}$	1
1 LC50 (marine or freshwater organism)	$PNEC_{sed,marine,ep} < LC50sed_{min}/1000$ $PNEC_{sed,marine,ep} \geq LC50sed_{min}/10000$	$PNEC_{sed,marine,ep}$ $LC50sed_{min}$	1 10000
2 LC50 (incl. one marine organism of sensitive taxa)	$PNEC_{sed,marine,ep} < LC50sed_{min}/1000$ $PNEC_{sed,marine,ep} \geq LC50sed_{min}/1000$	$PNEC_{sed,marine,ep}$ $LC50sed_{min}$	1 1000
1 NOEC/EC10		$NOECsed_{min}$/ $EC10sed_{min}$	1000
2 NOEC/EC10	With species representing different living and feeding conditions	$NOECsed_{min}$/ $EC10sed_{min}$	500
1 NOEC/EC10 and additional 1 NOEC/EC10 marine	With species representing different living and feeding conditions	$NOECsed_{min}$/ $EC10sed_{min}$	100
3 NOEC/EC10	With species representing different living and feeding conditions	$NOECsed_{min}$/ $EC10sed_{min}$	50
1 NOEC/EC10 and additional 2 NOEC/EC10 marine	With species representing different living and feeding conditions	$NOECsed_{min}$/ $EC10sed_{min}$	10
3 NOEC/EC10 marine	With species representing different living and feeding conditions	$NOECsed_{min}$/ $EC10sed_{min}$	10

[a] Where there is convincing evidence that the sensitivity of marine organisms is adequately covered by that available from freshwater species, the assessment factors used for freshwater sediment data may be applied. Such evidence may include data from long-term testing of freshwater and marine aquatic organisms, and must include data on specific marine taxa.

$$PNEC_{sed} = \frac{TOXsed}{AFsed} \quad \textbf{(250)}$$

$$PNEC_{sed,marine} = \frac{TOXsed}{AFsed_{marine}} \quad \textbf{(251)}$$

If $TOXsed = PNEC_{sed,ep}$ then $EPsed$ = 'yes'

Input			
Foc_{sed}	weight fraction of organic carbon in marine sediment	$[kg.kg^{-1}]$	D
Fom_{sed}	weight fraction of organic matter in marine sediment	$[kg.kg^{-1}]$	D/O
$Foc_{sed,exp}$	weight fraction of organic carbon in tested sediment	$[kg.kg^{-1}]$	S
$LC50sed_i$	LC50 for sediment-dwelling organisms, species *i*	$[kg_c.kg_{wwt}^{-1}]$	S
$NOECsed_i$	NOEC for sediment-dwelling organisms, species *i*	$[kg_c.kg_{wwt}^{-1}]$	S
$EC10sed_i$	EC10 for sediment-dwelling organisms, species *i*	$[kg_c.kg_{wwt}^{-1}]$	S
$LC50sed_{standard,i}$	Standardised LC50 for sediment-dwelling organisms, species *i*	$[kg_c.kg_{wwt}^{-1}]$	S/O
$NOECsed_{standard,i}$	Standardised NOEC for sediment-dwelling organisms, species *i*	$[kg_c.kg_{wwt}^{-1}]$	S/O
$EC10sed_{standard,i}$	Standardised EC10 for sediment-dwelling organisms, species *i*	$[kg_c.kg_{wwt}^{-1}]$	S/O
$PNEC_{water}$	PNEC for aquatic organisms	$[kg_c.m^{-3}]$	O[c]
$K_{susp-water}$	suspended matter-water partition coefficient	$[m^3.m^{-3}]$	O[c]
RHO_{susp}	bulk density of suspended matter	$[kg_{wwt}.m^{-3}]$	O[c]
$PNEC_{sed,ep}$	PNEC for sediment-dwelling organisms derived by eq. part.	$[kg_c.kg_{wwt}^{-1}]$	O[c]
Output			
TOXsed	toxicological data used for extrapolation of PNEC	$[kg_c.kg_{wwt}^{-1}]$	O
AFsed	assessment factor applied in extrapolation of PNEC	[-]	O
EPsed	equilibrium partitioning used for PNEC in sediment?	[yes/no]	O[c]
$PNEC_{sed}$	PNEC for sediment-dwelling organisms	$[kg_c.kg_{wwt}^{-1}]$	O

III.6.1.4 Micro-organisms

Chemicals may cause adverse effects on microbial activity in STPs and therefore it is necessary to derive a PNECmicro-organisms. Current test systems for measuring the effect of chemicals on microbial activity have different endpoints and different levels of sensitivity. A number of internationally accepted test systems exist. Available data suggest the following order of increasing sensitivities among particular test systems: respiration inhibition test < inhibition control in base-set tests < growth inhibition test with P. putida < inhibition of nitrification. Depending on the test system and toxicity data available for micro-organisms, assessment factors are selected for extrapolating results from toxicity tests to a PNEC for the sewage treatment plant.

Table III-99 *Assessment factors for deriving the $PNEC_{micro\text{-}organisms}$ for the STP.*

Test system	TOXmicro	AFmicro
Activated sludge, respiration inhibition tests		
Respiration inhibition tests EU Annex V C.11, OECD 209	$NOEC_{micro}$ or $EC10_{micro}$	10
	$EC50_{micro}$	100
Inhibition control in base-set tests		
Inhibition control in standard biodegradation test: ready or inherent tests	Tested conc. at which toxicity to inoculum can be ruled out [a]	10
Activated sludge, other tests		
Activated sludge growth inhibition tests, ISO-15522	$NOEC_{micro}$ or $EC10_{micro}$	10
	$EC50_{micro}$	100
Pilot scale activated sludge simulation tests OECD 303 A, ISO-11733	Expert judgement [b]	Case-by-case down to 1
Tests with specific populations of bacteria or protozoa		
Inhibition of nitrification, ISO-9509	$NOEC_{micro}$ or $EC10_{micro}$	1
	$EC50_{micro}$	10
Ciliate growth inhibition tests,	$NOEC_{micro}$ or $EC10_{micro}$	1
	$EC50_{micro}$	10
Growth inhibition tests with *Pseudomonas putida,* NF EN ISO 10712	$NOEC_{micro}$ or $EC10_{micro}$	1
	$EC50_{micro}$	10

[a] The tested concentration at which toxicity to the inoculum can be ruled out with sufficient reliability (cf. corresponding text section above) could be considered as a NOEC for the toxicity to micro-organisms of a STP;
[b] Based on case-by-case expert judgement, the tested concentration not impairing proper functioning of the continuous activated sludge unit could be considered as NOEC for micro-organisms in STPs

If more than one toxicity value is given, the lower of the resulting PNECs is used.

$$PNEC_{micro\text{-}organisms} = \frac{TOXmicro}{AFmicro} \qquad (252)$$

Input			
$EC50_{micro}$	EC50 for STP micro-organisms	$[kg_c.m^{-3}]$	S
$EC10_{micro}$	EC10 for STP micro-organisms	$[kg_c.m^{-3}]$	S
$NOEC_{micro}$	NOEC for STP micro-organisms	$[kg_c.m^{-3}]$	S
Output			
TOXmicro	toxicological data used for extrapolation of PNEC	$[kg_c.m^{-3}]$	O
AFmicro	assessment factor applied in extrapolation of PNEC	[-]	O
$PNEC_{micro\text{-}organisms}$	PNEC for STP micro-organisms	$[kg_c.m^{-3}]$	O^c

III.6.1.5 Secondary poisoning

For new substances, the results of mammalian repeated-dose toxicity test(s) are used to assess secondary poisoning effects. For existing substances, toxicity data for birds may also be present. Extrapolation from such test results gives a predicted no-effect concentration in food that should be protective of other mammalian and avian species. Acute lethal doses LD50 (rat, bird) are not acceptable for extrapolation to chronic toxicity, as these tests are not dietary tests. Acute effect concentrations (LC50, 5-day avian dietary studies) for birds are acceptable for extrapolation. The results of these tests may be expressed as a concentration in the food (mg/kg) or a dose (mg/kg body weight/day) causing no effect. For the assessment of secondary poisoning, the results are converted to the concentration in food (kg_c/kg food). NOECs converted from NOAELs have the same priority as direct NOECs. The table below gives some conversion factors for laboratory species.

Bird toxicity tests are not usually given for the test durations specified below (T_{bird}). This test duration is however only used to arrive at a representative assessment factor. The user therefore has to decide whether a longer-term bird toxicity test is comparable to 90 day or chronic mammal test.

Table III-100 *Assessment factors for deriving the $PNEC_{oral}$ for secondary poisoning.*

Available ecotox. Data	**Duration of (sub-)chronic test**	**TOXoral**	**AForal**
$LC50_{bird}$ only	5 days	$LC50_{bird}$	3000
$NOEC_{bird}$	Chronic	$NOEC_{bird}$	30
$NOEC_{mammal,food,chr}$	28 days 90 days chronic	$NOEC_{mammal,food,chr}$	300 90 30

If an NOEC for both birds and mammals is given, the lower of the resulting PNECs is used.

$$PNEC_{oral} = \frac{TOXoral}{AForal} \qquad \textbf{(253)}$$

Input			
$LC50_{bird}$	LC50 in avian dietary study (5 days)	$[kg_c.kg_{food}^{-1}]$	S
$NOEC_{bird}$	NOEC for birds	$[kg_c.kg_{food}^{-1}]$	S/O
$NOEC_{mammal,food,chr}$	NOEC for mammals	$[kg_c.kg_{food}^{-1}]$	S/O
T_{bird}	duration of (sub-)chronic test with birds	[d]	P
T_{mammal}	duration of (sub-)chronic test with mammals	[d]	P
Output			
TOXoral	toxicological data used for extrapolation of PNEC	$[kg_c.kg_{food}^{-1}]$	O
AForal	assessment factor applied in extrapolation of PNEC	[-]	O
$PNEC_{oral}$	PNEC for secondary poisoning of birds and mammals	$[kg_c.kg_{food}^{-1}]$	O[c]

If toxicity data are given as NOAEL only:

$$NOEC_{bird} = NOAEL_{bird} \cdot CONV_{bird} \quad \textbf{(254)}$$

$$NOEC_{mammal,\,food,chr} = NOAEL_{mammal,oral,chr} \cdot CONV_{mammal} \quad \textbf{(255)}$$

Input			
$NOAEL_{bird}$	NOAEL for birds	$[kg_c.kg_{bw}.d^{-1}]$	S
$NOAEL_{mammal,oral,chr}$	NOAEL for mammals	$[kg_c.kg_{bw}.d^{-1}]$	S/O
$CONV_{bird}$	conversion factor from NOAEL to NOEC	$[kg_{bw}.d.kg_{food}^{-1}]$	S
$CONV_{mammal}$	conversion factor from NOAEL to NOEC	$[kg_{bw}.d.kg_{food}^{-1}]$	P/S
Output			
$NOEC_{bird}$	NOEC for birds	$[kg_c.kg_{food}^{-1}]$	S/O
$NOEC_{mammal,food,chr}$	NOEC for mammals	$[kg_c.kg_{food}^{-1}]$	S/O

The conversion factors as published in the TGD and reproduced in **Table III-101**, with the addition of the factor for Guinea pig, can be traced back to Lehman (1954) and Romijn *et al.* (1993) and are based on default assumptions for body weights and daily food consumption. Other, more detailed values for body weights and food consumption can be found in the TGD, Part I, Appendix VI.

Table III-101 Conversion factors from NOAEL to NOEC for several mammalian species.

Species	**Conversion factor (BW/DFI) $CONV_{mammal}$ [$kg_{bw}.d.kg_{food}^{-1}$]**
Canis domesticus/ dog	40
Cavia cobaya/ guinea pig	25
Cricetus/ hamster	10
Macaca spp./ monkey	20
Microtus spp./ vole	8.3
Mus musculus/ mouse	8.3
Oryctolagus cuniculus/ rabbit	33.3
Rattus norvegicus (> 6 weeks)/ rat	20
Rattus norvegicus (≤ 6 weeks)/ rat	10
Gallus domesticus/ chick	8

III.6.1.6 Statistical extrapolation method

The statistical extrapolation method itself is not incorporated in EUSES 2.0.
The Aldenberg and Jaworska (2000) method within the ETX-program (Van Vlaardingen and Traas, 2002) can be used to support the effect assessment performed with assessment factors. The results of this method can be entered as input ($PNEC_{stat}$). For the statistical extrapolation method we refer to the ETX-program, which can be obtained from the RIVM (info@rivm.nl).

The no-effect level (HC_5) calculated according the Aldenberg and Jaworska (2000) method within ETX is the median concentration with the 90% confidence interval that protects 95% of the species in the system for which the experimental NOECs are a representative sample. The method is used for aquatic as well as terrestrial toxicity data. Values of the extrapolation constant k_s depend on the number of NOECs given and the desired confidence level. According to the TGD (2003) at least 10 NOECs from at least 8 different taxonomic groups must be present for this calculation. The TGD lists the taxonomical groups that are required. The TGD also documents data selection and data averaging, if more than one NOEC is available for each species.

In ETX it is checked whether the toxicity data deviate from the assumed normal distribution using the Anderson-Darling test (and the Kolmogorov Smirnov test). If a test statistic is above the 5% critical value, normality is rejected at the 5% critical value, indicating doubts about normality. If a GOF test statistic is below the 5% critical value, normality is accepted at the 5% critical value. If a higher critical value is accepted (e.g. at 2.5% significance level), then the probability that these data derive from a normal distribution is smaller than at 5%, but it is not impossible that the sample derives from a normal distribution. A GOF test does *not* say that a sample cannot derive from a normal distribution, just that it becomes less probable with decreasing significance levels.

Input

$PNECstat_{water}$	PNEC for aquatic organisms with statistical method	[$kg_c.m^{-3}$]	S
$PNECstat_{water, marine}$	PNEC for marine aquatic organisms with statistical method	[$kg_c.m^{-3}$]	S
$PNECstat_{soil}$	PNEC for terrestrial organisms with statistical method	[$kg_c.m^{-3}$]	S

III.6.1.7 PBT assessment

The PBT assessment (persistence, bioconcentration, toxicity) is not included in EUSES. It is referred to the TGD (2003) (Part II, chapter 4.4) for the criteria and the testing strategies.

III.6.2 Effects assessment for humans

III.6.2.1 Route-to-route extrapolation

For acute time scale effects it is not common to perform route-to-route extrapolations. When necessary and applicable, for (sub-)chronic time scale effects (repeated dose toxicity, carcinogenicity and reproductive toxicity (and within this endpoint a.o. fertility, maternal toxicity and developmental toxicity) route-to-route extrapolations may be performed.

Oral-to-dermal route

If oral and dermal absorption rates are known these should be used in the calculations. If these data are not known default values should be taken.

Table III-102 Defaults for oral-to-dermal extrapolation.

Parameter	**Symbol** [(a)]	**Unit**	**Value**
Bioavailability for oral uptake	$BIO_{oral,1}$	[-]	1
Bioavailability for dermal uptake	$BIO_{der,2}$	[-]	
MOLW >500 and [log Kow <-1 or >4]			0.10
MOLW ≤500 and [log Kow ≥-1 or ≤4]			1

These are parameters are already defined in the sub-modules on human exposure.
(a) "1" indicates starting route, "2" end route.

$$NOAEL_{mammal,der,i} = NOAEL_{mammal,oral,i} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \quad (256)$$

$$LOAEL_{mammal,der,i} = LOAEL_{mammal,oral,i} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \quad (257)$$

$$NOAEL_{man,der,i} = NOAEL_{man,oral,i} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \quad (258)$$

$$LOAEL_{man,der,i} = LOAEL_{man,oral,i} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \quad (259)$$

$$CED_{mammal,der,i} = CED_{mammal,oral,i} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \quad (260)$$

$$i \in \{repdose, carc, fert, mattox, devtox\}$$

$$T25_{mammal,der,nt} = T25_{mammal,oral,nt} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \quad (261)$$

$$CED_{mammal,der,nt} = CED_{mammal,oral,nt} \cdot \frac{BIO_{oral,1}}{BIO_{der,2}} \quad (262)$$

If absorption rates of humans and experimental animals differ and are known, the toxicity parameter estimated by EUSES should be corrected manually by multiplication with a factor $BIO_{der\text{-}animal}/BIO_{der\text{-}human}$.

Input			
$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint *i*	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint *i*	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$CED_{mammal,oral,nt}$	oral CED for mammals for non-threshold effects	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$BIO_{oral,1}$	bioavailability for oral uptake (starting route)	[-]	S/D
$BIO_{der,2}$	bioavailability for dermal uptake (end route)	[-]	S/D
Output			
$N(L)OAEL_{mammal,der,i}$	dermal N(L)OAEL for mammals for endpoint *i*	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$N(L)OAEL_{man,der,i}$	dermal N(L)OAEL for man for endpoint *i* $i \in$ {repdose,carc,fert,mattox,devtox}	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$CED_{mammal,der,i}$	dermal CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$CED_{mammal,der,nt}$	dermal CED for mammals for non-threshold effects	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O

Oral-to-inhalatory route

If oral and inhalation absorption rates are known these should be used in the calculations. If these data are not known default values should be taken. To err on the side of caution, the default value for the starting route (oral) is 50%. The respiratory rate used has to fulfill the requirements of allometric scaling and therefore the inhalatory rate (of humans) is multiplied with the allometric correction factor (AFallom). The TGD proposes the following values: rat 4, mice 7, guinea pig 3, rabbit 2.4, monkey 2, dog 1.4.

$$NOAEL_{mammal,inh,i} = NOAEL_{mammal,oral,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \quad \textbf{(263)}$$

$$LOAEL_{mammal,inh,i} = LOAEL_{mammal,oral,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \quad \textbf{(264)}$$

$$NOAEL_{man,inh,i} = NOAEL_{man,oral,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \quad \textbf{(265)}$$

$$LOAEL_{man,inh,i} = LOAEL_{man,oral,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \quad \textbf{(266)}$$

$$CED_{mammal,inh,i} = CED_{mammal,oral,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \quad \textbf{(267)}$$

$i \in \{repdose, carc, fert, mattox, devtox\}$

$$T25_{mammal,inh,nt} = T25_{mammal,oral,nt} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \quad \textbf{(268)}$$

$$CED_{mammal,inh,nt} = CED_{mammal,oral,nt} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{oral,1}}{BIO_{inh,2}} \quad \textbf{(269)}$$

If absorption rates of humans and experimental animals differ and are known, the toxicity parameter estimated by EUSES should be corrected manually by multiplication with a factor $BIO_{inh\text{-}animal}/BIO_{inh\text{-}human}$.

Table III-103 Defaults for oral-to-inhalation extrapolation.

Parameter	Symbol [(a)]	Unit	Value
Bioavailability for oral uptake	$BIO_{oral,1}$	[-]	0.50
Bioavailability for inhalation	$BIO_{inh,2}$	[-]	1
Body weight of the human considered	BW	$[kg_{bw}]$	70
Daily inhalation rate Consumer / Humans via the environment	IH_{air}	$[m^3.d^{-1}]$	 20

These are parameters are already defined in the sub-modules on human exposure.
(a) "1" indicates starting route, "2" end route.

Input

$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,\ nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$BIO_{oral,1}$	bioavailability for oral uptake (starting route)	[-]	S/D
$BIO_{inh,2}$	bioavailability for inhalation (end route)	[-]	S/D
BW	body weight of the human considered	$[kg_{bw}]$	D
IH_{air}	daily inhalation rate of humans	$[m^3.d^{-1}]$	D
AF_{allom}	allometric scaling factor	[-]	D

Output

$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,\ nt}$	inhalatory CED for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O

Dermal-to-oral route

If dermal and oral absorption rates are known these should be used in the calculations. If these data are not known default values should be taken.

Table III-104 Defaults for dermal-to-oral extrapolation.

Parameter	Symbol [(a)]	Unit	Value
Bioavailability for dermal uptake	$BIO_{der,1}$	[-]	
MOLW >500 and [log Kow <-1 or >4]			0.01
MOLW ≤500 and [log Kow ≥-1 and ≤4]			0.1
Bioavailability for oral uptake	$BIO_{oral,2}$	[-]	1

These are parameters are already defined in the sub-modules on human exposure.
(a) "1" indicates starting route, "2" end route.

$$NOAEL_{mammal,oral,i} = NOAEL_{mammal,der,i} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \quad (270)$$

$$LOAEL_{mammal,oral,i} = LOAEL_{mammal,der,i} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \quad (271)$$

$$NOAEL_{man,oral,i} = NOAEL_{man,der,i} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \quad (272)$$

$$LOAEL_{man,oral,i} = LOAEL_{man,der,i} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \quad (273)$$

$$CED_{mammal,oral,i} = CED_{mammal,der,i} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \quad (274)$$

$i \in \{repdose, carc, fert, mattox, devtox\}$

$$T25_{mammal,oral,nt} = T25_{mammal,der,nt} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \quad (275)$$

$$CED_{mammal,oral,nt} = CED_{mammal,der,nt} \cdot \frac{BIO_{der,1}}{BIO_{oral,2}} \quad (276)$$

If absorption rates of humans and experimental animals differ and are known, the toxicity parameter estimated by EUSES should be corrected manually by multiplication with a factor $BIO_{oral\text{-}animal}/BIO_{oral\text{-}human}$.

Input			
$N(L)OAEL_{mammal,der,i}$	dermal N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,der,i}$	dermal N(L)OAEL for man for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,i}$	dermal CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,\ nt}$	dermal CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$BIO_{der,1}$	bioavailability for dermal uptake (starting route)	[-]	S/D
$BIO_{oral,2}$	bioavailability for oral uptake (end route)	[-]	S/D
Output			
$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,\ nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O

Dermal-to-inhalatory route

If dermal and inhalation absorption rates are known these should be used in the calculations. If these data are not known default values should be taken. The respiratory rate used has to fulfill the requirements of allometric scaling and therefore the inhalatory rate (of humans) is multiplied with the allometric correction factor (AFallom). The TGD proposes the following values: rat 4, mice 7, guinea pig 3, rabbit 2.4, monkey 2, dog 1.4.

Table III-105 Defaults for dermal-to-inhalation extrapolation.

Parameter	**Symbol** [(a)]	**Unit**	**Value**
Bioavailability for dermal uptake	$BIO_{der,1}$	[-]	
MOLW >500 and [log Kow <-1 or >4]			0.01
MOLW ≤500 and [log Kow ≥-1 and ≤4]			0.1
Bioavailability for inhalation	$BIO_{inh,2}$	[-]	1
Body weight of the human considered	BW	$[kg_{bw}]$	70
Daily inhalation rate	IH_{air}	$[m^3.d^{-1}]$	
Consumer / Humans via the environment			20

These are parameters are already defined in the sub-modules on human exposure.
(a) "1" indicates starting route, "2" end route.

$$NOAEL_{mammal,inh,i} = NOAEL_{mammal,der,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \quad (277)$$

$$LOAEL_{mammal,inh,i} = LOAEL_{mammal,der,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \quad (278)$$

$$NOAEL_{man,inh,i} = NOAEL_{man,der,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \quad (279)$$

$$LOAEL_{man,inh,i} = LOAEL_{man,der,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \quad (280)$$

$$CED_{mammal,inh,i} = CED_{mammal,der,i} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \quad (281)$$

$i \in \{repdose, carc, fert, mattox, devtox\}$

$$T25_{mammal,inh,nt} = T25_{mammal,der,nt} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \quad (282)$$

$$CED_{mammal,inh,nt} = CED_{mammal,der,nt} \cdot \frac{BW}{IH_{air} \cdot AF_{allom}} \cdot \frac{BIO_{der,1}}{BIO_{inh,2}} \quad (283)$$

If absorption rates of humans and experimental animals differ and are known, the toxicity parameter estimated by EUSES should be corrected manually by multiplication with a factor $BIO_{inh\text{-}animal}/BIO_{inh\text{-}human}$.

Input			
$N(L)OAEL_{mammal,der,i}$	dermal N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,der,i}$	dermal N(L)OAEL for man for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,i}$	dermal CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,\ nt}$	dermal CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$BIO_{der,1}$	bioavailability for dermal uptake (starting route)	[-]	S/D
$BIO_{inh,2}$	bioavailability for inhalation (end route)	[-]	S/D
BW	body weight of the human considered	$[kg_{bw}]$	D
IH_{air}	daily inhalation rate	$[m^3.d^{-1}]$	D
AF_{allom}	allometric scaling factor	[-]	D
Output			
$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,\ nt}$	inhalatory CED for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O

Inhalatory-to-oral route

If inhalation and oral absorption rates are known these should be used in the calculations. If these data are not known default values should be taken. The respiratory rate used has to fulfill the requirements of allometric scaling and therefore the inhalatory rate (of humans) is multiplied with the allometric correction factor (AFallom). The TGD proposes the following values: rat 4, mice 7, guinea pig 3, rabbit 2.4, monkey 2, dog 1.4.

Table III-106 Defaults for inhalation-to-oral extrapolation.

Parameter	**Symbol** [(a)]	**Unit**	**Value**
Bioavailability for inhalation	$BIO_{inh,1}$	[-]	1
Bioavailability for oral uptake	$BIO_{oral,2}$	[-]	1
Daily inhalation rate Consumer / Humans via the environment	IH_{air}	$[m^3.d^{-1}]$	 20
Body weight of the human considered	BW	$[kg_{bw}]$	70

These are parameters are already defined in the sub-modules on human exposure.
(a) "1" indicates starting route, "2" end route.

Input			
$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,\ nt}$	inhalatory CED for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$BIO_{inh,1}$	bioavailability for inhalation (starting route)	[-]	S/D
$BIO_{oral,2}$	bioavailability for oral uptake (end route)	[-]	S/D
IH_{air}	daily inhalation rate	$[m^3.d^{-1}]$	D
BW	body weight of the human considered	$[kg_{bw}]$	D
AF_{allom}	allometric scaling factor	[-]	D
Output			
$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,\ nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O

$$NOAEL_{mammal,oral,i} = NOAEL_{mammal,inh,i} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \quad \textbf{(284)}$$

$$LOAEL_{mammal,oral,i} = LOAEL_{mammal,inh,i} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \quad \textbf{(285)}$$

$$NOAEL_{man,oral,i} = NOAEL_{man,inh,i} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \quad \textbf{(286)}$$

$$LOAEL_{man,oral,i} = LOAEL_{man,inh,i} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \quad \textbf{(287)}$$

$$CED_{mammal,oral,i} = CED_{mammal,inh,i} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \quad \textbf{(288)}$$

$$i \in \{repdose, carc, fert, mattox, devtox\}$$

$$T25_{mammal,oral,nt} = T25_{mammal,inh,nt} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \quad \textbf{(289)}$$

$$CED_{mammal,oral,nt} = CED_{mammal,inh,nt} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{oral,2}} \quad \textbf{(290)}$$

If absorption rates of humans and experimental animals differ and are known, the toxicity parameter estimated by EUSES should be corrected manually by multiplication with a factor $BIO_{oral\text{-}animal}/BIO_{oral\text{-}human}$.

Inhalatory-to-dermal route

If inhalation and dermal absorption rates are known these should be used in the calculations. If these data are not known default values should be taken. The respiratory rate used has to fulfill the requirements of allometric scaling and therefore the inhalatory rate (of humans) is multiplied with the allometric correction factor (AFallom). The TGD proposes the following values: rat 4, mice 7, guinea pig 3, rabbit 2.4, monkey 2, dog 1.4.

Table III-107 Defaults for inhalation-to-dermal extrapolation.

Parameter	**Symbol** [(a)]	**Unit**	**Value**
Bioavailability for inhalation	$BIO_{inh,1}$	[-]	1
Bioavailability for dermal uptake MOLW >500 and [log Kow <-1 or >4] MOLW ≤500 and [log Kow ≥-1 and ≤4]	$BIO_{der,2}$	[-]	 0.10 1
Daily inhalation rate Consumer / Humans via the environment	IH_{air}	$[m^3.d^{-1}]$	 20
Body weight of the human considered	BW	$[kg_{bw}]$	70

These are parameters are already defined in the sub-modules on human exposure.
(a) "1" indicates starting route, "2" end route.

$$NOAEL_{mammal,der,i} = NOAEL_{mammal,inh,i} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(291)}$$

$$LOAEL_{mammal,der,i} = LOAEL_{mammal,inh,i} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(292)}$$

$$NOAEL_{man,der,i} = NOAEL_{man,inh,i} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(293)}$$

$$LOAEL_{man,der,i} = LOAEL_{man,inh,i} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(294)}$$

$$CED_{mammal,der,i} = CED_{mammal,inh,i} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(295)}$$

$$i \in \{repdose, carc, fert, mattox, devtox\}$$

$$T25_{mammal,der,nt} = T25_{mammal,inh,nt} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(296)}$$

$$CED_{mammal,der,nt} = CED_{mammal,inh,nt} \cdot \frac{IH_{air} \cdot AF_{allom}}{BW} \cdot \frac{BIO_{inh,1}}{BIO_{der,2}} \quad \textbf{(297)}$$

If absorption rates of humans and experimental animals differ and are known, the toxicity parameter estimated by EUSES should be corrected manually by multiplication with a factor $BIO_{der\text{-}animal}/BIO_{der\text{-}human}$.

Input			
$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint *i*	$[kg_c.m^{-3}]$	S/O
$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,\ nt}$	inhalatory CED for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$BIO_{inh,1}$	bioavailability for inhalation (starting route)	[-]	S/D
$BIO_{der,2}$	bioavailability for dermal uptake (end route)	[-]	S/D
IH_{air}	daily inhalation rate	$[m^3.d^{-1}]$	D
BW	body weight of the human considered	$[kg_{bw}]$	D
AF_{allom}	allometric scaling factor	[-]	D
Output			
$N(L)OAEL_{mammal,der,i}$	dermal N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,der,i}$	dermal N(L)OAEL for man for endpoint *i* $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,i}$	dermal CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,\ nt}$	dermal CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O

For the route-to-route extrapolation for workers involving the inhalatory route an additional correction is used to account for the difference between the respiratory rate of the general population (default 20 m3 per 24 hrs), used in the route-to-route extrapolation, and the respiratory rate of workers (10 m3 in 8 hrs). The TGD recommends a factor of 0.5 for extrapolations from the dermal and oral route to the inhalatory route and 2 for extrapolations from the inhalatory route to the dermal and oral route. EUSES allows this correction in the derivation of the RMOS, RMOE and human equivalent dose for workers. The default is 1.

III.6.2.2 Conversion from $mg.kg_{food}^{-1}$ (diet studies) to $mg.kg_{bw}^{-1}.d^{-1}$

If NOAEL is absent and NOEC is available:

$$NOAEL_{mammal,oral,chr} = \frac{NOEC_{mammal,\ food,chr}}{CONV_{mammal}} \quad \textbf{(298)}$$

If LOAEL is absent and LOEC is available:

$$LOAEL_{mammal,oral,chr} = \frac{LOEC_{mammal,\ food,chr}}{CONV_{mammal}} \quad \textbf{(299)}$$

If T25 is only available from a diet study in mg/kg food:

$$T25_{mammal,oral,nt} = \frac{T25_{mammal,\ food,nt}}{CONV_{mammal}} \quad \textbf{(300)}$$

If CED is only available from a diet study in mg/kg food:

$$CED_{mammal,oral,nt} = \frac{CED_{mammal,\ food,nt}}{CONV_{mammal}} \qquad \textbf{(301)}$$

$i \in \{repdose, carc, fert, mattox, devtox\}$

Input

$N(L)OEC_{mammal,food,i}$	N(L)OEC via food for mammals for endpoint *i*	$[kg_c.kg_{food}^{-1}]$	S/O
$T25_{mammal,food,nt}$	T25 via food for mammals for non-threshold substances	$[kg_c.kg_{food}^{-1}]$	S/O
$CED_{mammal,food,i}$	CED via food for mammals for endpoint i	$[kg_c.kg_{food}^{-1}]$	S/O
$CED_{mammal,food,nt}$	CED via food for mammals for non-threshold substances	$[kg_c.kg_{food}^{-1}]$	S/O
$CONV_{mammal}$	conversion factor NOAEL to NOEC $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_{bw}.d.kg_{food}^{-1}]$	P/S [a]

Output

$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint *i*	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint i $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,\ nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O

[a] see **Table III-101** in Section III.6.1.5.

III.7 RISK CHARACTERISATION

In risk characterisation, exposure levels are compared to suitable no-effect levels to yield so-called Risk Characterisation Ratios (RCR) for each protection goal. For the environmental end-points, this is the ratio of PEC to PNEC. For the human end-points a distinction need to be made between threshold and non-threshold substances. For threshold substances the Margin Of Safety (MOS) is derived, i.e. the ratio of the effect parameter and the estimated exposure value. The MOS is compared to a reference-MOS. In addition, for biocides the Acceptable-Operator-Exposure-Level (AOEL) is compared to the internal exposure value. Risk characterisation of non-threshold substances entails a comparison between the estimated exposure and the T25 or BMD05, extrapolated to a lifetime cancer risk for humans. Additionally, the Margin of Exposure (MOE) approach is followed. This approach is equivalent to the MOS approach for threshold substances: the MOE is the ratio of the effect parameter (T25 or BMD05) and the estimated lifetime daily exposure level. The MOE is to be compared to the reference-MOE.. Environmental risk characterisation and human health risk characterisation are handled in separate sub-modules.

This module is divided into four specific sub-modules, which will be treated separately:
- Environment.
- Indirect human exposure.
- Consumer exposure.
- Workplace exposure.

III.7.1 Risk characterisation for the environment

Input

$PEClocal_{water}$	local PEC in surface water during emission episode	[$kg_c.m^{-3}$]	
$PEClocal_{water,marine}$	local PEC in marine surface water during emission episode	[$kg_c.m^{-3}$]	
$PECreg_{water}$	regional steady-state PEC in surface water	[$kg_c.m^{-3}$]	
$PECreg_{water,marine}$	regional steady-state PEC in marine surface water	[$kg_c.m^{-3}$]	
$PNEC_{water}$	PNEC for the aquatic compartment	[$kg_c.m^{-3}$]	c
$PNEC_{water,marine}$	PNEC for the marine aquatic compartment	[$kg_c.m^{-3}$]	c
$PEClocal_{soil}$	local PEC in agricultural soil, averaged over 30 days	[$kg_c.kg_{wwt}^{-1}$]	
$PECreg_{agric}$	regional steady-state PEC in agricultural soil	[$kg_c.kg_{wwt}^{-1}$]	
$PNEC_{soil}$	PNEC for the soil compartment	[$kg_c.kg_{wwt}^{-1}$]	c
TOXterr	toxicological data used for extrapolation of PNEC	[$kg_c.kg_{wwt}^{-1}$]	
EPterr	equilibrium partitioning used for PNEC for soil?	[yes/no]	c
Kow	octanol-water partition coefficient	[$m^3.m^{-3}$]	
$PEClocal_{sed}$	local PEC in sediment	[$kg_c.kg_{wwt}^{-1}$]	
$PEClocal_{sed,marine}$	local PEC in marine sediment	[$kg_c.kg_{wwt}^{-1}$]	
$PECreg_{sed}$	regional steady-state PEC in sediment	[$kg_c.kg_{wwt}^{-1}$]	
$PECreg_{sed,marine}$	regional steady-state PEC in marine sediment	[$kg_c.kg_{wwt}^{-1}$]	
$PNEC_{sed}$	PNEC for the sediment compartment	[$kg_c.kg_{wwt}^{-1}$]	
$PNEC_{sed,marine}$	PNEC for the marine sediment compartment	[$kg_c.kg_{wwt}^{-1}$]	
EPsed	equilibrium partitioning used for PNEC for sediment?	[yes/no]	c
$EPsed_{marine}$	equilibrium partitioning used for PNEC for marine sediment?	[yes/no]	c
PEC_{stp}	local PEC in STP during emission episode	[$kg_c.m^{-3}$]	
$PNEC_{micro\text{-}organisms}$	PNEC for STP micro-organisms	[$kg_c.m^{-3}$]	c
$PEC_{oral,fish}$	PEC in fish (local and regional combined)	[$kg_c.kg_{wwt}^{-1}$]	
$PEC_{oral,fish,marine}$	PEC in marine fish (local and regional combined)	[$kg_c.kg_{wwt}^{-1}$]	
$PEC_{oral,fish\ predator,marine}$	PEC in marine fish-eating predator (local and regional combined)	[$kg_c.kg_{wwt}^{-1}$]	
$PEC_{oral,worm}$	PEC in worm (local and regional combined)	[$kg_c.kg_{wwt}^{-1}$]	
$PNEC_{oral}$	PNEC for birds and mammals	[$kg_c.kg_{wwt}^{-1}$]	c
$PNECstat_{water}$	PNEC for aquatic organisms with statistical method	[$kg_c.m^{-3}$]	
$PNECstat_{water,\ marine}$	PNEC for marine aquatic organisms with statistical method	[$kg_c.m^{-3}$]	
$PNECstat_{soil}$	PNEC for terrestrial organisms with statistical method	[$kg_c.m^{-3}$]	

Output

$RCRlocal_{water}$	RCR for the local water compartment	[-]	c
$RCRlocal_{water,marine}$	RCR for the local marine water compartment	[-]	c
$RCRreg_{water}$	RCR for the regional water compartment	[-]	c
$RCRreg_{water,marine}$	RCR for the regional marine water compartment	[-]	c
$RCRlocal_{soil}$	RCR for the local soil compartment	[-]	c
$RCRreg_{soil}$	RCR for the regional soil compartment	[-]	c
$RCRlocal_{sed}$	RCR for the local sediment compartment	[-]	c
$RCRlocal_{sed,marine}$	RCR for the local marine sediment compartment	[-]	c
$RCRreg_{sed}$	RCR for the regional sediment compartment	[-]	c
$RCRreg_{sed,marine}$	RCR for the regional marine sediment compartment	[-]	c
RCR_{stp}	RCR for the sewage treatment plant	[-]	c
$RCR_{oral,fish}$	RCR for fish-eating birds and mammals	[-]	c
$RCR_{oral,fish,marine}$	RCR for fish-eating birds/mammals (marine environment)	[-]	c
$RCR_{oral,fish\ predator,marine}$	RCR for top-predators (marine environment)	[-]	c
$RCR_{oral,worm}$	RCR for worm-eating birds and mammals	[-]	c
$RCRstat_{water}$	RCR for aquatic organisms with statistical method	[-]	c
$RCRstat_{water,\ marine}$	RCR for marine aquatic organisms with statistical method	[-]	c
$RCRstat_{soil}$	RCR for terrestrial organisms with statistical method	[-]	c

III.7.1.1 Aquatic environment

The concentration of the chemical in surface water is compared to the no-effect concentration for aquatic organisms. This is done for the local as well as the regional freshwater and marine environment. On the local scale, the concentration during an emission episode is taken. It should be noted that the local ratios have to be defined for all relevant stages of the life cycle and for each application of the substance.

$$RCRlocal_{water} = \frac{PEClocal_{water}}{PNEC_{water}} \quad \textbf{(302)}$$

$$RCRlocal_{water,marine} = \frac{PEClocal_{water,marine}}{PNEC_{water,marine}} \quad \textbf{(303)}$$

$$RCRreg_{water} = \frac{PECreg_{water}}{PNEC_{water}} \quad \textbf{(304)}$$

$$RCRreg_{water,marine} = \frac{PECreg_{water,marine}}{PNEC_{water,marine}} \quad \textbf{(305)}$$

Input			
$PEClocal_{water}$	local PEC in surface water during emission episode	[$kg_c.m^{-3}$]	O
$PECreg_{water}$	regional steady-state PEC in surface water	[$kg_c.m^{-3}$]	O
$PEClocal_{water,marine}$	local PEC in marine water during emission episode	[$kg_c.m^{-3}$]	O
$PECreg_{water,marine}$	regional steady-state PEC in marine surface water	[$kg_c.m^{-3}$]	O
$PNEC_{water}$	PNEC for aquatic compartment	[$kg_c.m^{-3}$]	O^c
$PNEC_{water,marine}$	PNEC for marine aquatic compartment	[$kg_c.m^{-3}$]	O^c
Output			
$RCRlocal_{water}$	RCR for local water compartment	[-]	O^c
$RCRreg_{water}$	RCR for regional water compartment	[-]	O^c
$RCRlocal_{water,marine}$	RCR for local marine water compartment	[-]	O^c
$RCRreg_{water,marine}$	RCR for regional marine water compartment	[-]	O^c

III.7.1.2 Terrestrial compartment

The concentration of the chemical in agricultural soil is compared to the no-effect concentration for terrestrial organisms. This is done for the local as well as the regional environment. On the local scale, the concentration averaged over 30 days is used. It should be noted that the local ratios have to be defined for all relevant stages of the life cycle and for each application of the substance. For substances with a log *Kow* greater than 5, the equilibrium-partitioning method is used in a modified way. For these substances, the PEC/PNEC in soil is increased by a factor of 10 to account for uptake via ingestion of soil.

$$RCRlocal_{soil} = \frac{PEClocal_{soil}}{PNEC_{soil}} \quad \textbf{(306)}$$

$$RCRreg_{soil} = \frac{PECreg_{agric}}{PNEC_{soil}} \quad \textbf{(307)}$$

If *EPterr* = yes and log *Kow* > 5 then

$$RCRlocal_{soil} = \frac{PEClocal_{soil}}{PNEC_{soil}} \cdot 10 \quad \textbf{(308)}$$

If *EPterr* = yes and log *Kow* > 5 then

$$RCRreg_{soil} = \frac{PECreg_{agric}}{PNEC_{soil}} \cdot 10 \quad \textbf{(309)}$$

Input			
$PEClocal_{soil}$	local PEC in agricultural soil, averaged over 30 days	[$kg_c.kg_{wwt}^{-1}$]	O
$PECreg_{agric}$	regional steady-state PEC in agricultural soil	[$kg_c.kg_{wwt}^{-1}$]	O
$PNEC_{soil}$	PNEC for soil compartment	[$kg_c.kg_{wwt}^{-1}$]	O[c]
EPterr	equilibrium partitioning used for PNEC?	[yes/no]	O[c]
Kow	octanol-water partition coefficient	[$m^3.m^{-3}$]	S
Output			
$RCRlocal_{soil}$	RCR for local soil compartment	[-]	O[c]
$RCRreg_{soil}$	RCR for regional soil compartment	[-]	O[c]

III.7.1.3 Sediment compartment

The concentration of the chemical in sediment is compared to the no-effect concentration for sediment-dwelling organisms. This is done for the local as well as the regional freshwater and marine environment. It should be noted that the local ratios have to be defined for all relevant stages of the life cycle and for each application of the substance. For substances with a log *Kow* greater than 5, the equilibrium-partitioning method is used in a modified way. For these substances, the PEC/PNEC in sediment is increased by a factor of 10 to account for uptake via ingestion of sediment. It should be noted that a risk characterisation for sediment is only feasible if measured data are used to overwrite the estimates for PEC and/or PNEC in sediment (otherwise, equilibrium partitioning is applied to derive both PEC and PNEC).

$$RCRlocal_{sed} = \frac{PEClocal_{sed}}{PNEC_{sed}} \quad \textbf{(310)}$$

$$RCRlocal_{sed,marine} = \frac{PEClocal_{sed,marine}}{PNEC_{sed,marine}} \quad \textbf{(311)}$$

$$RCRreg_{sed} = \frac{PECreg_{sed}}{PNEC_{sed}} \quad \textbf{(312)}$$

$$RCRreg_{sed,marine} = \frac{PECreg_{sed,marine}}{PNEC_{sed,marine}} \quad \textbf{(313)}$$

If *EPsed* = yes and log *Kow* > 5 then:

$$RCRlocal_{sed} = \frac{PEClocal_{sed}}{PNEC_{sed}} \cdot 10 \quad \textbf{(314)}$$

$$RCRreg_{sed} = \frac{PECreg_{sed}}{PNEC_{sed}} \cdot 10 \quad \textbf{(315)}$$

If $EPsed_{marine}$ = yes and log *Kow* > 5 then:

$$RCRlocal_{sed,marine} = \frac{PEClocal_{sed,marine}}{PNEC_{sed,marine}} \cdot 10 \quad \textbf{(316)}$$

$$RCRreg_{sed,marine} = \frac{PECreg_{sed,marine}}{PNEC_{sed,marine}} \cdot 10 \quad \textbf{(317)}$$

Input			
$PEClocal_{sed}$	local PEC in sediment	[$kg_c.kg_{wwt}^{-1}$]	O
$PEClocal_{sed,marine}$	local PEC in marine sediment	[$kg_c.kg_{wwt}^{-1}$]	O
$PECreg_{sed}$	regional steady-state PEC in sediment	[$kg_c.kg_{wwt}^{-1}$]	O
$PECreg_{sed,marine}$	regional steady-state PEC in marien sediment	[$kg_c.kg_{wwt}^{-1}$]	O
$PNEC_{sed}$	PNEC for the sediment compartment	[$kg_c.kg_{wwt}^{-1}$]	O
$PNEC_{sed,marine}$	PNEC for the marine sediment compartment	[$kg_c.kg_{wwt}^{-1}$]	O
EPsed	equilibrium partitioning used for PNEC for sediment?	[yes/no]	O[c]
$EPsed_{marine}$	equilibrium partitioning used for PNEC for marine sediment?	[yes/no]	O[c]
Kow	octanol-water partition coefficient	[$m^3.m^{-3}$]	S
Output			
$RCRlocal_{sed}$	RCR for local sediment compartment	[-]	O[c]
$RCRlocal_{sed,marine}$	RCR for local marine sediment compartment	[-]	O[c]
$RCRreg_{sed}$	RCR for regional sediment compartment	[-]	O[c]
$RCRreg_{sed,marine}$	RCR for regional marine sediment compartment	[-]	O[c]

III.7.1.4 Micro-organisms in STP

The concentration of the chemical in the sewage treatment plant is compared to the no-effect concentration for micro-organisms. This is done for the local environment only. The concentration during an emission episode is used. It should be noted that the ratios have to be defined for all relevant stages of the life cycle and for each application of the substance.

$$RCR_{stp} = \frac{PEC_{stp}}{PNEC_{micro\text{-}organisms}} \quad \textbf{(318)}$$

Input			
PEC_{stp}	local PEC in STP during emission episode	[$kg_c.m^{-3}$]	O
$PNEC_{micro\text{-}organisms}$	PNEC for STP micro-organisms	[$kg_c.m^{-3}$]	O[c]
Output			
RCR_{stp}	RCR for sewage treatment plant	[-]	O[c]

III.7.1.5 Predators in freshwater and marine environment

The concentration of the chemical in fish and in fish-eating predator is compared to the no-effect concentration for birds and mammals. Local and regional concentrations are combined for calculating the concentration in fish and fish-eating predator . It should be noted that the ratios have to be defined for all relevant stages of the life cycle and for each application of the substance.

$$RCR_{oral,fish} = \frac{PEC_{oral,fish}}{PNEC_{oral}} \quad \textbf{(319)}$$

$$RCR_{oral,fish,marine} = \frac{PEC_{oral,fish,marine}}{PNEC_{oral}} \quad \textbf{(320)}$$

$$RCR_{oral,\,fish\ predator,\,marine} = \frac{PEC_{oral,\,fish\ predator,\,marine}}{PNEC_{oral}} \quad \textbf{(321)}$$

put			
$PEC_{oral,fish}$	PEC in fish (local and regional combined)	[$kg_c.kg_{wwt}^{-1}$]	O
$PEC_{oral,fish,marine}$	PEC in marine fish (local and regional combined)	[$kg_c.kg_{wwt}^{-1}$]	O
$PEC_{oral,fish\ predator,marine}$	PEC in marine fish-eating predator (local and regional combined)	[$kg_c.kg_{wwt}^{-1}$]	O
$PNEC_{oral}$	PNEC for birds and mammals	[$kg_c.kg_{wwt}^{-1}$]	O[c]
Output			
$RCR_{oral,fish}$	RCR for fish-eating birds/mammals (freshwater environment)	[-]	O[c]
$RCR_{oral,fish,marine}$	RCR for fish-eating birds/mammals (marine environment)	[-]	O[c]
$RCR_{oral,fish\ predator,marine}$	RCR for top-predators (marine environment)	[-]	O[c]

III.7.1.6 Worm-eating predators

The concentration of the chemical in earthworms is compared to the no-effect concentration for birds and mammals. There is only one concentration in earthworms as local and regional are combined in this concentration. It should be noted that the ratios have to be defined for all relevant stages of the life cycle and for each application of the substance.

$$RCR_{oral,worm} = \frac{PEC_{oral,worm}}{PNEC_{oral}} \quad \textbf{(322)}$$

Input			
$PEC_{oral,worm}$	PEC in worm (local and regional combined)	[$kg_c.kg_{wwt}^{-1}$]	O
$PNEC_{oral}$	PNEC for birds and mammals	[$kg_c.kg_{wwt}^{-1}$]	O[c]
Output			
$RCR_{oral,worm}$	RCR for worm-eating birds and mammals	[-]	O[c]

III.7.2 Risk characterisation for human health

For threshold-based effects, the quantitative risk characterisation is carried out by calculating 'Margins Of Safety' (MOS) and comparing this to a reference-MOS (MOS approach). This MOS approach is not applicable for non-threshold based effects. Next to the MOS approach, **for biocides** an Acceptable Operator Exposure Level (AOEL) is to be derived, which should be compared to the estimated exposure values. For non-threshold effects, i.e. genotoxic carcinogens, lifetime cancer risk is calculated based on T25 or CED05. Additionally, the Margin of Exposure (MOE) is calculated and compared to a reference-MOE (RMOE).

Table III-108 Defaults factors

Assessment factor	**Symbol**	**Unit**	**Value**
Allometric scaling factor	AF_{allom}	[-]	1[a]
Remaining interspecies differences	AF_{inter}	[-]	1[b]
Intraspecies differences	AF_{intra}	[-]	1[c]
Differences in exposure duration	AF_{expdur}	[-]	1[d]
Differences in exposure route	AF_{exprt}	[-]	1[e]
Dose-response relationship	$AF_{dose\text{-}resp}$	[-]	1[f]
Low risk extrapolation factor	AF_{lr}	[-]	250,000[g]
Correction factors workers			
Correction factor for route-to route extrapolation to account for difference in ventilation rate between workers and general population	CF_{occup1}	[-]	1[h]
Correction factor for duration and frequency of exposure	CF_{occup2}	[-]	2.8

[a] Correction for differences in metabolic size: the TGD recommends 4 for rats, 7 for mice, 3 for guinea pigs, 2.4 for rabbits, 2 for monkeys and 1.4 for dogs
[b] The TGD recommends 2.5
[c] The TGD recommends 5 for workers and 10 for the general population
[d]The TGD recommends 3 for subacute to sub/semi-chronic extrapolation, 2 for sub/semi-chronic to chronic extrapolation amd 6 for subacute to chronic extrapolation
[e] Factor to account for uncertainty in the route-to-route extrapolation
[f] Factor to account for uncertainty in the dose-response extrapolation; includes uncertainty regarding the nature of the effect and the quality of the database
[g] Factor, used for the calculation of the reference-MOE for non-threshold substances, accounting for the extrapolation for the high risk related to the T25 (25:100) to a low reference level, default chosen to be $1{:}10^6$
[h] Factor accounting for the difference between the respiratory rate of the general population (default 20 m^3 per 24 hrs) used in the route-to-route extrapolation and the respiratory rate of workers (10 m^3 in 8 hrs). The TGD recommends a factor of 0.5 for extrapolations from the dermal and oral route to the inhalatory route and 2 for extrapolations from the inhalatory route to the dermal and oral route.

III.7.2.1 Risk characterisation for humans exposed via the environment

III.7.2.1.1 Threshold substances

Calculation of scenario-specific MOS

Under the assumption that man is exposed throughout his or her lifetime, the total daily intake of a substance in food, drinking water and air is compared to the oral N(L)OAEL from repeated dose toxicity studies, carcinogenicity studies (unless carcinogenicity is via a non-threshold mode of action) and/or reproductive toxicity studies, resulting in a Risk Characterisation Ratio (RCR) called the Margin Of Safety, MOS. This comparison is made for both the local and the regional scale. If both an N(L)OAEL for man and an N(L)OAEL for mammals are available, the former one is used in this risk characterisation. In addition, the air concentration estimated for man in the standard environment is compared to the inhalatory N(L)OAEL for these endpoints.

Depending on the available data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOSman\text{-}env_{local,tot,i}$	$DOSElocal_{tot}$	$NOAEL_{mammal,oral,i}$ $LOAEL_{mammal,oral,i}$ $NOAEL_{man,oral,i}$ $LOAEL_{man,oral,i}$ $CED_{mammal,oral,i}$
$MOSman\text{-}env_{reg,tot,i}$	$DOSEreg_{tot}$	$NOAEL_{mammal,oral,i}$ $LOAEL_{mammal,oral,i}$ $NOAEL_{man,oral,i}$ $LOAEL_{man,oral,i}$ $CED_{mammal,oral,i}$
$MOSman\text{-}env_{local,inh,i}$	$PEClocal_{air,ann}$	$NOAEL_{mammal,inh,i}$ $LOAEL_{mammal,inh,i}$ $NOAEL_{man,inh,i}$ $LOAEL_{man,inh,i}$ $CED_{mammal,inh,i}$
$MOSman\text{-}env_{reg,inh,i}$	$PECreg_{air}$	$NOAEL_{mammal,inh,i}$ $LOAEL_{mammal,inh,i}$ $NOAEL_{man,inh,i}$ $LOAEL_{man,inh,i}$ $CED_{mammal,inh,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint of concern	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint of concern	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint of concern	$[kg_c.m^{-3}]$	S
$DOSElocal_{tot}$	local total daily intake for humans	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$DOSEreg_{tot}$	regional total daily intake for humans	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$PEClocal_{air,ann}$	annual average local PEC in air (total)	$[kg_c.m^{-3}]$	O
$PECreg_{air}$	regional PEC in air (total)	$[kg_c.m^{-3}]$	O
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MOSman\text{-}env_{local,tot,i}$	MOS local, total exposure via all media, for endpoint of concern	[-]	O[c]
$MOSman\text{-}env_{local,inh,i}$	MOS local, exposure via air, for endpoint of concern	[-]	O[c]
$MOSman\text{-}env_{reg,tot,i}$	MOS regional, total exposure via all media, for endpoint of conc.	[-]	O[c]
$MOSman\text{-}env_{reg,inh,i}$	MOS regional, exposure via air, for endpoint of concern	[-]	O[c]
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Derivation of scenario-specific reference-MOS

In order to account for the various uncertainties and variabilities in the extrapolation from experimental data to the human situation and in the available data set, per scenario under consideration a reference-MOS is to be derived. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOS (RMOS).

$$RMOSman - env_{x,y,i} = AF_{inter} \cdot AF_{allom} \cdot AF_{intra} \cdot AF_{expdur} \cdot AF_{exprt} \cdot AF_{dose-resp} \quad \textbf{(323)}$$

$x \in$ {local,reg}
$y \in$ {tot,inh}
$i \in$ {repdose,carc,fert,mattox,devtox}

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{inter}	assessment factor for remaining interspecies differences	[-]	S/D
AF_{intra}	assessment factor for intraspecies differences	[-]	S/D
AF_{expdur}	assessment factor for differences in exposure duration	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose\text{-}resp}$	assessment factor for dose-response relationship	[-]	S/D

Output

$RMOSman\text{-}env_{local,tot,i}$	reference-MOS local, total exposure via all media, for endpoint of concern	[-]	O[c]
$RMOSman\text{-}env_{local,inh,i}$	reference-MOS local, exposure via air, for endpoint of concern	[-]	O[c]
$RMOSman\text{-}env_{reg,tot,i}$	reference-MOS regional, total exposure via all media, for endpoint of concern	[-]	O[c]
$RMOSman\text{-}env_{reg.inh,i}$	reference-MOS regional, exposure via air, for endpoint of concern	[-]	O[c]
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Comparison of MOS with reference-MOS

In judging the acceptability of the MOS, in a second step of the quantitative risk characterisation the MOS is compared to the reference-MOS, resulting in a MOS/reference-MOS ratio (MRR).

Depending on the available data the following MRRs are possible:

RCR / reference-MOS	**RCR**	**Reference-MOS**
MRRman-$env_{local,tot,i}$	MOSman-$env_{local,tot,i}$	RMOSman-$env_{local,tot,i}$
MRRman-$env_{reg,tot,i}$	MOSman-$env_{reg,tot,i}$	RMOSman-$env_{reg,tot,i}$
MRRman-$env_{local,inh,i}$	MOSman-$env_{local,inh,i}$	RMOSman-$env_{local,inh,i}$
MRRman-$env_{reg,inh,i}$	MOSman-$env_{reg,inh,i}$	RMOSman-$env_{reg,inh,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

MOSman-$env_{local,tot,i}$	MOS local, total exposure via all media, for endpoint of concern	[-]	O^c
MOSman-$env_{local,inh,i}$	MOS local, exposure via air, for endpoint of concern	[-]	O^c
MOSman-$env_{reg,tot,i}$	MOS regional, total exposure via all media, for endpoint of conc.	[-]	O^c
MOSman-$env_{reg,inh,i}$	MOS regional, exposure via air, for endpoint of concern	[-]	O^c
RMOSman-$env_{local,tot,i}$	reference-MOS local, total exposure via all media, for endpoint of concern	[-]	O^c
RMOSman-$env_{local,inh,i}$	reference-MOS local, exposure via air, for endpoint of concern	[-]	O^c
RMOSman-$env_{reg,tot,i}$	reference-MOS regional, total exposure via all media, for endpoint of concern	[-]	O^c
RMOSman-$env_{reg.inh,i}$	reference-MOS regional, exposure via air, for endpoint of concern $i \in$ {repdose,carc,fert,mattox,devtox}	[-]	O^c

Output

MRRman-$env_{local,tot,i}$	ratio MOS/reference-MOS local, total exposure via all media, for endp. of concern	[-]	O^c
MRRman-$env_{local,inh,i}$	ratio MOS/reference-MOS local, exposure via air, for endpoint of concern	[-]	O^c
MRRman-$env_{reg,tot,i}$	ratio MOS/reference-MOS regional, total exposure via all media, for endp. of conc.	[-]	O^c
MRRman-$env_{reg.inh,i}$	ratio MOS/reference-MOS regional, exposure via air, for endpoint of concern $i \in$ {repdose,carc,fert,mattox,devtox}	[-]	O^c

III.7.2.1.2 Non-threshold substances

A. Lifetime carcinogenic risk

Starting point is the T25 which first needs to be converted to an equivalent human dose descriptor, the HT25, applying allometric assessment factors and, possibly, an assessment factor for route-to-route extrapolation.

$$AFman - env_{x,y,nt} = AF_{allom} \cdot AF_{\exp rt}$$

$x \in$ {local,reg}

$y \in$ {tot,inh}

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D

Output

AFman-$env_{local,tot,nt}$	assessment factor local, exposure via all media, non-thr.	[-]	S/O
AFman-$env_{reg,tot,nt}$	assessment factor regional, exposure via all media, non-thr.	[-]	S/O
AFman-$env_{local,inh,nt}$	assessment factor local, exposure via air, non-thr.	[-]	S/O
AFman-$env_{local,inh,nt}$	assessment factor regioanl, exposure via air, non-thr.	[-]	S/O

$$HT25man-env_{x,tot,nt} = \frac{T25_{mammal,oral,nt}}{AFman-env_{x,tot,nt}} \quad (324)$$

$$HT25man-env_{x,inh,nt} = \frac{T25_{mammal,inh,nt}}{AFman-env_{x,inh,nt}} \quad (325)$$

$x \in$ {local,reg}

Input

$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	[$kg_c.m^{-3}$]	S/O
AFman-$env_{local,tot,nt}$	assessment factor local, exposure via all media, non-thr.	[-]	S/O
AFman-$env_{reg,tot,nt}$	assessment factor regional, exposure via all media, non-thr.	[-]	S/O
AFman-$env_{local,inh,nt}$	assessment factor local, exposure via air, non-thr.	[-]	S/O
AFman-$env_{local,inh,nt}$	assessment factor regioanl, exposure via air, non-thr.	[-]	S/O

Output

HT25man-$env_{local,tot,nt}$	human equivalent dose local, exposure via all media, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
HT25man-$env_{reg,tot,nt}$	human equivalent dose regional, exposure via all media, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
HT25man-$env_{local,inh,nt}$	human equivalent dose local, exposure via air media, non-thr.	[$kg_c.m^{-3}$]	O
HT25man-$env_{reg,inh,nt}$	human equivalent dose regional, exposure via air media, non-thr.	$kg_c.m^{-3}$]	O

Subsequently the lifetime cancer risk is calculated for total exposure to and inhalation of ambient air at each spatial scale.

$$cLRman-env_{local,tot,nt} = \frac{DOSElocal_{tot}}{HT25man-env_{local,tot,nt}} \cdot 0.25 \quad (326)$$

$$cLRman-env_{reg,tot,nt} = \frac{DOSEreg_{tot}}{HT25man-env_{reg,tot,nt}} \cdot 0.25 \quad (327)$$

$$cLRman-env_{local,inh,nt} = \frac{PEClocal_{air,ann}}{HT25man-env_{local,inh,nt}} \cdot 0.25 \quad (328)$$

$$cLRman-env_{reg,inh,nt} = \frac{PECreg_{air}}{HT25man-env_{reg,inh,nt}} \cdot 0.25 \quad (329)$$

Input

$DOSElocal_{tot}$	local total daily intake for humans	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$DOSEreg_{tot}$	regional total daily intake for humans	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$PEClocal_{air,ann}$	annual average local PEC in air (total)	[$kg_c.m^{-3}$]	O
$PECreg_{air}$	regional PEC in air (total)	[$kg_c.m^{-3}$]	O
$HT25man\text{-}env_{local,tot,nt}$	human equivalent dose local, exposure via all media, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$HT25man\text{-}env_{reg,tot,nt}$	human equivalent dose regional, exposure via all media, non-thr.	$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$HT25man\text{-}env_{local,inh,nt}$	human equivalent dose local, exposure via air media, non-thr.	[$kg_c.m^{-3}$]	O
$HT25man\text{-}env_{reg,inh,nt}$	human equivalent dose regional, exposure via air media, non-thr.	[$kg_c.m^{-3}$]	O

Output

$cLRman\text{-}env_{local,tot,nt}$	lifetime cancer risk local, exposure via all media, non-thr.	[-]	O
$cLRman\text{-}env_{reg,,tot,nt}$	lifetime cancer risk regional, exposure via all media, non-thr.	[-]	O
$cLRman\text{-}env_{local,inh,nt}$	lifetime cancer risk local, exposure via air, non-thr.	[-]	O
$cLRman\text{-}env_{local,inh,nt}$	lifetime cancer risk regional, exposure via air, non-thr.	[-]	O

B. Margin Of Exposure

Calculation of scenario-specific MOE

Under the assumption that man is exposed throughout his or her lifetime, the total daily intake of a substance in food, drinking water and air is compared to the oral T25 or CED (BMD05), resulting in a Risk Characterisation Ratio (RCR) called the Margin Of Exposure. This comparison is made for both the local and the regional scale. In addition, the air concentration estimated for man in the standard environment can be compared to the inhalatory T25 or CED.

Depending on the available data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOEman\text{-}env_{local,tot,i}$	$DOSElocal_{tot}$	$T25_{mammal,oral,nt}$ $CED_{mammal,oral,,nt}$
$MOEman\text{-}env_{reg,tot,i}$	$DOSEreg_{tot}$	$T25_{mammal,oral,nt}$ $CED_{mammal,oral,nt}$
$MOEman\text{-}env_{local,inh,i}$	$PEClocal_{air,ann}$	$T25_{mammal,inh,nt}$ $CED_{mammal,inh,nt}$
$MOEman\text{-}env_{reg,inh,i}$	$PECreg_{air}$	$T25_{mammal,inh,nt}$ $CED_{mammal,inh,nt}$

Input

$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,nt}$	inhalatory CED for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$DOSElocal_{tot}$	local total daily intake for humans	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$DOSEreg_{tot}$	regional total daily intake for humans	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$PEClocal_{air,ann}$	annual average local PEC in air (total)	$[kg_c.m^{-3}]$	O
$PECreg_{air}$	regional PEC in air (total)	$[kg_c.m^{-3}]$	O
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MOEman\text{-}env_{local,tot,i}$	MOE local, total exposure via all media, non-thr.	[-]	O[c]
$MOEman\text{-}env_{local,inh,i}$	MOE local, exposure via air, non-thr.	[-]	O[c]
$MOEman\text{-}env_{reg,tot,i}$	MOE regional, total exposure via all media, non-thr.	[-]	O[c]
$MOEman\text{-}env_{reg,inh,i}$	MOE regional, exposure via air, non-thr.	[-]	O[c]

Derivation of scenario-specific reference-MOE

In order to account for the various uncertainties and variabilities in the extrapolation from experimental data to the human situation and in the available data set, per scenario under consideration a reference-MOE is to be derived. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOE (RMOE).

$$RMOEman-env_{x,y,nt} = AF_{inter} \cdot AF_{allom} \cdot AF_{exprt} \cdot AF_{dose-resp} \cdot AF_{lr} \quad \textbf{(330)}$$

$x \in$ {local,reg}

$y \in$ {tot,inh}

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{inter}	assessment factor for remaining interspecies differences	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose\text{-}resp}$	assessment factor for dose-response relationship	[-]	S/D
AFlr	assessment factor for extrapolation to a low risk level	[-]	S/D

Output

$RMOEman\text{-}env_{local,tot,nt}$	reference-MOE local, total exposure via all media, non-thr.	[-]	O[c]
$RMOEman\text{-}env_{local,inh,nt}$	reference-MOE local, exposure via air, non-thr.	[-]	O[c]
$RMOEman\text{-}env_{reg,tot,nt}$	reference-MOE regional, total exposure via all media, non-thr.	[-]	O[c]
$RMOEman\text{-}env_{reg.inh,nt}$	reference-MOE regional, exposure via air, non-thr.	[-]	O[c]

Comparison of MOE with reference-MOE

The MOE is compared to the reference-MOE, resulting in a MOE/reference-MOE ratio (MRR).

Depending on the available data the following MRRs are possible:

RCR / reference-MOS	**RCR**	**Reference-MOS**
$MRRman\text{-}env_{local,tot,nt}$	$MOEman\text{-}env_{local,tot,nt}$	$RMOEman\text{-}env_{local,tot,nt}$
$MRRman\text{-}env_{reg,tot,nt}$	$MOEman\text{-}env_{reg,tot,nt}$	$RMOEman\text{-}env_{reg,tot,nt}$
$MRRman\text{-}env_{local,inh,nt}$	$MOEman\text{-}env_{local,inh,nt}$	$RMOEman\text{-}env_{local,inh,nt}$
$MRRman\text{-}env_{reg,inh,nt}$	$MOEman\text{-}env_{reg,inh,nt}$	$RMOEman\text{-}env_{reg,inh,nt}$

Input

MOEman-env$_{local,tot,,nt}$	MOE local, total exposure via all media, non-thr.	[-]	O^c
MOEman-env$_{local,inh,nt}$	MOE local, exposure via air, non-thr.	[-]	O^c
MOEman-env$_{reg,tot,nt}$	MOE regional, total exposure via all media, non-thr.	[-]	O^c
MOEman-env$_{reg,inh,nt}$	MOE regional, exposure via air, non-thr.	[-]	O^c
RMOEman-env$_{local,tot,nt}$	reference-MOE local, total exposure via all media, non-thr.	[-]	O^c
RMOEman-env$_{local,inh,nt}$	reference-MOE local, exposure via air, non-thr.	[-]	O^c
RMOEman-env$_{reg,tot,nt}$	reference-MOE regional, total exposure via all media, non-thr.	[-]	O^c
RMOEman-env$_{reg.inh,nt}$	reference-MOE regional, exposure via air, non-thr.	[-]	O^c

Output

MRRman-env$_{local,tot,nt}$	ratio MOE/RMOE local, total exposure via all media, non-thr.	[-]	O^c
MRRman-env$_{reg,tot,nt}$	ratio MOE/RMOE regional, total exposure via all media, non-thr.	[-]	O^c
MRRman-env$_{local,inh,nt}$	ratio MOE/RMOE local, exposure via air, non-thr.	[-]	O^c
MRRman-env$_{reg.inh,nt}$	ratio MOE/RMOE regional, exposure via air, non-thr.	[-]	O^c

III.7.2.2 Risk characterisation for consumers

III.7.2.2.1 Threshold substances

MOS approach: Calculation of scenario-specific MOS

The concentration of the substance in air, a medium swallowed or on the skin is compared to effect or no-effect concentrations of corresponding time scale and route of exposure. Likewise, a potential dermal uptake rate for a substance in contact with the skin and an intake rate for a substance in a medium swallowed are compared to effect or no-effect doses of corresponding time scale and route of exposure. See Section III.6.2.2 for decision rules on the choice of the effect parameter in the risk characterisation for human health. If both an N(L)OAEL for man and an N(L)OAEL for mammals are available, the former one is used in this risk characterisation.

Note: Although in theory it is possible to calculate MOSs for the endpoints irritation/corrosivity and sensitisation, in practice the available toxicological database does not allow the derivation of a threshold for these endpoints. Therefore, MOS calculations for these endpoints have not been implemented in EUSES, but EUSES allows the user to flag substances for these properties (see Section III.6.2.2).

Inhalation exposure

Depending on the time scale of the exposure scenario and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOScons_{inh,acute}$	C_{inh}	$LC50_{mammal,inh}$ $NOAEL_{man,inh,acute}$ $LOAEL_{man,inh,acute}$
$MOScons_{inh,i}$	$C_{inh,ann}$	$NOAEL_{mammal,inh,i}$ $LOAEL_{mammal,inh,i}$ $NOAEL_{man,inh,i}$ $LOAEL_{man,inh,i}$ $CED_{mammal,inh,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$LC50_{mammal,inh}$	inhalatory LC50 for mammals	$[kg_c.m^{-3}]$	S
$N(L)OAEL_{man,inh,acute}$	inhalatory N(L)OAEL for man for acute effects	$[kg_c.m^{-3}]$	S
$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint of concern	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint of concern	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint of concern	$[kg_c.m^{-3}]$	S
C_{inh}	concentration in air of room	$[kg_c.m^{-3}]$	O
$C_{inh,ann}$	annual average inhalation exposure concentration $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.m^{-3}]$	O

Output

$MOScons_{inh,acute}$	MOS acute, inhalatory exposure	[-]	O^c
$MOScons_{inh,i}$	MOS for endpoint of concern, inhalatory exposure $i \in$ {repdose,carc,fert,mattox,devtox}	[-]	O^c

Dermal exposure

Depending on the time scale of the exposure scenario and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOScons_{der,acute}$	$U_{der,pot}$	$LD50_{mammal,der}$ $NOAEL_{man,der,acute}$ $LOAEL_{man,der,acute}$
	C_{der}	$NOEC_{man,medium,acute}$ $LOEC_{man,medium,acute}$
$MOScons_{der,i}$	$U_{der,pot}$	$NOAEL_{mammal,der,i}$ $LOAEL_{mammal,der,i}$ $NOAEL_{man,der,i}$ $LOAEL_{man,der,i}$ $CED_{mammal,der,i}$
	$C_{der,ann}$	$NOEC_{man,medium,i}$ $LOEC_{man,medium,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$LD50_{mammal,der}$	dermal LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{man,der,acute}$	dermal N(L)OAEL for man for acute effects	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OEC_{man,medium,acute}$	dermal N(L)OEC in a medium for man for acute effects	$[kg_c.m^{-3}]$	S
$N(L)OAEL_{mammal,der,i}$	dermal N(L)OAEL for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,der,i}$	dermal N(L)OAEL for man for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,i}$	dermal CED for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$N(L)OEC_{man,medium,i}$	dermal N(L)OEC in a medium for man for endpoint of concern	$[kg_c.m^{-3}]$	S
$U_{der,pot}$	potential dermal uptake rate	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
C_{der}	concentration of substance in product on skin	$[kg_c.m^{-3}]$	O
$C_{der,ann}$	annual average dermal exposure concentration	$[kg_c.m^{-3}]$	O
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MOScons_{der,acute}$	MOS acute, dermal exposure	[-]	O^c
$MOScons_{der,i}$	MOS for endpoint of concern, dermal exposure	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Oral exposure

Depending on the time scale of the exposure scenario and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOScons_{oral,acute}$	I_{oral}	$LD50_{mammal,oral}$ $DD_{mammal,oral}$ $NOAEL_{man,oral,acute}$ $LOAEL_{man,oral,acute}$
$MOScons_{oral,i}$	I_{oral}	$NOAEL_{mammal,oral,i}$ $LOAEL_{mammal,oral,i}$ $NOAEL_{man,oral,i}$ $LOAEL_{man,oral,i}$ $CED_{mammal,oral,i}$
	$C_{oral,ann}$ / RHO_{prod}	$NOEC_{mammal,food,i}$ $LOEC_{mammal,food,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$LD50_{mammal,oral}$	oral LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$DD_{mammal,oral}$	oral Discriminating Dose for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{man,oral,acute}$	oral N(L)OAEL for man for acute effects	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$N(L)OEC_{mammal,food,i}$	N(L)OEC via food for mammals for endpoint of concern	$[kg_c.kg_{food}^{-1}]$	S
RHO_{prod}	density of product before dilution	$[kg.m^{-3}]$	S
I_{oral}	ingestion rate of substance	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$C_{oral,ann}$	annual average oral exposure concentration $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.m^{-3}]$	O

Output

$MOScons_{oral,acute}$	MOS acute, oral exposure	[-]	O[c]
$MOScons_{oral,i}$	MOS for endpoint of concern, oral exposure $i \in$ {repdose,carc,fert,mattox,devtox}	[-]	O[c]

Total exposure via all routes

Depending on the time scale and available effects data the following RCRs are possible:

Effects / Exposure	Exposure	Available effects data
$MOScons_{tot,acute}$	U_{tot} / $BIO_{oral,2}$	$LD50_{mammal,oral}$ $DD_{mammal,oral}$ $NOAEL_{man,oral,acute}$ $LOAEL_{man,oral,acute}$
$MOScons_{tot,i}$	U_{tot} / $BIO_{oral,2}$	$NOAEL_{mammal,oral,i}$ $LOAEL_{mammal,oral,i}$ $NOAEL_{man,oral,i}$ $LOAEL_{man,oral,i}$ $CED_{mammal,oral,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$LD50_{mammal,oral}$	oral LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$DD_{mammal,oral}$	oral Discriminating Dose for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{man,oral,acute}$	oral N(L)OAEL for man for acute effects	$[kg_c.kg_{bw}^{-1}]$	S
$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint of concern	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$BIO_{oral,2}$	bioavailability for oral uptake (starting route)	[-]	S/D
U_{tot}	total uptake for one product via different routes $i \in$ {repdose,carc,fert,mattox,devtox}	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

Output

$MOScons_{tot,acute}$	MOS acute, total exposure	[-]	O[c]
$MOScons_{tot,i}$	MOS for endpoint of concern, total exposure $i \in$ {repdose,carc,fert,mattox,devtox}	[-]	O[c]

Derivation of scenario-specific reference-MOS

In order to account for the various uncertainties and variabilities in the extrapolation from experimental data to the human situation and in the available data set, per scenario under consideration a reference-MOS is to be derived. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOS (RMOS).

$$RMOScons_{y,acute} = AF_{inter} \cdot AF_{allom} \cdot AF_{intra} \cdot AF_{expdur} \cdot AF_{exprt} \cdot AF_{dose-resp} \quad (331)$$

$$RMOScons_{y,i} = AF_{inter} \cdot AF_{allom} \cdot AF_{intra} \cdot AF_{expdur} \cdot AF_{exprt} \cdot AF_{dose-resp} \quad (332)$$

$y \in$ {inh,der,oral,tot}
$i \in$ {repdose,carc,fert,mattox,devtox}

Input			
AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{inter}	assessment factor for remaining interspecies differences	[-]	S/D
AF_{intra}	assessment factor for intraspecies differences	[-]	S/D
AF_{expdur}	assessment factor for differences in exposure duration	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose\text{-}resp}$	assessment factor for dose-response relationship	[-]	S/D
AF_{nature}	assessment factor for nature of effect	[-]	S/D
AF_{data}	assessment factor for adequacy of/confidence in database	[-]	S/D
Output			
$RMOScons_{inh,acute}$	reference-MOS inhalatory exposure, for acute toxicity	[-]	O^c
$RMOScons_{der,acute}$	reference-MOS dermal exposure, for acute toxicity	[-]	O^c
$RMOScons_{oral,acute}$	reference-MOS oral exposure, for acute toxicity	[-]	O^c
$RMOScons_{tot,acute}$	reference-MOS total exposure, for acute toxicity	[-]	O^c
$RMOScons_{inh,i}$	reference-MOS inhalatory exposure, for endpoint of concern	[-]	O^c
$RMOScons_{der,i}$	reference-MOS dermal exposure, for endpoint of concern	[-]	O^c
$RMOScons_{oral,i}$	reference-MOS oral exposure, for endpoint of concern	[-]	O^c
$RMOScons_{tot,i}$	reference-MOS total exposure, for endpoint of concern	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Comparison of MOS with reference-MOS

In judging the acceptability of the MOS, in a second step of the quantitative risk characterisation the MOS is compared to the reference-MOS, resulting in a MOS/reference-MOS ratio (MRR).

Depending on the available data the following MRRs are possible:

RCR / reference-MOS	**RCR**	**reference-MOS**
$MRRcons_{inh,acute}$	$MOScons_{inh,acute}$	$RMOScons_{inh,acute}$
$MRRcons_{inh,i}$	$MOScons_{inh,i}$	$RMOScons_{inh,i}$
$MRRcons_{der,acute}$	$MOScons_{der,acute}$	$RMOScons_{der,acute}$
$MRRcons_{der,i}$	$MOScons_{der,i}$	$RMOScons_{der,i}$
$MRRcons_{oral,acute}$	$MOScons_{oral,acute}$	$RMOScons_{oral,acute}$
$MRRcons_{oral,i}$	$MOScons_{oral,i}$	$RMOScons_{oral,i}$
$MRRcons_{tot,acute}$	$MOScons_{tot,acute}$	$RMOScons_{tot,acute}$
$MRRcons_{tot,i}$	$MOScons_{tot,i}$	$RMOScons_{tot,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input			
$MOScons_{inh,acute}$	MOS acute, inhalatory exposure	[-]	O^c
$MOScons_{inh,i}$	MOS for endpoint of concern, inhalatory exposure	[-]	O^c
$MOScons_{der,acute}$	MOS acute, dermal exposure	[-]	O^c
$MOScons_{der,i}$	MOS for endpoint of concern, dermal exposure	[-]	O^c
$MOScons_{oral,acute}$	MOS acute, oral exposure	[-]	O^c
$MOScons_{oral,i}$	MOS for endpoint of concern, oral exposure	[-]	O^c
$MOScons_{tot,acute}$	MOS acute, total exposure	[-]	O^c
$MOScons_{tot,i}$	MOS for endpoint of concern, total exposure	[-]	O^c
$RMOScons_{inh,acute}$	reference-MOS inhalatory exposure, for acute toxicity	[-]	O^c
$RMOScons_{der,acute}$	reference-MOS dermal exposure, for acute toxicity	[-]	O^c
$RMOScons_{oral,acute}$	reference-MOS oral exposure, for acute toxicity	[-]	O^c
$RMOScons_{tot,acute}$	reference-MOS total exposure, for acute toxicity	[-]	O^c
$RMOScons_{inh,i}$	reference-MOS inhalatory exposure, for endpoint of concern	[-]	O^c
$RMOScons_{der,i}$	reference-MOS dermal exposure, for endpoint of concern	[-]	O^c
$RMOScons_{oral,i}$	reference-MOS oral exposure, for endpoint of concern	[-]	O^c
$RMOScons_{tot,i}$	reference-MOS total exposure, for endpoint of concern $i \in$ {repdose,carc,fert,mattox,devtox}	[-]	O^c
Output			
$MRRcons_{inh,acute}$	ratio MOS/reference-MOS inhalatory exposure, for acute toxicity	[-]	O^c
$MRRcons_{der,acute}$	ratio MOS/reference-MOS dermal exposure, for acute toxicity	[-]	O^c
$MRRcons_{oral,acute}$	ratio MOS/reference-MOS oral exposure, for acute toxicity	[-]	O^c
$MRRcons_{tot,acute}$	ratio MOS/reference-MOS total exposure, for acute toxicity	[-]	O^c
MRRconsinh,i	ratio MOS/reference-MOS inhalatory exposure, for endpoint of concern	[-]	Oc
MRRconsder,i	ratio MOS/reference-MOS dermal exposure, for endpoint of concern	[-]	Oc
MRRconsoral,i	ratio MOS/reference-MOS oral exposure, for endpoint of concern	[-]	Oc
MRRconstot,i	ratio MOS/reference-MOS total exposure, for endpoint of concern $i \in$ {repdose,carc,fert,mattox,devtox}	[-]	Oc

III.7.2.2.2 Method for non-threshold based effects

A. Lifetime carcinogenic risk

Starting point is the T25 which first needs to be converted to an equivalent human dose descriptor, the HT25, applying allometric assessment factors and, possibly, an assessment factor for route-to-route extrapolation.

$$AFcons_{x,nt} = AF_{allom} \cdot AF_{exprt} \quad \textbf{(333)}$$

$x \in$ {inh,der,oral,tot}

Input			
AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
Output			
$AFcons_{linh,nt}$	assessment factor for inhalatory exposure, non-thr.	[-]	S/O
$AFcons_{der,nt}$	assessment factor for dermal exposure, non-thr.	[-]	S/O
$AFcons_{oral,nt}$	assessment factor for oral exposure, non-thr.	[-]	S/O
$AFcons_{tot,nt}$	assessment factor for total exposure, non-thr.	[-]	S/O

$$HT25cons_{x,nt} = \frac{T25_{mammal,x,nt}}{AFcons_{x,nt}} \quad \textbf{(334)}$$

$x \in$ {inh, der,oral,tot}

Input

$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	[$kg_c.m^{-3}$]	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$AFcons_{linh,nt}$	assessment factor for inhalatory consumer exposure, non-thr.	[-]	S/O
$AFcons_{der,nt}$	assessment factor for dermal consumer exposure, non-thr.	[-]	S/O
$AFcons_{oral,nt}$	assessment factor for oral consumer exposure, non-thr.	[-]	S/O
$AFcons_{tot,nt}$	assessment factor for total consumer exposure, non-thr.	[-]	S/O

Output

$HT25cons_{inh,nt}$	human equivalent dose inhalatory consumer exposure, non-thr.	[$kg_c.m^{-3}$]	O
$HT25cons_{der,nt}$	human equivalent dose dermal consumer exposure, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$HT25cons_{oral,nt}$	human equivalent dose oral consumer exposure, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$HT25cons_{tot,nt}$	human equivalent dose total consumer exposure, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O

Subsequently the lifetime cancer risk is calculated for each route of exposure.

$$cLRcons_{inh,nt} = \frac{C_{inh,ann}}{HT25cons_{inh,nt}} \cdot 0.25 \quad (335)$$

$$cLRcons_{der,nt} = \frac{U_{der,pot}}{HT25cons_{der,nt}} \cdot 0.25 \quad (336)$$

$$cLRcons_{oral,nt} = \frac{I_{oral}}{HT25cons_{oral,nt}} \cdot 0.25 \quad (337)$$

$$cLRcons_{tot,nt} = \frac{U_{tot}}{HT25cons_{tot,nt}} \cdot 0.25 \quad (338)$$

Input

C_{inh}	annual average inhalation exposure concentration	[$kg_c.m^{-3}$]	O
$U_{der,pot}$	potential dermal uptake rate	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
I_{oral}	ingestion rate of substance	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
U_{tot}	total uptake for one product via different routes	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$HT25cons_{inh,nt}$	human equivalent dose inhalatory consumer exposure, non-thr.	[$kg_c.m^{-3}$]	O
$HT25cons_{der,nt}$	human equivalent dose dermal consumer exposure, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$HT25cons_{oral,nt}$	human equivalent dose oral consumer exposure, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$HT25cons_{tot,nt}$	human equivalent dose total consumer exposure, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O

Output

$cLRcons_{inh,nt}$	lifetime cancer risk, inhalatory consumer exposure, non-thr.	[-]	O
$cLRcons_{der,nt}$	lifetime cancer risk, dermal consumer exposure, non-thr.	[-]	O
$cLRcons_{oral,nt}$	lifetime cancer risk oral consumer exposure, non-thr.	[-]	O
$cLRcons_{tot,nt}$	lifetime cancer risk, total consumer exposure, non-thr.	[-]	O

B. Margin Of Exposure

Calculation of scenario-specific MOE

Under the assumption that man is exposed throughout his or her lifetime, consumer exposure to a substance is compared to the T25 or CED (BMD05), resulting in a Risk Characterisation Ratio (RCR) called the Margin Of Exposure. This comparison is made for all routes of exposure.

Depending on the available data the following RCRs are possible:

Effects / Exposure	Exposure	Available effects data
$MOECons_{inh,nt}$	$C_{inh,ann}$	$T25_{mammal,inh,nt}$ $CED_{mammal,inh,,nt}$
$MOECons_{der,nt}$	$U_{der,pot}$	$T25_{mammal,der,nt}$ $CED_{mammal,der,nt}$
$MOECons_{oral,nt}$	I_{oral}	$T25_{mammal,oral,nt}$ $CED_{mammal,oral,nt}$
$MOECons_{tot,nt}$	$U_{tot}/BIO_{oral,2}$	$T25_{mammal,oral,nt}$ $CED_{mammal,oral,nt}$

Input

$T25_{mammal,inh,nt}$	inhalatory T25 for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$CED_{mammal,inh,nt}$	inhalatory CED for mammals for non-threshold effects	$[kg_c.m^{-3}]$	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,der,nt}$	dermal CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$T25_{mammal,oral,nt}$	oral T25 for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$CED_{mammal,oral,nt}$	oral CED for mammals for non-threshold effects	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
C_{inh}	annual average inhalation exposure concentration	$[kg_c.m^{-3}]$	O
$U_{der,pot}$	potential dermal uptake rate	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
I_{oral}	ingestion rate of substance	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
U_{tot}	total uptake for one product via different routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
$BIO_{oral,2}$	bioavailability for oral uptake, starting route		

Output

$MOECons_{inh,nt}$	MOE inhalatory consumer exposure, non-thr.	[-]	O^c
$MOECons_{der,nt}$	MOE dermal consumer exposure, non-thr.	[-]	O^c
$MOECons_{oral,nt}$	MOE oral consumer exposure, non-thr.	[-]	O^c
$MOECons_{tot,nt}$	MOE total consumer exposure, non-thr.	[-]	O^c

Derivation of scenario-specific reference-MOE

In order to account for the various uncertainties and variabilities in the extrapolation from experimental data to the consumer situation and in the available data set, per scenario under consideration a reference-MOE is to be derived. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOE (RMOE).

$$RMOECons_{x,nt} = AF_{inter} \cdot AF_{allom} \cdot AF_{exprt} \cdot AF_{dose-resp} \cdot AF_{lr} \qquad \textbf{(339)}$$

$x \in \{inh,der,oral,tot\}$

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{inter}	assessment factor for remaining interspecies differences	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose\text{-}resp}$	assessment factor for dose-response relationship	[-]	S/D
AFlr	assessment factor for extrapolation to a low risk level	[-]	S/D

Output

$RMOEcons_{inh,nt}$	reference-MOE inhalatory consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{der,nt}$	reference-MOE dermal consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{oral,nt}$	reference-MOE oral consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{tot,nt}$	reference-MOE total consumer exposure, non-thr.	[-]	O^c

Comparison of MOE with reference-MOE

The MOE is compared to the reference-MOE, resulting in a MOE/reference-MOE ratio (MRR).

Depending on the available data the following MRRs are possible:

RCR / reference-MOS	**RCR**	**Reference-MOS**
$MRRcons_{inh,nt}$	$MOEcons_{inh,nt}$	$RMOEcons_{inh,nt}$
$MRRcons_{der,nt}$	$MOEcons_{der,nt}$	$RMOEcons_{der,nt}$
$MRRcons_{oral,nt}$	$MOEcons_{oral,nt}$	$RMOEcons_{oral,nt}$
$MRRcons_{tot,nt}$	$MOEcons_{tot,nt}$	$RMOEcons_{tot,nt}$

Input

$MOEcons_{inh,nt}$	MOE inhalatory consumer exposure, non-thr.	[-]	O^c
$MOEcons_{der,nt}$	MOE dermal consumer exposure, non-thr.	[-]	O^c
$MOEcons_{oral,nt}$	MOE oral consumer exposure, non-thr.	[-]	O^c
$MOEcons_{tot,nt}$	MOE total consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{inh,nt}$	reference-MOE inhalatory consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{der,nt}$	reference-MOE dermal consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{oral,nt}$	reference-MOE oral consumer exposure, non-thr.	[-]	O^c
$RMOEcons_{tot,nt}$	reference-MOE total consumer exposure, non-thr.	[-]	O^c

Output

$MRRcons_{inh,nt}$	ratio MOE/RMOE, inhalatory consumer exposure, non-thr.	[-]	O^c
$MRRcons_{der,nt}$	ratio MOE/RMOE, dermal consumer exposure, non-thr.	[-]	O^c
$MRRcons_{oral,nt}$	ratio MOE/RMOE, oral consumer exposure, non-thr.	[-]	O^c
$MRRcons_{tot,nt}$	ratio MOE/RMOE, total consumer exposure, non-thr.	[-]	O^c

III.7.2.3 Risk characterisation for workers

III.7.2.3.1 Threshold substances

MOS approach: Calculation of scenario-specific MOS

For the (sub-)chronic endpoints, the output of the EASE model is compared to effect or no-effect concentrations of corresponding route of exposure. For the acute endpoints, MOS calculations are based on acute exposure data, which have been introduced in EUSES separately. See Section III.6.2.2 for decision rules on the choice of the effect parameter in the risk characterisation for human health. If both an N(L)OAEL for man and an N(L)OAEL for mammals are available, the former one is used in this risk characterisation.
Note: Although in theory it is possible to calculate MOSs for the endpoints irritation/corrosivity and sensitisation, in practice the available toxicological database does not allow the derivation of a threshold for these endpoints. Therefore, MOS calculations for these endpoints have not been implemented in EUSES, but EUSES allows the user to flag substances for these properties.

Inhalation exposure

Depending on the time scale of the exposure scenario and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOSworker_{inh,acute}$	$C_{inh,worker,acute}$	$LC50_{mammal,inh}$ $NOAEL_{man,inh,acute}$ $LOAEL_{man,inh,acute}$
$MOSworker_{inh,vapour,i}$	$C_{inh,worker,vapour}$	$NOAEL_{mammal,inh,i}$ $LOAEL_{mammal,inh,i}$ $NOAEL_{man,inh,i}$ $LOAEL_{man,inh,i}$ $CED_{mammal,inh,i}$
$MOSworker_{inh,fibre,i}$	$C_{inh,worker,fibre}$	$NOAEL_{mammal,inh,fibre,i}$ $LOAEL_{mammal,inh,fibre,i}$ $NOAEL_{man,inh,fibre,i}$ $LOAEL_{man,inh,fibre,i}$ $CED_{mammal,inh,fibre,i}$
$MOSworker_{inh,dust,i}$	$C_{inh,worker,dust}$	$NOAEL_{mammal,inh,i}$ $LOAEL_{mammal,inh,i}$ $NOAEL_{man,inh,i}$ $LOAEL_{man,inh,i}$ $CED_{mammal,inh,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$LC50_{mammal,inh}$	inhalatory LC50 for mammals	[$kg_c.m^{-3}$]	S
$N(L)OAEL_{man,inh,acute}$	inhalatory N(L)OAEL for man for acute effects	[$kg_c.m^{-3}$]	S
$N(L)OAEL_{mammal,inh,i}$	inhalatory N(L)OAEL for mammals for endpoint of concern	[$kg_c.m^{-3}$]	S/O
$N(L)OAEL_{man,inh,i}$	inhalatory N(L)OAEL for man for endpoint of concern	[$kg_c.m^{-3}$]	S/O
$CED_{mammal,inh,i}$	inhalatory CED for mammals for endpoint of concern	[$kg_c.m^{-3}$]	S
$N(L)OAEL_{mammal,inh,fibre,i}$	inh. N(L)OAEL for mammals exposed to fibers for endpoint of concern	[$fibers.m^{-3}$]	S
$N(L)OAEL_{man,inh,fibre,i}$	inh. N(L)OAEL for man exposed to fibers for endpoint of concern	[$fibers.m^{-3}$]	S
$CED_{mammal,inh,fibre,i}$	inh. CED for mammals exposed to fibers for endpoint of concern	[$fibers.m^{-3}$]	S
$C_{inh,worker,acute}$	concentration in air for workers, acute exposure	[$kg.m^{-3}$]	S
$C_{inh,worker,vapour}$	vapour concentration in air for workers	[$kg.m^{-3}$]	O
$C_{inh,worker,fibre}$	fibre concentration in air for workers	[$fibers.m^{-3}$]	O
$C_{inh,worker,dust}$	dust concentration in air for workers	[$kg.m^{-3}$]	O
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MOSworker_{inh,acute}$	MOS acute, inhalatory exposure	[-]	O[c]
$MOSworker_{inh,vapour,i}$	MOS for endpoint of concern, inhalatory exposure of vapour	[-]	O[c]
$MOSworker_{inh,fibre,i}$	MOS for endpoint of concern, inhalatory exposure of fibers	[-]	O[c]
$MOSworker_{inh,dust,i}$	MOS for endpoint of concern, inhalatory exposure of dust	[-]	O[c]
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Dermal exposure

Depending on the time scale of the exposure scenario and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOSworker_{der,acute}$	$U_{der,pot,worker,acute}$	$LD50_{mammal,der}$ $NOAEL_{man,der,acute}$ $LOAEL_{man,der,acute}$
	$W_{der,worker,acute} / (TH_{der,worker} \cdot n_{worker})$	$NOEC_{man,medium,acute}$ $LOEC_{man,medium,acute}$
$MOSworker_{der,i}$	$U_{der,pot,worker}$	$NOAEL_{mammal,der,i}$ $LOAEL_{mammal,der,i}$ $NOAEL_{man,der,i}$ $LOAEL_{man,der,i}$ $CED_{mammal,der,i}$
	$W_{der,worker} / (TH_{der,worker} \cdot n_{worker})$	$NOEC_{man,medium,i}$ $LOEC_{man,medium,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$LD50_{mammal,der}$	dermal LD50 for mammals	[$kg_c.kg_{bw}^{-1}$]	S
$N(L)OAEL_{man,der,acute}$	dermal N(L)OAEL for man for acute effects	[$kg_c.kg_{bw}^{-1}$]	S
$N(L)OEC_{man,medium,acute}$	dermal N(L)OEC in a medium for man for acute effects	[$kg_c.m^{-3}$]	S
$N(L)OAEL_{mammal,der,i}$	dermal N(L)OAEL for mammals for endpoint of concern	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$N(L)OAEL_{man,der,i}$	dermal N(L)OAEL for man for endpoint of concern	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$CED_{mammal,der,i}$	dermal CED for mammals for endpoint of concern	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S
$N(L)OEC_{man,medium,i}$	dermal N(L)OEC in a medium for man for endpoint of concern	[$kg_c.m^{-3}$]	S
$U_{der,pot,worker,acute}$	potential dermal uptake for workers, acute exposure	[$kg.kg_{bw}^{-1}.d^{-1}$]	S
$W_{der,worker,acute}$	dermal weight of substance on skin of worker per day, acute exp.	[$kg.m^{-2}.d^{-1}$]	S
$U_{der,pot,worker}$	potential dermal uptake for workers	[$kg.kg_{bw}^{-1}.d^{-1}$]	O
$W_{der,worker}$	dermal weight of substance on skin of worker per day	[$kg.m^{-2}.d^{-1}$]	O
$TH_{der,worker}$	thickness of product	[m]	D
n_{worker}	mean number of events per day	[d^{-1}]	S
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MOSworker_{der,acute}$	MOS acute, dermal exposure	[-]	O[c]
$MOSworker_{der,i}$	MOS for endpoint of concern, dermal exposure	[-]	O[c]
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Total exposure

For certain scenarios there may be both dermal and inhalation exposure. Depending on the time scale of the exposure scenario and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOSworker_{tot,acute}$	$U_{tot,worker,acute}$ / $BIO_{oral,2}$	$LD50_{mammal,oral}$ $DD_{mammal,oral}$ $NOAEL_{man,oral,acute}$ $LOAEL_{man,oral,acute}$
$MOSworker_{tot\text{-}v/d,i}$	$U_{tot\text{-}v/d,worker}$ / $BIO_{oral,2}$	$NOAEL_{mammal,oral,i}$ $LOAEL_{mammal,oral,i}$ $NOAEL_{man,oral,i}$ $LOAEL_{man,oral,i}$ $CED_{mammal,oral,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$LD50_{mammal,oral}$	oral LD50 for mammals	[$kg_c.kg_{bw}^{-1}$]	S
$DD_{mammal,oral}$	oral Discriminating Dose for mammals	[$kg_c.kg_{bw}^{-1}$]	S
$N(L)OAEL_{man,oral,acute}$	oral N(L)OAEL for man for acute effects	[$kg_c.kg_{bw}^{-1}$]	S
$N(L)OAEL_{mammal,oral,i}$	oral N(L)OAEL for mammals for endpoint of concern	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$N(L)OAEL_{man,oral,i}$	oral N(L)OAEL for man for endpoint of concern	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$CED_{mammal,oral,i}$	oral CED for mammals for endpoint of concern	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S
$BIO_{oral,2}$	bioavailability for oral uptake (starting route)	[-]	S/D
$U_{tot,worker,acute}$	total uptake for one scenario via different routes, for acute effects	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$U_{tot\text{-}v/d,worker}$	total uptake (vapour + dermal) for one scenario via diff. routes	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Output

$MOSworker_{tot,acute}$	MOS acute, total exposure	[-]	O^c
$MOSworker_{tot\text{-}v/d,i}$	MOS for endpoint of concern, total exposure (vapour + dermal)	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

Derivation of scenario-specific reference-MOS

In order to account for the various uncertainties and variabilities in the extrapolation from experimental data to the human situation and in the available data set, per scenario under consideration a reference-MOS is to be derived. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOS (RMOS).

$$RMOSworker_{y,acute} = AF_{inter} \cdot AF_{allom} \cdot AF_{intra} \cdot AF_{expdur} \cdot AF_{exprt} \cdot AF_{dose-resp} \quad (340)$$

$$RMOSworker_{z,i} = AF_{inter} \cdot AF_{allom} \cdot AF_{intra} \cdot AF_{expdur} \cdot AF_{exprt} \cdot AF_{dose-resp} \cdot CF_{occup1} \quad (341)$$

$y \in$ {inh,der,tot}
$z \in$ {inh-vapour,inh-fibre,inh-dust,der,tot-v/d}
$i \in$ {repdose,carc,fert,mattox,devtox}

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{inter}	assessment factor for remaining interspecies differences	[-]	S/D
AF_{intra}	assessment factor for intraspecies differences	[-]	S/D
AF_{expdur}	assessment factor for differences in exposure duration	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose\text{-}resp}$	assessment factor for dose-response relationship	[-]	S/D
AF_{nature}	assessment factor for nature of effect	[-]	S/D
AF_{data}	assessment factor for adequacy of/confidence in database	[-]	S/D
CF_{occup1}	correction factor for respiratory rate in route-to-route extrapolation	[-]	S/D

Output

$RMOSworker_{inh,acute}$	reference-MOS inhalatory exposure, for acute toxicity	[-]	O^c
$RMOSworker_{der,acute}$	reference-MOS dermal exposure, for acute toxicity	[-]	O^c
$RMOSworker_{tot,acute}$	reference-MOS total exposure, for acute toxicity	[-]	O^c
$RMOSworker_{inh\text{-}vapour,i}$	reference-MOS inhalatory exposure of vapour, for endpoint of concern	[-]	O^c
$RMOSworker_{inh\text{-}fibre,i}$	reference-MOS inhalatory exposure of fibers, for endpoint of concern	[-]	O^c
$RMOSworker_{inh\text{-}dust,i}$	reference-MOS inhalatory exposure of dust, for endpoint of concern	[-]	O^c
$RMOSworker_{der,i}$	reference-MOS dermal exposure, for endpoint of concern	[-]	O^c
$RMOSworker_{tot\text{-}v/d,i}$	reference-MOS total exposure (vapour + dermal), for endpoint of concern	[-]	O^c
	$i \in$ {repdose,carc,fert,mattox,devtox}		

For the route-to-route extrapolation for workers involving the inhalatory route an additional

correction is used to account for the difference between the respiratory rate of the general population (default 20 m3 per 24 hrs) used in the route-to-route extrapolation and the respiratory rate of workers (10 m3 in 8 hrs). The TGD recommends a factor of 0.5 for extrapolations from the dermal and oral route to the inhalatory route and 2 for extrapolations from the inhalatory route to the dermal and oral route. EUSES allows this correction in the derivation of the RMOS, RMOE and human equivalent dose for workers. The default is 1.

Comparison of MOS with reference-MOS

In judging the acceptability of the MOS, in a second step of the quantitative risk characterisation the MOS is compared to the reference-MOS, resulting in a MOS/reference-MOS ratio (MRR).

Depending on the available data the following MRRs are possible:

RCR / reference-MOS	**RCR**	**reference-MOS**
$MRRworker_{inh,acute}$	$MOSworker_{inh,acute}$	$RMOSworker_{inh,acute}$
$MRRworker_{inh\text{-}vapour,i}$	$MOSworker_{inh\text{-}vapour,i}$	$RMOSworker_{inh\text{-}vapour,i}$
$MRRworker_{inh\text{-}fibre,i}$	$MOSworker_{inh\text{-}fibre,i}$	$RMOSworker_{inh\text{-}fibre,i}$
$MRRworker_{inh\text{-}dust,i}$	$MOSworker_{inh\text{-}dust,i}$	$RMOSworker_{inh\text{-}dust,i}$
$MRRworker_{der,acute}$	$MOSworker_{der,acute}$	$RMOSworker_{der,acute}$
$MRRworker_{der,i}$	$MOSworker_{der,i}$	$RMOSworker_{der,i}$
$MRRworker_{tot,acute}$	$MOSworker_{tot,acute}$	$RMOSworker_{tot,acute}$
$MRRworker_{tot\text{-}v/d,i}$	$MOSworker_{tot\text{-}v/d,i}$	$RMOSworker_{tot\text{-}v/d,i}$

$i \in$ {repdose,carc,fert,mattox,devtox}

Input

$MOSworker_{inh,acute}$	MOS acute, inhalatory exposure	[-]	O^c
$MOSworker_{inh,vapour,i}$	MOS for endpoint of concern, inhalatory exposure of vapour	[-]	O^c
$MOSworker_{inh,fibre,i}$	MOS for endpoint of concern, inhalatory exposure of fibers	[-]	O^c
$MOSworker_{inh,dust,i}$	MOS for endpoint of concern, inhalatory exposure of dust	[-]	O^c
$MOSworker_{der,acute}$	MOS acute, dermal exposure	[-]	O^c
$MOSworker_{der,i}$	MOS for endpoint of concern, dermal exposure	[-]	O^c
$MOSworker_{tot,acute}$	MOS acute, total exposure	[-]	O^c
$MOSworker_{tot-v/d,i}$	MOS for endpoint of concern, total exposure (vapour + dermal)	[-]	O^c
$RMOSworker_{inh,acute}$	reference-MOS inhalatory exposure, for acute toxicity	[-]	O^c
$RMOSworker_{der,acute}$	reference-MOS dermal exposure, for acute toxicity	[-]	O^c
$RMOSworker_{tot,acute}$	reference-MOS total exposure, for acute toxicity	[-]	O^c
$RMOSworker_{inh-vapour,i}$	reference-MOS inhalatory exposure of vapour, for endpoint of concern	[-]	O^c
$RMOSworker_{inh-fibre,i}$	reference-MOS inhalatory exposure of fibers, for endpoint of concern	[-]	O^c
$RMOSworker_{inh-dust,i}$	reference-MOS inhalatory exposure of dust, for endpoint of concern	[-]	O^c
$RMOSworker_{der,i}$	reference-MOS dermal exposure, for endpoint of concern	[-]	O^c
$RMOSworker_{tot-v/d,i}$	reference-MOS total exposure (vapour + dermal), for endpoint of concern $i \in$ {repdose,carc,fert,mattox,devtox}	[-]	O^c

Output

$MRRworker_{inh,acute}$	ratio MOS/reference-MOS inhalatory exposure, for acute toxicity	[-]	O^c
$MRRworker_{der,acute}$	ratio MOS/reference-MOS dermal exposure, for acute toxicity	[-]	O^c
$MRRworker_{tot,acute}$	ratio MOS/reference-MOS total exposure, for acute toxicity	[-]	O^c
$MRRworker_{inh-vapour,i}$	ratio MOS/reference-MOS inhalatory exposure of vapour, for endpoint of concern	[-]	O^c
$MRRworker_{inh-fibre,i}$	ratio MOS/reference-MOS inhalatory exposure of fibers, for endpoint of concern	[-]	O^c
$MRRworker_{inh-dust,i}$	ratio MOS/reference-MOS inhalatory exposure of dust, for endpoint of concern	[-]	O^c
$MRRworker_{der,i}$	ratio MOS/reference-MOS dermal exposure, for endpoint of concern	[-]	O^c
$MRRworker_{tot-v/d,i}$	ratio MOS/reference-MOS total exposure (vapour + dermal), for endpoint of concern $i \in$ {repdose,carc,fert,mattox,devtox}	[-]	O^c

III.7.2.3.2 Non-threshold substances

A. Lifetime carcinogenic risk

Starting point is the T25 which first needs to be converted to an equivalent human dose descriptor, the HT25, applying allometric assessment factors and, possibly, an assessment factor for route-to-route extrapolation.

$$AFwor\,\mathrm{ker}_{x,nt} = AF_{allom} \cdot AF_{\exp rt} \cdot CF_{occup1} \qquad \textbf{(342)}$$

$x \in$ {inh-vapour,inh-fibre, inh-dust, der,tot-v/d}

Input

AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
CF_{occup1}	correction factor for respiratory rate in route-to-route extrapolation	[-]	S/D

Output

$AFworker_{linh-vaour,nt}$	assessment factor for inhalatory worker vapour exposure, non-thr.	[-]	S/O
$AFworker_{linh-fibre,nt}$	assessment factor for inhalatory worker fibre exposure, non-thr.	[-]	S/O
$AFworker_{linh-dust,nt}$	assessment factor for inhalatory worker dust exposure, non-thr.	[-]	S/O
$AFworker_{der,nt}$	assessment factor for dermal worker exposure, non-thr.	[-]	S/O
$AFworker_{tot-v/d,nt}$	assessment factor for total worker exposure, non-thr.	[-]	S/O

$$HT25wor\,ker_{x,nt} = \frac{T25_{mammal,x,nt}}{AFwor\,ker_{x,nt}} \quad (343)$$

$x \in$ {inh-vapour,inh-fibre, inh-dust, der,tot-v/d}

Input			
$T25_{mammal,inh,,nt}$	inhalatory T25 for mammals for non-threshold effects	[$kg_c.m^{-3}$]	S/O
$T25_{mammal,inh,fibre,nt}$	inhalatory T25 (fibre)for mammals for non-threshold effects	[$fibres.m^{-3}$]	S/O
$T25_{mammal,inh,dust,nt}$	inhalatory T25 (dust) for mammals for non-threshold effects	[$kg_c.m^{-3}$]	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$AFworker_{inh\text{-}vapour,nt}$	assessment factor for inhalatory worker vapour exposure, non-thr.	[-]	S/O
$AFworker_{inh\text{-}fibre,nt}$	assessment factor for inhalatory worker fibre exposure, non-thr.	[-]	S/O
$AFworker_{inh\text{-}dust,nt}$	assessment factor for inhalatory worker dust exposure, non-thr.	[-]	S/O
$AFworker_{der,nt}$	assessment factor for dermal worker exposure, non-thr.	[-]	S/O
$AFworker_{tot\text{-}v/d,nt}$	assessment factor for total worker exposure, non-thr.	[-]	S/O
Output			
$HT25worker_{inh,vapour,nt}$	human equivalent dose inhalatory worker vapour exposure, non-thr.	[$kg_c.m^{-3}$]	O
$HT25worker_{inh,fibr,nt}$	human equivalent dose inhalatory worker fibre exposure, non-thr.	[$fibres.m^{-3}$]	O
$HT25worker_{inh,dust,nt}$	human equivalent dose inhalatory worker dust exposure, non-thr.	[$kg_c.m^{-3}$]	O
$HT25worker_{der,nt}$	human equivalent dose dermal worker exposure, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$HT25worker_{tot\text{-}v/d,nt}$	human equivalent dose total worker exposure, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O

For the route-to-route extrapolation for workers involving the inhalatory route an additional correction is used to account for the difference between the respiratory rate of the general population (default 20 m3 per 24 hrs) used in the route-to-route extrapolation and the respiratory rate of workers (10 m3 in 8 hrs). The TGD recommends a factor of 0.5 for extrapolations from the dermal and oral route to the inhalatory route and 2 for extrapolations from the inhalatory route to the dermal and oral route. EUSES allows this correction in the derivation of the RMOS, RMOE and human equivalent dose for workers. The default is 1.

Subsequently the lifetime cancer risk is calculated for each route of exposure. The exposure is corrected for differences between occupational and lifetime conditions by dividing by a factor of 2.8 (default = 7/5 . 52/48 . 75/40 = 2.8).

$$cLRwor\,ker_{inh,vapour,nt} = \frac{C_{inh,wor\,ker,vapour}}{HT25wor\,ker_{inh,vapour,nt}} \cdot 0.25. \frac{1}{CF_{occup2}} \quad (344)$$

$$cLRwor\,ker_{inh,fibre,nt} = \frac{C_{inh,wor\,ker,fibre}}{HT25wor\,ker_{inh,fibre,nt}} \cdot 0.25. \frac{1}{CF_{occup2}} \quad (345)$$

$$cLRwor\,ker_{inh,dust,nt} = \frac{C_{inh,wor\,ker,dust}}{HT25wor\,ker_{inh,dust,nt}} \cdot 0.25. \frac{1}{CF_{occup2}} \quad (346)$$

$$cLRwor\,ker_{der,nt} = \frac{U_{der,pot,wor\,ker}}{HT25wor\,ker_{der,nt}} \cdot 0.25. \frac{1}{CF_{occup2}} \quad (347)$$

$$cLRwor\,ker_{tot-v/d,nt} = \frac{U_{tot-v/d,wor\,ker}}{HT25wor\,ker_{tot-v/d,nt}} \cdot 0.25. \frac{1}{CF_{occup2}} \quad (348)$$

Input

$C_{inh,worker,\ vapour}$	vapour concentration in air for workers	[$kg_c.m^{-3}$]	O
$C_{inh,worker,\ fibre}$	fibre concentration in air for workers	[$fibres.m^{-3}$]	O
$C_{inh,worker,\ dust}$	dust concentration in air for workers	[$kg_c.m^{-3}$]	O
$U_{der,pot,worker}$	potential dermal uptake rate for workers	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$U_{tot\text{-}v/d,worker}$	total uptake for one scenario via different routes	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$HT25worker_{inh,vapour,nt}$	human equivalent dose inhalatory worker vapour exposure, non-thr.	[$kg_c.m^{-3}$]	O
$HT25worker_{inh,fibr,nt}$	human equivalent dose inhalatory worker fibre exposure, non-thr.	[$fibres.m^{-3}$]	O
$HT25worker_{inh,dust,nt}$	human equivalent dose inhalatory worker dust exposure, non-thr.	[$kg_c.m^{-3}$]	O
$HT25worker_{der,nt}$	human equivalent dose dermal worker exposure, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$HT25worker_{tot\text{-}v/d,nt}$	human equivalent dose total worker exposure, non-thr.	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
CF_{occup2}	correction factor for duration and frequency of exposure	[-]	D

Output

$cLRcons_{inh,vaour,nt}$	lifetime cancer risk, inhalatory worker vapour exposure, non-thr.	[-]	O
$cLRcons_{inh,fibre,nt}$	lifetime cancer risk, inhalatory worker fibre exposure, non-thr.	[-]	O
$cLRcons_{inh,dust,nt}$	lifetime cancer risk, inhalatory worker dust exposure, non-thr.	[-]	O
$cLRcons_{der,nt}$	lifetime cancer risk, dermal worker exposure, non-thr.	[-]	O
$cLRcons_{tot,nt}$	lifetime cancer risk, total worker exposure, non-thr.	[-]	O

B. Margin Of Exposure

Calculation of scenario-specific MOE

Under the assumption that man is exposed throughout his or her lifetime, exposure of workers to a substance is compared to the T25 or CED (BMD05), resulting in a Risk Characterisation Ratio (RCR) called the Margin Of Exposure. This comparison is made for all relevant routes of exposure.

Depending on the available data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$MOEworker_{inh,vapour,nt}$	$C_{inh,worker,vapour} \cdot 1/CF_{occup2}$	$T25_{mammal,inh,nt}$ $CED_{mammal,inh,nt}$
$MOEworker_{inh,fibre,nt}$	$C_{inh,worker,fibre} \cdot 1/CF_{occup2}$	$T25_{mammal,inh,fibre,nt}$ $CED_{mammal,inh,fibre,nt}$
$MOEworker_{inh,dust,nt}$	$C_{inh,worker,dust} \cdot 1/CF_{occup2}$	$T25_{mammal,inh,dust,nt}$ $CED_{mammal,inh,,dust,nt}$
$MOEworker_{der,nt}$	$U_{der,pot,worker} \cdot 1/CF_{occup2}$	$T25_{mammal,der,nt}$ $CED_{mammal,der,nt}$
$MOEworker_{tot\text{-}v/d,nt}$	$U_{tot\text{-}v/d,worker}/(BIO_{oral,2} \cdot CF_{occup2})$	$T25_{mammal,oral,nt}$ $CED_{mammal,oral,nt}$

Input			
$T25_{mammal,inh,,nt}$	inhalatory T25 for mammals for non-threshold effects	[$kg_c.m^{-3}$]	S/O
$T25_{mammal,inh,fibre,nt}$	inhalatory T25 (fibre)for mammals for non-threshold effects	[$fibres.m^{-3}$]	S/O
$T25_{mammal,inh,dust,nt}$	inhalatory T25 (dust) for mammals for non-threshold effects	[$kg_c.m^{-3}$]	S/O
$CED_{mammal,inh,nt}$	inhalatory CED for mammals for non-threshold effects	[$kg_c.m^{-3}$]	S/O
$CED_{mammal,inh,fibre,nt}$	inhalatory CED (fibe) for mammals for non-threshold effects	[$fibres.m^{-3}$]	S/O
$CED_{mammal,inh,dust,nt}$	inhalatory CED (dust) for mammals for non-threshold effects	[$kg_c.m^{-3}$]	S/O
$T25_{mammal,der,nt}$	dermal T25 for mammals for non-threshold effects	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$CED_{mammal,der,nt}$	dermal CED for mammals for non-threshold effects	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	S/O
$C_{inh,worker,\ vapour}$	vapour concentration in air for workers	[$kg_c.m^{-3}$]	O
$C_{inh,worker,\ fibre}$	fibre concentration in air for workers	[$fibres.m^{-3}$]	O
$C_{inh,worker,\ dust}$	dust concentration in air for workers	[$kg_c.m^{-3}$]	O
$U_{der,,pot,worker}$	potential dermal uptake rate for workers	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$U_{tot\text{-}v/d,worker}$	total uptake for one scenario via different routes	[$kg_c.kg_{bw}^{-1}.d^{-1}$]	O
$BIO_{oral,2}$	bioavailability for oral uptake, starting route	[-]	D
CF_{occup2}	correction factor for duration and frequency of exposure	[-]	D
Output			
$MOEworker_{inh,vapour,nt}$	MOE inhalatory worker vapour exposure, non-thr.	[-]	O[c]
$MOEworker_{inh,fibre,nt}$	MOE inhalatory worker fibre exposure, non-thr.	[-]	O[c]
$MOEworker_{inh,dust,nt}$	MOE inhalatory worker dust exposure, non-thr.	[-]	O[c]
$MOEworker_{der,nt}$	MOE dermal worker exposure, non-thr.	[-]	O[c]
$MOEworker_{tot\text{-}v/d,nt}$	MOE total worker exposure, non-thr.	[-]	O[c]

Derivation of scenario-specific reference-MOE

In order to account for the various uncertainties and variabilities in the extrapolation from experimental data to the worker situation and in the available data set, per scenario under consideration a reference-MOE is to be derived. All aspects that can be dealt with quantitatively (as assessment factors) are combined to form the overall assessment factor or reference-MOE (RMOE).

$$RMOEwor\,\mathrm{ker}_{x,nt} = AF_{\mathrm{int}\,er} \cdot AF_{allom} \cdot AF_{\mathrm{exp}\,rt} \cdot AF_{dose-resp} \cdot AF_{lr} \cdot CF_{occup1} \quad \textbf{(349)}$$

$x \in$ {inh-vapour,inh-fibre, inh-dust, der,tot-v/d}

Input			
AF_{inter}	assessment factor for interspecies differences	[-]	S/D
AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose\text{-}resp}$	assessment factor for dose-response relationship	[-]	S/D
AFlr	assessment factor for extrapolation to a low risk level	[-]	S/D
CF_{occup1}	correction factor for respiratory rate in route-to-route extrapolation	[-]	S/D
Output			
$RMOEworker_{inh,vapour,nt}$	reference-MOE inhalatory worker vapour exposure, non-thr.	[-]	O[c]
$RMOEworker_{inh,fibre,nt}$	reference-MOE inhalatory worker fibre exposure, non-thr.	[-]	O[c]
$RMOEworker_{inh,dust,nt}$	reference-MOE inhalatory worker dust exposure, non-thr.	[-]	O[c]
$RMOEworker_{der,nt}$	reference-MOE dermal worker exposure, non-thr.	[-]	O[c]
$RMOEworker_{tot,nt}$	reference-MOE total worker exposure, non-thr.	[-]	O[c]

For the route-to-route extrapolation for workers involving the inhalatory route an additional correction is used to account for the difference between the respiratory rate of the general population (default 20 m3 per 24 hrs) used in the route-to-route extrapolation and the respiratory rate of workers (10 m3 in 8 hrs). The TGD recommends a factor of 0.5 for extrapolations from the dermal and oral route to the inhalatory route and 2 for extrapolations

from the inhalatory route to the dermal and oral route. EUSES allows this correction in the derivation of the RMOS, RMOE and human equivalent dose for workers. The default is 1.

Comparison of MOE with reference-MOE
The MOE is compared to the reference-MOE, resulting in a MOE/reference-MOE ratio (MRR).

Depending on the available data the following MRRs are possible:

RCR / reference-MOS	**RCR**	**Reference-MOS**
$MRRworker_{inh,vapour,nt}$	$MOEworker_{inh,vapour,nt}$	$RMOEworker_{inh,vapour,nt}$
$MRRworker_{inh,fibre,nt}$	$MOEworker_{inh,fibre,nt}$	$RMOEworker_{inh,fibre,nt}$
$MRRworker_{inh,dust,nt}$	$MOEworker_{inh,dust,nt}$	$RMOEworker_{inh,dust,nt}$
$MRRworker_{der,nt}$	$MOEworker_{der,nt}$	$RMOEworker_{der,nt}$
$MRRworker_{tot\text{-}v/d,nt}$	$MOEworker_{tot\text{-}v/d,nt}$	$RMOEworker_{tot\text{-}v/d,nt}$

Input

$MOEworker_{inh,vapour,nt}$	MOE inhalatory worker vapour exposure, non-thr.	[-]	O^c
$MOEworker_{inh,fibre,nt}$	MOE inhalatory worker fibre exposure, non-thr.	[-]	O^c
$MOEworker_{inh,dust,nt}$	MOE inhalatory worker dust exposure, non-thr.	[-]	O^c
$MOEworker_{der,nt}$	MOE dermal worker exposure, non-thr.	[-]	O^c
$MOEworker_{tot\text{-}v/d,nt}$	MOE total worker exposure, non-thr.	[-]	O^c
$RMOEworker_{inh,vapour,nt}$	reference-MOE inhalatory worker vapour exposure, non-thr.	[-]	O^c
$RMOEworker_{inh,fibre,nt}$	reference-MOE inhalatory worker fibre exposure, non-thr.	[-]	O^c
$RMOEworker_{inh,dust,nt}$	reference-MOE inhalatory worker dust exposure, non-thr.	[-]	O^c
$RMOEworker_{der,nt}$	reference-MOE dermal worker exposure, non-thr.	[-]	O^c
$RMOEworker_{tot,nt}$	reference-MOE total worker exposure, non-thr.	[-]	O^c

Output

$MRRworker_{inh,vapour,nt}$	ratio MOE/RMOE, inhalatory worker vapour exposure, non-thr.	[-]	O^c
$MRRworker_{inh,fibre,nt}$	ratio MOE/RMOE, inhalatory worker fibre exposure, non-thr.	[-]	O^c
$MRRworker_{inh,dust,nt}$	ratio MOE/RMOE, inhalatory worker dust exposure, non-thr.	[-]	O^c
$MRRworker_{der,nt}$	ratio MOE/RMOE, dermal worker exposure, non-thr.	[-]	O^c
$MRRworker_{tot\text{-}v/d,nt}$	ratio MOE/RMOE, total worker exposure, non-thr.	[-]	O^c

III.7.2.3.3 Derivation of AOEL for biocides with a threshold

Risk characterisation of biocides should be performed by the MOS-approach as well by comparing the AOEL to the internal operator/bystander exposure values of corresponding time scale, resulting in an AOEL/exposure ratio (AER). The MOS-approach has already been described above. This section describes the default AOEL-procedure in EUSES.
Exposure estimated for biocides can be derived by measuring and by the application of various models. EUSES offers the possibility to use the TGD-consumer exposure models or to enter monitoring data. The EASE model results are generally not applicable to biocides since the scenarios relate to industrial use of chemicals. Other models may be used and the relevant exposure results entered in EUSES.

Derivation of AOEL and reference-MOS
As default-procedure, the AOEL (Acceptable Operator Exposure Level) is based on the NOAEL

(or exceptionally, LOAEL) from an oral short-term toxicity study (28- or 90-day study), which is to be converted to an internal dose by correction for systemic bioavailability. EUSES also performs the AOEL procedure on the basis of inhalatory and dermal N(L)OAELs from short-term toxicity studies. If both an N(L)OAEL for man and an N(L)OAEL for mammals are available, the former one is used. The user may decide to deviate from the default procedure and to base the AOEL on a NOAEL from other studies than the 28- or 90-day study. The internal N(L)OAEL is then divided by the overall assessment factor or reference-MOS (RMOS), to

$$RMOSaoel_{x,y} = AF_{inter} \cdot AF_{allom} \cdot AF_{intra} \cdot AF_{expdur} \cdot AF_{exprt} \cdot AF_{dose-resp} \cdot CF_{occup1} \quad \textbf{(350)}$$

account for uncertainties in the extrapolation from experimental data to the human situation.

$x \in$ {oral,inh,der}
$y \in$ {repdose, fert,carc} (repdose is default)

Input			
AF_{allom}	assessment factor for allometric scaling	[-]	S/D
AF_{inter}	assessment factor for remaining interspecies differences	[-]	S/D
AF_{intra}	assessment factor for intraspecies differences	[-]	S/D
AF_{expdur}	assessment factor for differences in exposure duration	[-]	S/D
AF_{exprt}	assessment factor for differences in exposure route	[-]	S/D
$AF_{dose\text{-}resp}$	assessment factor for dose-response relationship	[-]	S/D
AF_{nature}	assessment factor for nature of effect	[-]	S/D
AF_{data}	assessment factor for adequacy of/confidence in database	[-]	S/D
CF_{occup1}	correction factor for respiratory rate in route-to-route extrapolation	[-]	S/D
Output			
$RMOSaoel_{oral,y}$	reference-MOS oral exposure for endpoint y	[-]	O[c]
$RMOSaoel_{inh,,y}$	reference-MOS inhalatory exposure for endpoint y	[-]	O[c]
$RMOSaoel_{der,y}$	reference-MOS dermal exposure for endpoint y	[-]	O[c]

If only a N(L)OAEL for mammals is available:

$$AOEL_{1,x} = \frac{N(L)OAEL_{mammal,x,y} \cdot BIO_{x,2}}{RMOSaoel_{x,y}} \quad \textbf{(351)}$$

If a N(L)OAEL for man is available:

$$AOEL_{2,x} = \frac{N(L)OAEL_{man,x,y} \cdot BIO_{x,2}}{RMOSaoel_{x,y}} \quad \textbf{(352)}$$

$x \in$ {oral,inh,der}

$y \in$ {repdose, fert,carc} repdose is default

Input

$N(L)OAEL_{mammal,oral,y}$	oral N(L)OAEL for mammals for endpoint y	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{mammal,inh,y}$	inhalatory N(L)OAEL for mammals for endpoint y	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{mammal,der,y}$	oral N(L)OAEL for mammals for endpoint y	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,y}$	oral N(L)OAEL for man for endpoint y	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,inh,y}$	inhalatory N(L)OAEL for man for endpoint y	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,der,y}$	dermal N(L)OAEL for man for endpoint y	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$BIO_{oral,2}$	bioavailability for oral uptake (end route)	[-]	S/D
$BIO_{inh,2}$	bioavailability for inhalatory uptake (end route)	[-]	S/D
$BIO_{der,2}$	bioavailability for dermal uptake (end route)	[-]	S/D
$RMOSaoel_{oral,,y}$	reference-MOS oral exposure for endpoint y	[-]	O[c]
$RMOSaoel_{inh,,y}$	reference-MOS inhalatory exposure for endpoint y	[-]	O[c]
$RMOSaoel_{der,y}$	reference-MOS dermal exposure for endpoint y	[-]	O[c]

Output

$AOEL_{1,oral}$	AOEL, based on oral study in mammals	$[kg.kg_{bw}^{-1}.d^{-1}]$	O[c]
$AOEL_{1,inh}$	AOEL, based on inhalatory study in mammals	$[kg_c.m^{-3}]$	O[c]
$AOEL_{1,der}$	AOEL, based on dermal study in mammals	$[kg.kg_{bw}^{-1}.d^{-1}]$	O[c]
$AOEL_{2,oral}$	AOEL, based on oral study in man	$[kg.kg_{bw}^{-1}.d^{-1}]$	O[c]
$AOEL_{2,inh}$	AOEL, based on inhalatory study in man	$[kg_c.m^{-3}]$	O[c]
$AOEL_{2,der}$	AOEL, based on dermal study in man	$[kg.kg_{bw}^{-1}.d^{-1}]$	O[c]

2. Comparison of AOEL with exposure

Depending on the available data the following AERs are possible:

AOEL / Exposure	**AOEL**	**Exposure**
$AER_{1,oral}$	$AOEL_{1,oral}$	I_{oral} . $BIO_{oral,2}$
$AER_{1,inh}$	$AOEL_{1,inh}$	I_{inh} · $BIO_{inh,2}$
$AER_{1,der}$	$AOEL_{1,der}$	$U_{der,pot}$ · $BIO_{der,2}$
$AER_{1,tot}$	$AOEL_{1,oral}$	U_{tot}
$AER_{2,oral}$	$AOEL_{2,oral}$	I_{oral} . $BIO_{oral,2}$
$AER_{2,inh}$	$AOEL_{2,inh}$	I_{inh} · $BIO_{inh,2}$
$AER_{2,der}$	$AOEL_{2,der}$	$U_{der,pot}$ · $BIO_{der,2}$
$AER_{2,tot}$	$AOEL_{2,oral}$	U_{tot}

Input			
$AOEL_{1,oral}$	AOEL, based on oral study in mammals	$[kg.kg_{bw}^{-1}.d^{-1}]$	O^c
$AOEL_{1,inh}$	AOEL, based on inhalatory study in mammals	$[kg_c.m^{-3}]$	O^c
$AOEL_{1,der}$	AOEL, based on dermal study in mammals	$[kg.kg_{bw}^{-1}.d^{-1}]$	O^c
$AOEL_{2,oral}$	AOEL, based on oral study in man	$[kg.kg_{bw}^{-1}.d^{-1}]$	O^c
$AOEL_{2,inh}$	AOEL, based on inhalatory study in man	$[kg_c.m^{-3}]$	O^c
$AOEL_{2,der}$	AOEL, based on dermal study in man	$[kg.kg_{bw}^{-1}.d^{-1}]$	O^c
I_{oral}	ingestion rate of substance	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
I_{inh}	inhalatory intake of substance	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$U_{der,pot}$	amount of substance that potentially can be taken up	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
U_{tot}	total uptake via different routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$BIO_{oral,2}$	bioavailability for oral uptake (end route)	[-]	S/D
$BIO_{der,2}$	bioavailability for dermal uptake (end route)	[-]	S/D
$BIO_{inh,2}$	bioavailability for inhalation (end route)	[-]	S/D
Output			
$AER_{1,oral}$	ratio oral $AOEL_1$ / internal oral exposure	[-]	O^c
$AER_{1,inh}$	ratio inhalatory $AOEL_1$ / internal inhalator exposure	[-]	O^c
$AER_{1,der}$	ratio dermal $AOEL_1$ / internal dermal y exposure	[-]	O^c
$AER_{1,tot}$	ratio oral $AOEL_1$ / internal total exposure	[-]	O^c
$AER_{2,oral}$	ratio oral $AOEL_2$ / internal oral exposure	[-]	O^c
$AER_{2,inh}$	ratio inhalatory $AOEL_2$/ internal inhalatory exposure	[-]	O^c
$AER_{2,der}$	ratio dermal $AOEL_2$ / internal dermal exposure	[-]	O^c
$AER_{2,tot}$	ratio oral $AOEL_2$ / total internal exposure	[-]	O^c

III.8 HYDROCARBON BLOCK METHOD (HBM)

The principal steps in the application of the Hydrocarbon Block Method (HBM) are:

- obtain compositional data for the substance that are sufficient to assign components to blocks;
- define blocks by grouping components on the basis of similar structural and/or physico-chemical and ecotoxicological properties. If desired, blocks can be defined as single components;
- obtain production and use data;
- establish release estimates for each block. A single release estimate for a petroleum substance may not always be adequate; blocks with markedly different physico-chemical properties may require different release estimates;
- assign representative values for physico-chemical properties, degradation-rate constants and LC/EC50s and NOECs to each block;
- determine the PEC for each compartment for each block (local as well as regional);
- determine the PNEC for each block;
- calculate the PEC/PNEC ratio for each block, and sum.

Once the blocks with their physico-chemical and ecotoxicological properties have been defined, the assessment follows the methods described in the following sections. This means that local and regional PECs can be calculated as described in the 'Environmental distribution module' and a PNEC can be derived as described in the 'Effects assessment module'.

III.9 ENVIRONMENTAL RISK ASSESSMENT FOR METALS AND METAL COMPOUNDS

In principle, the models and approaches for organic substances can also be used to estimate exposure to metals. However, there are several differences compared with the use of these models for organic substances. Below, the differences are described.

III.9.1 Exposure assessment

1. Physico-chemical properties (Input module)

In general, water solubility, boiling point and vapour pressure cannot be used. The octanol-water partition coefficient is not appropriate and measured partition coefficients (*Kp*) should be used instead.

2. Partition coefficients (Environmental distribution module, partition coefficients sub-module)

Adsorption to aerosol particles

Most of the metal present in the atmosphere will be bound to aerosols. Therefore, an extremely low value for the vapour pressure should be used to estimate the fraction bound to aerosol, e.g. 10^{-20} Pa. This leads to a value for $Fass_{aer}$ almost equal to one. If a valid measured value is available for the aerosol-bound fraction, this value can be used.

Volatilisation

Volatilisation can be ignored for metals, except for mercury compounds and several organometallo-compounds. Therefore, the Henry coefficient should generally be set to a very low value.

Adsorption/desorption

Formulae to estimate *Koc* cannot be used. Measured *Kp*-values must be used for water-soil, water-sediment and water-suspended matter. *Kp* is influenced by speciation and the speciation behaviour must therefore be accounted for in *Kp*.

3. Biotic and abiotic degradation rates (Environmental distribution module, Environmental degradation rates sub-module)

Not relevant for metals. The substances must be specified as non-biodegradable (very high DT50).

4. Elimination processes prior to the release in the environment (Environmental distribution module, Sewage treatment sub-module)

For applying the STP model, a partition coefficient is used for water-sludge. For metals, a measured *Kp*-value must be used.

5. Calculation of the regional PEC (Environmental distribution module, Regional environmental distribution sub-module)

The values applied for model parameters for the regional model, inter-media mass-transfer coefficients and model parameters for the continental concentration can be used.

III.9.2 Effects assessment

PNECs can be derived through the application of assessment factors on the basis of the available data. Evaluation of the toxicity data is critical (the reader is referred to the TGD; EC, 1996). Standard methods applied for organic compounds can be used for this (see Section III.6). However, because of the specific mode of action that metals may have for some species, care should be taken in extrapolating short term toxicity data to the PNEC using the standard assessment factors. For many metals, sufficient long term toxicity data for aquatic organisms may be present to enable statistical extrapolation, results of which can support the results of PNECs calculated using assessment factors. Calculated PNECs derived for essential metals may not be lower than natural background concentrations.

A prerequisite for the derivation of the PNEC is that it is done on the basis of the same level of availability as in exposure assessment:

- Results from aquatic toxicity tests are usually expressed as total concentrations. As a first approach, total concentrations have to be recalculated to dissolved concentrations using partition coefficients. If this is not possible, the total concentration can be set equal to the dissolved concentration. Differences in test systems, e.g. (semi-)static versus continuous flow systems and natural versus standard water, have to be considered.
- For the terrestrial compartment, many data exist, but most are only expressed as total concentration that has been added to the test media. This added amount will be partitioned among the aqueous and the solid phase. Application of partition coefficients to calculate the available concentration in soil can be applied. Soil type correction, using reference lines, should be applied to correct for differences among soil types (Slooff, 1992).
- Some of the metals are essential metals, having a function in biological processes at low concentrations. Shortage of micronutrients may cause malfunction. This implies that in setting the PNEC, information on deficiency levels should be taken into account. It should, however, be noted that often no information on deficiency levels of various metals for various species is available.

Though some exceptions exist, in general ionic metal species are considered to be the dominant metal species taken up, and are thus considered to be the metal species responsible for the toxic effect. Data on the concentration of ionic species in aquatic and terrestrial systems are not readily available, and cannot, as yet, be applied on a regular basis in risk assessment.

Bioaccumulation of essential metals

Metals are taken up by organisms. For essential metals, biota regulate their uptake by means of the general physiological mechanism of homeostasis. By this mechanism, organisms will keep, within a certain range of varying external concentrations, their intracellular levels relatively constant, in order to satisfy their requirements for that essential element. Homeostasis implies that organisms can actively concentrate essential elements if concentrations in the environment are very low. This may lead to high BCF values. On the other hand, the homeostatic regulation capacity will be exceeded at a given higher external concentration beyond which the element will accumulate and become toxic.

IV. REFERENCES

Aldenberg, T. and W. Slob (1993). Confidence limits for hazardous concentrations based on logistically distributed NOEC toxicity data. Ecotoxicol. Environ. Saf. 25, 48-63.

Aldenberg, T.; Jaworska, J.S. (2000). Uncertainty of the hazardous concentration and fraction affected for normal species sensitivity distributions. Review. Ecotoxicol. Environ. Saf. 46: 1-18.

Aldenberg, T.; Jaworska, J.S.; Traas T.P. (2002). Normal species sensitivity distributions and probabilistic ecological risk assessment. In: Species sensitivity distributions in ecotoxicology (Posthuma, L; Suter,G.W.; Traas, T.P. Eds.). Lewis publishers, Press, Boca Raton FL, USA.

Belfroid, A., W. Seinen, K. van Gestel, J. Hermens and K. van Leeuwen (1995). Modelling the accumulation of hydrophobic organic chemicals in earthworms. - Application of the equilibrium partitioning theory. Environ. Sci. Pollut. Res. 2, 5-15.

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

Berding, V. (2000) Validation of a regional distribution model in environmental risk assessment of substances. Univerity of Osnabrück, Germany, Doctoral Thesis.

Bodar, C.W.M., de Bruijn, J.H.M., Vermeire T.G. and van der Zandt, P.T.J. (2002) Trends in risk assessment of chemicals in the European Union.Human Ecol. Risk Assessm. 8: 1825-1843.

Brandes, L.J., D. van de Meent and H. den Hollander (1996). SimpleBox 2.0: a nested multimedia fate model for evaluating the environmental fate of chemicals. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 719101029.

Bredendiek-Kämper, S. (2001) Do EASE scenarios fir workplace reality? A validation study of the EASE model. Appl. Occup. Environ. Hygiene 16:182-187.

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

Cathie, K., J. Staves and N. Kirkpatrick (1991). Consultancy Report, Paper recycling industry: Review of processes and effluent. Composition PIRA International, 33/TENQ/012/588.

Connell, D.W. and R.D. Markwell (1990). Bioaccumulation in the soil to earthworm system. Chemosphere 20, 91-100.

Cowan, C.E., D. Mackay, T. Feijtel and D. Van de Meent (1995). The Multimedia Fate Model. SETAC Press. ISBN 1-880611-02-3.

De Greef, J., and A.C.M. De Nijs (1990). Risk assessment of new chemical substances. Dilution of effluents in the Netherlands. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 670208001.

De Nijs, A.C.M., C. Toet, T.G. Vermeire, P. van der Poel and J. Tuinstra (1993). Dutch risk assessment system for new chemicals: DRANC. Sci. Total Environ., Suppl. 1993, 1729-1747.

De Nijs, A.C.M., J.M. Knoop and T.G. Vermeire (1988). Risk assessment of new chemical substances. System realisation & validation. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 718703001.

Den Hollander, H. A. and D. van de Meent (2004). Model parameters and equations used in Simplebox 3.0. Bilthoven, RIVM, Report No. 601200 003, January 2004.

Di Toro, D.M., C.S. Zarba, D.J. Hansen, W.J. Berry, R.C. Schwarz, C.E. Cowan, S.P. Pavlou, H.E. Allen, N.A. Thomas and P.R. Paquin (1991). Technical basis of establishing sediment quality criteria

for nonionic organic chemicals using equilibrium partitioning. Environ. Toxicol. Chem. 10, 1541-1583.

EC (1967). Council Directive of 27 July 1967 on the approximation of the laws, regulations and administrative provisions relating to the classification, packaging and labelling of dangerous substances (67/548/EEC). Official Journal of the European Communities, No. 196.

EC (1973). First Programme of Action on the Environment. Official Journal of the European Communities 16, No. C112, December 20, 1973.

EC (1990). Environmental hazard and risk assessment in the context of Directive 79/831/EEC. Brussels, Commission of the European Communities, Directorate-General of Environment, Nuclear Safety and Civil Protection, XI/730/89.

EC (1992a). Chemicals control in the European Community. Luxembourgh, Commission of the European Communities, Publication No. EUR 14385 EN.

EC (1992b). Council Directive of 30 April 1992 amending for the seventh time Directive 67/548/EEC on the approximation of the laws, regulations and administrative provisions relating to the classification, packaging and labelling of dangerous substances (92/32/EEC). Official Journal of the European Communities, L154.

EC (1993a). Commission Directive 93/67/EEC of 20 July 1993, laying down the principles for the assessment of risks to man and the environment of substances notified in accordance with Council Directive 67/548/EEC. Official Journal of the European Communities, L227.

EC (1993b). Technical guidance documents in support of the risk assessment Directive (93/67/EEC) for new substances notified in accordance with the requirements of Council Directive 67/548/EEC. Brussels, Belgium, Commission of the European Communities.

EC (1993c). Council Regulation (EC) 793/93 of 23 March 1993 on the evaluation and control of the risks of existing substances. Official Journal of the European Communities, L84.

EC (1993d). Annexes I, II, III and IV to Commission Directive 93/21/EEC of 27 April 1993 adapting to technical progress for the 18th time Council Directive 67/548/EEC on the approximation of the laws, regulations and administrative provisions relating to the classification, packaging and labelling of dangerous substances. Official Journal of the European Communities, L110A, Volume 36, 4 May 1993.

EC (1994a). Commission Regulation (EC) 1488/94 of 28 June 1994, laying down the principles for the assessment of risks to man and the environment of existing substances in accordance with Council Regulation (EEC) No. 793/93. Official Journal of the European Communities, L161.

EC (1994b). Technical guidance documents in support of the risk assessment Regulation (1488/94) for existing substances in the context of Council Regulation 793/93/EEC. Brussels, Belgium, Commission of the European Communities.

EC (1996). Technical Guidance Documents in support of Directive 93/67/EEC on risk assessment of new notified substances and Regulation (EC) No. 1488/94 on risk assessment of existing substances (Parts I, II, III and IV). EC catalogue numbers CR-48-96-001, 002, 003, 004-EN-C. Office for Official Publications of the European Community, 2 rue Mercier, L-2965 Luxembourg.

EC (1998). Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market. Office for Official Publications of the European Community, Luxembourg.

EC (2001). Commission Directive 2001/59/EC of 6 August 2001 adapting to technical progress for the 28th time Council Directive 67/548/EEC on the approximation of the laws, regulations and administrative provisions relating to the classification, packaging and labelling of dangerous

substances (Text with EEA relevance). Official Journal of the European Communities, L225, 21.8.2001.]

EC (2002a) Technical Notes for Guidance. Human exposure to biocidal products – Guidance on exposure estimation. Ispra, Italy, European Chemicals Bureau.

EC (2002b) Technical Notes for Guidance on Annex I, IA and IB inclusion - Technical Notes for Guidance in Support of Directive 98/8/EC of the European Parliament and the Council concerning the placing of biocidal products on the market. Principles and Practical procedures for the inclusion of active substances in Annexes I, IA and IB. Ispra, Italy, European Chemicals Bureau.

EC (2003). Technical Guidance Document on Risk Assessment (TGD).(in support of Commission Directive 93/67/EEC, Commission Regulation (EC) No 1488/94 and Directive 98/8/EC) European Chemicals Bureau, Ispra (It.), 2003.

EC (2003a). Assessment of human exposures to biocides. In preparation.

EC (2003b) Technical Notes for Guidance on Annex I inclusion. Technical notes for guidance in support of Directive 98/8/EC of the European Parliament and the Council concerning the placing of biocidal products on the market. Principles and practical procedures for the inclusion of active substances in Annexes I, IA and IB. April 2002.

EC (2003c) Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on risk assessment for New Notified Substances and Commission Regulation (EC) No. 1488/94 on Risk Assessment for Existing Substances and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market.

ECETOC (1990). Hazard assessment of chemical contaminants in soil. Technical Report No. 40, ECETOC, Brussels.

ECETOC (1992). Estimating environmental concentrations of chemicals using fate and exposure models. Technical Report No. 50, ECETOC, Brussels.

ECETOC (1994). Technical Report No. 58: Assessment of Non-Occupational Exposure to Chemicals.

Emans, H.J.B., E.J. v.d. Plassche, J.H. Canton, P.C. Okkerman and P.M. Sparenburg (1993). Validation of some extrapolation methods used for effect assessment. Environ. Toxicol. Chem. 12, 2139-2154.

Emans, H.J.B., M.A. Beek and J.B.H.J. Linders (1992). Evaluation system for pesticides (ESPE), 1. Agricultural pesticides. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 679101004.

ETAD (1983). Project A 4007 Final report on extractability of dyestuffs from textiles.

Etienne, R.S., Ragas, A.M.J. and van de Meent, D. (1997) Operational uncertainties in Simplebox. Bilthoven, RIVM, Report no. 719101031.

Euromonitor, European Marketing Data and Statistics 1992, ISBN: 0 86338 403 X, Euromonitor Plc 1992.

Health Council (1991). Uniform assessment of substances? Report on the prototype of the Uniform System for the Evaluation of Substances. Committee on uniform assessment of substances. The Hague, Health Council of The Netherlands, publication No. 1991/08 (in Dutch).

Health Council (1993). Uniform assessment of substances? (2) Assessment of the second prototype of the Uniform System for the Evaluation of Substances. Committee on uniform assessment of substances. The Hague, Health Council of The Netherlands, publication no. 1993/18E.

Hofstee A.W.M., J. Meulenbelt and T.J.F. Savelkoul (1990). Informatieverstrekking bij vergiftigingen

door het Nationaal Vergiftigingen Informatie Centrum bebaseerd op gegevens van 1985-1989 (In Dutch). Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 348802011. (Information supply for intoxication by the National Intoxication Information Centre based on data of 1985-1989)

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

Huijbregt, M.A.J.; Thissen, U., Jager, T., van de Meent, D. and Ragas, A.M.J. (2000) Priority assessment of toxic substances in life cycle assessment. Part II: assessing parameter uncertainty and human variability in the calculation of toxicity potentials. Chemosphere 41: 575-588.

IPCS (1992). Workshop on Toxicological Data Quality Indicators, Atlanta, 16-18 September 1992. Geneva, International Programme on Chemical Safety, WHO, PCS/93.28.

Jager, D.T., T.G. Vermeire, W. Slooff and H. Roelfzema (1994a). Uniform System for the Evaluation of Substances II. Effects assessment. Chemosphere 29, 319-335.

Jager, D.T., C.J.M. Visser and D. van de Meent (1994b). Uniform System for the Evaluation of Substances IV. Distribution and intake. Chemosphere 29, 353-369.

Jager, D.T. (1995a). Feasibility of validating the Uniform System for the Evaluation of Substances (USES). Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 679102026.

Jager, D.T. (1995b). Uncertainty Analysis of the Uniform System for the Evaluation of Substances (USES): Example Calculations. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 679102032.

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

Jager, D.T., Rikken, M., Poel, P. van der (1997) Uncertainty analysis of EUSES: improving risk management by probabilistic risk assessment. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 679102039.

Jager, T. (1998) Uncertainty analysis of EUSES: interviews with representatives from Member States and industry. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 679102047.

Jager, D.T. (1998). Mechanistic approach for estimating bioconcentration of organic chemicals in earthworms (Oligochaeta). Environ. Toxicol. Chem. 17: 2080-2090.

Jager, T. ed. (1998) Evaluation of EUSES: inventory of experiences and validation activities. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 679102048

Jager, D.T., Vermeire, T,G., Rikken, M. and van der Poel, P. (2001a) Opportunities for a probabilistic risk assessment of chemicals in the European Union. Chemosphere 43: 257-264.

Jager, T., den Hollander, D.A., van der Poel,P., Rikken, M. and Vermeire, T. (2001b) Probabilistic environmental risk assessment of dibutylphthalate (DBP). J. Human and Ecol. Risk Assessment 7(6): 1681-1697.

Junge, C.E. (1977). In: Fate of pollutants in the air and water environment. I.H. Suffet (ed), Wiley interscience, New York, 7-25.

Lehman, A.J.(1954) Untitled. Association of Food and Drug Officials Quarterly Bulletin 18: 66.

Linders, J.B.H.J. and R. Luttik (1995). Uniform System for the Evaluation of Substances V. ESPE, Risk

Assessment for Pesticides. Chemosphere 31, 3237-3248.

Luit, R.J. , Beems, R.B., van Benthem, J., Bodar, C.W.M., van Engelen, J.G.M., Hulzebos, E.M/, van Loveren, H. , Maślankiewicz, L., Piersma, A.H., Pronk, J.E.M., Rennen, M.A.J., Sijm, T.H.M. and Zweers, P.G.P.C. (2003) Inventory of revisions in the EC Technical Guidance Documents (TGDs) on risk assessment of chemicals. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 601200001.

Luttik, R., H.J.B. Emans, P. van der Poel and J.B.H.J. Linders (1993). Evaluation system for pesticides (ESPE), 2. Non-agricultural pesticides. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 679102021.

Mackay, D. (1991). Multimedia environmental models. Lewis Publishers, Chelsea, MI.

Mackay, D., S. Paterson and W.Y. Shiu, (1992). Generic models for evaluating the regional fate of chemicals; Chemosphere 24, (6), 695-717.

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

Mikkelsen, J. (1995, in press). Fate Model for Organic Chemicals in an Activated Sludge Wastewater Treatment Plant - Modification of SimpleTreat. National Environmental Research Institute, Denmark. Prepared for the Danish EPA.

OECD (Organisation for Economic Co-operation and Development) (1989). Report of the OECD Workshop on ecological effects assessment. Paris, France, Organisation of Economic Cooperation and Development, OECD Environment Monographs No. 26.

OECD (Organisation for Economic Co-operation and Development) (1992b). Report of the Workshop on Effects Assessment of Chemicals in Sediment. OECD Environment Monographs No. 60.

OECD (Organisation for Economic Co-operation and Development) (1992c). The Rate of Photochemical Transformation of Gaseous Organic Compounds in Air Under Tropospheric Conditions, OECD Environment Monographs No. 61.

OECD (Organisation for Economic Cooperation and Development) (1993). Occupational and consumer exposure assessments, OECD Environment Monographs, OCDE/GD(93)128, Paris.

Paustenbach, D.J. (1995). The practice of health risk assessment in the United States (1975-1995): how the US and other countries can benefit from that experience. Human Ecol. Risk Assessment 1, 29-79.

Polder, M.D., E.M. Hulzebos and D.T. Jager (1995). Validation of models on uptake of organic chemicals by plant roots. Environ. Toxicol. Chem. 14, 1615-1623.

Polder, M.D., E.M. Hulzebos and D.T. Jager (1996). Bioconcentration of gaseous organic chemicals in plant leaves: comparison of experimental data with model predictions. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 679102034.

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

RIVM, VROM, WVC (1994). Uniform System for the Evaluation of Substances (USES), version 1.0. National Institute of Public Health and the Environment (RIVM), Ministry of Housing, Physical Planning and Environment (VROM), Ministry of Welfare, Health and Cultural Affairs (WVC). The Hague, Ministry of Housing, Physical Planning and Environment. Distribution No. 11144/150.

Romijn, C.A.F.M., R. Luttik, D. van de Meent, W. Slooff and J.H. Canton (1993). Presentation of a General Algorithm to Include Effect Assessment on Secondary Poisoning in the Derivation of

Environmental Quality Criteria. Part 1: Aquatic food chains. Ecotox. Environ. Saf. 26, 61-85.

Romijn, C.F.A.M., R. Luttik and J.H. Canton (1994). Presentation of a general algorithm to include effect assessment on secondary poisoning in the derivation of environmental quality criteria. Part 2. Terrestrial food chains. Ecotox. Environ. Saf. 27, 107-127.

Ros, J.P.M. and J.J. Bogte (1985). Beoordelingssysteem Nieuwe Stoffen; Onderdeel: Uitworpverwachting fotochemicaliën. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 851502002 (in dutch). (System for assessing new substances: Predicted emissions of photochemicals)

Ros, J.P.M. (1985). Beoordelingssysteem Nieuwe Stoffen; Onderdeel: Uitworpverwachting textielkleurstoffen. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 851502001 (in dutch). (System for assessing new substances: Expected emissions of textile dyes)

Ros, J.P.M. and J.A.S. Berns (1988). Beoordelingssysteem Nieuwe Stoffen; Onderdeel: Uitworpverwachting papierchemicaliën. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 738620002 (in dutch). (System for the assessment of new substances: Predicted emissions ofrom the paper industry)

Ros, J.P.M. and P. van der Poel (1989). Uitworpverwachting tussenstoffen in de farmaceutische industrie. Bilthoven, National Institute of Public Health and the Environment (RIVM), Internal note RIVM/LAE (in dutch). (Predicted emissions of intermediates in the pharmaceutical industry)

Sabljic, A., H. Güsten, H. Verhaar and J. Hermens (1995). QSAR modelling of soil sorption. Improvements and systematics of log Koc vs. log Kow correlations. Chemosphere 31, 4489-4514.

Schwartz, S. (2000) Quality assurance of exposure models for environmental risk assessment of substances. University of Osnabrück, Germany, Doctoral Thesis.

Schwartz, S., Berding, S., Trapp, S. and Matthies, M. (1998) Quality criteria for environmental risk assessment software – Using the example of EUSES. Environ.Sci. Pollut. Res. 5: 217-222.

Slooff, W. (1992). RIVM Guidance Document. Ecotoxicological effect assessment: Deriving Maximum Tolerable Concentrations (MTC) from single-species toxicity data. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 719102018.

Struijs, J., J. Stoltenkamp and D. van de Meent (1991). A Spreadsheet-based Model to Predict the Fate of Xenobiotics in a Municipal Wastewater Treatment Plant. Wat. Res. 25, (7), 91-900.

Struijs, J. (1996). SimpleTreat 3.0: a model to predict the distribution and elimination of chemicals by sewage treatment plants. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 719101025.

Struijs,J. and Peijnenburg, W.J.G.M. (2002). Predictions by SimpleBox compared to field observations. Intermedia concentration ratios of two phthalates. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 607220008

Toet, C. and F.A.A.M. de Leeuw (1992). Risk Assessment System for New Chemical Substances: Implementation of atmospheric transport of organic compounds. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 679102008.

Toet, C., A.C.M. de Nijs, T.G. Vermeire, P. van der Poel and J. Tuinstra (1991). Risk Assessment of New Chemical Substances; System Realisation and Validation II. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 679102004.

Trapp, S. and M. Matthies (1995). Generic one-compartment model for uptake of organic chemicals by foliar vegetation. Environ. Sci. Technol. 29, 2333-2338.

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

United Nations (1992). Environmentally sound management of toxic chemicals including prevention of illegal international traffic in toxic and dangerous products. Agenda 21, Chapter 19. United Nations Conference on Environment and Development, Rio de Janeiro, Brasil.

US-EPA (1980). Office of Toxic Substances. Chemical Use Standard Encoding System (ChemUSES), Volume 2: Function List and Function List Index (Draft) EPA 560/13-80-034b, August 1980, Washington, DC 20460.

US-EPA (1989). Exposure factors handbook. Washington DC, USA, Office of Health and Environmental Assessment, Exposure Assessment Group, US Environmental Protection Agency, EPA/600/8-89/043, PB90-106774.

Van de Meent, D. and C. Toet (eds.) (1992). Dutch Priority setting system for existing chemicals: a systematic procedure for ranking chemicals according to increasing estimated hazards. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 679120001.

Van de Meent, D. (1993). SimpleBox: A Generic Multimedia Fate Evaluation Model. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 672720 001.

Van de Meent, D., J.H.M. De Bruijn, F.A.A.M. De Leeuw, A.C.M. De Nijs, D.T. Jager and T.G. Vermeire (1995). Exposure Modeling, In: Risk Assessment of Chemicals: an introduction. C.J. van Leeuwen and J.L.M. Hermens (eds.). Kluwer Academic Publishers, ISBN 0-7923-3740-9.

Van der Poel, P. and J.P.M. Ros (1987). Uitworpverwachting snijvloeistoffen en hydraulische vloeistoffen. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 738620001 (in dutch). (Predicted emissions from cutter fluids and hydraulic fluids)

Van der Poel, P. (1994). Uniform System for the Evaluation of Substances III. Emission estimation. Chemosphere 29, 337-352.

Van der Poel, P. (1999) Supplement to the Uniform System for the Evaluation of Substances (USES): Emission scenarios for waste treatment (elaborated for biocides). Bilthoven, National Institute for Public Health and the Environment (RIVM), Report No. 601450003.

Van Gestel, C.A.M. (1992). The influence of soil characteristics on the toxicity of chemicals for earthworms: a review. In: Becker, H. *et al.* (eds.). Ecotoxicology of earthworms. pp. 44-54, Intercept Andover.

Van Gestel, C.A.M., and W. Ma (1993). Development of QSARs in soil ecotoxicology: earthworm toxicity and soil sorption of chlorophenols, chlorobenzenes and chloroanilines. Water, Air and Soil Pollution 69, 265-276.

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

Van Leeuwen, C.J. and J.L.M. Hermens (eds.) (1995). Risk assessment of chemicals: an introduction. Dordrecht, Kluwer Academic Publishers, ISBN 0-7923-3740-9.

Van Veen, M.P. (1995). CONSEXPO, a program to estimate consumer product exposure and uptake. Bilthoven, National Institute of Public Health and the Environment (RIVM), Report No. 612810002.

Van Veen, M.P. (2001) CONSEXPO 3.0, Consumer exposure and uptake models. Bilthoven, National Institute for Public Health and the Environment (RIVM). Report No. 612810 011, May 2001.

Van Vlaardingen P., Traas T.P. (2002). ETX-2000. A program to calculate normal distribution based hazardous concentrations and the potentially affected fraction. Version 1.407, RIVM Bilthoven, The Netherlands (available through www.rivm.nl).

Veith, G.D., D.L. Defoe and B.V. Bergstedt (1979). Measuring and estimating the bioconcentration factor of chemicals in fish. J. Fish Board Can. 36, 1040-1048.

Velvart J. (1993). Toxicologie der Haushaltsproducte, Aus der Kasuistik der Schweizerischen Toxicologische Informationszentrums [in German]. Verlag H. Hubner, Bern.

Vermeire T.G., P. van der Poel, R.T.H. Van de Laar and H. Roelfzema (1993). Estimation of consumer exposure to chemicals: application of simple models. Science of the Total Environment 136, 155-176.

Vermeire, T.G., P.T.J. van der Zandt, H. Roelfzema and C.J. van Leeuwen (1994). Uniform System for the Evaluation of Substances I: Principles and Structure. Chemosphere 29, 23-38.

Vermeire,T., Jager T., Janssen, G., Bos, P. and Pieters, M. (2001). A probabilistic human health risk assessment for environmental exposure to dibutylphthalate. J. Human and Ecol. Risk Assessment 7(6): 1663-1679.

Versar Inc. (1991). Screening-Level Consumer Inhalation Exposure Software (SCIES): description and User's Manual Version 3.0, Draft Report. US-EPA 68-D9-0166.

Versar Inc. (1992). DERMAL Exposure Model Description and User's Manual, Final Draft Report. US-EPA 68-D6-0166.

Appendix I Glossary of abbreviations

AOEL	Acceptable Operator Exposure Level: the maximum amount of active substance to which the operator may be exposed without any adverse health effects
BAF	BioAccumulation Factor: ratio between concentration in (part of) organism and exposure level (see Section II.5)
BCF	BioConcentration Factor: ratio between the concentration in an organism and the concentration in an environmental compartment (water-borne exposure only) (see Section II.5)
CAS	Chemical Abstracts Service
CED	Critical Effect Dose: dose at which the average animal shows the (postulated) critical-effect-size defined for a particular endpoint, below which there is no reason for concern]
DD	oral Discriminatory Dose for mammals
EASE	Estimation and Assessment of Substance Exposure (see Section II.5.4)
EC	European Commission
EC50	median Effective Concentration: 1. the concentration resulting in a 50% change in a parameter (e.g. algal growth) relative to the control 2. the concentration at which a particular effect (e.g. Daphnia immobilisation) is observed in 50% of the organism population relative to the control
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
EINECS	European Inventory of Existing Commercial chemical Substances: lists all chemical substances defined as ‘existing’ prior to 18 September 1981
EU	European Union
EUSES	European Union System for the Evaluation of Substances
GLP	Good Laboratory Practice: a set of rules describing how a laboratory should work, how it should be organised and how it can produce valid data; GLP principles are described by OECD
HEDSET	Harmonised Electronic Data SET
HBM	Hydrocarbon Block Method: method for assessment of mixtures of hydrocarbons (see Section II.8)

IC	Industrial Category: classification of substance use (Section II.3.3)
IC50	median Inhibitory Concentration: the concentration resulting in a 50% inhibition of growth relative to the control
IUCLID	International Uniform ChemicaL Information Database
LC50	median Lethal Concentration: a statistically derived concentration that can be expected to cause death in 50% of animals exposed for a specified time
LD50	median Lethal Dose: statistically derived single dose that can be expected to cause death in 50% of dosed animals
LOAEL	Lowest-Observed-Adverse Effect Level: the lowest concentration or amount of a substance, found by experiment or observation, which causes an adverse alteration of morphology, functional capacity, growth, development, or life span of the target organism under defined conditions of exposure (WHO, 1979)
MC	Main Category: classification of substance use (Section II.3.3)
MMAD	Mass Median Aerodynamic Diameter; measure for particle size
MOS	Margin Of Safety: the risk characterisation ratio (RCR) of a suitable effect or no-effect level to a human exposure value
PNEC	Predicted No-Effect Concentration for a particular ecosystem or population
NOAEL	No-Observed-Adverse-Effect Level: the highest concentration or amount of a substance, found by experiment or observation, which causes no detectable adverse alteration of morphology, functional capacity, growth, development, or life span of the target organism under defined conditions of exposure (WHO, 1979)
NOEC	No-Observed-Effect-Concentration: the highest concentration without adverse effects
NOEL	No-Observed-Effect Level: the exposure level without any effect
OECD	Organisation for Economic Co-operation and Development
OPS	Operational Priority Substances atmospheric transport model; calculates long-term average concentrations in air resulting from emissions from point sources

PEC	Predicted Environmental Concentration
PMN	Pre-Marketing Notification
QA	Quality Assurance: internal laboratory control system to ascertain that tests are in compliance with GLP principles
QSAR	Quantitative Structure-Activity Relationship
RBT	Ready Biodegradability Test
RCR	Risk Characterisation Ratio: quantitative comparison of exposure and effects, can be a PEC/PNEC ratio or a MOS
SAR	Structure-Activity Relationship
SNIF	Substance Notification Interchange Format
SSD	Species Sensitivity Distribution
STP	Sewage Treatment Plant (see Section II.4.3)
TGD	Technical Guidance Document of the European Commission
UC	Use or function Category: classification of substance use (Section II.3.3)

Reference:

WHO (1979). Agreed terms on health effects evaluation and risk and hazard assessment of environmental agents. Internal report of a working group. (EHE/EHC/79.19). World Health Organisation, Geneva. In: Duffus J.F. (1993). Glossary for chemists of terms used in toxicology. Pure & Appl. Chem. **65(9)**, 2003-2122.

Appendix II. Data items incorporated in the EEC-OECD HEDSET

1. General information

1.01 Substance Identification

CAS-N^{o}
IUPAC-Name
EINECS-No.
Molecular Formula
Structural Formula (in Smiles code)
Molecular Weight

1.02 ID of Diskette Submitter

Company name
Type
Address

1.03 ID of the submitter of the full HEDSET

Company name
Type
Address

1.04 OECD/Company Information

Type
Name
Partner
Date
Address

1.1 General Substance Information

Substance Type
Physical State
Purity (% w/w)

1.2 Synonyms

1.3 Impurities

CAS-No
EINECS-No
IUPAC-Name
Value (% w/w)

1.4 Additives

CAS-No
EINECS-No
IUPAC-Name
Value (% w/w)

1.5 Quantity

Quantity produced or imported (tonnes in year)
Year - For the purpose of the EEC regulation
Indicate if the substance has been produced during the 12 months after adoption of the EEC regulation on existing substances
Indicate if the substance has been produced during the 12 months after adoption of the EEC regulation on existing substances

1.6. Labelling and classification

1.6.1 Labelling

Is the substance Labelled by -
Specific Limits
Symbols
Nota
R Phrases
S Phrases
Text

1.6.2 Classification

Classification
Category of Danger
R Phrases

1.7 Use Pattern

Type of Use
Category for the type of Use

1.8 Occupational Exposure Limit Value

Exposure Limit Value
Short Term Exposure Limit Value

1.9 Sources of Exposure

1.10 Additional Remarks

2. Physico-chemical Data

2.1 Melting Point

Value (degree C)
Decomposition
Sublimation
Method
Year
GLP

2.2 Boiling Point

Value (degree C)
Pressure
Decomposition
Method
Year
GLP

2.3 Density

Type
Value
Temperature (degree C)
Method
Year
GLP

2.4 Vapour Pressure

Value
Temperature (degree C)
Method
Year
GLP

2.5 Partition Coefficient

log Pow (base 10)
Temperature (degree C)
Method
Year
GLP

2.6 Water Solubility

Value
Temperature (degree C)
pH value
pKa at 25 degree C
Description
Method
Year
GLP

2.7 Flash Point

Value (degree C)
Type of Test
Method
Year
GLP

2.8 Auto Flammability

Value (degree C)
Pressure
Method
Year
GLP

2.9 Flammability

Results
Method
Year
GLP

2.10 Explosive Properties

Result
Method
Year
GLP

2.11 Oxidizing Properties

Result
Method
Year
GLP

2.12 Additional Remarks

3. Environmental Fate and Pathway

3.1 Stability

3.1.1 Photodegradation

Type
Light Source
Light Spectrum
Relative Intensity (based on Intensity of Sunlight)
Spectrum of Substance
Concentration of Substance
Temperature (degree C)

DIRECT PHOTOLYSIS
- t1/2 (Halflife)
- Degradation (% w/w)
- Quantum yield

INDIRECT PHOTOLYSIS
- Type Sensitizer
- Concentration of Sensitizer
- Rate Constant (radical)
- Degradation (% w/w)

Method
Year
GLP
Test Substance

3.1.2 Stability in Water

Type
t1/2 (Half life) at pH 4, 7, 9 or at given pH
Degradation
Degradation products
Method
Year
GLP
Test Substance

3.1.3 Stability in Soil

Type
Radiolabel
Concentration
Soil Temperature (degree C)
Soil Humidity
Soil Classificat.
Year
Content of Clay, Silt and Sand (w/w %)
Organic Carbon (w/w %)
pH
Cation Exchange Capacity
Microbial Biomass
Dissipation Time DT50/DT90
Dissipation (w/w %)
Method
Year
GLP
Test Substance

3.2 Monitoring Data (Environment)

Type of Measurement
Media

3.3 Transport and distribution between environmental compartments

3.3.1 Transport

Type
Media
Method
Year
Results

3.3.2 Distribution

Media
Method
Year
Results

3.4 Mode of Degradation in Actual Use

3.5 Biodegradation

Type
Inoculum
Concentration
Degradation (w/w %)
Degradation Products
Results
Kinetic (e.g. Zahn-Wellens-Test)
Method
Year
GLP
Test Substance

3.6 BOD_5, COD or BOD_5/COD Ratio

BOD_5
- Method
- Year
- Concentration
- BOD_5 (mg/l)
- GLP

COD
- Method
- Year
- COD (mg/g substance)
- GLP

Ratio BOD_5/COD

3.7 Bioaccumulation

Species
Exposure Period
Temperature (degree C)
Concentration
Bioconcentration Factor (BCF)
Elimination
Method
Year
GLP
Test Substance

3.8 Additional Remarks

4. Ecotoxicity

4.1 Acute/Prolonged Toxicity to Fish

Type
Species
Exposure Period
Unit of Measurement
NOEC, LC0, LC50, LC100 and other
Analytical Monitoring
Method
Year
GLP
Test Substance

4.2 Acute/prolonged Toxicity to Aquatic Invertebrates

Species
Exposure Period
Unit of measurement
NOEC, EC0, EC50, EC100 and other
Analytical Monitoring
Method
Year
GLP
Test Substance

4.3 Toxicity to Aquatic Plants e.g. Algae

Species
End-point
Exposure Period
Unit of Measurement
EC0, EC10, EC50, NOEC, LOEC and other
Analytical Monitoring
Method
Year
GLP
Test Substance

4.4 Toxicity to Bacteria

Type
Species
Exposure Period
Unit of Measurement
EC0, EC10, EC50 and other
Analytical Monitoring
Method
Year
GLP
Test Substance

4.5 Chronic Toxicity to Aquatic Organism

4.5.1 Chronic Toxicity to Fish

Species
End-point
Exposure Period
Unit of measurement
LLC, NOEC, LOEC and other
Analytical Monitoring
Results
Method
Year
GLP
Test Substance

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species
End-point
Exposure period
Unit of Measurement
EC50, NOEC, LOEC and other
Analytical Monitoring
Results
Method
Year
GLP
Test Substance

4.6 Toxicity to Terrestrial Organisms

4.6.1 Toxicity to Soil Dwelling Organisms

Type
Species
End-point
Exposure Period
Unit of Measurement
NOEC, LC0, LC50, LC10 and other
Method
Year
GLP
Test Substance

4.6.2 Toxicity to Terrestrial Plants

Species
End-point
Exposure Period
Unit of Measurement
NOEC, EC50, LC50 and other
Method
Year
GLP
Test Substance

4.6.3 Toxicity to Other Non-Mammalian Terrestrial Species

Species
End-point
Exposure Period
Unit of measurement
NOEC, LC0, LC50, LC100 and other
Method
Year
GLP
Test Substance

4.7 Biological Effects Monitoring (including Biomagnification)

4.8 Biotransformation and Kinetics in Environmental Species

4.9 Additional Remarks

5. Toxicity

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type
Species
Value
Method
Year
GLP
Test Substance

5.1.2 Acute Inhalation Toxicity

Type
Species
Exposure Time
Value
Method
Year
GLP
Test Substance

5.1.3 Acute Dermal Toxicity

Type
Species
Value
Method
Year
GLP
Test Substance

5.1.4 Acute Toxicity, Other Routes of Administration

Type
Species
Route of Administration
Exposure Time
Value
Method
Year
GLP
Test Substance

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species
Results
Classification
Method
Year
GLP
Test Substance

5.2.2 Eye Irritation

Species
Results
Classification
Method
Year
GLP
Test Substance

5.3 Sensitization

Type
Species
Result
Classification
Method
Year
GLP
Test Substance

5.4 Repeated Dose Toxicity

Species
Strain
Sex
Route of Administration
Exposure Period
Frequency of Treatment
Post Exposure Observation Period
Doses
Control Group
NOEL, LOEL
Results
Method
Year
GLP
Test Substance

5.5 Genetic Toxicity in Vitro

Type
System of Testing
Concentration
Metabolic Activation
Results
Method
Year
GLP
Test Substance

5.6 Genetic Toxicity in Vivo

Type
Species
Strain
Sex
Route of Administration
Exposure Period
Doses
Results
Method
Year
GLP
Test Substance

5.7 Carcinogenicity

Species
Strain
Sex
Route of Administration
Exposure Period
Frequency of Treatment
Post Exposure Observation Period
Doses
Control Group
Method
Year
GLP
Test Substance

5.8 Toxicity to Reproduction

Type
Species
Strain
Sex
Route of Administration
Exposure Period
Frequency of Treatment
Premating Exposure Period
Duration of Test
Doses
Control Group
NOEL Parental
NOEL F1 Offspring
NOEL F2 Offspring
Results
Method
Year
GLP
Test Substance

5.9 Developmental Toxicity/Teratogenicity

Species
Strain
Sex
Route of Administration
Exposure Period
Frequency of Treatment
Doses
Control Group
NOEL Maternal Toxicity
NOEL Teratogenicity
Results
Method
GLP
Test Substance

5.10 Other Relevant Information

Type

5.11 Experience with Human Exposure

Appendix III. Emission factors for different use categories

Contents

Introduction to the release tables
For all industrial categories distinguished in Section II.3 estimates have been generated for:

1. The emission factors for all (relevant) stages of the life cycle, i.e. (1) production, (2) formulation, (3) industrial use, (4) private use, service life(5), and waste treatment; these estimates have been collected in the 'A-tables'. When possible defaults occurring in emission scenario documents of the TGD have been implemented.

2. The fraction of the main source and the number of emission days (point sources); these estimates have been collected in the 'B-tables'. When possible data on the model source of emission scenario documents of the TGD have been implemented.

Many tables are applied for more than one category, but are given only once (at the first occurrence). For other categories, reference is made to the number of those tables. It should be noted that only for a limited number of industrial categories and specific applications (use categories) have studies been performed (resulting in so-called use-category documents) to provide a solid basis for the estimates.

Types of substances and levels of production and use
New substances are usually produced at a rather low level. For existing substances high production-volume chemicals (HPVC) will also have to be considered. Non-HPVCs will be indicated in the tables with NSEC (New Substances and Existing Chemicals). In 1990 the OECD list of HPVCs contained about 1600 chemicals which are either produced in excess of 10,000 tonnes in any one member country or in two or more countries in excess of 1,000 tonnes. For the B-tables, default values have been introduced for every industrial category, above which a chemical is considered to be an HPVC (unless the chemical is considered as an HPVC by the notifier or when a tonnage is indicated for a HPVC in the relevant emission scenario document of the TGD). If the (production) volume of a substance is rather high (HPVC), it may be unrealistic to use the standard size for the STP. A correction may be made in a more refined stage of the assessment.

In the text the term 'volume' will be used instead of 'production volume', as the volume applied

in the EU is now considered. This means that the volume (or tonnage) equals the production volume + the volume imported in the EU - the volume exported from the EU (the substance as such, not the quantities imported in products). It should be noted that the regional production or tonnage volume is used as input for the emission tables.
A chemical may have applications in more than one industrial category (IC) and/or use category (UC). As an assessment has to be made for all relevant applications of the chemical, the input of fractions for different industrial- and use-category combinations must be realised.

Aspects of production
If specific data on emissions at production are known, these can be used instead of the tables. Specific data may also be entered for the fraction of the main source, either as the capacity (tonnes/day) or as the period (days/year) in which the chemical is produced.

Aspects of formulation
For this stage of the life cycle, too, specific data may be entered on the fraction of the main source and the emissions/emission factors. For the emissions, a refinement may be achieved by discriminating between cleaning with/without water and soap. This has not yet been done. If a substance is applied in a formulation at a rather low level, unrealistic values for the fraction of the main source and the number of days will be derived from the tables using the tonnage as such. Therefore a correction is made for the tonnage used as input for the B-tables: if the percentage of substance in the formulation is 0.1, the volume (tonnes/year) is multiplied by 100/0.1. This tonnage may then be used to estimate the fraction of the main source and the number of days. It is possible to calculate an average if a range of contents has been specified.

Aspects of industrial use
Specific data on the fraction of the main source and the emissions may be used as input. This will be repeated for every specified IC-UC combination. If there is a specific scenario for an IC-UC combination, specific data will be requested. An interesting point that has not been elaborated yet is the possible emissions of chemicals present in articles after industrial use. These articles will be used for periods ranging from days up to many years. Examples are plasticizers in PVC articles. The number of these articles will build up over the years, and the diffuse emissions due to migration followed by evaporation and leaching will hence increase.

Aspects of service life
The life cycle stage service life is only considered for articles produced in textile industry.

Aspects of private use
Specific data on the fraction of the main source and the emissions may be used. This will be possible for every specified IC-UC combination for which the stage of private use is relevant.

Aspects of waste treatment
Specific data on the fraction of the main source and the emissions may be used. This will be possible for every specified IC-UC combination for which the stage of waste treatment is relevant. For waste treatment only situations where a material – which contains the chemical of interest – is recovered and processes to make it suitable for reuse in its original application (recycling) or another application are mentioned.

A-tables: Estimates for the emission factors (fractions released)

IC = 1: AGRICULTURAL INDUSTRY

PRODUCTION Table A1.1

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors All MC's	MC=1b	MC=1c	MC=3 (1)
Air		<1		0	0	0.00001
		1-10		0	0.00001	0.0001
		10-100		0.00001	0.0001	0.001
		100-1,000		0.0001	0.001	0.01
		1,000-10,000		0.001	0.005	0.05
		≥10,000		0.005	0.01	0.05
	T (tonnes/year)					
Waste water	<1,000		0.02			
	≥1,000		0.003			
Soil			0.0001			

(1) Default

FORMULATION Table A2.1

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors All MC's	MC=1b	MC=1c	MC=3 (1)
Air		<10		0.0005	0.001	0.0025
		10-100		0.001	0.0025	0.005
		100-1,000		0.0025	0.005	0.01
		≥1,000		0.005	0.01	0.025
		T (tonnes/year)				
Waste water		<1,000	0.02			
		≥1,000	0.003			
Soil			0.0001			

(1) Default

INDUSTRIAL USE Table A3.1

UC's	Description	Emission factors to:	Air	Surface water	Industrial soil
Default other UCs than specified below			0.1	0.1	0*
3	aerosol propellants		1	0	0
9, 10, 36	cleaning/washing agents and additives + colorants + odour agents		0	0.1	0.4
19	fertilisers		0	0.05	0.95
26	food/feedstuff additives		0	0	0.05
38, 50	pesticides + surfactants		0.05	0.1	0.85
41	pharmaceuticals (external application)		0	0	0.1
41	pharmaceuticals (internal application)	0	0	0	
48	solvents		1	0	0

Fertilisers and pesticides + surfactants go to agricultural soil on the regional and continental scale, the others go to industrial soil

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC=2: CHEMICAL INDUSTRY: BASIC CHEMICALS

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.2

Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors Air	Waste water	Soil
<100	<100	0.65	0.25	0.0005
	100-1,000	0.8	0.1	0.0025
	≥1,000	0.95	0.05	0.001
100-1,000	<100	0.4	0.5	0.005
	100-1,000	0.55	0.35	0.002
	≥1,000	0.65	0.25	0.001
1,000-10,000	<100	0.25	0.65	0.005
	100-1,000	0.35	0.55	0.002
	≥1,000	0.5	0.4	0.001
≥10,000	<100	0.05	0.85	0.005
	100-1,000	0.1	0.8	0.002
	≥1,000	0.25	0.65	0.001

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable
(Emissions at recovery of chemicals such as catalysts are included in the emissions at industrial use)

IC = 3: CHEMICAL INDUSTRY: CHEMICALS USED IN SYNTHESIS

PRODUCTION Table A1.1 for UC ≠ 33 (intermediates)
Table A1.2 for UC = 33 (intermediates)

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors All MC's	MC=1a	MC=1b	MC=1c
Air		<1		0	0	0
		1-10		0	0	0.00001
		10-100		0	0.00001	0.0001
		100-1,000		0.00001	0.0001	0.001
		1,000-10,000		0.0001	0.001	0.01
		≥10,000		0.001	0.01	0.025
	Process	T (tonnes/year)				
Waste water	Wet	<1,000	0.02			
		≥1,000	0.003			
	Dry		0			

PRODUCTION Table A1.2 for UC = 33 (intermediates)

Compartment	Conditions	Emission factors All MC's	MC=1a	MC=1b	MC=1c
Soil			0	0.00001	0.0001

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.3

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors All MC's	MC = 1b	MC = 1c	MC = 3 (1)
Air		<1		0	0	0.00001
		1-10		0	0	0.0001
		10-100		0	0.00001	0.001
		100-1,000		0.00001	0.0001	0.01
		1,000-10,000		0.0001	0.001	0.025
		≥10,000		0.001	0.005	0.05
	Process	T (tonnes/year)				
Waste water	Wet	<1,000	0.02			
		≥1,000	0.007	0.0005		
	Dry		0			
Soil			0.0001			

(1) Default

Remark: The releases at industrial use for use category 33 (intermediates) should be added to the releases at production **unless** the notifier states that the substance is processed elsewhere

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 4: ELECTRICAL/ELECTRONIC INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.4

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors MC = 2	MC = 3 (1)
Air		<100	0.0005	0.0005
		≥100	0.0005	0.001
Waste water			0.0001	0.005

INDUSTRIAL USE Table A3.4 **Continued**

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors MC = 2	MC = 3 (1)
Soil			0.0001	0.01

(1) Default

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 5: PERSONAL /DOMESTIC

PRODUCTION Table A1.1 for UC ≠ 9 (cleaning/washing agents) and 15 (cosmetics)
PRODUCTION Table A1.2 for UC = 9 and 15 (if production volume < 1000 tonnes/year Table A1.1 applies)

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors Batch process [1)]	Continuous process [2)]
Air			0.000 001	0.000 001
Wastewater			. [3)]	. [4)]
Solid waste			0	0

1) E.g., ethoxilation to nonionic surfactants and production of amphoteric and cationic surfactants
2) E.g., sulphonation and sulphation to anionic surfactants
3) According to the emission scenario document < 0.3 % (worst case = 0.003)
4) According to the emission scenario document < 0.1 % (worst case = 0.001)

FORMULATION Table A2.1 for UC ≠ 9 (cleaning/washing agents) and 15 (cosmetics)
FORMULATION Table A2.2 for UC = 9 (cleaning/washing agents) and UC15 (cosmetics)

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors Regular powder	Compact powder	Liquid	Unknown
Air			0.000 2	0.000 2	0.000 02	0.000 2
Wastewater			0.000 1	0.000 01	0.000 9	0.000 9
Solid waste			0.007 3	0.008 1	0.003 2	0.008 1

INDUSTRIAL USE Not applicable

PRIVATE USE Table A4.1

Compartment	Conditions Use category	Sol. (mg/l)	Vap. (Pa)	Emission factors
Air	2, 7, 8, 9, 10, 11, 15			
	41,47, 50			0
	3			1
	5			0.0005
	26		<5,000	0
			≥5,000	0.01
	35		<5,000	0
			≥5,000	0.05
	36		<100	0.05
			100-2,500	0.2
			2,500-10,000	0.5
			≥10,000	0.9
	38 (herbicides)		0.01	
	(pesticides, garden)			0.05
	(pesticides, pets)		<100	0.05
			100-5,000	0.1
			≥5,000	0.8
	48, 55	<10	<10	0.005
			10-100	0.015
			100-1,000	0.15
			1,000-10,000	0.4
			≥10,000	0.6
Air	48, 55	10-100	<10	0.0015
			10-100	0.075
			100-1,000	0.125
			1,000-10,000	0.25
			≥10,000	0.4
		100-1,000	<10	0.0015
			10-100	0.025
			100-1,000	0.1
			1,000-10,000	0.15
			≥10,000	0.225
		≥1,000	<10	0.00075
			10-100	0.03
			100-1,000	0.075
			1,000-10,000	0.125
			≥10,000	0.175
Surface water	5, 35 (car products)		0.0005	

PRIVATE USE Table A4.1 **Continued**

Compartment	Conditions Use category	Sol. (mg/l)	Vap. (Pa)	Emission factors
Waste water	2	<25		0
		≥25		0.005
	3, 5, 19, 35			0
	7			0.01
	8 (household products)			0.95
	(cosmetics)			0.8
	9, 15			1
	50			0.99
	10 (cleaning products)			1
	(cosmetics)			0.8
	(else)			0.5
	11			0.8
	26			0.025
	36 (cosmetics)		<2,500	0.8
			2,500-10,000	0.5
			≥10,000	0.1
	(cleaning products, etc.)		<100	0.9
			100-2,500	0.8
			2,500-10,000	0.5
			≥10,000	0.1
	(else)		<100	0.5
			100-2,500	0.3
			2,500-10,000	0.2
			≥10,000	0.05
	38 (herbicides)			0
	(pesticides, garden)			0
	(pesticides, pets)			0.1
	41 (external)			0.25
	(oral)			0.05
	47			0.9
	48, 55	<10		0.1
		10-100		0.2
		100-1,000		0.4
		≥1,000		0.6

PRIVATE USE Table A4.1 **Continued**

Compartment	Conditions Use category	Sol. (mg/l)	Vap. (Pa)	Emission factors
Soil	2			0.0001
	3, 36, 41			0
	5			0.0005
	7			0.001
	8 (household products)			0.01
	(cosmetics)			0.001
	9, 15			0
	47, 50			0.01
	10 (cleaning products)			0.002
	(cosmetics)			0.0001
	(else)			0.01
	11			0.0001
	19			1
	26, 35			0.002
	38 (garden: herbicides, pesticides)			0.9
	(pesticides, pets)		<100	0.05
			100-5,000	0.01
			≥5,000	0.002
	48, 55		<10	0.2
			10-100	0.1
			100-1,000	0.05
			1,000-10,000	0.005
			≥10,000	0.002

WASTE TREATMENT Not applicable

IC = 6: PUBLIC DOMAIN

PRODUCTION	Table A1.1 for UC ≠ 9 (cleaning/washing agents) and 15 (cosmetics)
PRODUCTION	Table A1.2 for UC = 9 and 15 (if production volume < 1000 tonnes/year Table A1.1 applies)
FORMULATION	Table A2.1 for UC ≠ 9 (cleaning/washing agents)
FORMULATION	Table A2.2 for UC = 9 (cleaning/washing agents)
INDUSTRIAL USE	Table A3.5

Conditions Use categories		Emission factors Air	Waste water	Soil
9	(cleaning/washing agents)			
	≤ 1000 tonnes/year	0.0025	0.9	0.05
	> 1000 tonnes/year	0	1	0
39	(pesticides, non-agricultural)	0.1	0.05	0.8
All	other	0.05	0.45	0.45

PRIVATE USE	Not applicable
WASTE TREATMENT	Not applicable

IC = 7: LEATHER PROCESSING INDUSTRY

PRODUCTION Table A1.1 for UC ≠ 10 (colorants)
Table A1.3 for UC = 10 (colorants)

UC = 10 (Colorants)

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors
Air			0.0008
Waste water	<2,000		0.015
	2,000-10,000		0.02
	10,000-100,000		0.03
	100,000-500,000		0.05
	≥500,000		0.06
Soil			0.0001

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.6

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors All MC's	MC = 2	MC = 3 (1)
Air	<100	<100	0.001		
	<100	≥100	0.01		
	≥100		0		
Waste water	<100			0.05	0.9
	100-1,000			0.15	0.99
	≥1,000			0.25	0.99
Soil			0.01		

(1) Default

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 8: METAL EXTRACTION, REFINING AND PROCESSING INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1 for UC ≠ 29 & 35
Table A2.2 for UC = 29 & 35

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors
Air		<1	0.00005
		1-10	0.00001
		10-100	0.0005
		100-1,000	0.0025
		≥1,000	0.025
Waste water			0.002
Soil			0.00001

(1) Default

INDUSTRIAL USE Table A3.7

Compartment	Conditions UC≠29&35	Sol. (mg/l)	Emission factors MC = 2	MC = 3 (1)
Air			0	0.25
Waste water		<100	0.05	0.5
		100-1,000	0.1	0.5
		≥1,000	0.25	0.5
Soil			0	0.05

Compartment	Conditions UC=29&35	log Henry	Emission factors
Air		<2	0.0002
		≥2	0.002
Waste water	Pure oils		0.185
	Water based + unknown		0.316
Soil			0.0001

(1) Default
UC 29 = heat transferring agents, UC 35 = lubricants and additives; both are used in metalworking fluids

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 9: MINERAL OIL AND FUEL INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.8

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors
Air		<1	0.0001
		1-10	0.0005
		10-100	0.001
		100-1,000	0.005
		≥1,000	0.01
Waste water			0.0005
Soil			0.001

PRIVATE USE Table A4.2

Compartment	Conditions	Vap. (Pa)	Emission factors
Air		<10	0.005
		10-100	0.015
		100-1,000	0.15
		1,000-10,000	0.4
		≥10,000	0.6
Waste water			0.0005
Surface water			0.0001
Soil			0.0001

WASTE TREATMENT Not applicable

IC = 10: PHOTOGRAPHIC INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1 default for formulations to be used in photographic baths (aqueous solutions)
Table A2.3 for UC=42, and other UC's in the manufacture of solid materials

Compartment	Conditions	Vap. (Pa)	Emission factors
Air	Control of crystal growth		0
	Other functions	<1	0.0001
		1-10	0.001
		10-100	0.3
		100-1,000	0.7
		≥1,000	0.99

FORMULATION Table A2.3 for UC=42, and other UC's in the manufacture of solid materials **Continued**

Compartment	Conditions	Emission factors
Waste water	Control of crystal growth Other functions	0.99 0.002
Soil		0.00025

(1) Default

INDUSTRIAL USE Table A3.9

Compartment	Conditions	Emission factors	
		Vap. (Pa)	MC=2	MC=3 (1)
Air	Solid materials (e.g. films)		0	
	Else	<1 1-10 10-100 100-1,000 ≥1,000		0.000035 0.00025 0.0075 0.025 0.075
Waste water	Solid materials (e.g. fims)		0	
	Aqueous solutions: - coupler of dye - else			0.15 0.8
Soil	Solid materials (e.g. fims) Else		0	0.00025

(1) Default

PRIVATE USE Table A4.3

Compartment	Conditions UC=42 (photochemicals), for aqueous solutions only!	Emission factors
Air		0
Waste water		0.4
Soil		0

WASTE TREATMENT Table A5.1

Compartment	Conditions UC=42 (photochemicals), for aqueous solutions only!	Vap. (Pa)	Emission factors
Air		<1 1-10 10-100 100-1,000 ≥1,000	0.000005 0.000025 0.00075 0.0025 0.01
Waste water			0.2
Soil			0

IC = 11: POLYMERS INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.10 for polymerization processes

In the polymers industry polymers are produced by:
A) Polymerisation reactions: A.1) "Wet" (e.g. emulsion polymerization)
A.2) "Dry" (e.g. gas phase polymerization)
B) Other (e.g. polyadditions, polycondensations)

The Use category (HEDSET) for all types of chemicals is: 43 Process regulators,

which can be subdivided into:

Type	Type of function
I	Monomers (UC 43 Process regulators)
II	Catalysts (UC 43 Process regulators)
III	Initiators, Inhibitors, Retarders, Chain transfer agents (UC 43 Process regulators),
	Vulcanising agents (UC 53 Vulcanising agents), etc.

N.B. 1. In principle this might be considered as stage 1. Production!
2. As no good information is available Process types "A.1" and "B" have been considered to have the same emission factors

INDUSTRIAL USE Table A3.10 for polymerisation processes

Compartment	Conditions	Emission factors					
		Type I		Type II		Type III	
	Vap. (Pa)	"Wet"	"Dry"	"Wet"	"Dry"	"Wet"	"Dry"
Air	<1	0.00001	0.00001	0	0	0	0
	1-10	0.0001	0.0001	0	0	0	0
	10-100	0.001	0.001	0	0	0	0
	100-1,000	0.01	0.01	0.0005	0.0005	0	0
	1,000-10,000	0.05	0.05	0.001	0.001	0.0005	0.0005
	≥10,000	0.05	0.05	0.01	0.01	0.001	0.001

INDUSTRIAL USE Table A3.10 for polymerisation processes **Continued**

Compartment	Conditions	Emission factors					
		Type I		Type II		Type III	
	Sol. (mg/l)	"Wet"	"Dry"	"Wet"	"Dry"	"Wet"	"Dry"
Waste water	<10	0.00001	0	0.005	0	0.0005	0
	10-100	0.0001	0	0.01	0	0.001	0
	100-1,000	0.001	0	0.025	0	0.0025	0
	≥1,000	0.01	0	0.05	0	0.005	0
	Vap. (Pa)						
Soil	<5,000	0	0	0.0005	0.0005	0.00025	0.00025
	≥5,000	0	0	0	0	0	0

INDUSTRIAL USE Table A3.11 for polymer processing

Processing of polymers ("shaping" by all kind of techniques) occurs in many Industrial categories

Two categories of polymer processing are distinguished:

A Processing of thermoplastics
B Processing of thermosetting resins (prepolymers)

For the emission factors the following types of chemicals used are considered:

I	(A, B)	Additives	UC 7 (Anti-static agents), 22 (Flame retardants), 49 (Stabilizers) & 55 Others (e.g. antioxidants)
		Pigments	UC 10 (colorants)
		Fillers	UC 20
II	(A)	Plasticizers	UC 47 (softeners)
III	(A, B)	Solvents	UC 48
IV	(A, B)	Processing aids	UC 6 (Anti-set off and anti-adhesive agents) & 35 (lubricants and additives)
V	(B)	Curing agents	UC 43 (Process regulators, e.g. initiators)
		Cross-linking agents	UC 43 (Process regulators: monomers)

INDUSTRIAL USE Table A3.11 for polymer processing

Compartment	Conditions		Emission factors		Type of
	Vap. (Pa)	Boiling point (°C)	A	B	chemicals
Air	<1	<300/unknown	0.001	0	I
		≥300	0.0005	0	
	1-100	<300/unknown	0.0025	0	
		≥300	0.001	0	
	≥100	<300/unknown	0.01	0	
		≥300	0.005	0	
		<400/unknown	0.01		II
		≥400	0.005		
	<100		0.1	0.1	III
	100-1,000		0.25	0.25	
	1,000-10,000		0.5	0.5	
	≥10,000		0.75	0.75	

INDUSTRIAL USE Table A3.11 for polymer processing **Continued**

Compartment	Conditions Vap. (Pa)	Boiling point (°C)	Emission factors A	B	Type of chemicals
Air	<1	<300/unknown	0.01	0	IV
		≥300	0.005	0	
	1-100	<300/unknown	0.025	0	
		≥300	0.01	0	
	≥100	<300/unknown	0.1	0	
		≥300	0.05	0	
	<100			0.075	V
	100-1,000			0.15	
	1,000-10,000			0.25	
	≥10,000			0.35	
Waste water			0.0005	0.0005	I
			0.001	0	II
			0	0	III
			0.0005	0.0005	IV
				0.00005	V
Soil			0.0001	0.0001	I
			0.0005	0	II
			0.00001	0.00001	III
			0.001	0.001	IV
				0.00001	V

PRIVATE USE Not applicable

WASTE TREATMENT Not considered yet

IC = 12: PULP, PAPER AND BOARD INDUSTRY

PRODUCTION Table A1.1 for UC ≠ 10 (colorants)
Table A1.3 for UC = 10 (colorants)

FORMULATION Table A2.1 for UC ≠ 45 (reprographic agents)
Table A2.1 for UC = 45 (reprographic agents)

INDUSTRIAL USE Table A3.12 for printing and allied processes

Compartment	Conditions Use categories	Vap. (Pa)	Emission factors MC = 2	MC = 3 (1)
Air	Default	<100	0	0.01
		100-1,000	0.05	0.2
		1,000-10,000	0.25	0.5
		≥10,000	0.5	0.75
	10 & 45		0	
	48	<100		0.05
		100-1,000		0.3
		1,000-10,000		0.65
		≥10,000		0.85
		Sol. (mg/l)	MC = 2	MC = 3 (1)
Waste water	Default	<100	0.0001	0.01
		100-1,000	0.005	0.05
		≥1,000	0.001	0.1
	9			0.9
	10 & 45		0.0005	
	48	<100		0.0005
		100-1,000		0.001
		≥1,000		0.005
		Vap. (Pa)	MC = 2	MC = 3 (1)
Soil	All	<100	0.0015	0.0015
		100-1,000	0.0001	0.0001
		1,000-10,000	0.00001	0.00001
		≥10,000	0	0

(1) Default

INDUSTRIAL USE Table A3.13 for pulp, paper and board production

Compartment	Conditions Use category	Sol. (mg/l)	Emission factors Vap. (Pa)	MC=2	MC=3 (1)	
Air	All		<100	<100	0	0.0001
				100-1,000	0.00001	0.001
				≥1,000	0.0001	0.01
			100-1,000	<100	0	0.00001
				100-1,000	0	0.0001
				≥1,000	0.00001	0.001
			≥1,000	<100	0	0
				100-1,000	0	0.0001
				≥1,000	0	0.001

INDUSTRIAL USE Table A3.13 for pulp, paper and board production **Continued**

Compartment	Conditions Use category	Emission factors Sol. (mg/l)	Vap. (Pa)	MC=2	MC=3 (1)
Waste water	Default	<100	<100	0.85	0.85
			100-500	0.75	0.75
			≥500	0.5	0.5
		100-1,000	<100	0.875	0.875
			100-500	0.85	0.85
			≥500	0.75	0.75
		1,000-10,000	<100	0.9	0.9
			100-500	0.875	0.875
			≥500	0.85	0.85
		≥10,000	-	0.95	0.95
	10:				
	- Basic dye, anion			0.023	0.023
	- Direct dye			0.04	0.04
	- Direct dye, kation			0.055	0.055
	- Direct dye, anion/kation			0.028	0.028
	- Acid dye, kation/unknown			0.079	0.079
	- Brightener			0.064	0.064
	20 & 31			0.05	0.05
Soil	All		<100	0.0015	0.0015
			100-1,000	0.0001	0.0001
			1,000-10,000	0.00001	0.00001
			≥10,000	0	0

(1) Default

PRIVATE USE Not applicable

WASTE TREATMENT Table A5.2

Compartment	Conditions	Emission factors
Air		0
Waste water	Use category = 10 (Colourants)	0.1
	Use category 45, for paper type:	
	- graphic	0.2
	- cardboard	0.01
	- newspaper	0.15
	- sanitary	0.01
	- packing	0.1
	- archives	0.05
	- other, or >1 application	0.2
Soil		0

IC = 13: TEXTILE PROCESSING INDUSTRY

PRODUCTION Table A1.1 for UC ≠ 10 (colourants)
Table A1.3 for UC = 10 (colourants)

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.14

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors UC<>10	UC = 10
Air	<100	<100	0.05	
		100-1,000	0.15	
		≥1,000	0.4	
	100-1,000	<100	0.025	
		100-1,000	0.05	
		≥1,000	0.15	
	1,000-10,000	<100	0.01	
		100-1,000	0.025	
		≥1,000	0.05	
	≥10,000	<100	0.005	
		100-1,000	0.01	
		≥1,000	0.025	
	Conditions			
	Batch dyeing			0.0007
	Continuous dyeing			
	- thermosol/unknown			0.05
	- other			0.0025
	- printing			0.0025
	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors UC<>10	
Waste water	<100	<100	0.85	
		100-1,000	0.75	
		≥1,000	0.5	
	100-1,000	<100	0.875	
		100-1,000	0.85	
		≥1,000	0.75	
	1,000-10,000	<100	0.9	
		100-1,000	0.875	
		≥1,000	0.85	
	≥10,000	-	0.95	

WASTE WATER for UC = 10 (colorants):
Emission factor (EF) = Emission factor dyeing process (E.1) + Emission factor "handling, washing out and cleaning" (E.2)

E.1 = A / (1 + K * B) B = 1 / liquor ratio (liquor ratio: default = 10 kg fibres / 1 l solution)
A = constant
K = equilibrium constant

INDUSTRIAL USE Table A3.14 **Continued**

Conditions Type of dye	(**UC = 10**) Type of dyeing	K	A	B	E.2
Disperse	Continuous	115	5	1	0.055
"	Printing	115	2	0.5	0.12
Direct	Batch	73	1	0.1 (1)	0.01
Reactive - wool	Batch	190	1	0.1 (1)	0.01
Reactive - cotton	Batch	23	1	0.1 (1)	0.01
Reactive - general	Batch	57	1	0.1 (1)	0.01
Vat	Continuous	190	5	1	0.055
	Printing	190	2	0.5	0.12
Sulfur	Continuous	40	5	1	0.055
	Printing	40	2	0.5	0.12
Acid - one SO3	Batch	90	1	0.1 (1)	0.01
Acid - > 1 SO3	Batch	190	1	0.1 (1)	0.01
Basic	Batch	990	1	0.1 (1)	0.01
Azoic (naphtole)	Continuous	30	5	1	0.055
	Printing	30	2	0.5	0.12
Metal complex	Batch	150	1	0.1 (1)	0.01
Pigment	Continuous	5000	5	1	0.055
	Printing	5000	2	0.5	0.12
Unknown, low solubility	Continuous	190	5	1	0.055
	Printing	190	2	0.5	0.12
Unknown, acid groups	Batch	90	1	0.1 (1)	0.01

(1) Default

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors UC<>10	UC=10
Soil				0.005
	<100	<100	0.005	
		100-500	0.0025	
		≥500	0.001	
	≥100	<100	0.005	
		100-500	0.002	
		≥500	0.001	

PRIVATE USE Table A4.4

Compartment	Conditions Sol. (mg/l)	Emission factors UC<>10	UC=10 (1)
Air			0
Waste water	<250		0.1
	250-1,000		0.15
	1,000-5,000		0.2
	≥5,000		0.3
Soil			0

(1) For UC = 10 (Colorants) only, i.e. types used normally by industry for batch dyeing

5. WASTE TREATMENT Not applicable

IC = 14: PAINTS, LACQUERS AND VARNISHES INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.15

Compartment	Conditions Use category	Vap. (Pa)	Emission factors Water based	Solvent based
Air	3			1
	10, 14, 20		0	0
	50		0	
	47, 52, 55	<10	0	0
		10-500	0	0.001
		500-5,000	0.01	0.05
		≥5,000	0.05	0.15
	48		0.8	0.9
		Sol. (mg/l)		
Waste water	3			0
	10, 14, 20		0.005	0.001
	50	<10	0.005	
		10-100	0.01	
		≥100	0.05	
	47, 52, 55	<10	0.005	0.001
		10-100	0.01	0.005
		≥100	0.05	0.01
	48		0.1	0.02
Soil	3			0
	10, 14, 20		0.005	0.005
	50		0.005	
	47, 52, 55		0.005	0.005
	48		0.001	0.001

PRIVATE USE Table A4.5

Compartment	Conditions Use category	Vap. (Pa)	Emission factors Water based	Solvent based
Air	3			1
	10, 14, 20		0	0
	50		0	
	47, 52, 55	<10	0	0
		10-500	0	0.001
		500-5,000	0.01	0.05
		≥5,000	0.05	0.15
	48		0.8	0.95

PRIVATE USE Table A4.5 **Continued**

	Conditions Use category	Sol. (mg/l)	Emission factors Water based	Solvent based
Waste water	3			0
	10, 14, 20		0.005	0.001
	50	<10	0.005	
		10-100	0.01	
		≥100	0.05	
	47, 52, 55	<10	0.005	0.001
		10-100	0.01	0.005
		≥100	0.05	0.01
	48		0.15	0.04
Soil	3			0
	10, 14, 20		0.005	0.005
	50		0.005	
	47, 52, 55		0.005	0.005
	48		0.01	0.01

WASTE TREATMENT Not applicable

IC = 16: ENGINEERING INDUSTRY: CIVIL AND MECHANICAL

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.16

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors MC=2	MC=3 (1)	MC =4
Air	<100	<10	0.0001	0.001	0.01
		10-100	0.001	0.01	0.1
		100-1,000	0.01	0.1	0.25
		1,000-10,000	0.1	0.5	0.7
		≥10,000	0.5	0.75	0.9
	100-1000	<10	0.00001	0.0001	0.001
		10-100	0.0001	0.001	0.05
		100-1,000	0.001	0.05	0.1
		1,000-10,000	0.05	0.1	0.5
		≥10,000	0.25	0.5	0.75
	≥1,000	<10	0	0.00001	0.0001
		10-100	0.00001	0.0001	0.001
		100-1,000	0.0001	0.001	0.01
		1,000-10,000	0.001	0.01	0.1
		≥10,000	0.01	0.1	0.5

INDUSTRIAL USE Table A3.16 **Continued**

Compartment	Conditions Sol. (mg/l)	Vap. (Pa)	Emission factors MC=2	MC=3 (1)	MC =4
Waste water	<100	<10	0.01	0.1	0.5
		10-100	0.001	0.01	0.1
		100-1,000	0.0001	0.001	0.01
		1,000-10,000	0.00001	0.0001	0.001
		≥10,000	0	0.00001	0.0001
	100-1000	<10	0.25	0.5	0.75
		10-100	0.05	0.1	0.5
		100-1,000	0.001	0.01	0.1
		1,000-10,000	0.0001	0.001	0.05
		≥10,000	0.00001	0.0001	0.001
	≥1,000	<10	0.5	0.75	0.9
		10-100	0.1	0.5	0.7
		100-1,000	0.01	0.1	0.25
		1,000-10,000	0.001	0.01	0.1
		≥10,000	0.0001	0.001	0.01
Soil	<100	<10	0.005	0.01	0.05
		10-100	0.001	0.005	0.01
		100-1,000	0.0005	0.001	0.005
		1,000-10,000	0	0.0005	0.001
		≥10,000	0	0	0.0005
	100-1000	<10	0.001	0.005	0.01
		10-100	0.0005	0.001	0.005
		100-1,000	0	0.0005	0.001
		1,000-10,000	0	0	0.0005
		≥10,000	0	0	0.0001
	≥1,000	<10	0.0005	0.001	0.005
		10-100	0	0.0005	0.001
		100-1,000	0	0	0.0005
		1,000-10,000	0	0	0.0001
		≥10,000	0	0	0

(1) Default

4. PRIVATE USE Table A3.16

WASTE TREATMENT Not applicable

IC = 0: OTHERS

PRODUCTION Table A1.1

FORMULATION Table A2.1

INDUSTRIAL USE Table A3.16

B-tables: Estimates for the fraction of the main source and

IC = 1: AGRICULTURAL INDUSTRY

PRODUCTION	Table B1.1 for new substances and existing substances other than HPVC for UC ≠ 38 & 41	
T (tonnes/year)	f main source	No. of days
<1,000	1	0.1f*T
1,000-2,000	0.9	0.1f*T
2,000-4.000	0.75	0.1f*T
≥4,000	0.7	300

PRODUCTION	Table B1.2 for new substances and existing substances other than HPVC for UC = 38 & 41	
T (tonnes/year)	f main source	No. of days
<10	1	f*T
10-50	0.9	f*T
50-100	0.8	0.6667f*T
100-1,000	0.75	0.4f*T
1,000-2,500	0.6	0.2f*T
≥2,500	0.6	300

PRODUCTION	Table B1.3 for HPVC (default ≥10,000) for UC ≠ 38 & 41	
T (tonnes/year)	f main source	No. of days
<25,000	1	300
25,000-100,000	0.75	300
>100,000	0.6	300

PRODUCTION	Table B1.4 for HPVC (default ≥3,500) for UC = 38 & 41	
T (tonnes/year)	f main source	No. of days
<5,000	1	300
5,000-25,000	0.8	300
25,000-100,000	0.6	300
≥100,000	0.4	300

FORMULATION	Table B2.1 for new substances and existing substances other than HPVC	
T (tonnes/year)	f main source	No. of days
<100	1	2f*T
100-500	0.6	f*T
500-1,000	0.6	0.5f*T
≥1,000	0.4	300

FORMULATION Table B2.2 for HPVC for UC ≠ 38 & 41

T (tonnes/year)	f main source	No. of days
<15,000	1	300
15,000-50,000	0.75	300
≥50,000	0.6	300

FORMULATION Table B2.3 for HPVC for UC = 38 & 41

T (tonnes/year)	f main source	No. of days
<3,500	1	300
3,500-10,000	0.8	300
10,000-25,000	0.7	300
25,000-50,000	0.6	300
≥50,000	0.4	300

INDUSTRIAL USE Table B3.1

T (tonnes/year)	f main source	No. of days for use categories:			
		3,19,39,48,50	41	9,10,36	26
<10	0.05	2	10	50	300
10-100	0.01	2	10	50	300
100-1,000	0.005	2	10	50	300
1,000-10,000	0.001	2	10	50	300
10,000-50,000	0.0005	2	10	50	300
≥50,000	0.00001	2	10	50	300

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 2: CHEMICAL INDUSTRY: BASIC CHEMICALS

PRODUCTION Table B1.1 for NSEC
Table B1.5 for HPVC (default ≥10,000)

T (tonnes/year)	f main source	No. of days
<25,000	1	300
25,000-100,000	0.75	300
100,000-500,000	0.6	300
≥500,000	0.5	300

FORMULATION Table B2.4 for NSEC
If applicable!

T (tonnes/year)	f main source	No. of days
<10	1	2f*T
10-50	0.9	f*T
50-500	0.8	0.4f*T
500-2,000	0.75	0.2f*T
≥2,000	0.65	300

FORMULATION Table B2.5 for HPVC
If applicable!

T (tonnes/year)	f main source	No. of days
<25,000	1	300
25,000-50,000	0.75	300
≥50,000	0.4	300

INDUSTRIAL USE Table B3.2

T (tonnes/year)	f main source	No. of days
<10	0.8	2f*T
10-50	0.65	f*T
50-500	0.5	0.4f*T
500-2,000	0.4	0.25f*T
2,000-5,000	0.3	0.2f*T
5,000-25,000	0.25	300
25,000-75,000	0.2	300
≥75,000	0.15	300

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 3: CHEMICAL INDUSTRY: CHEMICALS USED IN SYNTHESIS

PRODUCTION Table B1.2 for NSEC
Table B1.6 for HPVC (default ≥7,000)

T (tonnes/year)	f main source	No. of days
<10,000	1	300
10,000-50,000	0.75	300
50,000-250,000	0.6	300
≥250,000	0.5	300

FORMULATION Table B2.4 for NSEC
Table B2.3 for HPVC
If applicable!

INDUSTRIAL USE Table B3.2

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 4: ELECTRICAL/ELECTRONIC INDUSTRY

PRODUCTION Table B1.7 for NSEC

T (tonnes/year)	f main source	No. of days
<100	1	0.1f*T
100-1,000	0.9	0.1f*T
1,000-2,500	0.8	0.1f*T
≥2,500	0.75	300

PRODUCTION Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.4 for NSEC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.2

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 5: PERSONAL/DOMESTIC

PRODUCTION Table B1.7 for NSEC
Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.1 for NSEC
Table B2.3 for HPVC

INDUSTRIAL USE Not applicable

PRIVATE USE Table B4.1 for UC ≠ 9 (cleaning/washing agents) and 15 (cosmetics)
Only for waste water!

T (tonnes/year)	f main source	No. of days:
	0.002	365

PRIVATE USE Table B4.2 for UC = 9 and 15 (if production volume < 1000 tonnes/year Table B4.1 applies)
A) Based on tonnage

T (tonnes/year)	No. inhabitants region	No. inhabitants feeding STP	No. of days:
	$2.0*10^7$	10,000	365

WASTE TREATMENT Not applicable

IC = 6: PUBLIC DOMAIN

PRODUCTION Table B1.7 for NSEC
Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.1 for NSEC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.3
Only for waste water!

T (tonnes/year)	f main source	No. of days for use categories:		
		9	39	Else
	0.002	200	15	50

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 7: LEATHER PROCESSING INDUSTRY

PRODUCTION Table B1.8 for NSEC for UC ≠ 6, 9 10 & 31

T (tonnes/year)	f main source	No. of days
<1,000	1	0.1f*T
1,000-4,000	0.9	0.1f*T
≥4,000	0.75	300

PRODUCTION Table B1.9 for NSEC for UC = 6, 9 10 & 31

T (tonnes/year)	f main source	No. of days
<10	1	f*T
10-50	0.9	f*T
50-500	0.5	f*T
500-1,500	0.2	f*T
≥1,500	0.2	300

PRODUCTION Table B1.4 for HPVC (default ≥5,000) for UC ≠ 6, 9 10 & 31
Table B1.4 for HPVC (default ≥2,500) for UC = 6, 9 10 & 31

FORMULATION Table B2.4 for NSEC
Table B2.3 for HPVC for UC ≠ 6, 9, 10 & 31
Table B2.6 for HPVC for UC = 6, 9, 10 & 31

T (tonnes/year)	f main source	No. of days
<100,000	1	300
100,000-250,000	0.7	300
≥250,000	0.4	300

INDUSTRIAL USE Table B3.4

T (tonnes/year)	f main source	No. of days
<10	0.8	2f*T
10-50	0.75	2f*T
50-500	0.6	f*T
500-1,500	0.5	0.4f*T
1,500-5,000	0.35	300
5,000-25,000	0.2	300
≥25,000	0.1	300

PRIVATE USE Not applicable

WASTE TREATMENT Not applicable

IC = 8: METAL EXTRACTION, REFINING AND PROCESSING INDUSTRY

PRODUCTION — Table B1.2 for NSEC for UC ≠ 29 & 35
Table B1.10 for NSEC for UC = 29 & 35

T (tonnes/year)	f main source	No. of days
<10	1	f*T
10-50	0.9	f*T
50-500	0.8	0.6667f*T
500-1,500	0.5	0.4f*T
≥1,500	0.5	300

PRODUCTION — Table B1.6 for HPVC (default ≥7,000) for UC ≠ 29 & 35
Table B1.4 for HPVC (default ≥2,500) for UC = 29 & 35

FORMULATION — Table B2.4 for NSEC
Table B2.3 for HPVC

INDUSTRIAL USE — Table B3.5 for UC = 29 & 35

T (tonnes/year)	No. of days	f main source:	Field of application: Primary steelworks	Else
<1,000	300		1	0.8
1,000-5,000	300		0.9	0.5
5,000-50,000	300		0.75	0.3
≥50,000	300		0.6	0.2

INDUSTRIAL USE — Table B3.6 for UC ≠ 29 & 35

T (tonnes/year)	f main source	No. of days
<10	1	2f*T
10-50	1	0.5f*T
50-500	0.9	0.4f*T
500-2,000	0.8	0.1875f*T
2,000-10,000	0.7	300
10,000-50,000	0.6	300
≥50,000	0.5	300

PRIVATE USE — Not applicable

WASTE TREATMENT — Not applicable

IC = 9: MINERAL OIL AND FUEL INDUSTRY

PRODUCTION Table B1.1 for NSEC for UC = 27
Table B1.2 for NSEC for UC = 28 and others <> 27
Table B1.4 for HPVC (default ≥3,000) for UC = 28 and others <> 27
Table B1.11 for HPVC (default ≥25,000) for UC = 27

T (tonnes/year)	f main source	No. of days
<100,000	1	300
100,000-500,000	0.75	300
≥500,000	0.5	300

FORMULATION Table B2.7 for NSEC for UC = 27

T (tonnes/year)	f main source	No. of days
<1,000	1	100
1,000-2,000	0.8	200
≥2,000	0.6	300

FORMULATION Table B2.8 for NSEC for UC = 28 and others <> 27

T (tonnes/year)	f main source	No. of days
<5	1	20
5-50	1	60
50-100	1	2f*T
100-500	0.8	f*T
500-1,000	0.6	0.5f*T
≥1,000	0.4	300

FORMULATION Table B2.6 for HPVC for UC = 27
Table B2.6 for HPVC for UC = 28

INDUSTRIAL USE Table B3.7

T (tonnes/year)	f main source	No. of days
<50	0.5	350
50-500	0.4	350
500-5,000	0.3	350
5,000-25,000	0.2	350
25000-100,000	0.05	350
≥100,000	0.02	350

PRIVATE USE Table 4.1
Only for waste water!

WASTE TREATMENT Not applicable

IC = 10: PHOTOGRAPHIC INDUSTRY

PRODUCTION Table B1.4 for HPVC (default ≥4,000)
Table B1.12 for NSEC

T (tonnes/year)	f main source	No. of days
<5	1	f*T
5-50	1	0.5f*T
50-250	0.75	0.4f*T
250-3,000	0.5	0.2f*T
≥3,000	0.5	300

FORMULATION Table B2.8 for NSEC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.8

Company size	f main source	No. of days	
One company	1	300	(No private use)
Large companies	0.333	300	(No private use)
Small companies	0.05	300	

PRIVATE USE Table B4.2
Only for waste water!
Only if company size at industrial use is small companies (otherwise f main source is zero)

f main source = 0.002 * f private use

T (tonnes/year)	f private use	f main source	No. of days:
<10	0	0	200
10-50	0.00002	4.10^{-8}	200
50-500	0.0001	2.10^{-7}	200
500-5,000	0.0005	1.10^{-6}	200
≥5,000	0.0025	5.10^{-6}	200

WASTE TREATMENT Table B5.1

T (tonnes/year)	f main source	No. of days	One company
<10	1	150	(No private use)
≥10	1	300	

T (tonnes/year)	f main source	No. of days	Large companies
<30	0.333	150	
≥30	0.333	300	

T (tonnes/year)	f main source	No. of days	Small companies
<200	0.2	150	
≥200	0.2	300	

IC = 11: POLYMERS INDUSTRY

PRODUCTION Table B1.9 for NSEC for UC ≠ 20, 47 & 43 (monomers, cross-linking agents & curing agents)
Table B1.13 for NSEC for UC = 20, 47 & 43 (monomers, cross-linking agents & curing agents; **not:** initiators, retarders & inhibitors)

T (tonnes/year)	f main source	No. of days
<50	0.9	0.4f*T
50-500	0.75	0.2F*T
500-5,000	0.6	0.1f*T
5,000-25,000	0.75	200
≥25,000	0.5	300

PRODUCTION Table B1.4 for HPVC (default ≥3,000) for UC ≠ 20, 47 & 43 (monomers, cross-linking agents & curing agents)

PRODUCTION Table B1.14 (default ≥60,000) for HPVC for UC = 20, 47 & 43 (monomers, cross-linking agents & curing agents; **not:** initiators, retarders & inhibitors)

T (tonnes/year)	f main source	No. of days
<100,000	1	300
100,000-250,000	0.65	300
≥250,000	0.4	300

FORMULATION Table B2.8 for NSEC
Table B2.3 for HPVC for UC ≠ 20, 47 & 43 (monomers, cross-linking agents & curing agents)
Table B2.9 for HPVC for UC = 20, 47 & 43 (monomers, cross-linking agents & curing agents; **not:** initiators, retarders & inhibitors)

T (tonnes/year)	f main source	No. of days
<25,000	1	300
25,000-50,000	0.75	300
≥50,000	0.4	300

INDUSTRIAL USE Table B3.9

T (tonnes/year)	f main source	No. of days
<10	0.5	2f*T
10-50	0.35	f*T
50-500	0.25	0.4f*T
500-5,000	0.15	0.4f*T
5,000-25,000	0.1	300
≥25,000	0.05	300

PRIVATE USE Not applicable

WASTE TREATMENT Not considered yet

IC = 12: PULP, PAPER AND BOARD INDUSTRY

PRODUCTION
Table B1.8 for NSEC for UC ≠ 10 & 45
Table B1.9 for NSEC for UC = 10 & 45
Table B1.4 for HPVC (default ≥4,500) for UC ≠ 10 & 45
Table B1.4 for HPVC (default ≥2,500) for UC = 10 & 45

FORMULATION
Table B2.1 for NSEC for UC ≠ 10 & 45
Table B2.8 for NSEC for UC = 10 & 45
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.10

T (tonnes/year)	f main source	No. of days
One company		
<10	1	2f*T
10-50	1	f*T
50-500	1	0.4f*T
≥500	1	300
Large companies		
<100	0.333	2f*T
100-250	0.333	f*T
250-600	0.333	0.5f*T
≥600	0.333	300
Small companies		
<200	0.05	2f*T
200-1,000	0.05	f*T
1,000-6,000	0.05	0.5f*T
6,000-25,000	0.05	300
≥25,000	0.02	300

PRIVATE USE Not considered yet

WASTE TREATMENT Table B5.2

T (tonnes/year)	f main source	No. of days
<100	0.5	150
100-1,000	0.4	200
1,000-10,000	0.3	250
10,000-100,000	0.2	300
≥100,000	0.1	300

IC =13: TEXTILE PROCESSING INDUSTRY

PRODUCTION Table B1.2 for NSEC
Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.3 for HPVC
Table B2.8 for NSEC

INDUSTRIAL USE Table B3.11 for UC = 10

T (tonnes/year)	f main source	No. of days
<10	0.9	10f*T
10-20	0.75	10f*T
20-100	0.6	5f*T
100-1,000	0.4	300
1,000-10,000	0.2	300
≥10,000	0.1	300

INDUSTRIAL USE Table B3.12 for UC ≠ 10

T (tonnes/year)	f main source	No. of days
<10	0.75	5f*T
10-100	0.4	5f*T
100-750	0.4	f*T
750-3,000	0.2	0.5f*T
3,000-25,000	0.2	300
≥25,000	0.1	300

PRIVATE USE Table B4.3
Only for waste water!
Only for UC = 10 (and only for types of dyes used for batch dyeing by industry) for all other UCs, the f main source is zero

f main source = 0.002 * f private use

T (tonnes/year)	f private use	f main source	No. of days:
<50	0	0	
50-500	0.000004	8.10^{-9}	300
≥500	0.00002	4.10^{-8}	300

WASTE TREATMENT Not applicable

IC = 14: PAINTS, LACQUERS AND VARNISHES INDUSTRY

PRODUCTION Table B1.2 for NSEC
Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.8 for NSEC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.13

T (tonnes/year)	f main source	No. of days
<10	0.9	20f*T
10-50	0.6	6.667f*T
50-300	0.3	3.333f*T
300-5,000	0.15	300
5,000-25,000	0.1	300
≥25,000	0.05	300

PRIVATE USE Table B4.4
Only for waste water!
Only for paints classified as 'do-it-yourself'

f main source = 0.002 * f private use

T (tonnes/year)	f private use	f main source	No. of days:
<500	1	0.002	150
≥500	1	0.002	300

PRIVATE USE Table B4.5
Only for waste water!
Only for paints classified as 'constructions, maintenance', etc.

f main source = 0.002 * f private use

T (tonnes/year)	f private use	f main source	No. of days:
<50	0	0	
50-500	0.00002	4.10^{-8}	200
500-2,500	0.0004	8.10^{-7}	300
2,500-10,000	0.002	4.10^{-6}	300
10,000-50,000	0.01	2.10^{-5}	300
≥50,000	0.05	1.10^{-4}	300

WASTE TREATMENT Not applicable

IC = 16: ENGINEERING INDUSTRY: CIVIL AND MECHANICAL

PRODUCTION Table B1.2 for NSEC
Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.8 for NSEC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.14

T (tonnes/year)	f main source	No. of days
<10	1	2f*T
10-50	0.9	f*T
50-500	0.8	0.4f*T
500-2,000	0.75	0.2f*T
2,000-5,000	0.6	0.1f*T
5,000-25,000	0.5	300
≥25,000	0.3	300

PRIVATE USE Table B4.5

WASTE TREATMENT Not applicable

IC = 0 (Others)

PRODUCTION Table B1.2 for NSEC
Table B1.6 for HPVC (default ≥7,000)

FORMULATION Table B2.8 for NSEC
Table B2.3 for HPVC

INDUSTRIAL USE Table B3.14

PRIVATE USE Table B4.5

WASTE TREATMENT Table B5.3

T (tonnes/year)	f main source	No. of days
<100	0.5	150
100-1,000	0.3	150
1,000-10,000	0.2	150
≥10,000	0.2	150

IIIa. Synonyms for functions according to ChemUSES (US-EPA, 1980)

No.	USE CATEGORY	No.	Function (ChemUSES)
1	Absorbents and adsorbents	131	Absorbents
		60	Adsorbents
		213	Dehumidifiers
2	Adhesive, binding agents	302	Adhesives
		143	Binders
		145	Food additives
		92	Spreaders
		165	Stickers
		280	Tackifiers
3	Aerosol propellants	178	Aerosol propellents
4	Anti-condensation agents		
5	Anti-freezing agents	77	Antifreezes
		74	Deicers
		52	Deodorants
		313	Functional fluids
6	Anti-set-off and anti-adhesive agents	104	Abherents
		63	Antiblocking agents
		188	Anticaking agents
		300	Detackifiers
		233	Dusting agents
		144	Parting agents
		7	Soil retardants
7	Anti-static agents	328	Antistatic agents
		89	Electroconductive coating agents
		318	Humectants
8	Bleaching agents	304	Bleaching assistants
		132	Bleaching agents
9	Cleaning/washing agents and additives	293	Antiredeposition agents
		180	Boil-off assistants
		242	Cleaners
		173	Detergents
		78	Pre-spotting agents
		274	Scouring agents
		261	Shrinkage controllers
		14	Soaping-off assistants
		294	Soil release agents
10	Colouring agents	5	Bloom agents
		86	Colouring agents
		174	Coupling agents (dyes)
		267	Dyes

No.	USE CATEGORY	No.	Function (ChemUSES)
10	Colouring agents (continued)	20	Fluorescent agents
		248	Lakes
		381	Luminiscent agents
		235	Mercerizing assistants
		128	Opacifiers
		139	Pearlizing agents
		125	Pigments
		83	Stains
11	Complexing agents	177	Antiprecipitants
		124	Complexing agents
		10	Sequestering agents
12	Conductive agents	161	Electrical conductive agents
		383	Electrode materials
		245	Electrolytes
		313	Functional fluids
13	Construction materials and additives	324	Case-hardening agents
		355	Concrete additives
		361	Embrittlement inhibitors
		375	Materials for shaping
		250	Reinforcing agents
		349	Water-reducing agents
14	Corrosion inhibitors	230	Antioxidants
		64	Antiscaling agents
		323	Corrosion inhibitors
15	Cosmetics	301	Antiperspirants
		167	Cosmetic ingredients
16	Dust binding agents	26	Dust control agents
17	Electroplating agents	353	Brighteners
		32	Fume suppressants
18	Explosives	179	Detonators
		363	Explosion inhibitors
		158	Explosives
		27	Incendiaries
19	Fertilizers	34	Fertilizers
20	Fillers	351	Fillers (augmentation)
		212	Fillers (patching)
		371	Surface coating additives
		127	Swelling agents
		58	Weighting agents (textile technology)

No.	USE CATEGORY	No.	Function (ChemUSES)
21	Fixing agents	291	Anticrock agents
		347	Antistripping agents
		268	Barrier coating agents
		295	Fixatives
		134	Fixing agents (fragrances)
		112	Fixing agents (textile technology)
		227	Mordants
22	Flame retardants and fire preventing agents	25	Fire extinguishing agents
		332	Flame retardants
23	Flotation agents	163	Activators (ore processing)
		190	Flocculating agents
		297	Flotation agents
		360	Modifiers
24	Flux agents for casting		
25	Foaming agents	358	Blowing agents
		133	Chemical blowing agents
		94	Frothers
		50	Physical blowing agents
26	Food/feedstuff additives	214	Acidulants
		66	Feed additives
		80	Sweeteners (taste)
27	Fuels	247	Fuels
28	Fuel additives	329	Antifouling agents
		76	Antiknock agents
		183	Deposit modifiers
		306	Fuel additives
		138	Sweeteners (petroleum technology)
29	Heat transferring agents	72	Coolants
		313	Functional fluids
		199	Heat transfer agents
		216	Quenchers
		208	Refrigerants
30	Hydraulic fluids and additives	313	Functional fluids
		65	Hydraulic fluids
		256	Transmission fluids
31	Impregnation agents	102	Delustrants
		98	Sizes
		258	Water repellents
		23	Waterproofing agents

No.	USE CATEGORY	No.	Function (ChemUSES)
32	Insulating materials	254	Acoustical insulating material
		311	Electrical insulating material
		314	Heat insulating materials
		162	Insulating materials
33	Intermediates	146	Inorganic intermediates
		115	Monomers
		290	Organic intermediates
		43	Prepolymers
34	Laboratory chemicals	238	Analytical and product testing
		122	Chelating agents
		107	Deionizers
		373	Extraction agents
		69	Indicators
		325	Oxidation-reduction indicators
		374	Reagents
35	Lubricants and additives	119	Antiseize agents
		313	Functional fluids
		148	Internal lubricating agents
		195	Lubricant additives
		364	Lubricating agents
		346	Oiliness agents
		249	Penetrants
		312	Slip agents
36	Odour agents	79	Flavors and fragrances
		339	Odorants
37	Oxidizing agents	149	Oxidizers
38	Plant protection products, agricultural	166	Animal repellents
		333	Bactericides
		108	Biocides
		97	Decontaminats
		270	Fumigants
		362	Fungicides
		275	Herbicides
		155	Insect attractants
		348	Insect repellents
		330	Insecticides
		252	Nematocides
		253	Pesticides
		264	Rodenticides
39	Biocides, non-agricultural	287	Algicides
		1	Antifouling agents
		140	Disinfectants
		118	Preservatives
		116	Slime preventatives

No.	USE CATEGORY	No.	Function (ChemUSES)
40	PH-regulating agents	172	Laundry sours
		266	pH control agents
		191	pH indicators
41	Pharmaceuticals		
42	Photochemicals	122	Chelating agents
		198	Desensitizers (explosives)
		299	Desensitizers (photography)
		182	Developers
		286	Intensifiers (photography)
		285	Light stabilizers
		344	Photosensitive agents
		303	Sensitizers
43	Process regulators	321	Accelerators
		46	Activators (chemical processes)
		239	Activators (enzymes)
		110	Adhesion promoters
		4	Antifelting agents
		352	Antislip finishing agents
		206	Antistaining agents
		194	Antiwebbing agents
		281	Builders
		222	Carbonizing agents
		164	Carriers
		19	Catalyst supports
		170	Catalysts
		31	Chain extenders
		113	Chain terminators
		141	Chain transfer agents
		122	Chelating agents
		114	Coagulants
		278	Coalescents
		357	Coalescing agents
		315	Crabbing assistants
		228	Crosslinking agents
		226	Curing agents (concrete)
		369	Curing agents (polymer technology)
		18	Currying agents
		236	Deasphalting agents
		342	Defoamers
		365	Degumming agents
		137	Dehairing agents
		73	Dehydrating agents
		366	De-inkers
		84	Delignification agents
		30	Depolymerization agents
		367	Depressants
		292	Desizing agents
		259	Dispersants
		317	Driers

No.	USE CATEGORY	No.	Function (ChemUSES)
43	Process regulators (continued)	150	Dye carriers
		255	Dye leveling agents
		307	Dye retardants
		211	Dye retention aids
		341	Enzyme inhibitors
		157	Enzymes
		284	Finishing agents
		337	Formation aids
		331	Fuel oxidizers
		117	Fulling agents
		103	Initiators
		359	Intensifiers (printing)
		171	Kier boiling assistants
		24	Nucleating agents
		96	Peptizing agents
		75	Pitch control agents
		121	Polymerization additives
		209	Polymerization inhibitors
		21	Prevulcanization inhibitors
		153	Refining agents
		223	Repulping aids
		136	Retarders
		296	Retention aids
		338	Rubber compounding agents
		51	Scavengers
		326	Solubilizing agents
		310	Weighting agents (petroleum technology)
44	Reducing agents	244	Reducers
45	Reprographic agents	225	Toners
46	Semiconductors	202	Semiconductors
		378	Photovoltaic agents
47	Softeners	269	Bates
		231	Devulcanizing agents
		28	Elasticizers
		265	Emollients
		185	Plasticizers
		29	Softeners
		147	Water softeners
48	Solvents	229	Degreasers
		82	Dewaxing solvents
		373	Extraction agents
		320	Paint and varnish removers
		16	Reaction media
		271	Solvents
49	Stabilizers	277	Anticracking agents
		12	Antifume agents

No.	USE CATEGORY	No.	Function (ChemUSES)
49	Stabilizers (continued)	129	Antihydrolysis agents
		168	Antiozonants
		230	Antioxidants
		120	Antilivering agents
		282	Antiplasticizers
		160	Antisagging agents
		68	Antisettling agents
		88	Bloom inhibitors
		123	Coupling agents (polymers)
		159	Emulsifiers
		87	Heat stabilizers
		54	Stabilizers
		36	Ultraviolet absorbers
50	Surface-active agents	41	Antifloating agents
		234	Antifogging agents
		109	Surfactants
		243	Wetting agents
51	Tanning agents	316	Tanning agents
52	Viscosity adjustors	152	Antiflooding agents
		120	Antilivering agents
		343	Antiskinning agents
		221	Gelling agents
		262	Pour point depressants
		272	Thickeners
		334	Thixotropic agents
		240	Turbulence suppressors
		135	Viscosity adjustors
		15	Viscosity index improvers
53	Vulcanizing agents	288	Vulcanizing agents
54	Welding and soldering agents	101	Brazing agents
		22	Fluxing agents
0	Other	204	Ablatives
		105	Abrasives
		196	Activators (luminiscence)
		354	Aerating agents
		47	Air entraining agents
		376	Alloying agents
		90	Anticratering agents
		48	Anticreasing agents
		99	Antifogging agents
		218	Antipilling agents
		350	Antiskid agents
		6	Blasting abrasives
		70	Bluing agents
		220	Bright dips
		93	Chemical raw materials

No.	USE CATEGORY	No.	Function (ChemUSES)
0	Other (continued)	298	Clarifiers
		260	Cloud point depressants
		130	Coating agents
		283	Collectors
		335	Coupling agents (solutions)
		215	Culture nutrients
		81	Deaerating agents
		309	Deblooming agents
		85	Dechlorinating agents
		73	Dehydrating agents
		107	Deionizers
		232	Demulsifiers
		200	Denaturants
		49	Descaling agents
		205	Dewatering aids
		356	Discharge printing agents
		38	Drainage aids
		44	Drilling mud additives
		322	Dry strength additives
		39	Dye stripping agents
		100	Electron emission agents
		340	Eluting agents
		372	Embalming agents
		186	Encapsulating agents
		57	Enhanced oil recovery agents
		308	Entraining agents
		319	Etching agents
		336	Evaporation control agents
		373	Extraction agents
		207	Fiber-forming compounds
		368	Filtration aids
		56	Flatting agents
		79	Flavors and fragrances
		142	Fluid loss additives
		313	Functional fluids
		193	Greaseproofing agents
		184	"Grinding, lapping, sanding and"
		192	Hormones
		246	Humidity indicators
		210	Hydrotropic agents
		181	Impact modifiers
		380	Incandescent agents
		69	Indicators
		2	Ion exchange agents
		91	Lachrymators
		33	Latex compounding agents
		53	Leaching agents
		156	Leather processing agents
		370	Liquid crystals
		381	Luminiscent agents
		379	Magnetic agents
		67	Mar proofing agents

No.	USE CATEGORY	No.	Function (ChemUSES)
0	Other (continued)	289	Metal conditioners
		95	Metal strippers
		37	Metal treating agents
		327	Milling aids
		237	Obscuring agents
		197	Oil repellents
		62	Optical quenchers
		382	Osmotic membranes
		17	Papermaking agents
		55	Phosphatizing agents
		203	Phosphorescent agents
		59	Pickling agents
		217	Pickling inhibitors
		251	Plant growth regulators
		176	Plastics additives
		224	Plastics for shaping
		169	Plating agents
		8	Poison gas decontaminants
		3	Polymer strippers
		111	Pore forming agents
		151	Precipitating agents
		106	Protective agents
		45	Radioactivity decontaminants
		374	Reagents
		219	Refractive index modifiers
		241	Refractories
		154	Resists
		9	Rinse aids
		71	Ripening agents
		187	Rubber for shaping
		201	Rubber reclaiming agents
		189	Rubbing fastness agents
		276	Rust inhibitors
		11	Rust removers
		263	Scrooping agents
		42	Sealants
		98	Sizes
		126	Slime control agents
		305	Soil conditioners
		61	Strippers
		40	Tar removers
		345	Tarnish inhibitors
		13	Tarnish removers
		279	Textile specialities
		257	Vat printing assistants
		273	Wax strippers
		35	Well treating agents
		175	Wet strength additives
		377	X-ray absorbents

IIIb. Synonyms for functions according to ChemUSES (US-EPA, 1980)

No.	ChemUSES Function	Use category EU (No.)
104	Abherents	6
204	Ablatives	55
105	Abrasives	0
131	Absorbents	1
321	Accelerators	43
214	Acidulants	26
254	Acoustical insulating material	32
46	Activators (chemical processes)	43
163	Activators (ore processing)	23
196	Activators (luminiscence)	55
239	Activators (enzymes)	43
110	Adhesion promoters	43
302	Adhesives	2
60	Adsorbents	1
354	Aerating agents	0
178	Aerosol propellents	3
47	Air entraining agents	0
287	Algicides	39
376	Alloying agents	0
238	Analytical and product testing	34
166	Animal repellents	38
63	Antiblocking agents	6
188	Anticaking agents	6
277	Anticracking agents	49
90	Anticratering agents	0
48	Anticreasing agents	0
291	Anticrock agents	21
4	Antifelting agents	43
41	Antifloating agents	50
152	Antiflooding agents	52
234	Antifogging agents	50
99	Antifogging agents	0
1	Antifouling agents	39
329	Antifouling agents	28
77	Antifreezes	5
12	Antifume agents	49
129	Antihydrolysis agents	49
76	Antiknock agents	28
120	Antilivering agents	49, 52
230	Antioxidants	14, 49
168	Antiozonants	49
301	Antiperspirants	15
218	Antipilling agents	55
282	Antiplasticizers	49
177	Antiprecipitants	11
293	Antiredeposition agents	9
160	Antisagging agents	49
64	Antiscaling agents	14
119	Antiseize agents	35
68	Antisettling agents	49
350	Antiskid agents	0
343	Antiskinning agents	52
352	Antislip finishing agents	43
206	Antistaining agents	43
328	Antistatic agents	7
347	Antistripping agents	21
194	Antiwebbing agents	43
333	Bactericides	38
268	Barrier coating agents	21
269	Bates	47
143	Binders	2
108	Biocides	38
6	Blasting abrasives	0
132	Bleaching agents	8
304	Bleaching assistants	8
5	Bloom agents	10
88	Bloom inhibitors	49
358	Blowing agents	25
70	Bluing agents	0
180	Boil-off assistants	9
101	Brazing agents	54
220	Bright dips	0
353	Brighteners	17
281	Builders	43
222	Carbonizing agents	43
164	Carriers	43
324	Case-hardening agents	13
170	Catalysts	43
19	Catalyst supports	43
31	Chain extenders	43
113	Chain terminators	43
141	Chain transfer agents	43
122	Chelating agents	34, 42, 43
133	Chemical blowing agents	25
93	Chemical raw materials	0
298	Clarifiers	0
242	Cleaners	9
260	Cloud point depressants	0
114	Coagulants	43
278	Coalescents	43
357	Coalescing agents	43
130	Coating agents	0
283	Collectors	0
86	Coloring agents	10
124	Complexing agents	11
355	Concrete additives	13
72	Coolants	29
323	Corrosion inhibitors	14
167	Cosmetic ingredients	15
123	Coupling agents (polymers)	49
174	Coupling agents (dyes)	10
335	Coupling agents (solutions)	55
315	Crabbing assistants	43
228	Crosslinking agents	43
215	Culture nutrients	0
226	Curing agents (concrete)	43
369	Curing agents (polymer technology)	43
18	Currying agents	43
366	De-inkers	43
81	Deaerating agents	0
236	Deasphalting agents	43
309	Deblooming agents	0
85	Dechlorinating agents	55
97	Decontaminats	38
342	Defoamers	43
229	Degreasers	48
365	Degumming agents	43
137	Dehairing agents	43
213	Dehumidifiers	1
73	Dehydrating agents	0, 34
74	Deicers	5
107	Deionizers	0, 34
84	Delignification agents	43
102	Delustrants	31
232	Demulsifiers	0
200	Denaturants	0
52	Deodorants	5
30	Depolymerization agents	43
183	Deposit modifiers	28
367	Depressants	43

No. ChemUSES Function Use category EU (No.)

No.	ChemUSES Function	Use category EU (No.)
49	Descaling agents	0
198	Desensitizers (explosives)	42
299	Desensitizers (photography)	42
292	Desizing agents	43
300	Detackifiers	6
173	Detergents	9
179	Detonators	18
182	Developers	42
231	Devulcanizing agents	47
205	Dewatering aids	0
82	Dewaxing solvents	48
356	Discharge printing agents	0
140	Disinfectants	39
259	Dispersants	43
38	Drainage aids	0
317	Driers	43
44	Drilling mud additives	0
322	Dry strength additives	0
26	Dust control agents	16
233	Dusting agents	6
150	Dye carriers	43
255	Dye leveling agents	43
307	Dye retardants	43
211	Dye retention aids	43
39	Dye stripping agents	0
267	Dyes	10
28	Elasticizers	47
161	Electrical conductive agents	12
311	Electrical insulating material	32
89	Electroconductive coating agen	7
383	Electrode materials	12
245	Electrolytes	12
100	Electron emission agents	0
340	Eluting agents	0
372	Embalming agents	0
361	Embrittlement inhibitors	13
265	Emollients	47
159	Emulsifiers	49
186	Encapsulating agents	0
57	Enhanced oil recovery agents	0
308	Entraining agents	0
341	Enzyme inhibitors	43
157	Enzymes	43
319	Etching agents	0
336	Evaporation control agents	0
363	Explosion inhibitors	18
158	Explosives	18
373	Extraction agents	34, 48
66	Feed additives	26
34	Fertilizers	19
207	Fiber-forming compounds	0
212	Fillers (patching)	20
351	Fillers (augmentation)	20
368	Filtration aids	0
284	Finishing agents	43
25	Fire extinguishing agents	22
295	Fixatives	21
112	Fixing agents (textile technology)	21
134	Fixing agents (fragrances)	21
332	Flame retardants	22
56	Flatting agents	0
79	Flavors and fragrances	0, 36
190	Flocculating agents	23
297	Flotation agents	23
142	Fluid loss additives	0
20	Fluorescent agents	10
22	Fluxing agents	54
145	Food additives	2
337	Formation aids	43
94	Frothers	25
306	Fuel additives	28
331	Fuel oxidizers	43
247	Fuels	27
117	Fulling agents	43
32	Fume suppressants	17
270	Fumigants	38
313	Functional fluids	0, 5, 12, 29, 30, 35
362	Fungicides	38
221	Gelling agents	52
193	Greaseproofing agents	0
184	Grinding, lapping, sanding and polishing abrasives	0
199	Heat transfer agents	29
314	Heat insulating materials	32
87	Heat stabilizers	49
275	Herbicides	38
192	Hormones	0
318	Humectants	7
246	Humidity indicators	0
65	Hydraulic fluids	30
210	Hydrotropic agents	0
181	Impact modifiers	0
380	Incandescent agents	0
27	Incendiaries	18
69	Indicators	0, 34
103	Initiators	43
146	Inorganic intermediates	33
155	Insect attractants	38
348	Insect repellents	38
330	Insecticides	38
162	Insulating materials	32
286	Intensifiers (photography)	42
359	Intensifiers (printing)	43
148	Internal lubricating agents	35
2	Ion exchange agents	0
171	Kier boiling assistants	43
91	Lachrymators	0
248	Lakes	10
33	Latex compounding agents	0
172	Laundry sours	40
53	Leaching agents	0
156	Leather processing agents	0
285	Light stabilizers	42
370	Liquid crystals	0
195	Lubricant additives	35
364	Lubricating agents	35
381	Luminiscent agents	0, 10
379	Magnetic agents	0
67	Mar proofing agents	55
375	Materials for shaping	13
235	Mercerizing assistants	10
289	Metal conditioners	0
37	Metal treating agents	0
95	Metal strippers	0
327	Milling aids	0
360	Modifiers	23
115	Monomers	33
227	Mordants	21
252	Nematocides	38
24	Nucleating agents	43
237	Obscuring agents	0
339	Odorants	36
197	Oil repellents	0
346	Oiliness agents	35
128	Opacifiers	10
62	Optical quenchers	0

No.	ChemUSES Function	Use category EU (No.)
290	Organic intermediates	33
382	Osmotic membranes	0
325	Oxidation-reduction indicators	34
149	Oxidizers	37
320	Paint and varnish removers	48
17	Papermaking agents	0
144	Parting agents	6
139	Pearlizing agents	10
249	Penetrants	35
96	Peptizing agents	43
253	Pesticides	38
191	pH indicators	40
266	pH control agents	40
55	Phosphatizing agents	0
203	Phosphorescent agents	0
344	Photosensitive agents	42
378	Photovoltaic agents	42
50	Physical blowing agents	25
217	Pickling inhibitors	0
59	Pickling agents	0
125	Pigments	10
75	Pitch control agents	43
251	Plant growth regulators	0
185	Plasticizers	47
176	Plastics additives	0
224	Plastics for shaping	0
169	Plating agents	0
8	Poison gas decontaminants	0
3	Polymer strippers	0
121	Polymerization additives	43
209	Polymerization inhibitors	43
111	Pore forming agents	0
262	Pour point depressants	52
78	Pre-spotting agents	9
151	Precipitating agents	0
43	Prepolymers	33
118	Preservatives	39
21	Prevulcanization inhibitors	43
106	Protective agents	0
216	Quenchers	29
45	Radioactivity decontaminants	0
16	Reaction media	48
374	Reagents	0, 34
244	Reducers	44
153	Refining agents	43
219	Refractive index modifiers	0
241	Refractories	0
208	Refrigerants	29
250	Reinforcing agents	13
223	Repulping aids	43
154	Resists	0
136	Retarders	43
296	Retention aids	43
9	Rinse aids	0
71	Ripening agents	0
264	Rodenticides	38
338	Rubber compounding agents	43
187	Rubber for shaping	0
201	Rubber reclaiming agents	0
189	Rubbing fastness agents	0
11	Rust removers	0
276	Rust inhibitors	0
51	Scavengers	43
274	Scouring agents	9
263	Scrooping agents	0
42	Sealants	0
202	Semiconductors	46
303	Sensitizers	42
10	Sequestering agents	11
261	Shrinkage controllers	9
98	Sizes	0, 31
126	Slime control agents	0
116	Slime preventatives	39
312	Slip agents	35
14	Soaping-off assistants	9
29	Softeners	47
305	Soil conditioners	0
294	Soil release agents	9
7	Soil retardants	6
326	Solubilizing agents	43
271	Solvents	48
92	Spreaders	2
54	Stabilizers	49
83	Stains	10
165	Stickers	2
61	Strippers	0
371	Surface coating additives	20
109	Surfactants	50
138	Sweeteners (petroleum technology)	28
80	Sweeteners (taste)	26
127	Swelling agents	20
280	Tackifiers	2
316	Tanning agents	51
40	Tar removers	0
13	Tarnish removers	0
345	Tarnish inhibitors	0
279	Textile specialities	0
272	Thickeners	52
334	Thixotropic agents	52
225	Toners	45
256	Transmission fluids	30
240	Turbulence suppressors	52
36	Ultraviolet absorbers	49
257	Vat printing assistants	0
135	Viscosity adjustors	52
15	Viscosity index improvers	52
288	Vulcanizing agents	53
147	Water softeners	47
258	Water repellents	31
349	Water-reducing agents	13
23	Waterproofing agents	31
273	Wax strippers	0
310	Weighting agents (petroleum technology)	43
58	Weighting agents (textile technology)	20
35	Well treating agents	0
175	Wet strength additives	0
243	Wetting agents	50
377	X-ray absorbents	0

Appendix IV. Flow diagrams of EASE

Appendix 1

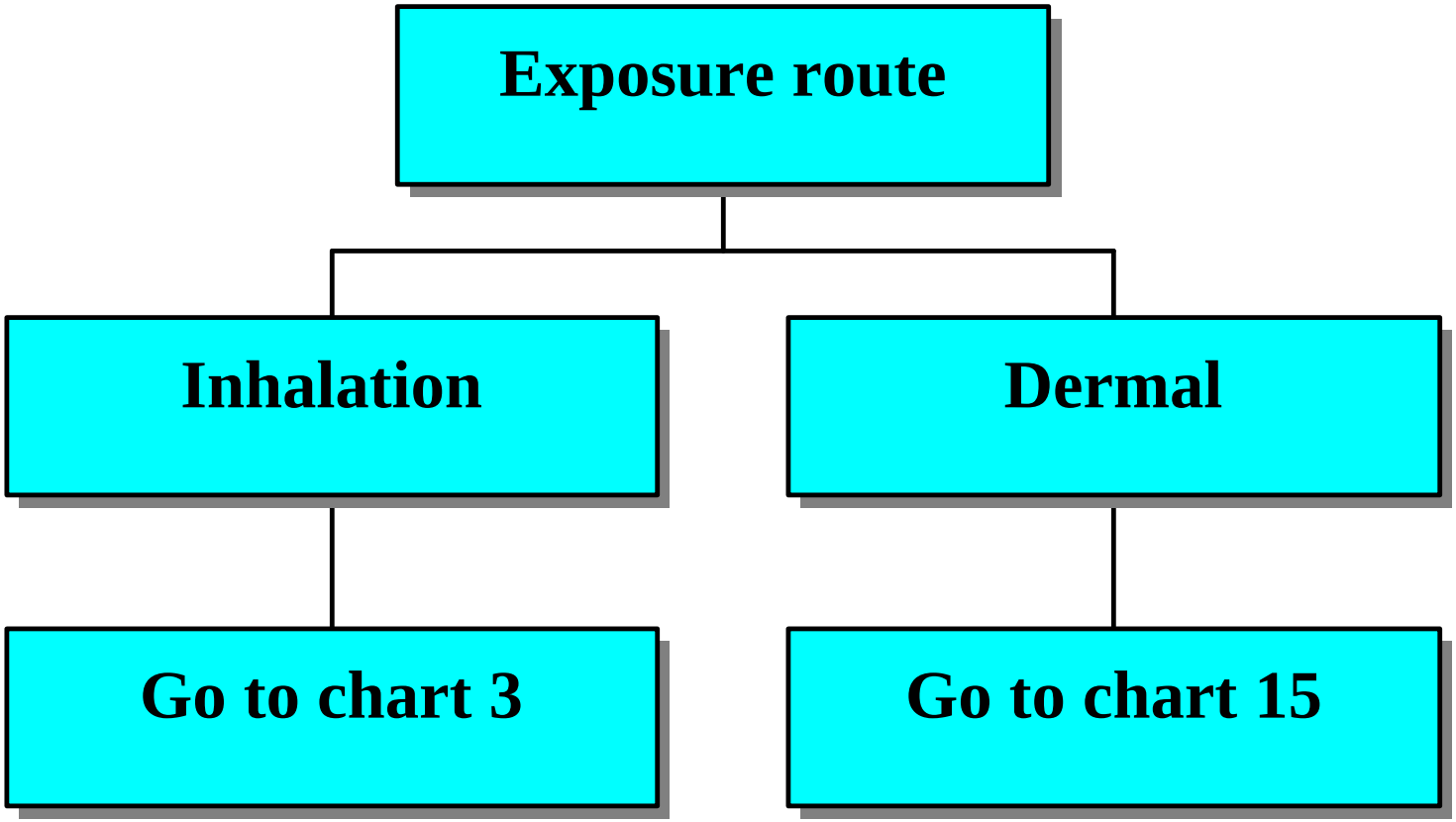
Logic diagrams for EASE

(version 2 for windows)

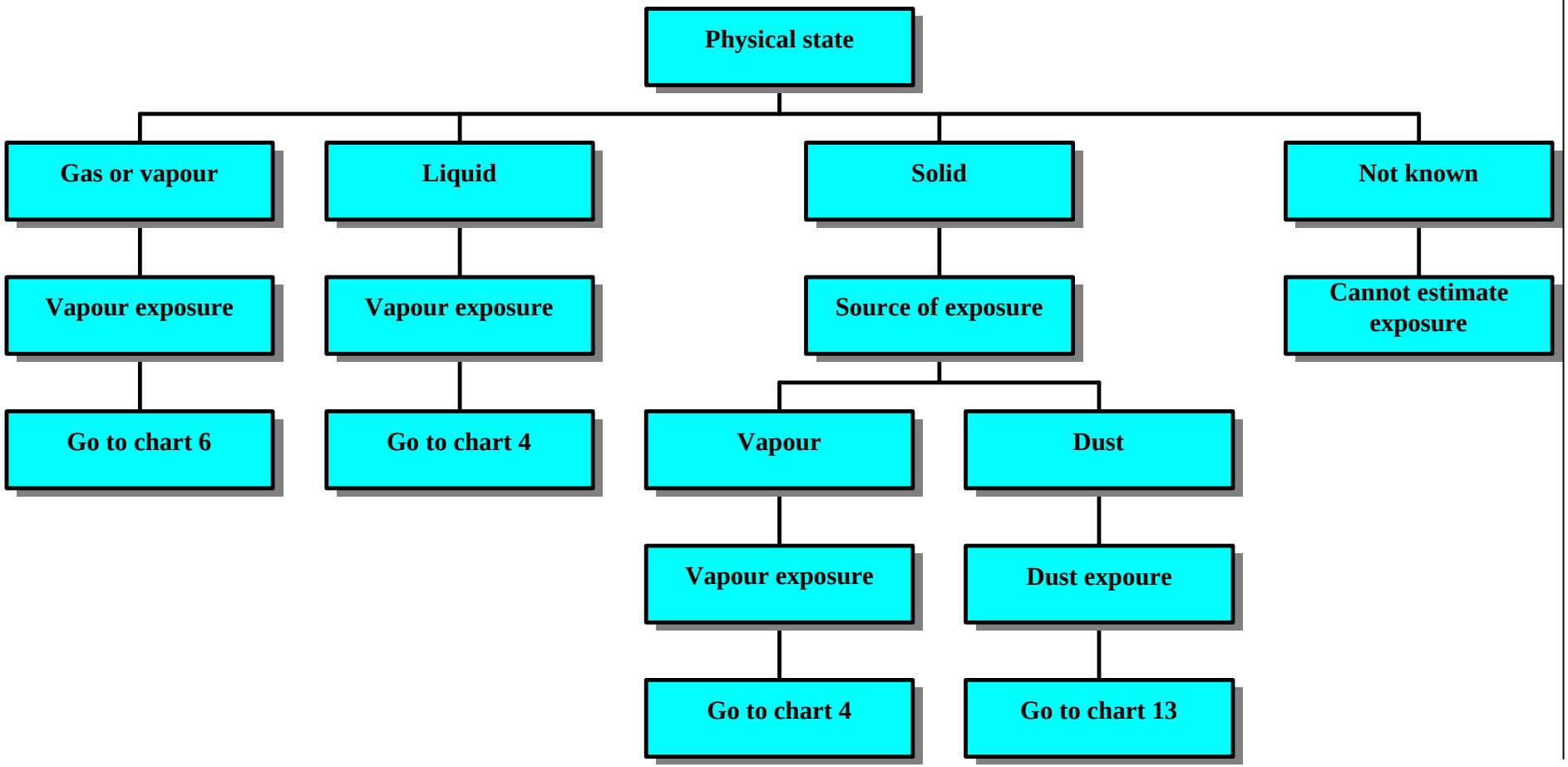
Abbreviations

P.T	Process temperature
B.P.	Boiling point
M.P.	Melting point
V.P.	Vapour pressure
TBA	Tendency to become airborne
Mod	Moderate
p	Page
LEV	Local exhaust ventilation
Seg	Segregation
dil vent	Dilution ventilation
DC&G	Dry crushing and grinding
DM	Dry manipulation
LDT	Low dust techniques

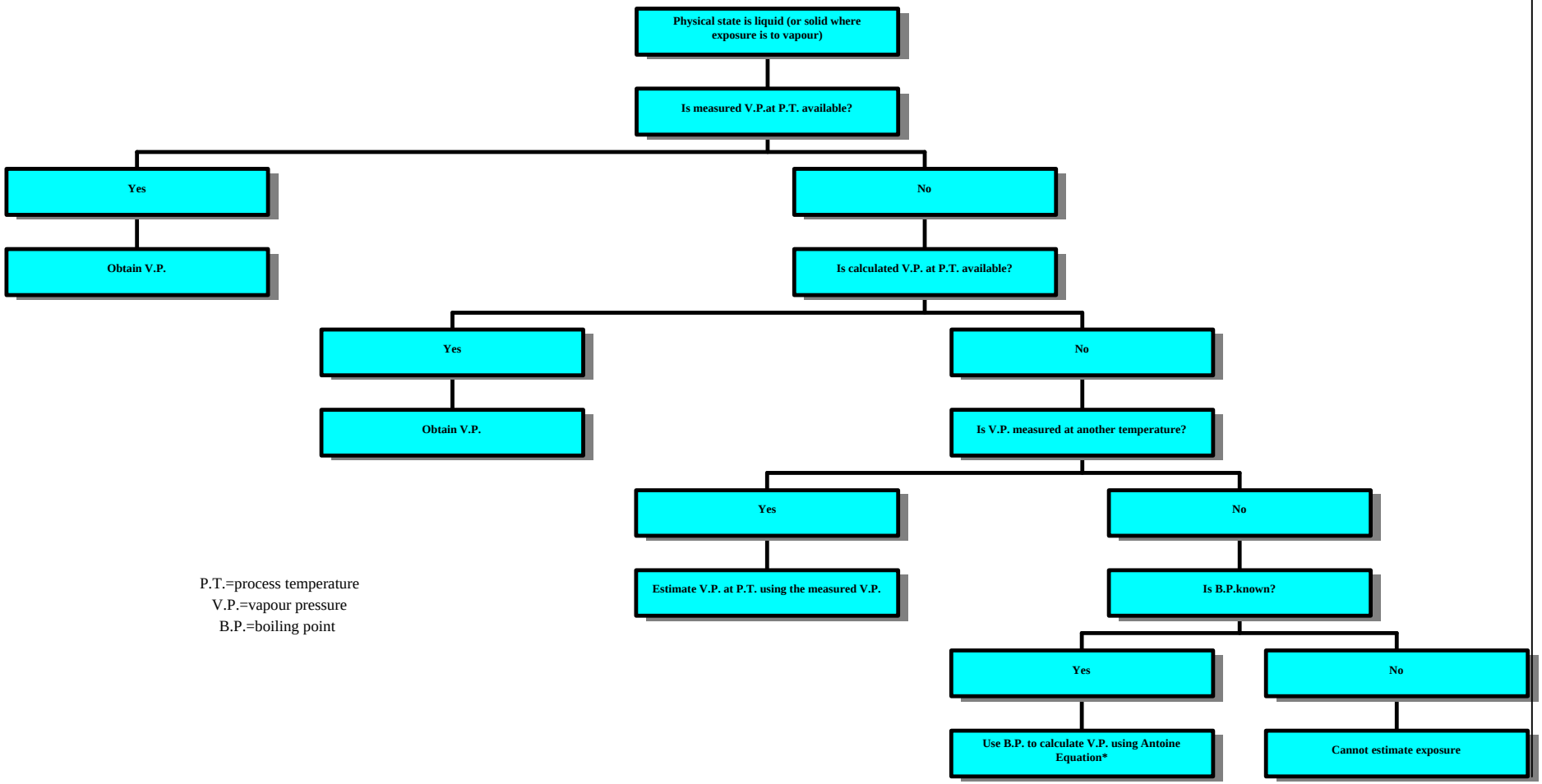
Route of exposure



Determination of type of inhalation exposure



Determination of vapour pressure

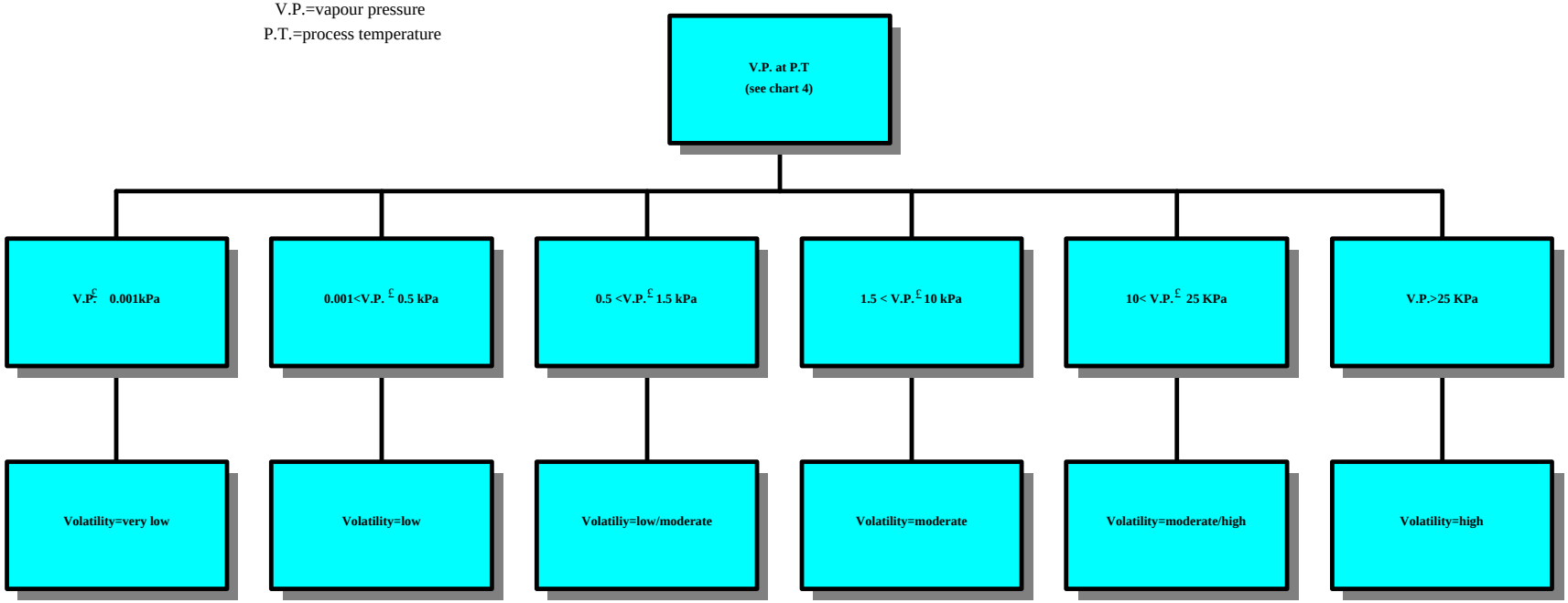


P.T.=process temperature
V.P.=vapour pressure
B.P.=boiling point

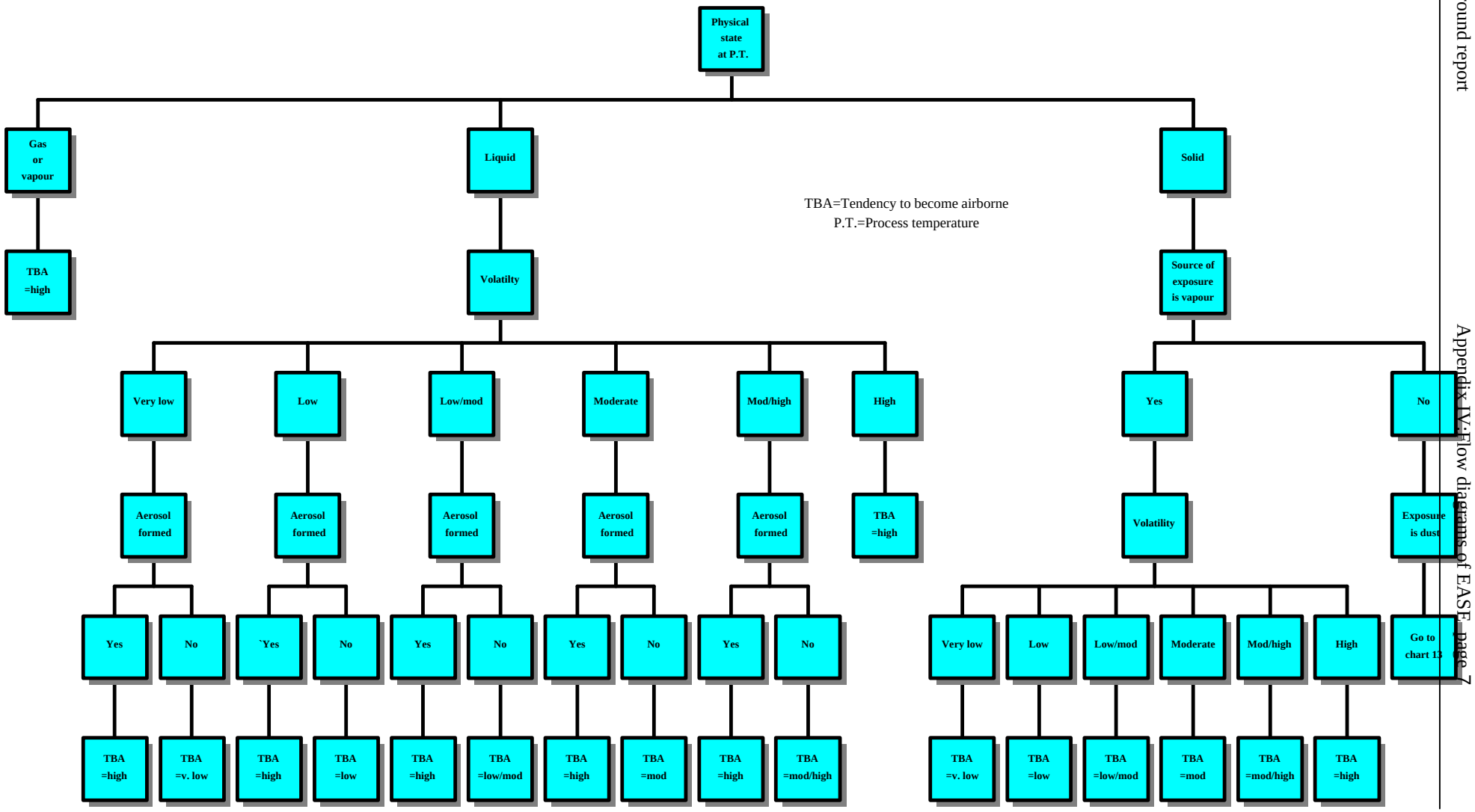
* applies only to certain classes of organic chemicals

Determination of volatility

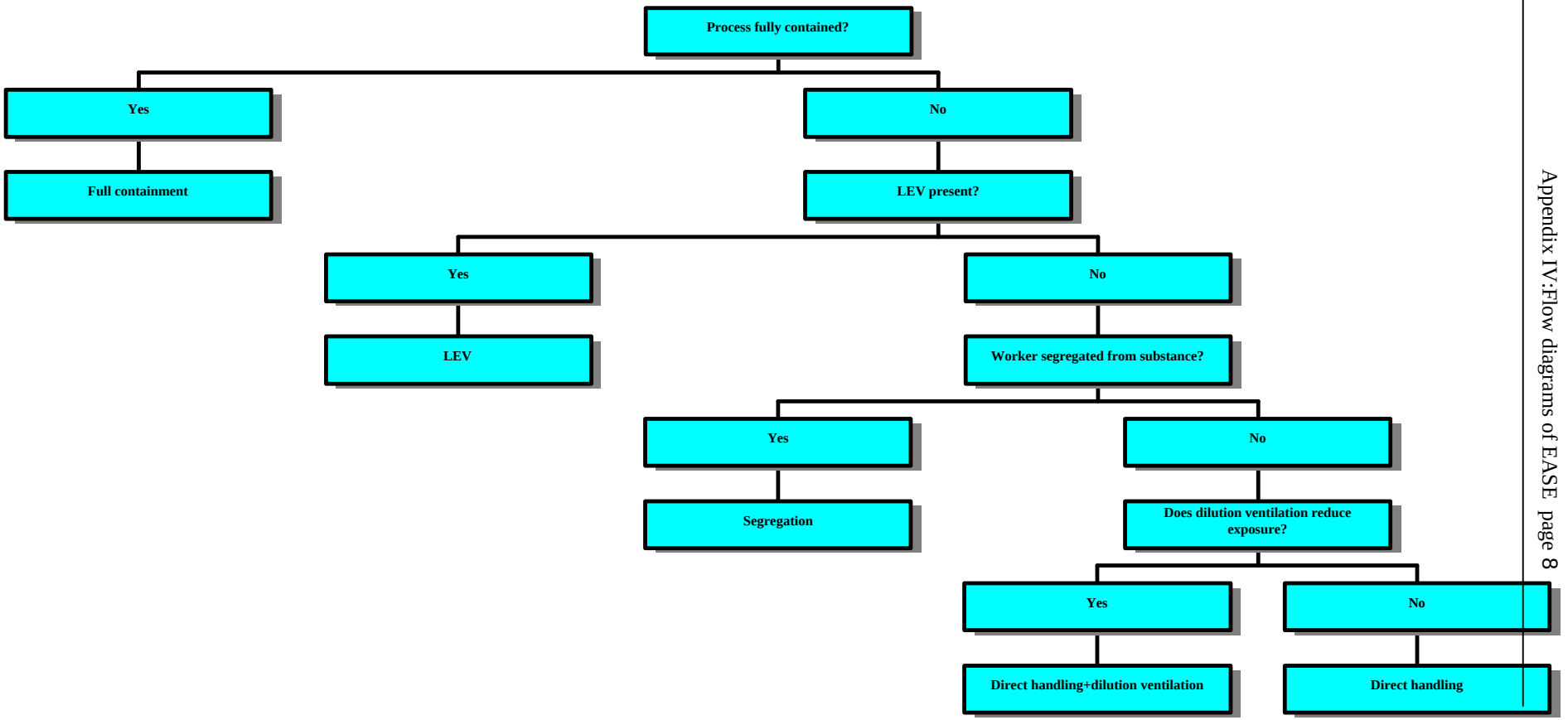
V.P.=vapour pressure
P.T.=process temperature



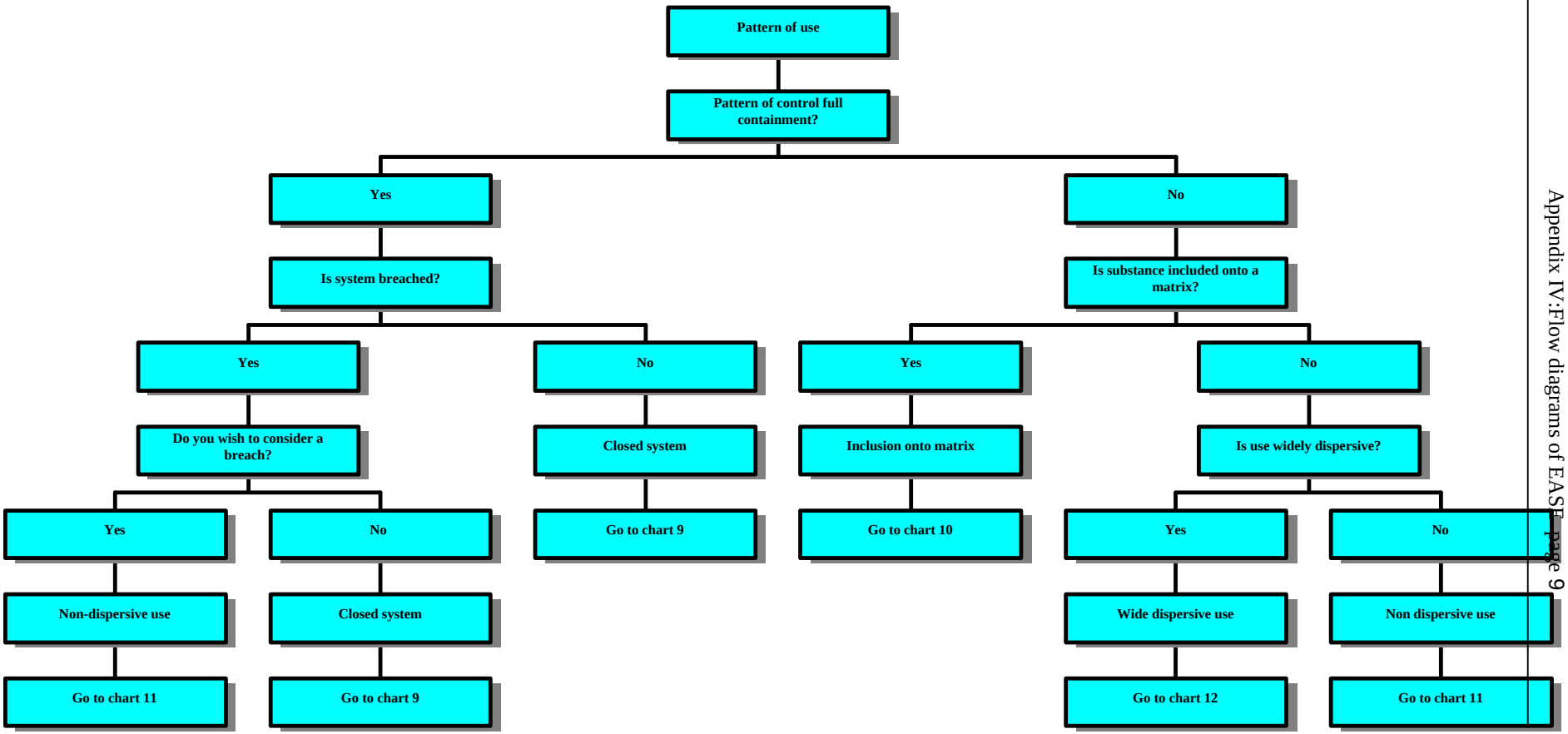
Determination of tendency to become airborne



Determination of pattern of control



Determination of pattern of use

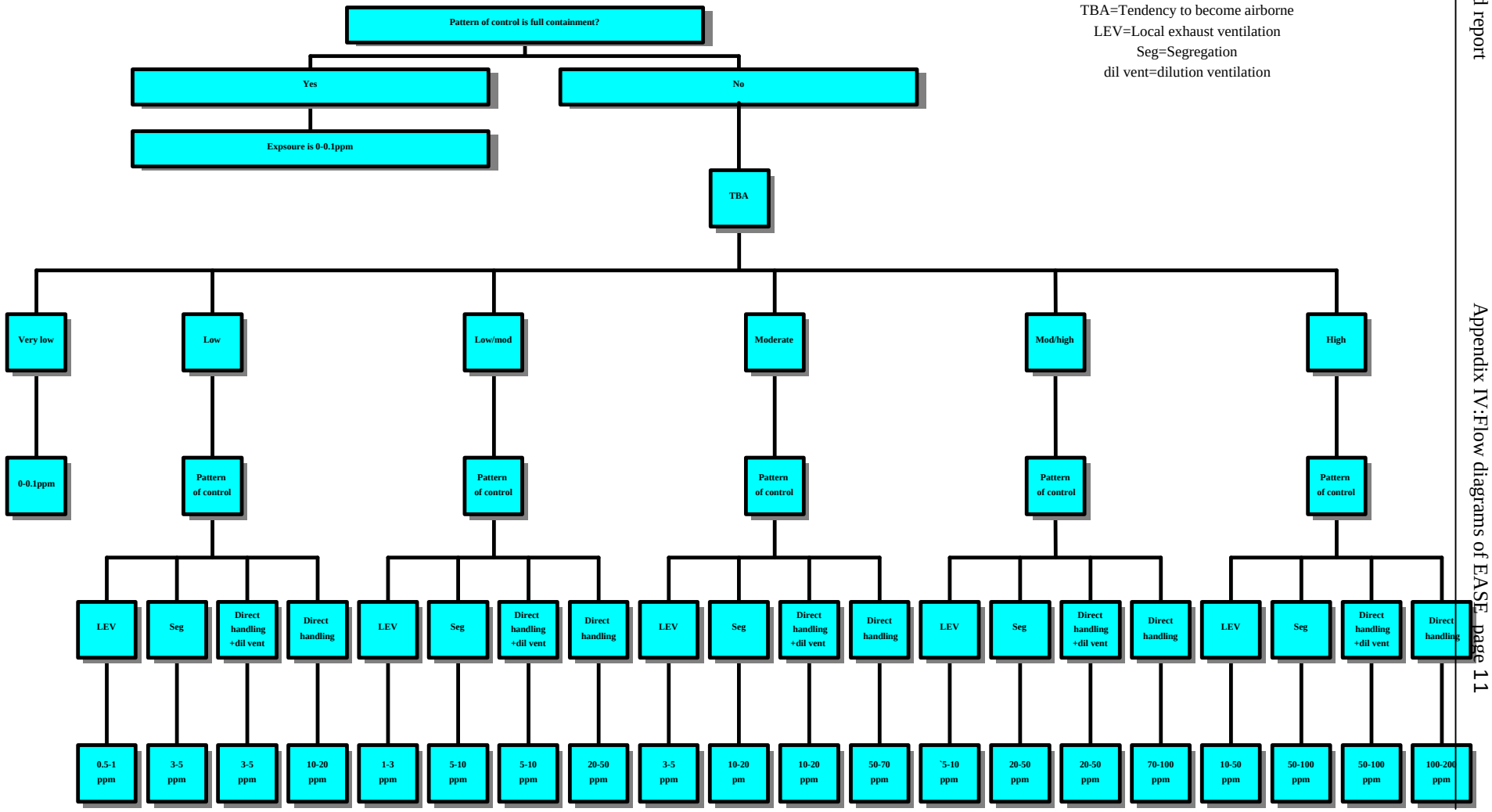


Determination of vapour exposure use pattern is closed system

Exposure = 0-0.1 ppm

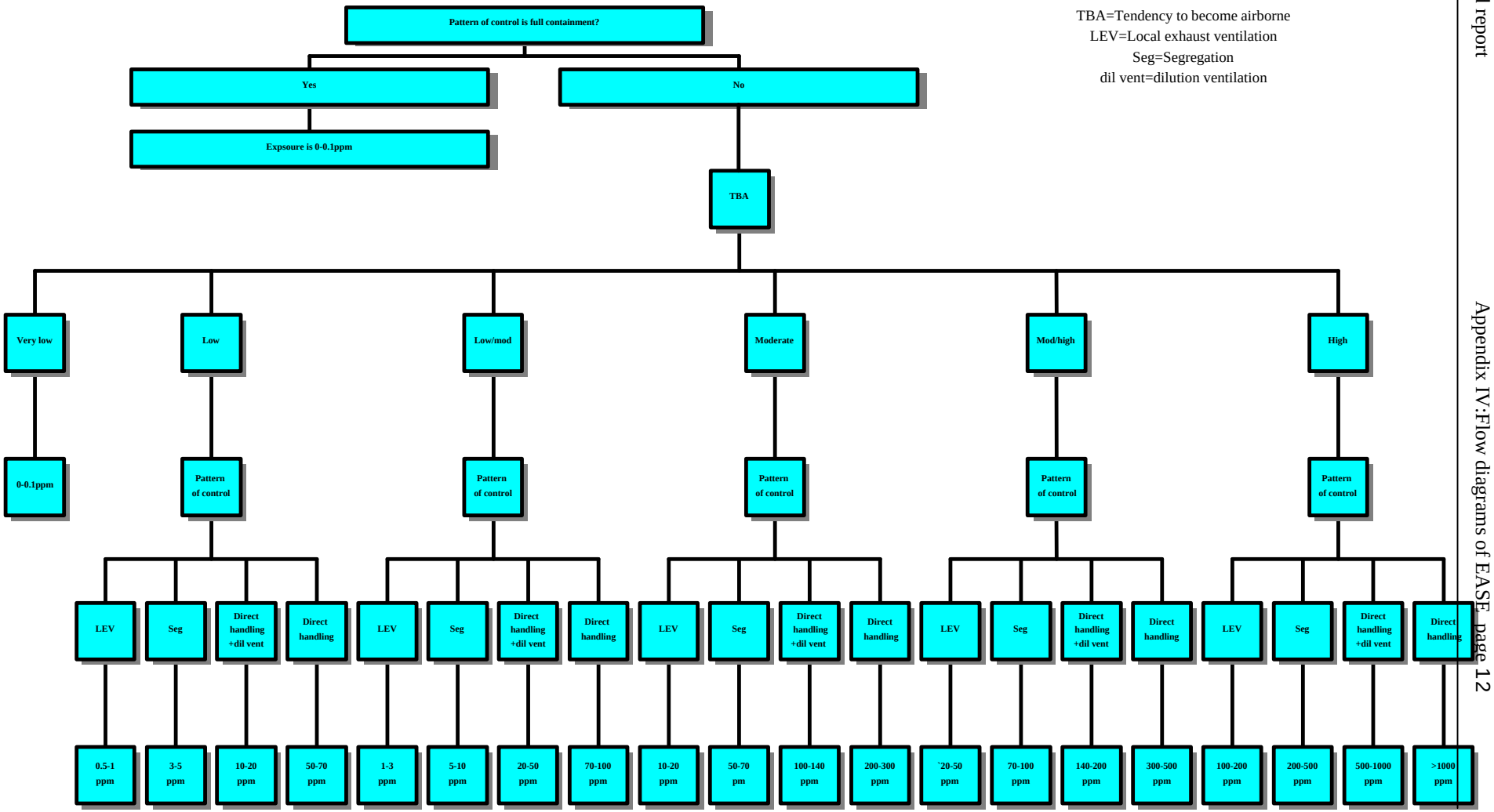
Determination of vapour exposure use pattern is inclusion onto a matrix

TBA=Tendency to become airborne
LEV=Local exhaust ventilation
Seg=Segregation
dil vent=dilution ventilation



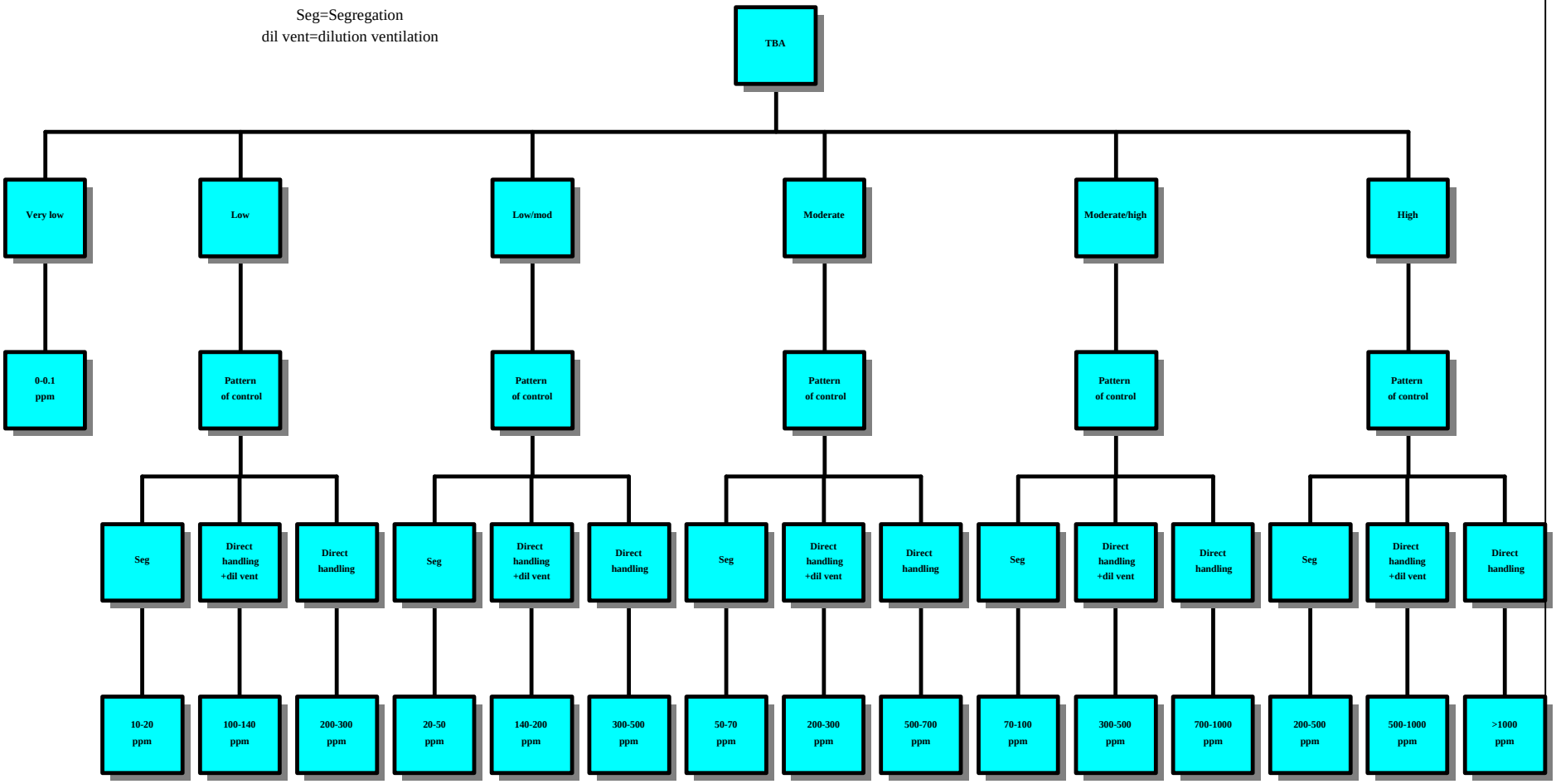
Determination of vapour exposure use pattern is non-dispersive

TBA=Tendency to become airborne
LEV=Local exhaust ventilation
Seg=Segregation
dil vent=dilution ventilation



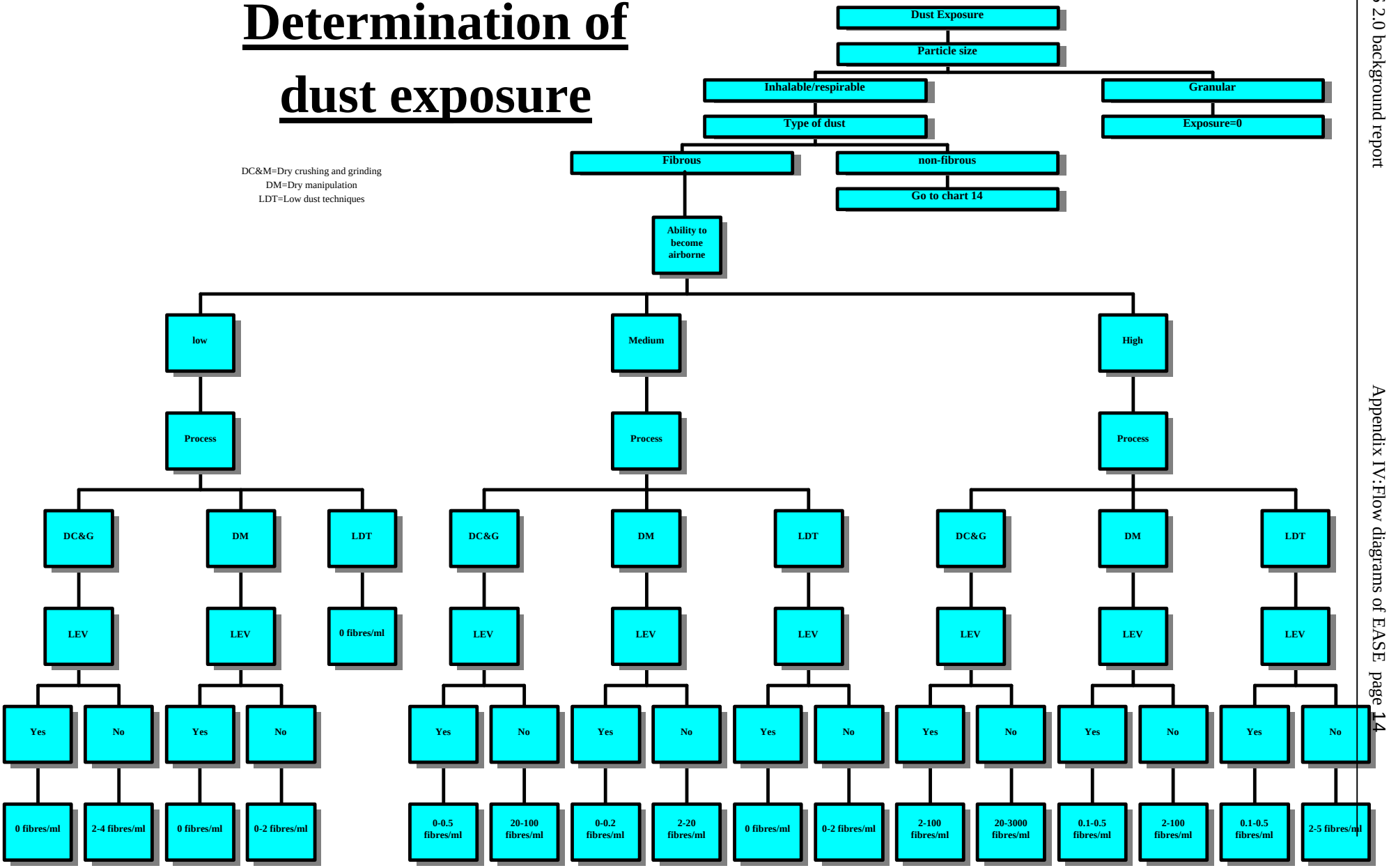
Determination of vapour exposure use pattern is widely dispersive

TBA=Tendency to become airborne
LEV=Local exhaust ventilation
Seg=Segregation
dil vent=dilution ventilation

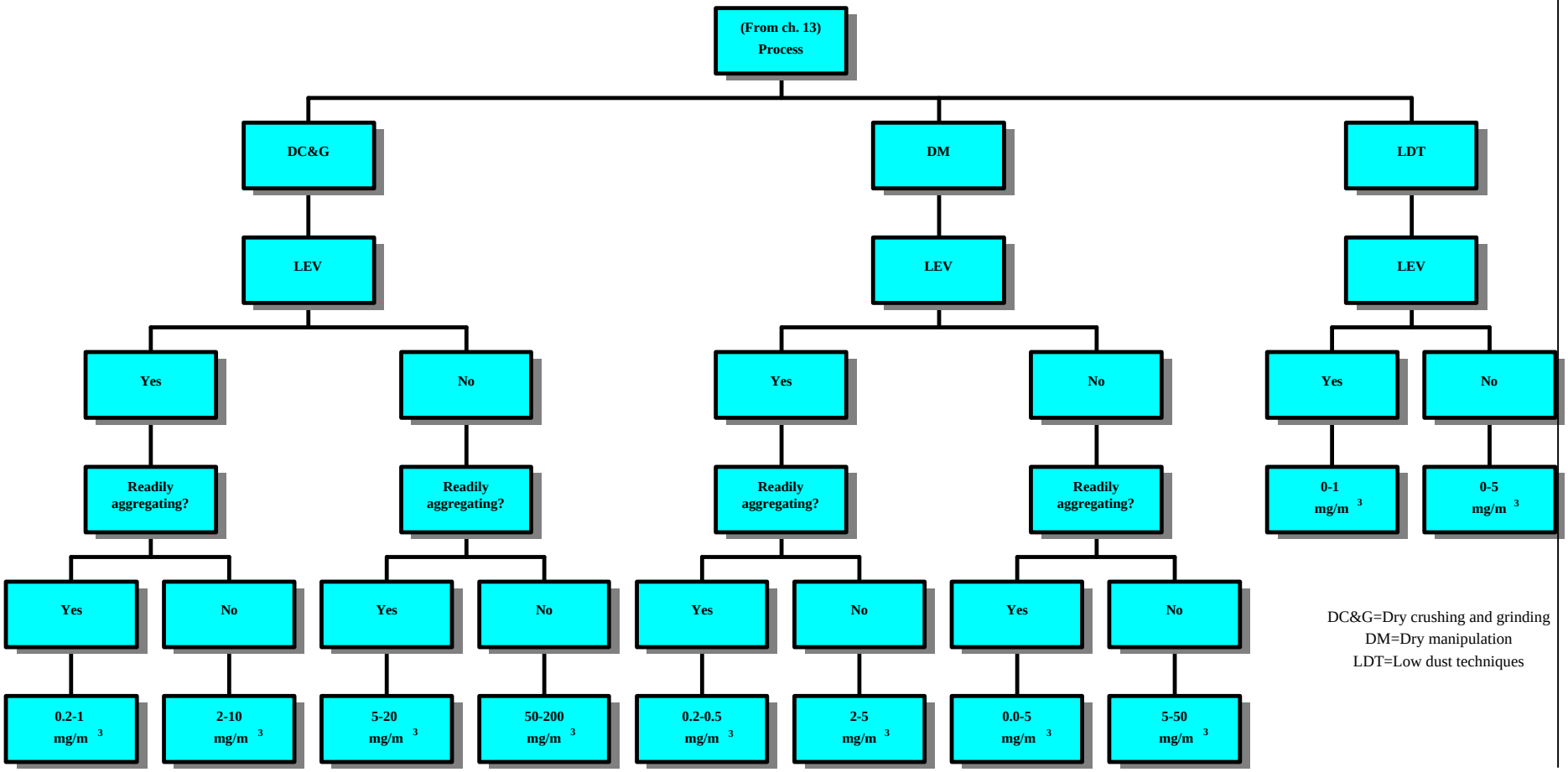


Determination of dust exposure

DC&M=Dry crushing and grinding
DM=Dry manipulation
LDT=Low dust techniques



Determination of dust exposure
Dust is non-fibrous



DC&G=Dry crushing and grinding
DM=Dry manipulation
LDT=Low dust techniques

Determination of dermal exposure