Uniform System for the Evaluation of Substances (USES), version 4.0

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PREFACE

Risk assessment of chemical substances has become a key element in the international substances policy. It is the basis for risk management, aimed at the protection of man and the environment against dangerous chemical substances. Consequently, methodologies for risk assessment of substances were developed and harmonised during the past decade.

In the framework of their first National Environmental Policy Plan, the government of the Netherlands developed the first version of the Uniform System for the Evaluation of Substances (USES 1.0). USES 1.0 became available in 1994 and harmonised the risk assessment of new and existing substances, biocides and plant protection products. USES 1.0 was tailored to the corresponding EC and national legislation.

USES 1.0 was subsequently used as one of the base documents for the development of the EU Technical Guidance Document for the risk assessment of new and existing substances in support of the corresponding EC legislation. The Netherlands Ministry of Housing Spatial Planning and the Environment (VROM) took the initiative, supported by several EU member states, the European Commission and the European Centre for Ecotoxicology and Toxicology of Chemicals for the chemical industry, to further attune USES 1.0 to these EU Technical Guidance Documents. In 1997 this led to the first version of the European Union System for Evaluation of Substances (EUSES 1.00).

Simultaneously with the development of EUSES a second version of USES has been developed by VROM in 1998, mainly for use in the Netherlands. USES 2.0 comprises risk assessment methods for biocides and plant protection products in addition to those for new and existing substances. The risk assessment methods for biocides and plant protection products are in accordance with the corresponding national legislation and as much as possible with the corresponding EC legislation. In USES 2.0, the risk assessment methods for new and existing substances are fully equivalent to EUSES 1.00.

The third version of USES has been prepared by the National Institute of Public Health and the Environment (RIVM) in the Netherlands. It was supervised by a Steering Committee and guided by an Advisory Group, representing government and industry. USES 3.0 is an update of USES 2.0 with regard to the risk assessment system for plant protection products and was released in 1999.

This report describes the USES 4.0 system, which is an update of USES 3.0 with regard to the risk assessment of biocides mainly. It has been prepared by the National Institute of Public Health and the Environment (RIVM) in the Netherlands.

Users are encouraged to report any errors found and to suggest recommendations for improvement. A blacklist of USES 4.0 with all bugs reported, will be available from the RIVM (http://www.rivm.nl/csr/risk.html).

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SUMMARY

This report describes the fourth version of the Uniform System for the Evaluation of Substances, USES 4.0 an integrated risk assessment system for new and existing substances and agricultural and non-agricultural pesticides. The risk assessment system for new and existing substances in USES 4.0 is equivalent to EUSES 1.00, the European Union System for the Evaluation of Substances. USES is a decision-support system for use by central governments, research institutes and the chemical industry for rapid, quantitative assessments of the general risks of substances.

The Netherlands Ministry of Housing, Spatial Planning and the Environment (VROM) made USES 1.0, the first version of the Uniform System for the Evaluation of Substance, available in 1994. USES 1.0, developed at the National Institute of Public Health and the Environment (RIVM) during the previous decade, included risk assessment systems for new and existing substances and for plant protection products and biocides. This version was integrated as much as possible. Since then, the assessment system for new and existing substances in USES 1.0 has been updated to an EU-harmonised risk assessment system, EUSES 1.00, within the framework of EC Regulation (EC) 793/93 and Directive 92/32/EC. The risk assessment system for pesticides (USES 2.0) was independently updated at the national level in the Netherlands, taking into account Annex VI, the “Uniform Principles”, of EC Directive 91/414/EC (Directive 97/57/EC) and further technical developments for both plant protection products and biocides. With regard to biocides, the recently adopted Biocides Directive (Directive 98/8/EC) including Annex VI the “Common Principles”, was taken into account as much as possible. Further to this directive, more adjustments of USES will have to be made in the future. Technical developments and adaptation to national legislation resulted in USES 2.0, released in 1998. Further development of the distribution models for pesticides necessitated the update of USES 2.0 to USES 3.0 in 1999. The current update includes the ongoing work in the field of biocides, representing several new scenarios and technical updates in response to a black list.

The risk assessment was carried out in a stepwise procedure starting with data input and estimation, and further, going on to the estimation of emissions, prediction of environmental distribution, calculation of human and environmental exposure, derivation of no-effect levels and risk characterisation. USES aims at a quantitative comparison of the results of effects assessment and exposure assessment. This comparison is based on the Risk Characterisation Ratio: the ratio of the estimated exposure for the organism, population or ecosystem to be protected and a suitable no-effect or effect parameter for toxicity. The organisms, populations or ecosystems to be protected are: humans exposed via the environment, micro-organisms, the aquatic, terrestrial and sediment ecosystem, predators, fish, crustaceans, algae, mammals, birds, bees, earthworms, nitrifying bacteria and arthropods.

The exposure assessment for new and existing substances covers the whole life cycle of substances and their fate in all environmental compartments on three spatial scales. These are the personal scale, for consumers and workers, the local scale, for humans and ecosystems near point sources, and the regional scale, for humans and ecosystems

exposed as a result of all releases of substances in a large region. Pesticides are assessed for application on a local scale. For all substances, both short- and long-term exposure is considered where appropriate. The exposure assessment is performed departing from a screening level in which generic exposure scenarios are applied. Substances are assumed to be emitted into a standard environment with pre-defined environmental characteristics. Default values may be changed, however, and intermediate results replaced, for example, by measured data. Based on estimated emissions to water, soil and air, the distribution of the substance is modelled, leading to Predicted Environmental Concentrations (PECs) and an estimation of the intake by mammals, birds, predators and humans. Additionally, direct exposure of humans to substances in consumer products and the workplace can be estimated via separate screening modules.

The main differences found between USES 2.0 and USES 1.0 for the pesticide/biocide assessment are:

- Adjustment of the drift table;
- Inclusion of additional emission and distribution routes for non-agricultural pesticides;
- Inclusion of scenarios on use of pesticides as amenities;
- Estimation of local short-term atmospheric distribution of agricultural pesticides.

The main differences between USES 2.0/3.0 and USES 1.0 for the assessment of new and existing substances are:

- USES 2.0 includes a risk assessment for sediment organisms (also for pesticides);
- USES 2.0 includes a risk assessment system for workers (EASE - Estimation and Assessment of Substance Exposure).
- USES 2.0 includes a risk assessment system for complex mixtures (Hydrocarbon Block Method);
- Several models like the sewage treatment plant model, the plant accumulation model and the regional distribution model have been adapted;
- Many default values for such factors as emission rates, parameters describing the local or regional environment, intakes and assessment factors are different for USES 2.0 and USES 1.0 (also holds for pesticides).

The main differences between USES 3.0 and USES 2.0 are:

- The surface water model for pesticides SLOOT.BOX has been replaced by TOXSWA (TOXic substances in Surface WAter);
- The leaching model PESTLA for pesticides has been replaced by PEARL (PEsticides emission Assessment at the Regional and Local scale);
- Adaptation of the pesticide application scenario for granules and treated seeds.

The main differences between USES 4.0 and USES 3.0 are:

- New PEARL tables have been generated using PEARL version 1.0 for the plough layer in addition to the tables for upper groundwater;
- Existing TOXSWA tables have been extended by a fourteen days column, and new TOXSWA tables for sediment have been added;
- For product types 1 (human hygiene biocidal products), 2 (private area and public health area disinfectants and other biocidal products, except for swimming pools),

6 (in-can preservatives), 7 (film preservatives), 8 (wood preservatives, only waste treatment module added),
9 (fibre, leather, rubber and polymerised material preservatives), 12 (slimicides), 22 (embalming and taxidermist fluids), and 7 and 8 (a landfill module), new biocide scenarios have been added;

- Several bugs in USES 3.0 have been solved.

SAMENVATTING

Dit rapport beschrijft de vierde versie van het Uniforme Beoordelingssysteem Stoffen, USES 4.0. USES 4.0 bestaat uit een zoveel mogelijk geïntegreerd risicobeoordelingssysteem voor nieuwe en bestaande stoffen, landbouwbestrijdingsmiddelen (gewasbeschermingsmiddelen) en niet-landbouwbestrijdingsmiddelen (biociden). Het risicobeoordelingssysteem voor nieuwe en bestaande stoffen is volledig gelijk is aan EUSES 1.00 (European Union System for the Evaluation of Substances). USES is een beslissingsondersteunend instrument voor overheden, onderzoeksinstituten en chemische bedrijven bij het snel en efficiënt kwantitatief beoordelen van de algemene risico's van stoffen.

De eerste versie van USES kwam in 1994 beschikbaar als een uitgave van het Ministerie van Volkshuisvesting, Ruimtelijke Ordening en Milieubeheer (VROM). In USES 1.0 waren de gedurende een tiental jaren op het RIVM ontwikkelde risicobeoordelingsmethodieken voor nieuwe en bestaande stoffen en landbouw- en niet-landbouwbestrijdingsmiddelen geïntegreerd in één beoordelingsschema. Volgend op deze publicatie is het beoordelingssysteem voor nieuwe en bestaande stoffen in USES 1.0 opgewaardeerd en aangepast tot een op EU-niveau geharmoniseerd risicobeoordelingssysteem EUSES 1.00 in het kader van EC Verordening (EC) 793/93 en Richtlijn 92/32/EEC. Tegelijkertijd is op nationaal niveau het beoordelingssysteem voor bestrijdingsmiddelen in Nederland verder ontwikkeld met inachtneming van Annex VI, de "Uniform Principles", van EC Richtlijn 91/414/EC (Richtlijn 97/57/EC) en andere technische ontwikkelingen zowel ten aanzien van gewasbeschermingsmiddelen als van biociden. Wat betreft biociden is zoveel mogelijk ingespeeld op de Biocidenrichtlijn die recent is aangenomen (Richtlijn 98/8/EC) en de daarbijbehorende Annex VI, de "Common Principles". In de toekomst zal USES dienovereenkomstig verder ontwikkeld moeten worden. Deze ontwikkelingen hebben in 1998 geleid tot USES 2.0. Verdere ontwikkeling van de verspreidingsmodellen voor bestrijdingsmiddelen maakte een derde versie noodzakelijk in 1999. De vierde versie van USES bevat de resultaten van het voortgaande werk op het gebied van biociden en een aantal technische aanpassing.

De risicobeoordeling wordt stapsgewijs uitgevoerd, te beginnen met de invoer en schatting van gegevens welke wordt gevolgd door de schatting van emissies, de voorspelling van de verspreiding in het milieu, de berekening van de blootstelling van mens en milieu, de afleiding van geen-effect niveaus en de risicokarakterisering. Het doel van USES is een kwantitatieve vergelijking van de resultaten van de effectbeoordeling en de blootstellingsschatting. Deze vergelijking is gebaseerd op de Risk Characterisation Ratio: de verhouding van de geschatte blootstelling voor het te beschermen organisme, de te beschermen populatie of ecosysteem en een geschikte effect of geen-effect parameter voor toxiciteit. Beschermingsdoelen zijn: de mens, blootgesteld via het milieu, micro-organismen, het aquatische, terrestrische and sediment ecosysteem, predatoren, vissen, crustaceae, algen, zoogdieren, vogels, bijen, regenwormen, nitrificerende bacteriën en arthropoden.

De blootstellingsschatting voor nieuwe en bestaande stoffen beslaat de gehele levenscyclus van stoffen en hun lot in alle milieucompartimenten. Dit gebeurt op drie

schaalniveaus: de persoonlijke schaal voor consumenten en werknemers, de lokale schaal voor de mens en ecosystemen dichtbij puntbronnen en de regionale schaal voor de mens en ecosystemen wanneer ze blootgesteld worden ten gevolge van emissies in een groot gebied. Bestrijdingsmiddelen worden beoordeeld op risico's na gebruik op lokale schaal. Voor alle stoffen kunnen naar behoefte zowel korte- als lange-termijn blootstelling beschouwd worden. De blootstellingsschatting gaat uit van een screeningsniveau waarbij algemene blootstellingsscenario's worden toegepast. Aangenomen wordt dat de stoffen worden uitgestoten naar een standaard milieu met welomschreven milieukarakteristieken. De waarden van de standaardparameters kunnen echter aangepast worden en tussenresultaten kunnen worden overschreven door bijvoorbeeld gemeten getallen. Uitgaande van emissies naar water, bodem en lucht wordt de verspreiding van de stof gemodelleerd welke resulteert in Predicted Environmental Concentrations (PECs) en een schatting van de inname door zoogdieren, vogels, predatoren en de mens. Bovendien kan in aparte screeningsmodulen directe blootstelling van de mens aan stoffen in consumentenprodukten en op de werkplek geschat worden.

De voornaamste verschillen tussen de beoordeling van bestrijdingsmiddelen in USES 2.0 en USES 1.0 zijn:

- De drifttabel is aangepast;
- Voor niet-landbouwbestrijdingsmiddelen zijn emissie- en verspreidingsroutes toegevoegd;
- Blootstellingsscenario's voor het gebruik van pesticiden in openbaar groen zijn opgenomen;
- De berekening van de lokale korte-termijn verspreiding van bestrijdingsmiddelen via de atmosfeer is toegevoegd.

De voornaamste verschillen tussen de beoordeling van nieuwe en bestaande stoffen in USES 2.0/3.0 en USES 1.0 zijn:

- USES 2.0 bevat een risicobeoordeling voor sediment organismen (geldt ook voor pesticiden);
- USES 2.0 bevat een risicobeoordeling voor werknemers (EASE, Estimation and Assessment of Substance Exposure);
- USES 2.0 bevat een risicobeoordeling voor complexe mengsels (Hydrocarbon Block Method);
- Een aantal deelmodellen, onder meer het rioolwaterzuiveringsmodel, het plantenaccumulatiemodel en het regionale verspreidingsmodel zijn aangepast;
- Vele defaultwaarden voor onder meer emissiefactoren, parameters die het lokale en regionale milieu beschrijven, voedselinnamefactoren en assessmentfactoren verschillen tussen USES 2.0 en USES 1.0 (geldt ook voor bestrijdingsmiddelen).

De voornaamste verschillen tussen USES 3.0 en USES 2.0 zijn:

- Het oppervlaktewatermodel voor bestrijdingsmiddelen SLOOT.BOX is vervangen door TOXSWA (TOXic substances in Surface WAter);
- Het uitspoelingsmodel voor bestrijdingsmiddelen PESTLA is vervangen door PEARL (PEsticides emission Assessment at the Regional and Local scale);
- Aanpassing van het scenario voor de toepassing van granulaten en behandelde zaden;

De voornaamste verschillen tussen USES 4.0 en USES 3.0 zijn:

- Nieuwe tabellen gegenereerd met PEARL versie 1.0 voor de ploegvoor, naast de al bestaande tabellen voor het grondwater;
- Bestaande TOXSWA tabellen zijn uitgebreid met een kolom voor veertien dagen en nieuwe TOXSWA tabellen voor sediment zijn toegevoegd;
- Toevoeging van nieuwe biocide scenario's betreffende producttypes 1 (biocicen voor menselijke hygiëne), 2 (desinfecterende middelen voor privé-gebruik en voor de openbare gezondheidszorg en andere biociden), 6 (conserveringsmiddelen voor geconserveerde producten), 7 (filmconserveringsmiddelen), 8 (houtverduurzamingsmiddelen, alleen afvalverwerkingssmodule toegevoegd), 9 (conserveringsmiddelen voor vezels, leer, rubber en gepolymeriseerde materialen), 12 (slijmbestrijdingsmiddelen), 22 (vloeistoffen voor balsemen en opzetten) en een afvalstort module voor producttype 7 en 8;
- Het oplossen van verscheidene fouten in USES 3.0.

ACKNOWLEDGEMENTS

The development of a decision making tool such as USES requires the input of a number of experts in different scientific fields. USES 2.0 is the collective result of the work of experts from the RIVM, VROM and VWS who participated in USES projects since the early 1980s as well as from several national and international organisations and the chemical industry who participated in the development of EUSES. The development of the second, third and fourth version of USES at the RIVM has been carried out by a project team coordinated by T.G. Vermeire and J.B.H.J. Linders and further included J. Bakker, D.T. Jager, A.M.A. van der Linden, R. Luttik, B.J.W.G. Mensink, M.H.M.M. Montforts, J. van der Pol, W.A.J. van der Pul, M.G.J. Rikken and C.E. Smit. Contributions also came from J. Montfoort, P. van der Poel, P.T.J. van der Zandt (all RIVM), H. Kraaij (RIZA), G.G.C. Verstappen (RIZA), D.J. Bakker (TNO-MEP) and S. Teeuwisse (TNO-MEP).

TSA Group Delft BV was responsible for the operationalisation of USES 2.0, USES 3.0 and USES 4.0 in the present PC program.

The Evaluation Group Environment reviewed the risk assessment system for pesticides: B.A. Baumann (RIVM), P. van Beelen (RIVM), W.W.M. Brouwer (PD), A.M.A. van der Linden (RIVM), R. Luttik (RIVM) and M.A. Schrap (RIZA).

The overall scientific content of the USES 2.0 project was guided by an Advisory Group, chaired by M. Hof (RIVM), with the following members: M.L.C. van Assen (Nefyto), W.F. ten Berge (DSM), C. van de Guchte or M. Beek (RIZA), H. de Heer (LNV), K.H. den Haan (Shell), M. Lans (CTB), A.M.A. van der Linden (RIVM), J.B.H.J. Linders (RIVM), J.E. Prast (VROM), H. Roelfzema (VWS), T.G. Vermeire (RIVM), R.J. van Wijk (Akzo Nobel).

In USES 3.0 the surface water model TOXSWA and the leaching model PEARL are implemented. TOXSWA has been developed by the Agricultural Research Department of the Winand Staring Centre (SC-DLO) at Wageningen, The Netherlands. PEARL has been developed by RIVM and SC-DLO together.

The USES Steering Committee (until 2000), chaired by C.J. van Leeuwen, included F. Baerselman (LNV), H. van de Baan (LNV), J.S.M. Boleij (CTB), R. Faassen (RIZA), A.W. van der Wielen (VROM), M.A. van der Gaag (VROM), M. Hof (RIVM) G. de Mik (RIVM), T. Vermeire (RIVM) and H. Roelfzema (VWS).

The development of USES was commissioned by the Ministry of Housing, Spatial Planning and the Environment for which M. Hof coordinated this project.

The contributions of all persons to the USES project are gratefully acknowledged.

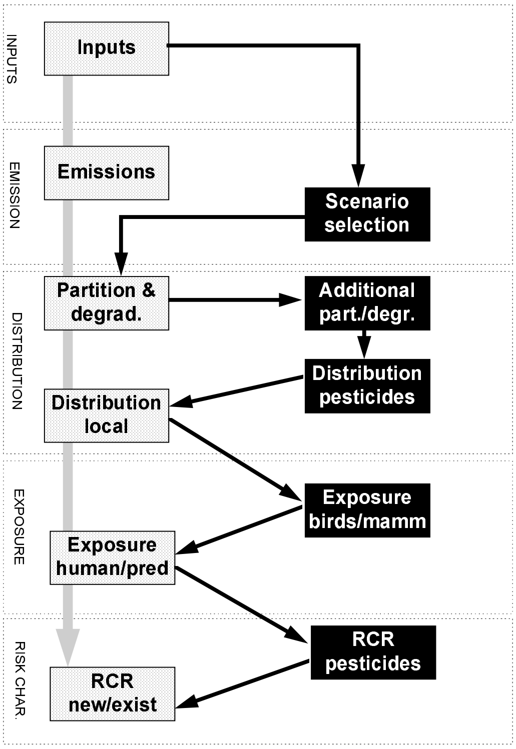
READERS GUIDE

This USES 4.0 documentation consists of additional pages which have been combined with the EUSES documentation (EC, 1996b). The additional documentation concerns the pesticide and biocide assessment and the optional global-scale calculations (SimpleBox 2.0). Although the page headers specify this report as the USES documentation, the text for the assessment of new and existing chemicals is identical to the EUSES text. Therefore, the text mentions "EUSES" on several occasions which can be read as "USES 4.0".

The following is done to improve readability:

- In Chapters II, III and IV, pages relevant for pesticide application are numbered with a P (e.g. page III-P1). Pages describing the additional global-scale calculations in Chapter III are numbered with an S proceeding the page number.
- These pages are recognisable by their deviating colour: green for pesticides and blue for global scale calculations and are not present in the report version, which is available from the internet (paper version only).
- Equations are also numbered with a P for pesticides and an S for the global scale calculations.

The figure on the right shows the program flow of USES 4.0. The light grey boxes and the large grey arrow indicate the EUSES modules for new and existing substances, the black boxes and arrows indicate the specific pesticide modules. The EUSES modules will also be used to assess the stages of production and formulation of pesticides. Furthermore, these modules will also be used in cases where pesticides are released through an STP and for exposure of humans through the environment.



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 the European Union (EU), environmental policy started in 1973 with the adoption of the first 5-year European Community Environmental Action Programme (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 first article of Directive 92/32/EEC (EC, 1992b) requires an evaluation of the potential hazards and risks of notified substances on the basis of a specified data set. This Directive also requires 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 lays 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).

Directive 91/414/EEC (EC, 1991) has been adopted for the placing on the market of plant protection products in the EEC. In Annex VI of this Directive (97/57/EC), Uniform Principles for the evaluation of these products have been laid down. Several items have been identified like groundwater pollution and toxicological effects on birds, water organisms and terrestrial organisms. If the criteria are met, authorisation of the pesticide is granted. If not, an additional adequate risk assessment is required. An EC Directive (98/8/EC) on the placing of biocidal products on the market has been adopted recently (EC, 1998). Related to this Directive, Common Principles for data requirements and risk assessment of biocides are being developed.

The corresponding national legislation comprises The Netherlands Chemical Substances Act of 1986 with regard to new and existing substances and The Netherlands Pesticide Act of 1962. The latter Act required the assessment of public health risks, but was amended in 1975 to include environmental risks as well. In addition to this Act, early 1995 an Administrative Order came into force in which more detailed regulations were stipulated on three criteria: persistence, leaching to groundwater and risks to water organisms (Staatsblad, 1995). Additional criteria were announced in relation to EU Directive 91/414/EEC, among which criteria for birds,

earthworms, bees and other beneficials, soil macro- and micro-organisms (EC, 1991).
It is against this background that USES (the Uniform 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, the first official version of the Dutch Risk Assessment System for New Chemicals (DRANC) became available in 1992 (De Nijs *et al.*, 1993) as well as test versions of the PRIority Setting system for Existing Chemicals (PRISEC; Van de Meent and Toet, 1992).

In The Netherlands, the Board for the Authorization of Pesticides, CTB (Dutch acronym: College Toelating Bestrijdingsmiddelen) takes the decisions on the approval of plant protection products and biocides on the basis of methods and criteria provided by the responsible Ministries. The risk assessment methodology as developed by the former CTB Environment Support Group for plant protection products was also described integrally and presented as the Evaluation System for Pesticides (ESPE, Emans *et al.*, 1992; Luttik *et al.*, 1992).

Prototypes of a risk assessment system integrating these three risk assessment tools (USES, the Uniform System for the Evaluation of Substances) were discussed at length by scientists and risk managers from governmental, industrial and private institutions. The Netherlands' Health Council also advised on two prototypes of USES (Health Council 1991, 1993) and several EC Member States took an active interest in this project, which 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 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 coordinated effort of EU Member States, the European Commission and its European Chemicals Bureau, and the European Chemical Industry.

At approximately the same time, the risk assessment methodology for plant protection products in The Netherlands was adapted to the Uniform Principles. Together with further technical developments in the risk assessment methodology for both plant protection products and biocides an update of the risk assessment system for pesticides in USES 1.0 was considered necessary. The EC Uniform Principles of Directive 91/414/EEC, including the so-called 'unless'-clauses and the Administrative Order on Plant Protection Products (Staatsblad, 1995), have been incorporated into USES 2.0, as much as possible. The 'unless'-clauses provide the applicant an opportunity to show that under field circumstances and after application of the substance according to Good Agricultural Practices the chemical does not show unacceptable hazards to the organism under consideration. The proof presented should be based on an appropriate risk assessment according the proposed conditions of use. Since no final decisions have been taken for the implementation and harmonisation of the Common Principles for biocides, a corresponding adjustment of USES will take place in the future. The integration of EUSES for new and existing substances with this updated system for pesticides has resulted in USES 2.0.

Soon after the release of USES 2.0, new distribution models for pesticides have become available which are approved and recommended for use in the risk assessment of pesticides by the Board for the Authorization of Pesticides, CTB. This development triggered the update, USES 3.0.

The biocidal Products Directive 98/8/EC (EC, 1998) has been developed to control the risk of biocides at EU level. To enforce the Directive emission estimation scenarios have been developed by the RIVM in the past and have been incorporated in USES versions 1, 2 and 3. The EUBEES working group Gathering, review and development of environmental emission scenarios for biocides''that supervised the project also produced several scenario documents. The most recently finalised emission scenarios have been incorporated in current version, USES 4.0

I.2. Objectives

The Uniform System for the Evaluation of Substances (USES 4.0) was developed for quantitative assessment of the risks posed by new and existing chemical substances, plant protection products and biocides to man and the environment. This assessment must be transparent to all users and easy to perform, and USES 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 the Uniform Principles for pesticides of the European Commission and the Administrative Order on Plant Protection Products (Stb., 1995). 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.

USES 4.0 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 USES 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 (EC, 1995).

Table I-1 *Assessment stages according to the OECD (1989). USES 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 USES can be used to carry out tiered risk assessments of increasing complexity, requiring additional data. Using OECD terminology, USES can specifically be used in the initial, or screening, and intermediate, or refined, stages of assessment (OECD, 1989; Table I-1). With USES, 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. USES 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. USES 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

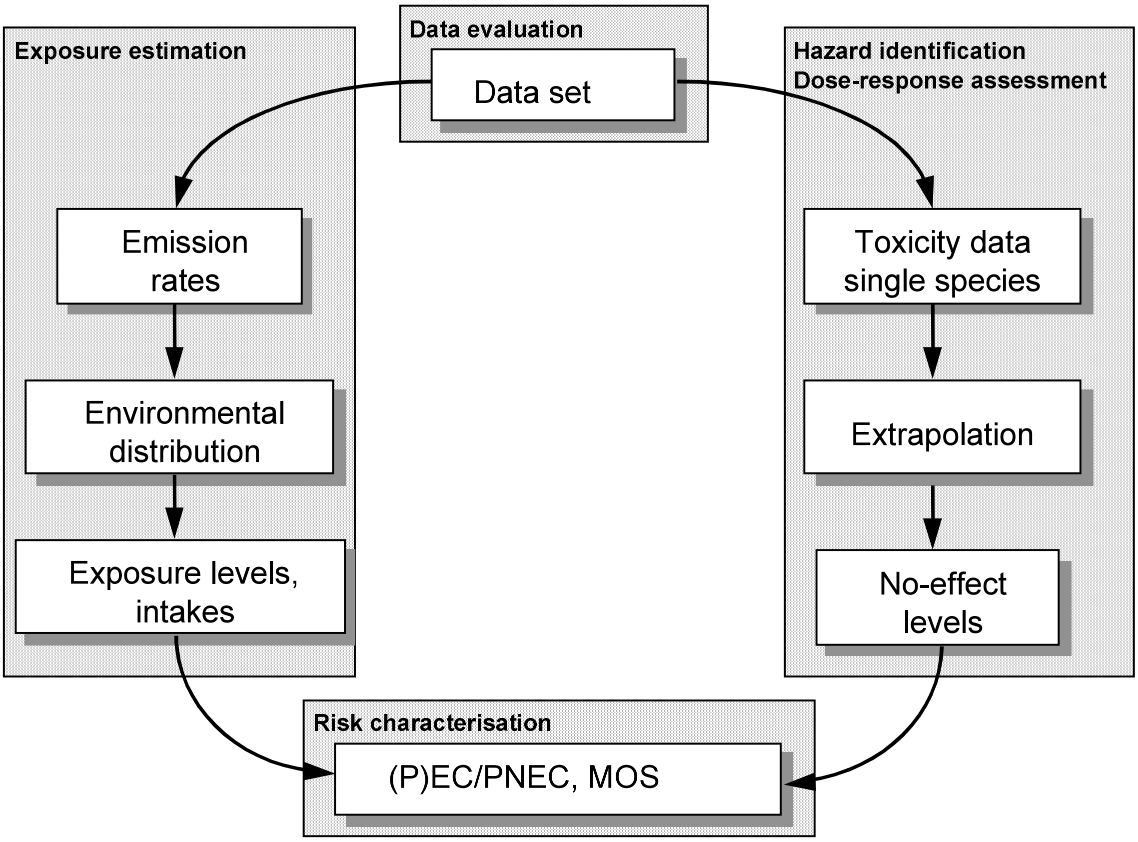


Figure I-1 *Basic steps in USES.*

Risk assessment in USES is carried out in a stepwise procedure encompassing the following stages (Figure I-1):

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.

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. With regard to pesticides, this comparison will be made on the basis of a PEC (Predicted Environmental Concentration) or a PED (Predicted Environmental Dose for mammals) and the non-extrapolated results of, usually single-species, toxicity tests such as L(E)C50-values and NOECs. In addition, the PEC in surface water and soil is compared to the extrapolated PNEC for aquatic and terrestrial organisms, respectively. In the Netherlands, the PNEC, after application of the appropriate extrapolation method, is considered to be equal to the Maximum Permissible Concentration (MPC, in Dutch: MTR). The generic name for PEC/PNEC, MOS, PEC/LC50, PED/LD50 etc. in USES 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.

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

For new and existing substances, the risk assessment for man aims at such a level of protection, expressed in the Margin of Safety, 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 severity of the effect(s). 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

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

Human populations:
- Workers [1]
- Consumers [1]
- Man exposed via the environment (also for pesticides)

Ecological systems and populations:
- Micro-organisms in sewage treatment systems
- Aquatic ecosystem
- Terrestrial ecosystem
- Sediment ecosystem
- Top predators

Species and populations (pesticides):
- Fish
- Crustaceans
- Algae
- Birds
- Mammals
- Bees
- Earthworms
- Nitrifying bacteria
- Arthropods

[1] does not apply to pesticides.

an unacceptable effect will most likely not occur (EC, 1995).
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For pesticides, the risk assessment for human exposure has to reveal that on the one hand the Acceptable Operator Exposure Level (AOEL) is not exceeded and on the other hand that because of intake of pesticide residues no exceedance is expected of the Acceptable Daily Intake (ADI). The environmental risk assessment for pesticides is also defined in several Toxicity-Exposure Ratios (TER) or Risk Characterisation Ratios (RCR) for specific organisms (EC, 1991 and EC, 1994). For biocides, EC Directive 98/8/EC (EC, 1998) requires a risk assessment which determines whether or not the risks of individual constituents of the biocide to man and the environment are acceptable or not.

Risk assessment with USES departs from a screening level in which so-called generic exposure scenarios are applied. It is assumed then that substances are emitted in a standard environment with predefined environmental characteristics. No measured data are used at this level. For new and existing substances, the resulting screening-level risk assessment is in principle valid for all EU countries, as required by the relevant EU regulations. Subsequently, in an iterative process, the risk assessment can 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 USES always shows the result of the standard assessment, in addition to the results of refined assessments made.

The exposure assessment in USES covers the whole life cycle of substances as well as their fate in all environmental compartments. As explained in more detail in Section I.5, three spatial scales and two time scales are distinguished. 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.

USES 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 USES, 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 USES and is based on the assumption that effects will be concentration-additive.

I.4. System structure

As outlined in Section I.2, USES 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 are predicted based on the volume produced or imported, 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.

I.4.3. The USES main modules

The main structure of USES 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.

Input module
The basic input data required to run USES will be entered in this module (substance identification and physico-chemical properties). There are no calculations in this module apart from the conversions from screen units to internal units.

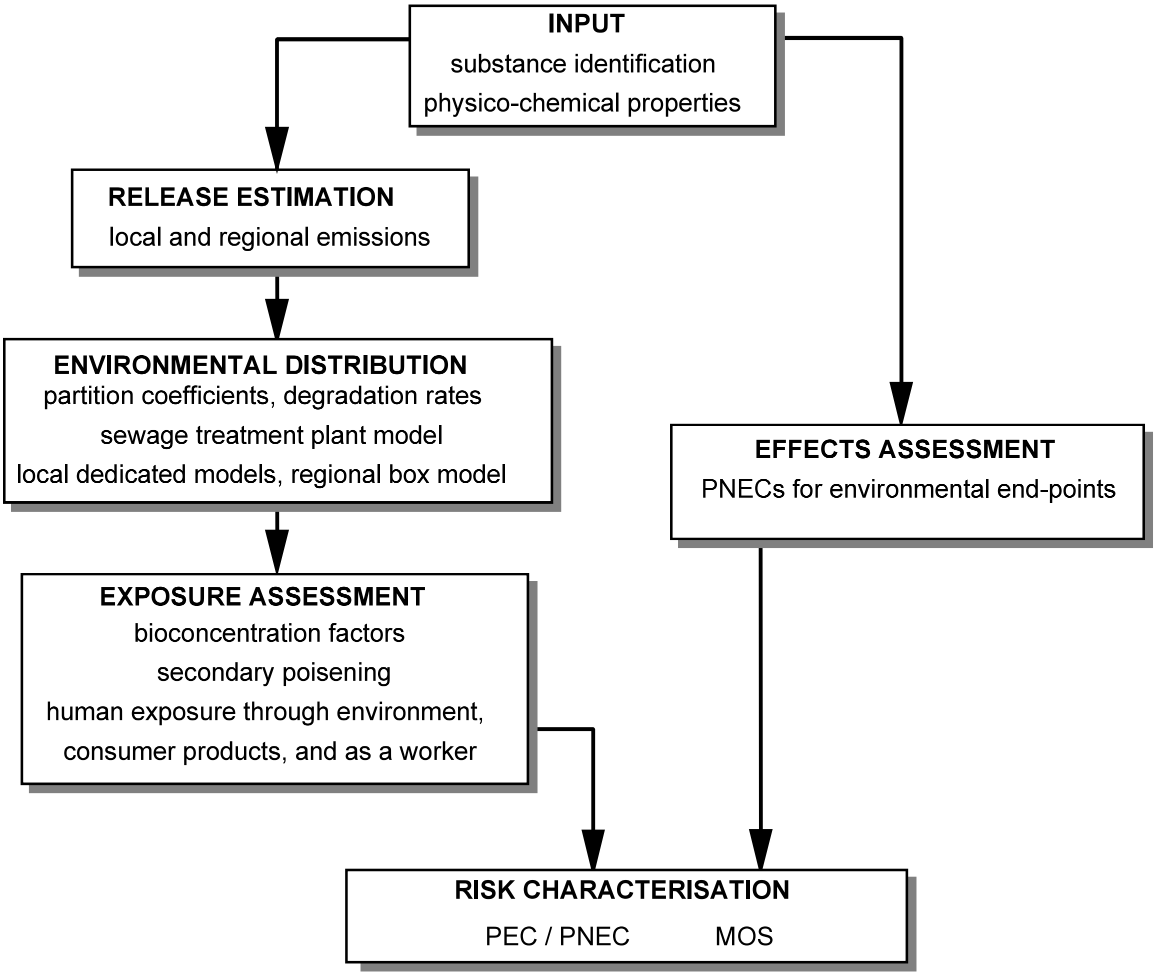


Figure I-2 *The main modules of USES.*

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.

Distribution module

his module contains all the models necessary to estimate the distribution of a substance in the environment at the appropriate scale (see Section I.5). End-points are concentrations in the relevant environmental compartments (air, surface 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, a distinction is made between indirect exposure through the environment, exposure through consumer products, and exposure in 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.

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. In the Uniform Principles, the ratio is defined as Toxicity Exposure Ratio (TER) which equals PNEC/PEC.

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

I.5. Model dimensions

Three factors determine the dimensions of USES: 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. USES 3.0 furthermore includes three overlying global scales (moderate, tropic and arctic) as option.

Table I-3 *The structure of USES.*

Module	Content
Input module	Data entry in HEDSET format: substance identification and physico-chemical properties
Emission module	Estimation of local emissions to wastewater and air for various life-cycle stages Estimation of regional emissions to wastewater, air and soil for various life-cycle stages Emission tables are used, given in Appendix IV
Distribution module	Local models: STP model: SimpleTreat Air model: OPS (new and existing substances), EPA-PAL (pesticides) Dilution and sorption in surface water One-compartment soil model (new and existing substances) Leaching and accumulation model PEARL (pesticides) Drift model TOXSWA (pesticides) 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 humans through the environment (including food products) Human exposure through use of consumer products 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 for new and existing substances
Risk characterisation module	Determination of RCRs for all end-points of the risk assessment

Abbreviations used: STP = Sewage Treatment Plant; OPS = Operational atmospheric transport model for Priority Substances; PEARL = PEsticides emission Assessment at the Regional and Local scale; TOXSWA = TOXic substances in Surface WAter; PNEC = Predicted No-Effect Concentration; RCR = Risk Characterisation Ratio

The concentrations at the continental and global scales are not used for risk characterisation. It should be kept in mind that pesticides are only evaluated at the local scale, the scale of the field where the substance is applied, contrary to new and existing substances which are also evaluated at the regional scale.

Figure I-3 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.

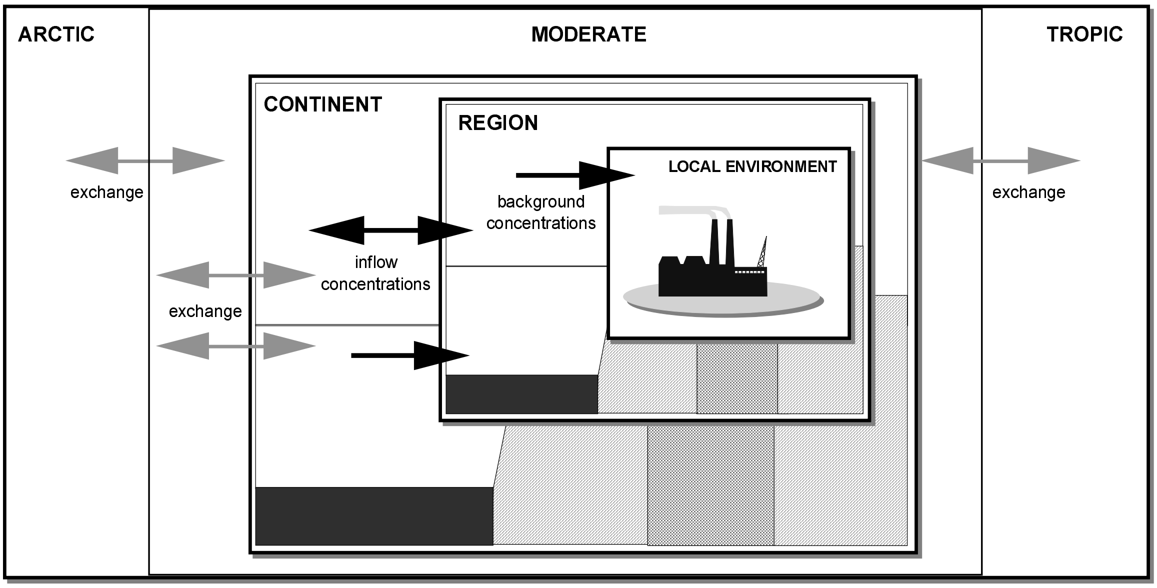


Figure I-3 *The relationships between the exposure assessments at the different spatial scales.*

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. Guiding for the evaluation of pesticides is the application scenario valid for the substance under consideration. Therefore, the dose applied during the growing season is calculated, taking into account e.g. degradation and sorption during the application interval. A herbicide for instance, may need only one application, while *Phytophtera* in potatoes may need up to 15 applications during the growing season.

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 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, 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 USES can therefore only give an approximation of the potential risk of a substance.

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 will, however, eventually lead to unrealistically high risk levels which are extremely unlikely to occur. The aim of USES is to perform a 'reasonable worst-case' risk assessment. The chosen standard exposure scenario represents an unfavourable, but not unrealistic, situation. For the model parameters, however, 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.

I.6. Model parameters

Input
USES 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. Data sets will also be available for pesticides. 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, USES 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) USES which parameters have been changed. However, as USES 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 USES 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

A model is always a simplified representation of reality. Therefore, model analysis is important to gain more insight into the model's behaviour. With USES 1.0, limited model analysis was performed: a framework for uncertainty analysis was defined (Jager and Slob, 1995), some example uncertainty analyses were performed (Jager, 1995b) and the validation status of the system and its sub-modules was discussed (Jager, 1995a). Validation is a crucial step in model analysis. In fact, it is the final check to assess whether the model produces results that are acceptable for its purpose. A definition of validation is shown in Table I-4. It should be recognised that several definition of validation are used. The FOCUS Steering group (FOrum for the Coordination of pesticide fate models and their USe) have adopted a slightly different definition. Here the definition given is used.

Model analysis of USES has not yet been performed in detail. Numerical validation of risk assessment systems, in the strictest sense, is impossible, as risks (or even PEC/PNEC ratios) cannot be measured. Nevertheless, the accuracy with which the system predicts exposure levels and effects may be expressed (semi-)quantitatively. Validation of a general system like USES is troublesome; the system should perform adequately for, in principle, all substances, in all situations. Furthermore, it is difficult to judge the degree of certainty that the decision-maker needs when assessing the risks of chemicals. In spite of this, the user of a system should be aware of the (in)accuracy of the model.

Table I-4 *Definition of validation.*

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

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

The major problem in using field data to validate environmental computer models is the large spatial and temporal variability of experimental data measured in the field. For instance, it is not abnormal for the concentration of a chemical in sediment samples from within the same square meter to vary by more than a factor 10 or even 100 (ECETOC, 1992). Therefore, care should be taken in interpreting field data and validation results. Moreover, even in the case of all sub-modules being satisfactorily validated, the combination of all sub-modules into a chain of models may not be valid if the models are inappropriately linked. It is clear that numerical validation only is not sufficient to validate a risk assessment system like USES. Individual models can be validated with measured data, but first, one has to check whether this particular model is appropriate (operational validation) and whether the assumptions and scenarios are acceptable and relevant (conceptual validation).

The Dutch Risk Assessment System for New Chemicals (DRANC, see Section I.1) was subjected to validation. The environmental concentrations and human intakes estimated with DRANC 1.0 were compared to measured data for 25 existing chemicals (Toet *et al.*, 1991; De Nijs *et al.*, 1988; De Nijs *et al.*, 1993; RIVM *et al.*, 1994). The following general conclusions could be drawn from these studies:

- The Sewage Treatment Plant (STP) model SimpleTreat performed satisfactorily in predicting concentrations in effluent and sludge from influent concentrations.
- The drinking water module performed quite well, even though a conservative approach was followed in the modelling process.
- The estimation of bioconcentration factors for fish, crops and cattle appears to be quite inaccurate.
- The concentrations calculated in fish, plants and cattle deviated even more from measured

values. It should be noted that in this version of the system, the air route to plants and cattle had not yet been implemented.

Several major problems concerning validation of risk assessment systems like USES and its predecessors have been identified by Toet *et al.* (1991):

- The Risk Characterisation Ratios cannot be measured directly. Only intermediate results of the exposure assessment can be measured, like emission fluxes, concentrations in the environment, bioconcentration factors and daily doses.
- One of the purposes of the model is to predict the risk of new chemicals, notified within the scope of EC Directive 67/548/EEC, before they enter the market. Measured data for comparison with intermediate model results are not available. A validation of the risk assessment system must therefore be carried out with existing chemicals, which are already in production.
- It is extremely difficult to find a consistent dataset of measurements over the same distribution pathways as described in USES. For example, measured concentrations in the environment cannot generally be related to a specific emission point. Moreover, substances may very well be released by other sources and distribution pathways than assumed in USES.
- The system makes use of a 'standard environment'. Reported data will invariably not only be non-representative for the standard environment, but also be incomplete and often ill-defined with respect to the time and spatial scales of the measurements. Measurements will often originate from many different locations.

Jager (1995a) has discussed the validation status of USES 1.0 in detail. Some of the major conclusions relevant to USES and some recent developments are summarised below:

- The validity of QSARs (Quantitative Structure-Activity Relationships) can be extracted from the original publications. Their application in the evaluation system needs to be given further consideration (e.g. when QSARs are applied outside their domain).
- The predictive capacity of the QSARs for estimating transfer to meat and milk is low. This is reflected in very high uncertainty factors (95% of the values are within a factor of 36 of the median estimate for milk and a factor of 64 for meat: Jager and Slob, 1995). The possibilities for improving this estimation were investigated by Van Eijkeren *et al.* (1998). These authors concluded that a more detailed model could, at this moment, not be applied.
- The uptake and translocation of chemicals from soil by plants has been extensively validated by Polder *et al.* (1995). The estimated concentration factor between root and soil was in good agreement with measured data. The estimated soil-leaf concentration ratio performed less well, with large deviations occurring, owing partly to inter-species differences and experimental design.
- Uptake of chemicals from air by plants was validated by Polder *et al.* (1996), showing, in general, good agreement between the model and measured data.
- For the sewage treatment plant model, extensive validation has been initiated. Experiments will be conducted in a pilot-scale activated sludge plant.
- Validation of the multi-media box model SimpleBox (on which the regional fate model of EUSES and USES 2.0 is based) was performed in 1997 (Bakker *et al.*, in prep). This project focused on concentration ratios. Only for a few chemicals, sufficient consistent data were available. For these compounds, the calculated water-sediment and air-water ratios were in good agreement with measured data, but the measured air-soil ratios were consistently lower

than computed ones.
- More detailed investigation of the uptake of chemicals by fish, earthworms and plants was also performed (Jager and Hamers, 1997), providing suggestions for further improvement.
- The extrapolation procedure from single-species toxicity tests to ecosystem no-effect levels has been validated by Emans *et al.* (1993) for the aquatic environment. The results indicated the applicability of the assessment factors (according to the modified EPA method) as they usually lead to a 'safe level'. However, the best estimates of 'safe levels' were obtained with the statistical extrapolation procedure (Aldenberg and Slob, 1993).

With respect to pesticides the European Commission has installed a group of experts from industry, government and research organisations called FOCUS. FOCUS stands for FOrum for the Coordination of pesticide fate models and their USe. Three working groups, Leaching, Soil and Surface water, have made an inventory of available models used in the registration of pesticides in Member States. Recently these working groups have established their final reports (EU Doc. 4952-VI-95, 7617-VI-96 and 6476-VI-96, respectively, Linders, pers.comm.). It can be concluded that the validation status of all models analysed must be considered as low. However, for several models currently validation is carried out, generally on a local basis. The EU-Directive 91/414/EEC requires model calculations in establishing Predicted Environmental Concentrations (PEC) using a mathematical model validated on a community level. The working groups have concluded that it still will take a while before the mathematical models currently used will reach such a status. For USES 2.0 it should be stated that the ground water model PESTLA is currently being validated at a local scale for the Dutch situation. Generally, the different models built in USES have to be considered as non-validated models, e.g. amenity use, water sediment, and the air module. Considering drift to surface water, it may be stated that the currently established drift table is based on state-of-the-art research on this phenomenon and therefore can be considered to be validated for the Dutch situation and under the circumstances of the study (Van de Zande et al., 1995).
At the transfer of USES 2.0 to USES 3.0, the models SLOOT.BOX and PESTLA have been replaced by TOXSWA and PEARL, as has been stated before. From the validation point of view it is clear that both models should not be considered as fully validated. The PEARL model should be given the same validation status as PESTLA. The TOXSWA-model is not yet validated but several efforts to validate TOXSWA are currently carried out. It is expected that the validation status will rise in the coming few years.

I.8. System limitations

Several limitations of USES 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. USES is not specifically designed for use in site-specific assessments.
3. The environmental risk assessment in USES 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. USES 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. Information may be found in Mensink *et al.* (1995).
7. Several hazards are not yet considered in USES: examples are global warming, ozone depletion, acidification, eutrophication, depletion of raw materials, effects on materials, calamities and hazardous waste.

I.9. USES 4.0 versus USES 1.0, USES 2.0 and USES 3.0

The indirect risks to man resulting from use of pesticides and biocides are not considered in EUSES but are included in USES 2.0, 3.0 and 4.0. The main differences between USES 2.0 and USES 1.0 for the pesticide/biocide assessment are:

- adjustment of the drift table (Table A-5 in Chapter III),
- inclusion of additional emission and distribution routes for non-agricultural pesticides,
- scenario on use of pesticides in amenity use,
- estimation of local short-term atmospheric distribution of agricultural pesticides,

The main differences between USES 2.0 and USES 1.0 for the assessment of new and existing substances are:

- USES 2.0 includes a risk assessment for sediment organisms (also for pesticides);
- USES 2.0 includes a risk assessment system for workers (EASE, Estimation and Assessment of Substance Exposure);
- USES 2.0 includes a risk assessment system for complex mixtures (Hydrocarbon Block Method);
- Several models, a.o. the sewage treatment plant model, the plant accumulation model and the regional distribution model, have been adapted;
- Many default values for a.o. emission rates, parameters describing the local or regional environment, intakes and assessment factors, differ between USES 2.0 and USES 1.0 (also for pesticides).

The main differences between USES 3.0 and USES 2.0 are:

- The surface water model for pesticides SLOOT.BOX has been replaced by TOXSWA (TOXic substances in Surface WAter);
- The leaching model PESTLA for pesticides has been replaced by PEARL (PEsticides emission Assessment at the Regional and Local scale);
- Adaptation of the pesticide application scenario for granules and treated seeds.

The main differences between USES 4.0 and USES 3.0 are:

- New PEARL tables have been generated using PEARL version 1.0 for the plough layer in addition to the tables for upper groundwater;

- Existing TOXSWA tables have been extended with a fourteen days column and new TOXSWA tables for sediment have been added.
- Addition of new biocides scenarios for product types 1 (human hygiene biocidal products), 2 (private area and public heatlh area disinfectants and other biocidal products except for swimming pools), 6 (In-can preservatvies), 7 film preservatives), 8 (wood preservatives,only waste treatment module added), 9 (fibre, leather, rubber and polymerised materials preservatives), 12 (slimicides), 22 (embalming and taxidermist fluids) and a landfill module for product types 7 and 8.
- Several bugs in USES 3.0 have been solved.

II. MODEL DESCRIPTION

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.

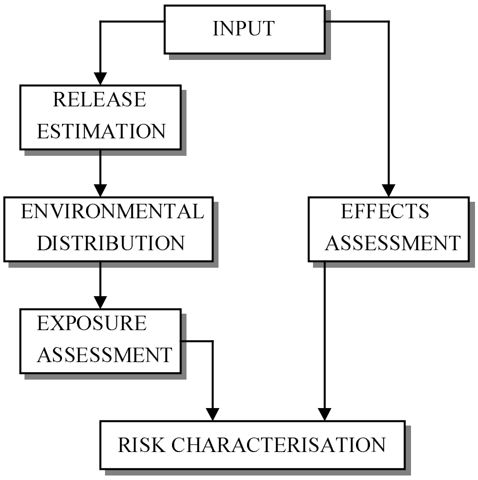


Figure II-1 *System structure.*

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, 1996).

The text for the assessment of new and existing chemicals is identical to the EUSES text. Therefore, the text mentions "EUSES" on several occcasions which can be read as "USES 4.0"

II.2. Input module and dataset

The input module requires the input of substance identification (name, CAS-number, etc.) and the primary data (physico-chemical properties) required to run USES. 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.

There are no calculations in this module. Since all required information should be available in the base set, no estimation routines are implemented. However, QSARs may be used in the evaluation of the measured data (e.g. see Chapter 4 of the TGD: EC, 1996).

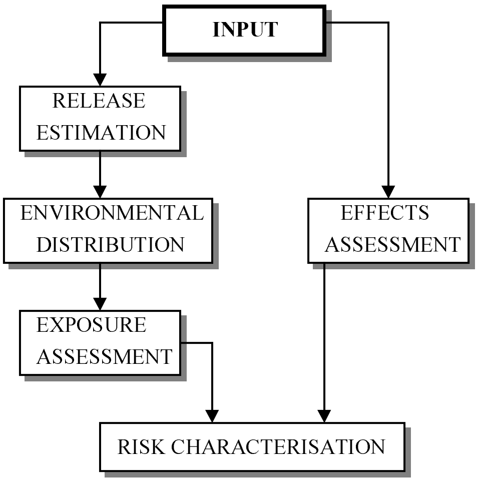


Figure II-2 *System structure.*

II.2.1. Data set for new and existing substances

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 'secondary 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 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. EUSES can import SNIF files directly from this database. 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-3). 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-3):

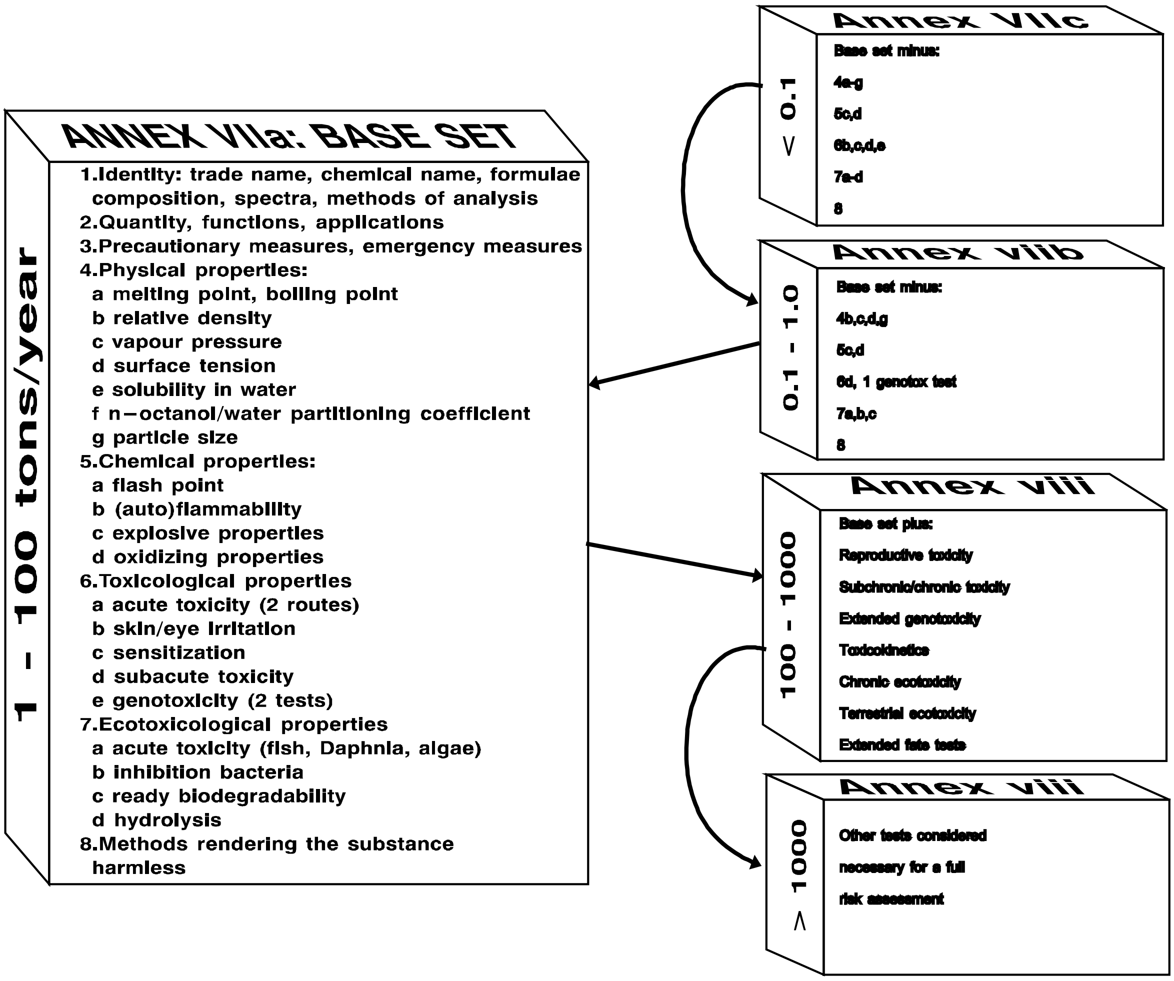


Figure II-3 *Data requirements for new chemicals, depending on the production or import volume.*

- 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, oxidizing properties, granulometry.
- Toxicological studies:
  acute toxicity (2 routes), skin and eye irritation, skin sensitization, 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 III) 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.2.2. 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.2.4. Data availability for agricultural and non-agricultural pesticides

When requesting registration of a new pesticide, provision of the data set for pesticides is obligatory. The required data set for pesticides is in agreement with regulations in the EU. Compared to the data availability for new and existing chemical, the data set for pesticides is usually quite extensive and includes more fate, toxicity and ecotoxicity data. This is necessary since pesticides, by definition, have an adverse effect on various organisms.

First, the data must refer to the active ingredient and its main metabolites (>10% of applied amount in fate studies). However, if necessary, data of the formulations can be required. The applicant must state why certain data do not need to be delivered.

Up to now, the data set required from the company which intends to market a pesticide or biocide consists of the following data (Anonymous, 1993):

- Identity:
- primary name, chemical names, trade names, CAS-number.
- Properties:
- structure and molecular weight, purity, additives and formulations, appearance, melting point, boiling point, density, Henry coefficient, surface tension, solubility in water, fat and other solvents, stability, spectra, vapour pressure (active ingredient and other substances), octanol/water partitioning coefficient, sediment/water partitioning coefficient, particle size, spraying patterns, degree of fixation to fibres, stability of baits.
- Analysis and detection:
- analytical methods for soil and water.
- Function and uses:
- application, frequency, dosage, description of processes in which the compound/formulation is used, estimation of concentration of the compound in the effluent (waste water of industry/plant).
- Chemobiokinetics and metabolism:
- in animals and plants.
- Ecotoxicology:
    - fate and degradation products of active ingredient (a.i.) in soil;
    - degradation rate in soil (a.i. and metabolites);
    - mobility in soil (a.i. and metabolites);
    - fate and degradation products of a.i. in water;
    - degradation rate in water (a.i. and metabolites);
    - adsorption of a.i. and metabolites to particles;
    - photochemical degradation;
    - hydrolysis;
    - data on flux of a.i. from paint or treated wood to the water phase;
    - emission to air;
    - acute oral toxicity study (LD50) with mammals;
    - chronic oral toxicity study (NOEC or NOAEL) with mammals;
    - acute oral toxicity study (LD50) with birds;
    - semi chronic oral toxicity study (LC50) with birds;
    - chronic oral toxicity study (NOEC) with birds;

- short-term toxicity study (EC50) with algae;
- short-term toxicity study (EC50) with daphnids;
- chronic toxicity study (NOEC) with daphnids;
- short-term toxicity study (LC50) with fish;
- chronic toxicity study (NOEC) with fish;
- short-term toxicity study (LD50 oral and contact) with bees;
- short-term toxicity study (LC50) with earthworms;
- sub-acute toxicity study (NOEC) with earthworms;
- study on the influence of a.i. (respiration) on the Municipal Sewage Treatment Plant (STP);
- study on the influence of a.i. on the nitrification in soil;
- study on the influence of a.i. on the respiration in soil;
- bioaccumulation;
- secondary poisoning.

II.3. Release estimation

II.3.1. Life cycle of substances

Releases into the environment can take place from processes at any stage of the life cycle of a substance (Figure II-5). The stages are discussed briefly below.

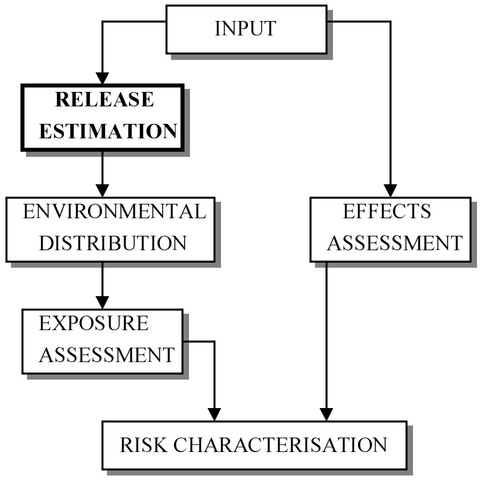


Figure II-4 *System structure.*

Production

Production is the stage in which the substance is manufactured, i.e. formed by chemical reaction(s), isolated, purified, drummed or bagged, etc. For intermediates (chemicals used to make other chemicals) a distinction is made between non-isolated intermediates, site-limited, and captive and other intermediates, as can be seen in Figure II-5. 'Non-isolated' means that the substance is not isolated from the reaction mixture but transformed directly into another substance in the same equipment in a subsequent reaction step. 'Site-limited' means that the substance is manufactured and consumed at the same site. This signifies that releases during production and processing (transformation into the next substance) occur at the same site. 'Captive' means that the intermediate is manufactured and shipped to other sites owned by the same company, but not sold to others. Therefore, releases during production of captive and other intermediates occur at a different site from where the substance is transformed into the next substance.

Formulation

Formulation is the stage in which chemicals are combined in a process of blending and mixing to obtain a product or preparation. This may be a formulation like a paint, or a product like a photographic film. Formulations are applied or used at the next stage of the life cycle (processing).

Processing

The processing stage (which is called 'industrial use' for applications in industry) consists of all kinds of processes whereby the substance as such, a formulation or an article containing the substance assessed is applied or used. Substances may be used as a processing aid or be incorporated in a product. An example of a processing aid is a developer used in a photographic bath which is disposed of after use. It should be noted that the manufacture of photographic film and paper might also be considered as processing of the chemicals involved. However, these materials will be processed again after exposure (developing and fixing). So, manufacture of photographic films and paper is considered as the stage of formulation. Articles like a plastic toy or articles with a coating layer containing the substance assessed will be used during a certain range of years. Releases into the environment during this period due to migration, leaching and evaporation will increase to a maximum after the introduction of the substance, and subsequently decrease. Processing can take place on a very large scale at one or only a few sites in industry or on a small professional scale.

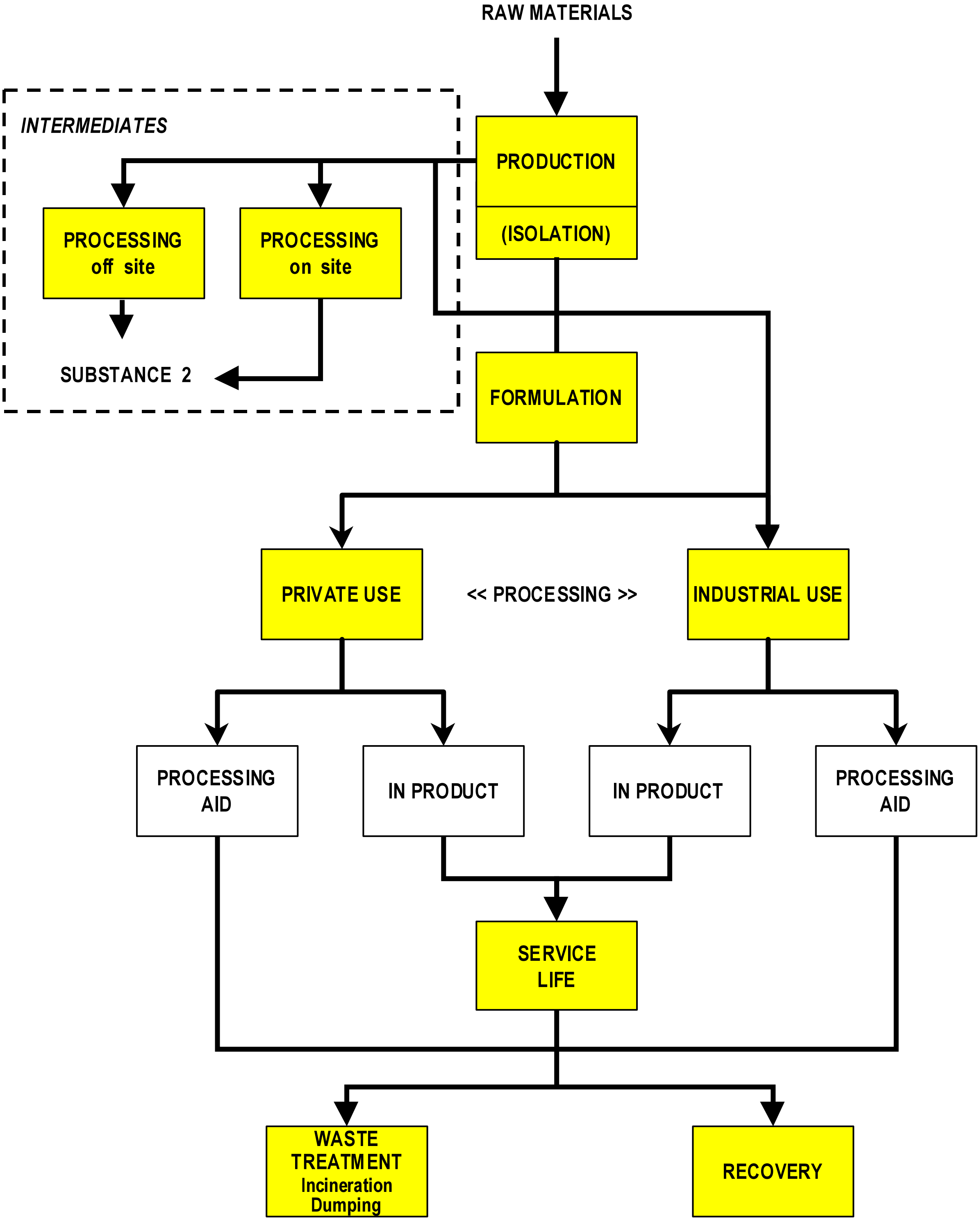


Figure II-5 *Schematic representation of the life cycle of a substance.*

Private use

This stage considers the use and application of substances (as such or in formulations such as cosmetics and biocides) on the scale of households (consumers). It should be noted that private use can be considered as the equivalent of processing for industrial use.

Service life

Many substances are used in products such as paints, inks, adhesives, etc., and many others as components (often called additives) in plastics and rubber. During the service life of the products in or on which they are used they may be released into the environment. An additive in paint or plastic may migrate to the surface of the paint layer or plastic article and be leached and volatilised. Another part may be released with small particles of the articles due to wear and abrasion. This aspect has not been covered in the first version of the TGD. In USES 4.0 the aspect of service life has only been covered for the application of biocides in wood preservatives.

Disposal (waste treatment and recovery)

At the stage of disposal, the substance (or the products containing the substance) is disposed of with waste or wastewater. Waste treatment may consist of incineration or dumping. Releases during these processes have not yet been taken into account, as there are no or insufficient data on leaching from landfills and escape of non-degraded substances during incineration. At this stage recovery processes may also occur. In recovery, two different situations have to be considered. Firstly, the substance assessed may be recovered and recycled. In this case releases will be limited. Secondly, another substance or product may be recycled, with the substance assessed being present in this product. Releases in this situation will be much higher as a rule, as attention is not focused on the substance assessed, but on the substance or product recovered. A substance present in a photographic bath for example, will be released during discharge after silver recovery, and a substance present in printing ink will be released with wastewater and de-inking sludge during paper recycling.

Note

Various stages of the life cycle are treated specifically for pesticides and biocides, see II.3.8 and II.3.9.

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 which 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, 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-3)
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 paint 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 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 IVa/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 (use category documents);
3) emission factors as included in the release tables of Appendix IV.

In many cases, little or no specific information on releases will be available, and emission scenario documents are scarce. Therefore use will have to be made of the emission factors of the release tables of Appendix IV, which have been implemented in EUSES. 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 IV.

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 IV 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 IV 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 IV, 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 IV, 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 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

New substances are usually produced in rather low volumes. For existing substances High-Production-Volume Chemicals (HPVC) 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. 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 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 IV.

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).

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.

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.

7. Leather processing industry

A general scenario is presented 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

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). The basis for the 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 documents for this IC.

10. Photographic industry

Several use-category documents are available for this IC. The values in the 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.

12. Pulp, paper and board industry
The 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.

13. Textile processing industry
The original scenario derived from the document of Ros (1985) has been used for the emission tables.

14. Paints, lacquers and varnishes industry
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 UCs, water-based and solvent-based types, and application by industries and households.

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.

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.3.8. Release estimation for agricultural pesticides on a local scale

For the releases of pesticides on a local scale, application-specific scenarios have been developed for the use/processing of agricultural pesticides (Emans *et al.*, 1992). Application of pesticides in areas of public use, referred to as amenity use, is reported separately (Kraaij and Verstappen, 1995). In Figure II-1 on Page II-P23, the emission and distribution routes of pesticides are indicated. The information given in Emans *et al.* (1992) is also provided in the current document.

As several scenarios require distribution parameters, all calculations for these scenarios are part of the distribution module (Section III.4.6). In fact, the emission estimation is covered with the entry of type, dosage and frequency of application. The emission of agricultural pesticides into the environment takes place during and after the application of the substance. There are three main applications of pesticides: 1. spray, 2. granular application and 3. seed treatment. A spray generally consists of water but also other carriers may be used e.g. mineral oil. The emission involves release into three environmental compartments; air, soil and water. Granular application and seed treatment are considered to be released to the target soil only. Often the particles are covered by a layer of soil after the application, which also limits the distribution to other compartments.

Another application area is the use of pesticides in amenity use. According to Kraaij and Verstappen (1995) amenity use can be divided into several
sectors of application:

- pavements; with possible discharges:
  - direct run-off to surface water,
  - discharge through rain water drain of a separated sewer system,
  - discharge through a storm overflow of a mixed sewer system and
  - discharge through a municipal sewage system connected to a mixed sewer
- system;
- planting, railways and water courses; with possible emission routes:
  - drift,
  - run-off and
  - leaching;
- paved dikes and slopes; two emission routes have been identified as relevant:
  - drift,
  - run-off.

The emission of pesticides during the applications mentioned is estimated using standard scenarios for representative towns and cities in the Netherlands. Additional information is given in the relevant sections of Chapter III.

II.3.9. Release estimation for non-agricultural pesticides on a local scale

Non-agricultural pesticides can be emitted to air, directly to surface water and/or soil, or via an STP to surface water and/or soil. For non-agricultural pesticides specific release and distribution scenarios have been provided by Luttik *et al.* (1992 and 1995). These scenarios were already incorporated in USES 1.0. They were implemented according to the classification in the Netherlands. The following groups of non-agricultural pesticides are distinguished at the time by the Dutch government: disinfectants, industrial biocides, preservatives, household products, wood preservatives and protectors, and antifoulings. Since the EU Directive on the placing of biocidal products on to the market (EC, 1998) has come into force, the existing scenarios have been rearranged according to the 23 product types distinguished in this directive.

Table II-1 presents an overview of the 23 product types – with subdivision where appropriate – and the status of the emission scenarios, which are present in this version of USES. The status denotes if the emission scenario is new or comes from USES 3.0. Where "EUBEES" has been stated, this signifies the EU working group on 'Gathering, review and development of environmental emission scenarios for biocides'. The emission scenarios have been implemented according to the report by Van der Poel and Bakker (2002). A brief description of the applications of biocidal products is presented in the following sections.

As several scenarios require distribution parameters, for model calculations, all scenarios are part of the distribution module (Section III.4.7). The emission estimation is finished with the selection of the scenario.

Table II-1 *Overview of emission scenarios according to their product type (Pt) of EU Directive 98/8/EC (EC, 1998), their status and remarks (EUBEES = EU working group supervising the project 'Gathering, review and development of environmental emission scenarios for biocides'.*

Pt	Description of product type	Life cycle stage	Status	Remark(s)
1	Human hygiene biocidal products	Private use	New	Existing generic EUSES scenario based on annual tonnage
		Private use	New	Based on average consumption
		Industrial use	New	Existing generic EUSES scenario based on annual tonnage
2	Private area and public health area disinfectants and other biocidal products:			
	- Swimming pools	Industrial use	USES 3.0	Public swimming pools; acute and chronic situations (Disinfectants_
		Industrial/Private use	USES 3.0	Public and private swimming pools; acute situation (Disinfectants)
	- Sanitary sector	Formulation	New	Existing emission scenario document 1 of TGD + generic B-tables for industrial category 5
		Private use	New	Based on annual tonnage
		Private use	New	Based on average consumption
	- Horticulture	Industrial use	New	Existing emission scenario of USES 3.0 for household products used for fogging
	- Tiles and surfaces	Formulation	New	Existing emission scenario document 1 of TGD + generic B-tables for industrial category 5
		Private/Industrial use	New	Existing generic EUSES scenario based on annual tonnage
	- Medical sector:			
	-- Disinfection of rooms, furniture and objects	Industrial use/Service life	New	Based on annual tonnage
		Industrial use/Service life	New	Based on average consumption
	-- Disinfection of instruments	Industrial use/Service life	New	Disinfection of scopes in washers
		Industrial use/Service life	New	Disinfection of other instruments

Table II-1 *Overview of emission scenarios, their status and remarks (continued).*

Pt	Description of product type	Life cycle stage	Status	Remark(s)
	- Medical sector continued:			
	-- Laundry disinfectants	Industrial use/Service life	New	Washing streets
		Industrial use/Service life	New	Tumbler washing machines
	-- Hospital waste disinfectants	-	Not available	
	-- Disinfectants with more than one application	-	See remark	Adding the outcomes of different scenarios for the medical sector
	- Disinfection of air conditioning systems	-	Not available	
	- Disinfection of industrial areas	-	Not available	
	- Disinfectants for sewage and wastewater	Industrial use	New	Preliminary emission scenario
	- Soil and other disinfectants, …..	-	Not available	
	- Disinfection of chemical toilets	-	Not available	
3	Veterinary hygiene biocidal products:			
	- Disinfection of animal housing	Industrial use	Not yet implemented	International harmonisation (EUBEES)
	- Disinfection of footwear and animals' feet	Industrial use	Not yet implemented	International harmonisation (EUBEES)
	- Disinfection of milk extraction systems	Industrial use	Not yet implemented	International harmonisation (EUBEES)
	- Disinfection of means of transport	Industrial use	Not yet implemented	International harmonisation (EUBEES)
	- Disinfection of hatcheries	Industrial use	Not yet implemented	International harmonisation (EUBEES)
	- Disinfection of fish farms	-	Not available	
4	Food and feed area disinfectants	-	Under development	EUBEES: RIVM
5	Drinking water disinfectants	-	Under development	EUBEES: Umweltbundesamt

Table II-1 *Overview of emission scenarios, their status and remarks (continued).*

Pt	Description of product type	Life cycle stage	Status	Remark(s)
6	In-can preservatives			
	- Washing and cleaning fluids, human	Private use	New	Based on annual tonnage
	hygienic products and cosmetics	Private use	New	Based on annual tonnage
	- Detergents	Private use	as previous product subtype	
	- Paints and coatings	Industrial use 1)	New	Existing emission scenario document 14 of TGD + generic B-tables for industrial category 14
		Industrial use 2)	New	Existing emission scenario document 14 of TGD + generic B-table for industrial category 14
		Waste treatment	New	
	- Fluids used in paper production	Industrial use	New	Drying sections after size-pressing (EUBEES)
		Industrial use		Broke (EUBEES)
		Recycling	New	EUBEES
	- Fluids used in textile production	Industrial use	New	EUBEES
	- Fluids used in leather production	Industrial use	New	EUBEES
	- Lubricants	-	Not available	
	- Machine oils	-	Not avialable	
	- Fuels	-	Not available	

1) product formulation) 2) product application

Table II-1 *Overview of emission scenarios, their status and remarks (continued).*

Pt	Description of product type	Life cycle stage	Status	Remark(s)
7	Film preservatives:			
	- Paints and coatings	Industrial use [1]	New	Existing emission scenario document 14 of TGD + generic B-tables for industrial category 14
		Industrial use [2]	New	Existing emission scenario document 14 of TGD + generic B-table for industrial category 14
		Waste treatment	New	
	- Plastics	-		
	- Glues and adhesives	Waste treatment	New	
	- Paper and cardboard	Industrial use	New	Drying sections after size-pressing (EUBEES)
		Industrial use	New	Broke (EUBEES)
		Recycling	New	EUBEES
8	Wood preservatives	Industrial use	USES 3.0	Preventive application: Creosote impregnation
		Industrial use	USES 3.0	Preventive application: Salt impregnation
		Industrial use	USES 3.0	Preventive application: Drenching and dipping
		Industrial use	USES 3.0	Curative application: Remedial timber treatment in buildings
		Service life	USES 3.0	Leaching from impregnated wood to surface water
		Service life	USES 3.0	Leaching from impregnated wood to sandy soil and groundwater
		Service life	USES 3.0	Leaching from impregnated wood to soil
		Waste treatment	New	

[1] product formulation) [2] product application

Table II-1 *Overview of emission scenarios, their status and remarks (continued).*

Pt	Description of product type	Life cycle stage	Status	Remark(s)
9	Fibre, leather, rubber and polymerised materials preservatives			Biocide present in imported material
	- Textile and fabrics	Industrial use	New	Application steps in textile (EUBEES)
		Industrial use	New	EUBEES
		Service life	New	EUBEES
	- Leather and hides	Industrial use	New	(EUBEES)
	- Rubber, plastics and other polymerised materials	-		
	- Paper and cardboard	Industrial use	New	Drying sections after size-pressing (EUBEES)
		Industrial use		Broke (EUBEES)
		Recycling		EUBEES
10	Masonry preservatives	-	Under development	EUBEES: INERIS
11	Preservatives for liquid-cooling and processing systems	Industrial use	USES 3.0	Revision expected (EUBEES)
12	Slimicides	Industrial use	USES 3.0	
		Industrial use	New	Draft report EUBEES
13	Metalworking-fluid preservatives	Industrial use	USES 3.0	
14	Rodenticides	Industrial use	USES 3.0	Fogging of buildings and silos
		Industrial use	Under development	EUBEES: MST Denmark (Baits)
15	Avicides	-	Not available	
16	Molluscicides	-	Not available	
17	Piscicides	-	Not available	

Table II-1 *Overview of emission scenarios, their status and remarks (continued).*

Pt	Description of product type	Life cycle stage	Status	Remark(s)
18	Insecticides, acaricides and products to control other arthropods:			
	- Insecticides for manure	Industrial use	Draft EUBEES report	i.e. manure storage systems
	- Insecticides for stables	Industrial use	Draft EUBEES report	i.e. animal housings
	- Refuse dumps	-	Not available	
	- Insecticides for empty spaces and spaces with stocks	Industrial use	New	Existing emission scenario of USES 3.0 for household products used for fogging
	- Aerosols/fumigants used outdoors	Industrial use	New	Existing emission scenario of USES 3.0 for household products used for fogging
	- Aerosols/fumigants used within fumigation installations	Industrial use	New	Existing emission scenario of USES 3.0 for household products used for fogging
	- Aerosols/fumigants used indoors	Industrial use	New	Existing emission scenario of USES 3.0 for household products used for fogging
19	Repellents and attractants	-	Not available	
20	Preservatives for food or feedstocks	-	Not available	
21	Antifouling products	Service life	USES 3.0	
22	Embalming and taxidermist fluids	Industrial use	New	Taxidermy (EUBEES)
		Industrial use	New	Embalming (EUBEES)
23	Control of other vertebrates	-	Not available	

MAIN GROUP 1: Disinfectants and general biocidal products
These product types exclude cleaning products that are not intended to have a biocidal effect, including washing liquids, powders and similar products.

II.3.9.1. Product-type 1: Human hygiene biocidal products

Products in this group are biocidal products used for human hygiene purposes.

The products that fall into this product type are, e.g., creams, lotions, soaps with biocides used as skin antiseptics, antimicrobial soaps, health care hand wash products, anti acne products, anti-dandruff shampoos, antiperspirants, and deodorants. There are four scenarios altogether, two for private use and two for professional use (industrial use). The user can – in both cases – choose between a scenario based on the annual tonnage of the active substance and a scenario based on the average consumption of the product involved. For the scenarios based on the tonnage the fraction of the active substance reaching the model STP is set at 0.002 for private use and at 0.007 for industrial use (in hospitals) by default. Appendix IX explains the difference and usefulness of scenarios based on tonnages and average consumption.

II.3.9.2. Product-type 2: Private area and public health area disinfectants and other biocidal products

Products used for the disinfection of air, surfaces, materials, equipment and furniture which are not used for direct food or feed contact in private, public and industrial areas, including hospitals, as well as products used as algaecides. Usage areas include, inter alia, swimming pools, aquariums, bathing and other waters; air-conditioning systems; walls and floors in health and other institutions; chemical toilets, waste water, hospital waste, soil or other substrates (in playgrounds).

As can be seen from the description above as stated in the biocidal products directive (EC, 1998) this product type comprises a variety of applications of disinfectants (see also Table II-1). The applications for which emission scenarios are present are described below.

Swimming pools
There are two scenarios, viz. one for public swimming pools discharging their water to the sewage system, and one for public and private pools discharging into surface water. The first scenario can be used either for the 'acute' situation (the whole pool is emptied completely in the STP) or for the 'chronic' situation (a fixed amount of water per visitor is discharged). The input to be specified by the user is the concentration of the active substance in the swimming water. There are defaults for the required parameters concerning the dimension of the swimming pool, the number of visitors and the amount of water replaced per visitor. The second scenario considers the release of the whole pool capacity (acute situation). The input to be specified by the user is the concentration of the active substance in the swimming water. There is a default for the parameter depth of the ditch (receiving surface water).

Sanitary sector
For this application scenarios for two stages of the life cycle are present, one for formulation and one for private use. The scenario for formulation uses the emission factors of the emission

scenario document for industrial categories 5 (Personal/domestic) and 6 (Public domain) and the generic B-tables for these industrial categories. For the stage of private use the user can choose between a scenario based on the annual tonnage of the active substance and a scenario based on the average consumption of the product. For the scenarios based on the tonnage the fraction of the active substance reaching the model STP is set at 0.002 by default. Appendix IX explains the difference and usefulness of scenarios based on tonnages and average consumption.

Horticulture

No specific scenario has been implemented for the application of disinfectants in horticulture in general. For the disinfection of greenhouses the same emission scenario for fogging of household products as present in USES 3.0 is used. This scenario uses the amount of active ingredient used, a retention in goods (predominantly soil in this application), and a fraction disintegrated.

Tiles and surfaces

This application covers small-scale applications at home and medium to large-scale applications in food processing industries (no direct contact with food). As it is not possible to distinguish between private use and industrial use one emission scenario is used, which is based on the annual tonnage of the active substance. The fraction of the active substance reaching the model STP is set at 0.002 by default.

It should be noted that this scenario is closely related to the scenario of USES 3.0 for disinfectants in accommodations (disinfectants applied in accommodations for man accommodations for preparing food and drinks). However, strictly speaking this application belongs largely to product type 4 (Food and feed area disinfectants). Furthermore, there is a specific application of disinfectants in accommodation for man in hospitals, which is covered in the next subsection.

Medical sector

The application of disinfectants applied in the medical sector falls apart into four specific parts:

i Disinfection of accommodations for man
ii Disinfection of medical instruments
iii Disinfection of laundry
iv Disinfection of hospital waste (infectious waste)

i Disinfection of accommodations for man

This includes disinfection of bathrooms, toilets, walls, and floors. There are two scenarios, one based on the annual tonnage and one based on the daily consumption. For the scenarios based on the tonnage the fraction of the active substance reaching the model STP is set at 0.007 by default. Appendix IX explains the difference and usefulness of scenarios based on tonnages and average consumption.

ii Disinfection of medical instruments

There are two scenarios, one for washers/disinfectors for disinfection of (endo)scopes, and one for the disinfection of other instruments. The scenario for scopes can be used for both washers/disinfectors with replacement of the biocidal product at regular intervals ('replacement') and for washers/disinfectors where a fresh disinfection solution is applied at every disinfection operation ('once-through'). It should be noted that if a biocide is notified for both disinfection of scopes and other instruments the results of both emission scenarios should be summed.

iii Disinfection of laundry
The first scenario for this application concerns the use of disinfectants in washing streets at commercial laundries where hospitals send their laundry. The other scenario is for laundries or hospitals using tumbler washing machines.

iv Disinfection of hospital waste (infectious waste)
There is no scenario available at present.

If a disinfectant has been notified for more than one application in the medical sector the results for the releases to wastewater of the scenarios that are applicable should be summed.

II.3.9.3 Product-type 3: Veterinary hygiene biocidal products

Products in this group are biocidal products used for veterinary hygiene purposes including products used in areas in which animals are housed, kept or transported.

The application of biocides for veterinary hygiene falls apart in five separate applications, for which emission scenarios have been developed but not yet implemented in this version of USES (see also Table II-1).

II.3.9.4 Product-type 4: Food and feed area disinfectants

Products used for the disinfection of equipment, containers, consumption utensils, surfaces or pipework associated with the production, transport, storage or consumption of food, feed or drink (including drinking water) for humans and animals.

An emission scenario has not been implemented in this version of USES. An emission scenario document will be developed by the EUBEES working group on the project 'Gathering, review and development of environmental emission scenarios for biocides'. It should be noted that the scenario of USES 3.0 for disinfectants in accommodations (disinfectants applied in accommodations for man accommodations for preparing food and drinks) might be used. It is not available for product type 4, but has been implemented for product type 2 (Private area and public health area disinfectants and other biocidal products) for the part 'Tiles and surfaces'.

II.3.9.5 Product-type 5: Drinking water disinfectants

Products used for the disinfection of drinking water (for both humans and animals).

An emission scenario document will be developed by the EUBEES working group on the project 'Gathering, review and development of environmental emission scenarios for biocides'.

MAIN GROUP 2: Preservatives

II.3.9.6 Product-type 6: In-can preservatives

Products used for the preservation of manufactured products, other than foodstuffs or feedingstuffs, in containers by the control of microbial deterioration to ensure their shelf life.

In-can preservatives are added to a variety of products, viz.:

i Washing and cleaning fluids, human hygienic products and cosmetics
ii Detergents
iii Paints and coatings
iv Fluids used in paper, textile and leather production
v Lubricants
vi Machine oils
vii Fuels

Only the products for which a scenario has been implemented are treated below.

i Washing and cleaning fluids, human hygienic products and cosmetics
The scenario for these products employs either the average consumption per inhabitant or the average consumption per application.

iii Paints and coatings
For three stages of the life cycle emission scenarios have been implemented. The first stage of the life cycle covered is formulation of paint products, i.e. the industrial application of biocides or formulations containing biocides in the manufacture of paints. The scenario uses the emission factors of the emission scenario document for industrial category 14 (Paints, lacquers and varnishes industry) of the TGD together with the appropriate B-tables of the TGD.
The stage industrial use – i.e. the professional application of paints and coatings – uses also the emission scenario document for industrial category 14 for the emission factors together with the appropriate B-table.
For waste treatment defaults for the required parameters of the landfill module (see also section II.3.9.24) are provided. The user can overwrite these values if more accurate information is known.

iv Fluids used in paper, textile and leather production
There are two scenarios for industrial use of products with an in-can preservative used in paper production, one for the releases from drying sections after size-pressing and coating, and one for releases from broke (scrap paper cuttings). Furthermore, there is a scenario for releases at paper recycling.
For textile production (industrial use of products containing an in-can preservative) there is one scenario. As different products with the same active ingredient may be used in the various treatment steps (i.e. desizing/scouring, dyeing and finishing) in textile production, the releases of the individual steps are summed. An identical scenario has been implemented for leather production. At leather production the steps curing, soaking, pickling, tanning, and finishing can be distinguished.

II.3.9.7 Product-type 7: Film preservatives

Products used for the preservation of films or coatings by the control of microbial deterioration in order to protect the initial properties of the surface of materials or objects such as paints, plastics, sealants, wall adhesives, binders, papers, art works.

As can be seen from the description above as stated in the biocidal products directive (EC, 1998) film preservatives may be used in many products in a variety of processes and for many materials. As far as film preservatives in plastics are concerned – so, not just at the surface or in a coating layer on the plastic subject – they belong to product type 9 (Fibre, leather and polymerised materials preservatives). The following applications have been provided with emission scenarios:

i Paints and coatings
ii Glues and adhesives
iii Paper and cardboard

i Paints and coatings

For formulation, industrial use, and waste treatment the scenarios for product type 6 (in-can preservatives) are used. Only for waste treatment one parameter has a different default.

ii Glues and adhesives

Only for the life cycle stage waste treatment a scenario is present. This is the general scenario for the landfill (see section II.3.9.24) applies, for which default values for the required parameters are provided, both for water-based adhesives and dispersion adhesives.

iii Paper and cardboard

For the stage of industrial use two scenarios have been implemented, one for the releases after size-pressing and coating, and one from broke (scrap paper cuttings) respectively.

II.3.9.8 Product-type 8: Wood preservatives

Products used for the preservation of wood, from and including the saw-mill stage, or wood products by the control of wood-destroying or wood-disfiguring organisms. This product type includes both preventive and curative products.

The same scenarios as present in USES 3.0 have been implemented, for the stages of the life cycle industrial use (4) and service life (3) respectively.

For industrial use the scenario choice depends on the type of preservative and whether the application is preventive or curative. The four scenarios deal with creosote impregnation, salt impregnation, drenching and dipping, and curative application respectively respectively. The defaults that have been used for the emission factors for creosote impregnation were originally estimated from some known data and available physico-chemical properties for common components of creosote. For the releases to to water and soil it is assumed that 1% of the releases goes to soil and 99% to wastewater, i.e. to an STP. For salt impregnation the amount of a specific substance has to be specified by the user. In both scenarios the defaults for the mean storage time are 10 weeks with 5 storage events per yearr per square meter, and for the storage densities of treated wood 0.76 m^3 wood per m^2. For the drenching and dipping scenario a distinction has been made between agents dissolved in water and agents dissolved in organic solvents. The defaults for storage time, numer of episodes and storage density are 5 weeks, 10 events per year and 0.5 m^3 wood m^{-2} respectively. For remedial timber treatment the relative toxicity index (RTI) is calculated as described in Luttik *et al.* (1992). The user has to specify the values of the parameters for solid or fluid application.

For wood in service (life cycle stage service life) the scenarios cover leaching from poles to surface water, leaching from impregnated wood to sandy soil and groundwater, and leaching from impregnated wood to soil respectively. For the scenario of leaching to surface water a small model waterway is used with the following characteristics/defaults:

- the model waterway is a rectangular box
- the residence time of the water in the watreway is 20 days
- there is complete mixing perpendicular to the direction of the water flow with no back-mixing
- length 1000 meters
- depth 1.5 meters
- width 5 meters
- at both sides along the complete length of the waterway impregnated wooden poles are placed (5 poles per meter of waterway). It is assumed that all poles have 100% contact with the surface water
- diameter of the poles is 0.1 meter.

For calculation of the concentration of the compound used for impregnating the wood in surface water it is necessary to have results from a lixiviation experiment (mean flux) over a certain period.

For the scenario dealing with the leaching to groundwater is is assumed that the leaching only occurs in the saturated zone, where the wood is in direct contact with the stagnant soil pore water. In this situation, the leached compounds are distributed over the solid and aqueous soil phase and concentrations will be determined by the substance specific partitioning coefficients. The diameter of the poles is 0.1 m, the part of the pole which is subjected to leaching is 0.1 m. The compound leaches with a constant flux in a sideways direction, over a maximum distance of 0.05 m from the pole. Vertical transport is not included in the calculations. The calculated initial concentration in the soil pore water can be used as a PEC for groundwater organisms. For the calculation of the concentration in groundwater used for production of drinking water, a correction factor is applied in which the soil area around the poles is related to the total soil area. The correction factor is based on the situation that an area of 100x100 m is fenced along four sides with 50 poles per side.

The model for leaching to soil describes the impact of leaching to soil from a fence due to rain. The fence consists of impregnated wooden poles and planks with a total area of 2 m^2 per meter length. Leaching occurs at one side only. The amount that is leached over one year is present in the soil beneath the fence. The soil compartment is a rectangular box, with a default value for the width of 0.025 m and a depth of 0.05 m. The default for the number of days that leaching occurs is set at 35 and is based on the day totals of rainfall in the Netherlands.

Furthermore, two sets of defaults for parameters of the general scenario for a landfill have been implemented for the stage of waste treatment (see also section II.3.9.24), one for wood preservatives applied by impregnation, immersion, drenching, dipping, etc., and one for wood preservatives in products for general-use surface protection (a kind of coating).

II.3.9.9 Product-type 9: Fibre, leather, rubber and polymerised materials preservatives

Products used for the preservation of fibrous or polymerised materials, such as leather, rubber or paper or textile products and rubber by the control of microbiological deterioration.

The following specific materials to be preserved can be distinguished:
i Textile and fabrics
ii Leather and hides
iii Rubber plastics and other polymerised materials
iv Paper and cardboard

Below, the items of the listing for which emission scenarios have been provided are described briefly.

i Textile and fabrics
For the stage of industrial use two new scenarios have been implemented, replacing the scenario of USES 3.0. The first scenario is for preservatives present on imported materials and the second for preservatives used in one or more application steps (desizing/scouring, dyeing, finishing). In cases that the same active substance is applied in more than one step, the releases have to be summed. This is added to the release from imported material as well if the same active substance is concerned. Furthermore, a scenario has been added for the stage of service life.

ii Leather and hides
A scenario has been implemented for the stage of industrial use, where the releases for the appropriate treatment steps (curing, soaking, pickling, tanning, and finishing) are summed.

iv Paper and cardboard
For industrial use scenarios, for releases from drying sections after size-pressing and coating, and from broke (scrap paper cuttings) respectively, have been implemented. It should be noted that in the draft emission scenario document of the EUBEES working group pulp preservatives are treated in a different way. As this has not been harmonised yet this has not been worked out in this version of USES (see also II.3.9.12 Product-type 12: Slimicides).

II.3.9.10 Product-type 10: Masonry preservatives

Products used for preservation and remedial treatment of masonry or other construction materials other than wood by the control of microbiological and algal attack.

An emission scenario document will be developed by the EUBEES working group on the project 'Gathering, review and development of environmental emission scenarios for biocides'.

II.3.9.11 Product-type 11: Preservatives for liquid-cooling and processing systems

Products used for the preservation of water or other liquids used in cooling and processing systems by the control of harmful organisms such as microbes, algae and mussels. Products used for the preservation of drinking water are not included in this product type.

The scenario of USES 3.0 has been implemented in this version of USES. It can handle biocides applied in continuous flow systems and in open circulation systems with open cooling towers.

II.3.9.12 Product-type 12: Slimicides

Products used for the prevention or control of slime growth on materials, equipment and structures, used in industrial processes, e.g. on wood and paper pulp, porous sand strata in oil extraction.

The simple scenario of USES 3.0 has been implemented but the default for the amount of wastewater has been revised (from 3000 to 5000 $m^3.d^{-1}$). Furthermore, the scenario has been extended in such a way that paper production process differences in respect to the pH – alkaline, neutral or acid – are taken into account. Also the most important differences found in wastewater treatment have been incorporated.

II.3.9.13 Product-type 13: Metalworking-fluid preservatives

Products used for the preservation of metalworking fluids by the control of microbial deterioration.

The scenario of USES 3.0 has been implemented. The model uses default values for the system capacity of the metalworking equipment, the fraction of that capacity that has to be supplemented every working day, and for the content of active ingredient in the diluted fluid (only water-based fluids contain preservatives and are divided in emulsions, dispersions, synthetics, and semi-synthetics).

MAIN GROUP 3: Pest control

II.3.9.14 Product-type 14: Rodenticides

Products used for the control of mice, rats or other rodents.

There is no model available yet; an emission scenario document will be developed by the EUBEES working group on the project 'Gathering, review and development of environmental emission scenarios for biocides'.

II.3.9.15 Product-type 15: Avicides

Products used for the control of birds.

There is no model available yet.

II.3.9.16 Product-type 16: Molluscicides

Products used for the control of molluscs.

There is no model available yet.

II.3.9.17 Product-type 17: Piscicides

Products used for the control of fish; these products exclude products for the treatment of fish diseases.

There is no model available yet.

II.3.9.18 Product-type 18: Insecticides, acaricides and products to control other arthropods

Products used for the control of arthropods (e.g. insects, arachnids and crustaceans).

The application of these kinds of biocides has been split in five application groups:
- Insecticides for manure
- Insecticides for stables
- Insecticides for refuse dumps
- Insecticides for empty spaces and spaces with stocks
- Aerosols/fumigants used outdoors
- Aerosols/fumigants used within fumigation installations
- Aerosols/fumigants used indoors

For the first two subgroups an emission scenario document has been developed by the EUBEES working group on the project 'Gathering, review and development of environmental emission scenarios for biocides'. The emission scenarios that have been developed have not yet been implemented in this version of USES.

For the application of insecticides on refuse dumps no emission scenario is available yet.

The last application groups have been treated together, assuming that the application of biocides outdoors will not occur as the chemicals will disappear almost completely before having the desired effect (the application of pesticides is not considered here). The emission scenario of USES 3.0 for household products for fogging has been implemented for these groups. The model uses an amount of the active substance applied and fractions of retention in goods and disintegration.

II.3.9.19 Product-type 19: Repellents and attractants

Products used to control harmful organisms (invertebrates such as fleas, vertebrates such as birds), by repelling or attracting, including those that are used for human or veterinary hygiene either directly or indirectly.

There is no model available yet.

MAIN GROUP 4: Other biocidal products

II.3.9.20 Product-type 20: Preservatives for food or feedstocks

Products used for the preservation of food or feedstocks by the control of harmful organisms.

There is no model available yet.

II.3.9.21 Product-type 21: Antifouling products

Products used to control the growth and settlement of fouling organisms (microbes and higher forms of plant or animal species) on vessels, aquaculture equipment or other structures used in water.

For the stage of the service life the emission scenario for a (freshwater) yacht-basin of USES 3.0 has been implemented. The defaults for the required parameters are for a middle-sized yacht-basin with 250 ships. Some defaults are 10 m^2 for the mean deck area, 2.5 m for the depth of the yacht-basin, and 3 for the ratio water/ship. It is preferred to have results of a lixiviation study. In case no data are available, a default of $2.5 \cdot 10^{-4}$ $kg.m^{-2}.d^{-1}$ is used.

II.3.9.22 Product-type 22: Embalming and taxidermist fluids

Products used for the disinfection and preservation of human or animal corpses, or parts thereof.

For taxidermy and embalming two scenarios developed by the EUBEES working group on the project 'Gathering, review and development of environmental emission scenarios for biocides' have been implemented. The scenario for taxidermy needs values for the parameters quantity of drained skin and of active substance used per day, and the degree of fixing. There are defaults for all parameters and if the same active substance is used in more than treatment steps (soaking, pickling, and tanning) the results of the individual steps are summed.

For embalming two scenarios have been implemented, one for the stage of industrial use (i.e. the application in the embalming process) and one for the stage of service life (the release in cemeteries after burial). For both models the user has to supply the concentrations for the solutions used for arterial injection and cavity treatment. There are defaults for the parameters volume of solutions used for arterial injection and cavity treatment, density of the solutions, and retention rates, which are used in both scenarios. For the cemetery model additional defaults are provided for the parameters factor for reaction with the body, number of embalmed corpses per year, dimensions of the cemetery, and density of soil.

II.3.9.23 Product-type 23: Control of other vertebrates

Products used for the control of vermin.

There is no model available yet.

II.3.9.24 Waste treatment: landfill model

The model of the landfill described in Van der Poel (1999) has been implemented and can be used for those product types of biocides, which have defaults for the required parameters. In this version of USES the stage of waste treatment can be assessed for product types 6 (In-can preservatives) for paints and coatings, 7 (Film preservatives) for paints and coatings, and glues and adhesives, and wood preservatives.

The model has a lot of parameters, which can be divided in parameters for the size of the landfill, the way the landfill is operated, precipitation, mass transfer and degradation, etc. The output for the amounts of the active substance considered reaching the STP, penetrating into the soil, volatised, and the concentrations of the active substance in percolating water and landfill gas are calculated for the period from the moment the landfill came into operation till five years after utilisation. The output of the calculations shown will consist of the maxima with the year the maxima occur.

The input parameter that has to be provided for the product type considered is the initial concentration of the biocide in the waste that is landfilled. Therefore, a separate calculation is carried out for the specific product type considered. For that calculation every product type has specific defaults for the parameters fraction of biocide in the product, quantity of the product in the region, fraction of the product with a biocide, penetration factor (market penetration), fraction lost due to diffuse releases, fraction lost due to degradation, fraction of product waste landfilled, fraction of total waste landfilled, and the total quantity of waste in the region.

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.

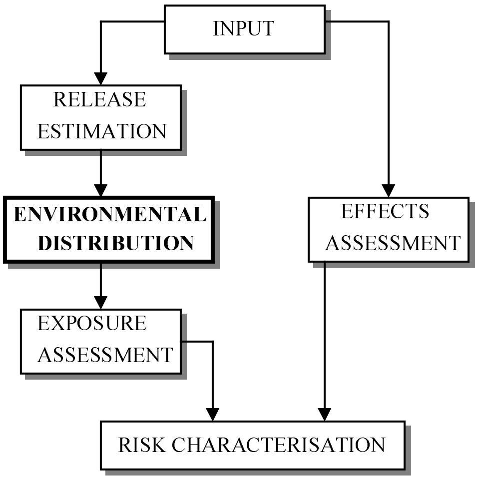


Figure II-6 *System structure.*

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 in EUSES. For specific groups of substances, other QSARs are given in the TGD. 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, 1996). It should be noted that for many substances, the rate of hydrolysis will be highly dependent on the specific environmental pH and 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 which 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 irradiance (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, 1996).

II.4.2.4. Biodegradation in the sewage treatment plant

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.

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 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 constants as those for soil are assumed.

II.4.3. Sewage treatment

Across the European Union, taken as a whole, approximately 70% of the municipal wastewater volume (domestic and industrial loads) is treated in a biological wastewater treatment plant (EC, 1996). 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 70% of the wastewater is treated in a biological STP and the remaining 30% 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* (*Koc* or more specific partition coefficients can also be used), Henry's Law constant and the results of biodegradation tests as input parameters. 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 3.0 (Struijs, 1996). Improvement 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-7a,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.

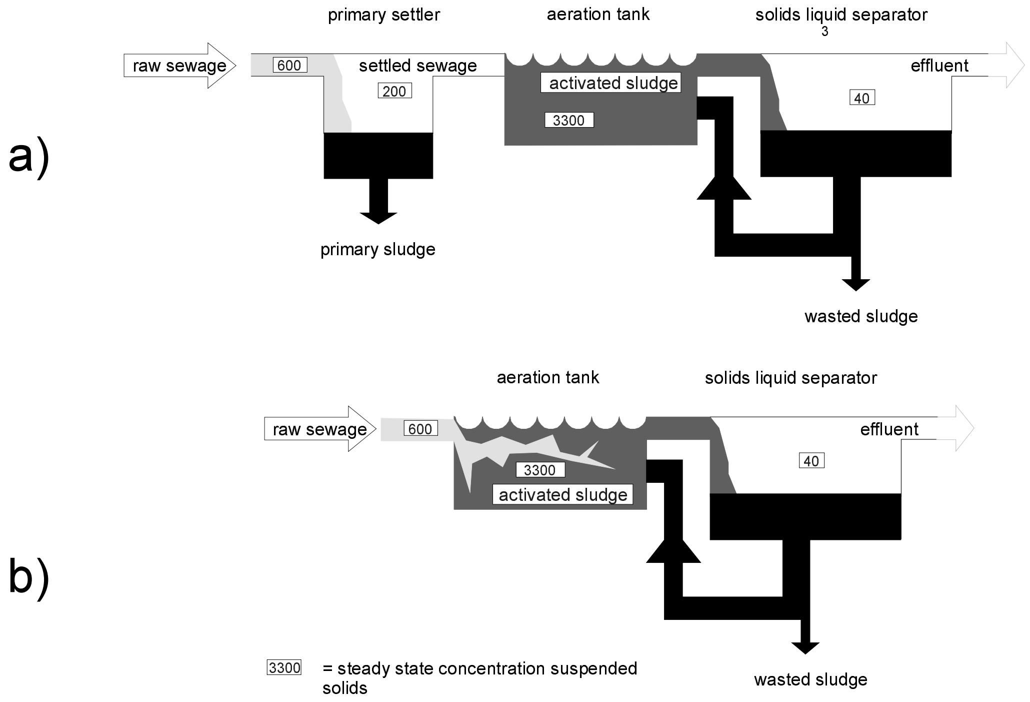


Figure II-7a,b *Schemes of communal biological sewage treatment plants; (a) with and (b) without primary sedimentation.*

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-8). 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.

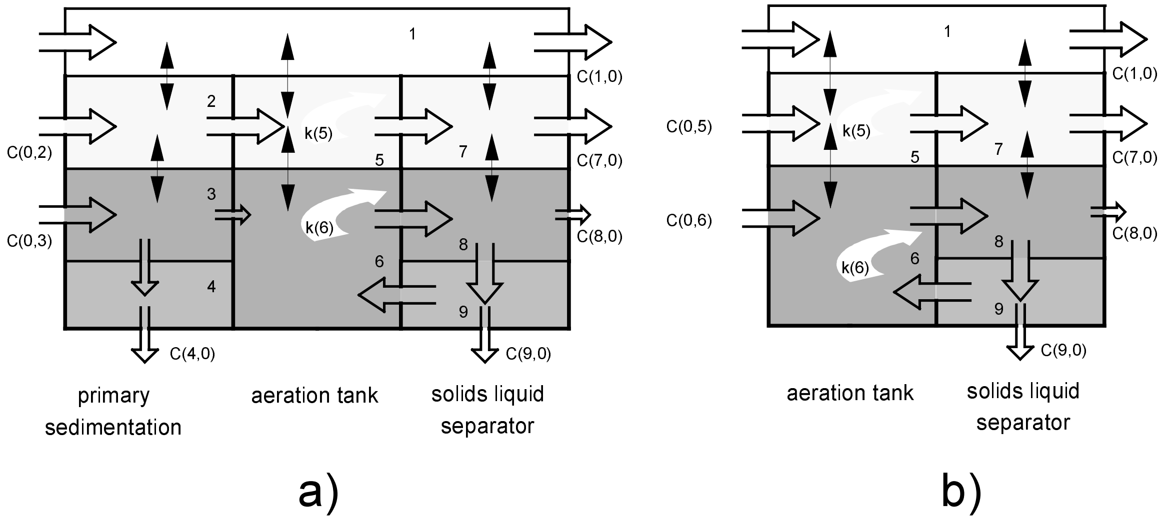


Figure II-8a,b *Box schemes of chemical fate in a communal sewage treatment plant (a) with and (b) without primary sedimentation.*

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

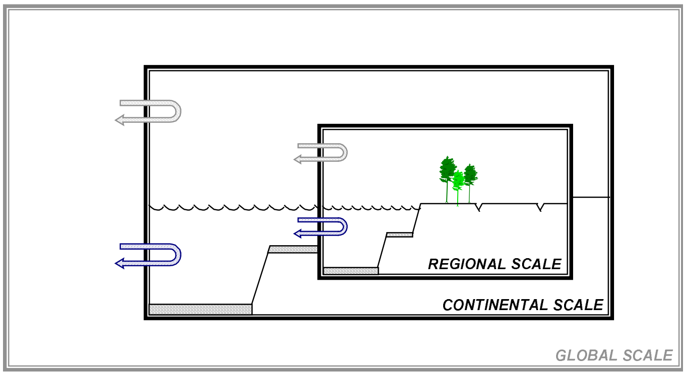


Figure II-9 *Nested multi-media fate model for calculating regional exposure concentrations according to SimpleBox version 2.0.*

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 incorporates a recent version of the SimpleBox model (Version 2.0; Brandes *et al.*, 1996; Figure II-9), in which the fate of chemicals is modelled on different spatial scales simultaneously. Of this model, only the two inner scales (regional and continental) are used; the outer (global) scales, as well as several other options (variable soil depth, vegetation compartment, temperature correction), are 'switched off'.

This 'nested' modelling approach recognizes 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-10. 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.
- 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.

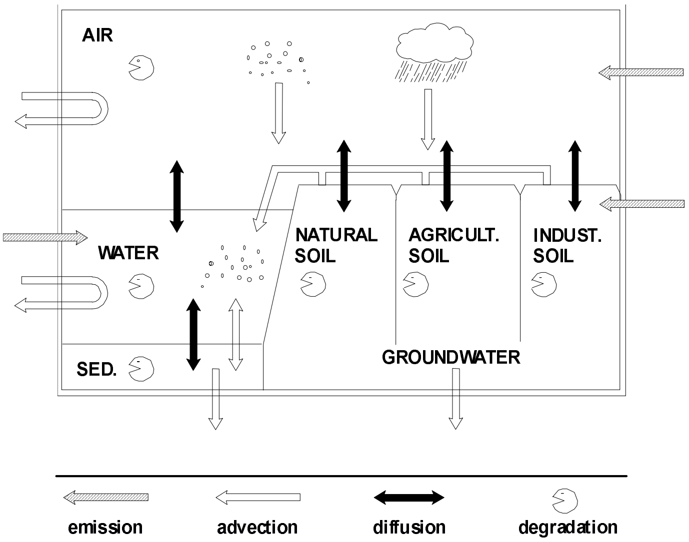


Figure II-10 *Schematic representation of the model for calculating the regional PEC.*

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':

<u>Atmosphere</u>

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 the larger spatial scale. Along with these air streams, chemicals are imported and exported from and to the larger 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

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 river 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

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 inflowing 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 (Van de Meent, 1993). The following processes (mass flows) are accounted for in the model (see Figure II-10):

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 modeled 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 II.4.2).

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 10 % 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-11 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.

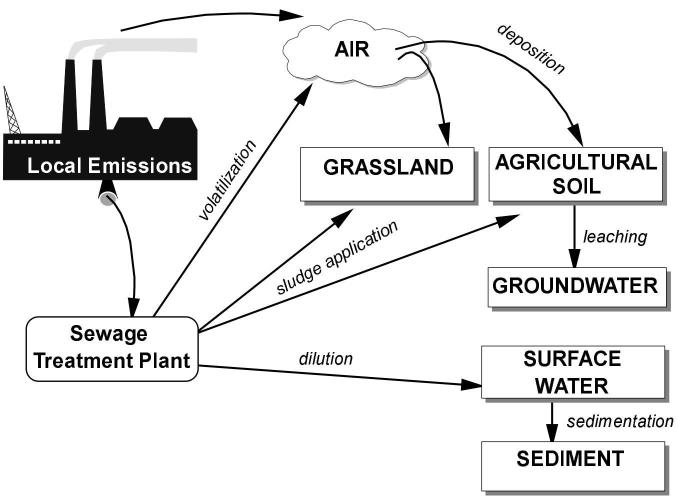


Figure II-11 *Local emission and distribution routes.*

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:

- 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-12.

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.

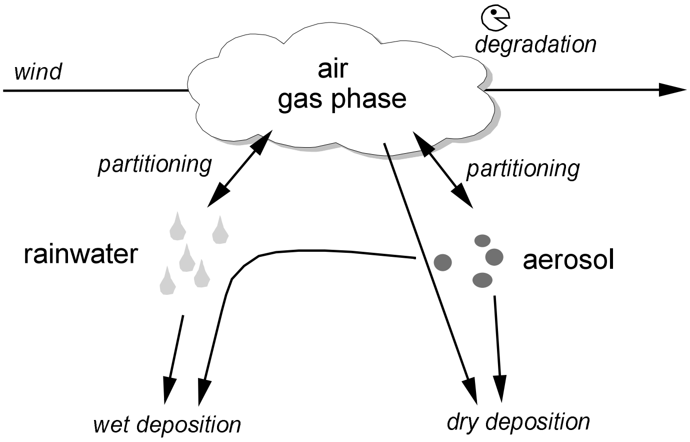


Figure II-12 *Possible fate processes in the air compartment.*

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

The effluent of the sewage treatment plant is diluted in the surface water. Figure II-13 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.

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 substance if no specific data are available.

For some substances 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 on the effects found in the aquatic toxicity tests.

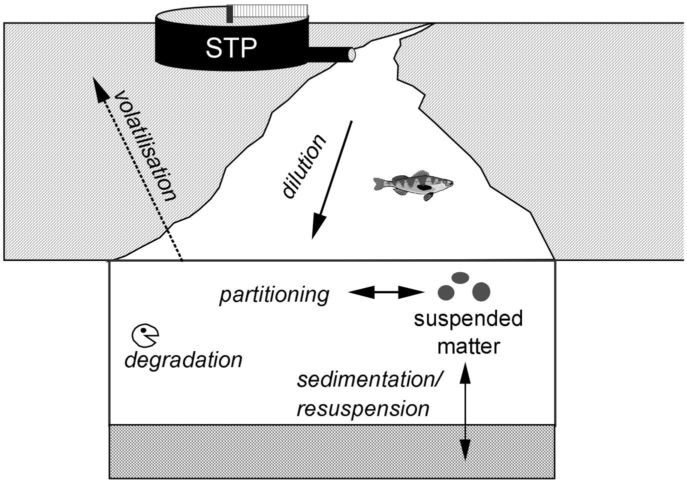


Figure II-13 *Possible fate processes in surface water.*

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-14 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.

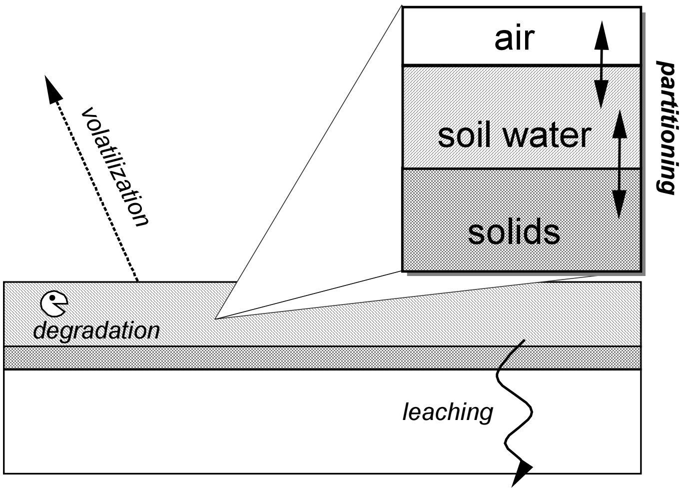


Figure II-14 *Possible fate processes in the soil compartment.*

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 applied over consecutive years. This is illustrated in Figure II-15. 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.

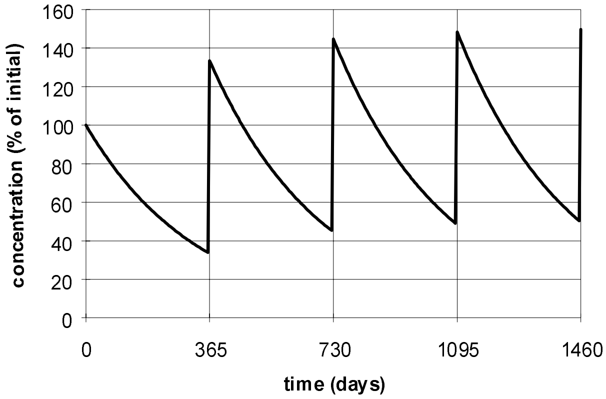


Figure II-15 *Accumulation in soil due to several years of sludge application.*

As shown in Figure II-15, 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-16 (the average concentration is given by the shaded area, divided by the number of days).

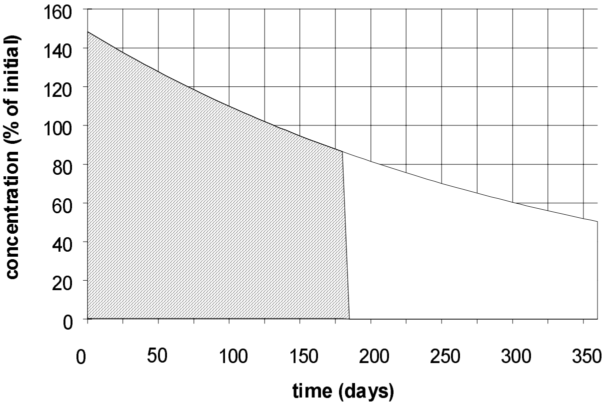


Figure II-16 *The concentration in soil after 10 years. The shaded area is the integrated concentration over a period of 180 days.*

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.4.6. Distribution routes for application of agricultural pesticides

For pesticides, the main route of exposure for terrestrial organisms is not through application of contaminated sludge but through direct application of the substance on soil (the application soil or target area). Application can occur through spraying of the substance, but also through application of granules or treated seeds. The distribution routes for agricultural pesticides are summarised in Figure II-1.

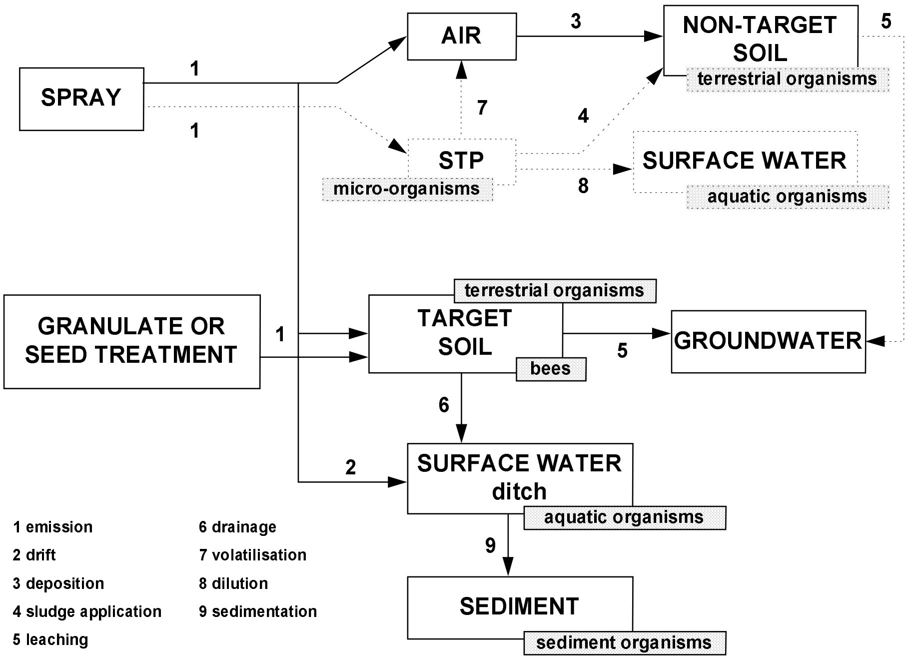


Figure II-1 *Distribution routes for agricultural pesticides. Grey boxes contain the endpoints, dotted lines and boxes are used if the only release is via STP.*

The standard environment in this case consists of a plot of target soil with a surface area of 1 hectare. Concentrations in soil and in surface water (in this case a ditch surrounding the area) are calculated averaged over different time periods (reflecting the exposure period in the toxicity tests for the species to be evaluated). Annual average concentrations in air will be calculated to evaluate indirect exposure of human beings as a consequence of the application of the pesticide as done for new and existing chemicals (Section II.4.5). The agricultural soil for new and existing substances is regarded as the non-target soil for pesticides.

The behaviour of pesticides in soil and surface water is described with the mathematical models PEARL and TOXSWA, resp. In the following paragraphs a short description of both models will be given.

PEARL

For the soil environment the model PEARL is used to calculate the concentration in the upper soil layer as well as the concentration in the upper groundwater (1 to 2 meter depth).

PEARL (Leistra *et al.*, 2000) is an acronym for Pesticide Emission Assessment at the Regional and Local scale. It is a one-dimensional model for simulating the behaviour of pesticides and other organic trace compounds in, and their emissions from, a plant – soil environment. PEARL is based on the models PESTLA v3.4 (Van den Berg and Boesten, 1999; Boesten and Van der Linden, 1991; Van der Linden and Boesten, 1989) and PESTRAS v3.1 (Freijer *et al*., 1996). The software design and the implementation in Fortran90 are, however, completely new. PEARL uses the model SWAP v2.0 (Van Dam *et al*., 1997) for calculating water and heat flow in the system and specified crop parameters. Because of the use of one integral input file and only one command to start the execution of both models, the user in general will hardly notice that in fact two models are run instead of one. A metamodel of PEARL is incorporated in USES v3.0.

The SWAP model calculates water flow in the soil system according to Richard's equation; heat transport is calculated according to a one-dimensional heat conduction equation. The upper boundary conditions are the daily precipitation and the daily average air temperature at the soil surface. The lower boundary conditions imply a fluctuating groundwater table and a zero heat flux at the bottom of the system.

The PEARL model encompasses the following features:

1. interception of substances dependent on the soil cover by the plants (optional);
2. first-order dissipation of substances from the canopy;
3. passive uptake of substances from the soil solution by plant roots;
4. volatilisation of substances from the soil surface;
5. transport of substances in the gas phase of the soil by diffusion;
6. equilibrium sorption in the soil system according to the Freundlich equation;
7. non-equilibrium sorption using a first-order sorption rate equation;
8. PEARL can handle rather complex metabolisation schemes;
9. transformation of compounds, dependent on temperature, moisture content and depth in the system, according to first–order kinetics; only the substances in the equilibrium domain of the soil are liable to transformation;
10. lateral drainage of substances to ditches.

Items 1, 2, 4, 7 and 10 were switched off when deriving the metamodel for USES v3. The metamodel is only applicable to single compounds; the leaching of metabolites can sometimes be approximated pretending they are parent substances.

In the pesticide registration evaluation process a standard scenario is used for calculating the leaching potential of substances. The standard scenario is described in detail by Van der Linden and Boesten (1989). The most important elements of the standard scenario are:

a standard dose of 1 kg/ha;
a sandy soil with an average organic matter content of 1.65% and an average groundwater table at 1 m depth (supposedly 80% vulnerable);
a 75% wet year (De Bilt, 1980); for longer lasting simulations this year is repeated;
maize as the standard crop;
the application of the substance at day 145 (26 May) assuming a 100% load of the soil;
the absence of a non-equilibrium sorption phase in the soil.

As a standard option USES contains now also the possibility to calculate an autumn application. The only difference with the standard spring scenario is the application date. In the autumn scenario the date of application is 1 November.

The user should start checking the volatility of a substance. If the substance is incorporated or injected into the soil because of its volatility, then the metamodel is no longer valid and the user should consider to run the PEARL model itself.

The input needed to run the metamodel is the half-life of the substance under reference conditions ($DT_{50bio,soil}$) and the sorption constant normalised to organic matter (K_{om}). The reference conditions for transformation are: soil collected freshly from the plough layer, a temperature of 20 °C and a moisture content equivalent to field capacity (pF = 2).

PEARL generates as a standard result:

the maximum (in time) of the average concentration of the substance in the uppermost metre of the groundwater (or in case of a shallower groundwater table during part of the year: the groundwater between 1 and 2 metres depth). The standard result is derived from the metamodel of PEARL, the interpolation tables for spring and autumn (see paragraph III.4.9.5).). The PEARL programm is required for substances with a Kair-water $>1.10^{-5}$ and under the condition of mixing with soil (MIX = yes). Whenever the DT50 □200 days or when the Kom > 200 $l.kg^{-1}$ and the DT50 □185 days the PEARL model is also used.

TOXSWA

TOXSWA (TOXic substances in Surface WAters) describes the fate of pesticides entering water bodies (Adriaanse, 1996). In the Dutch standard scenarios (Beltman and Adriaanse, 1999) TOXSWA simulates a single loading or repeated loadings via spray drift. The maximal values of the momentary concentration and of the Time Weighted Average Exposure Concentrations over 4, 21 and 28 days are calculated for evaluation of acute and chronic exposure, respectively.

The simulated water body system is two-dimensional and consists of two subsystems: a water layer containing suspended solids and macrophytes and a sediment layer whose properties (porosity, organic matter content and bulk density) vary with depth. The vertical cross section of the water subsystem has a trapezoidal shape. In the water layer subsystem, the pesticide concentration is assumed to be constant in the wetted cross section, so it is only a function of the horizontal direction. In the sediment subsystem, the pesticide concentration is a function of both the horizontal and vertical directions. Water and sediment exchange pesticide mass through the wetted perimeter of the water body.

TOXSWA considers four processes: (i) transport, (ii) transformation, (iii) sorption and (iv) volatilization (see Figure II-2). In the water layer, pesticides are transported by advection and dispersion, whereas in the sediment, diffusion is included as well. The transformation rate covers the combined effects of hydrolysis, photolysis and biodegradation; metabolites are not considered. Sorption to suspended solids and to sediment is described using the non-linear Freundlich equation. Sorption to macrophytes is described using a linear isotherm. (Note that the ditches of the Dutch standard scenarios described in USES 4.0 do not contain macrophytes.) Pesticides are transported across the water-sediment interface by advection (upward or downward see Page II-P26) and by diffusion.

Mass balances for an elemental volume in the water layer and in the sediment link all the processes together; the mass balances result in two mass conservation equations. These two differential equations are solved using a generalized finite-difference method. For the numerical solution, the water layer subsystem is divided into a number of segments in the horizontal direction. Below each segment, a number of segments are defined for the sediment subsystem. Segment lengths in the water and sediment subsystems are of the order of metres and millimetres, respectively.

Advection and water depth are the most important system parameters and transformation and volatilization are the most important process parameters in TOXSWA, that determine the exposure concentrations (Westein *et al,* 1998).

The standard scenarios for a spring and autumn application have been incorporated in USES with a metamodel which is presented in the tables of Appendix VIII (see paragraph III.4.9.3).

Air

Finally, the air module is based on the Dutch version of the EPA-PAL method described in Teeuwisse and Bakker (1996).

For some specific applications (for instance mushroom cultures) the substance will only reach the environment through a sewage treatment plant. The same STP-model and distribution models as for new and existing chemicals are used for this route (see Section II.4.5). This means that there will be no evaluation for target soil (the application area): the terrestrial organisms will be evaluated on non-target soil.

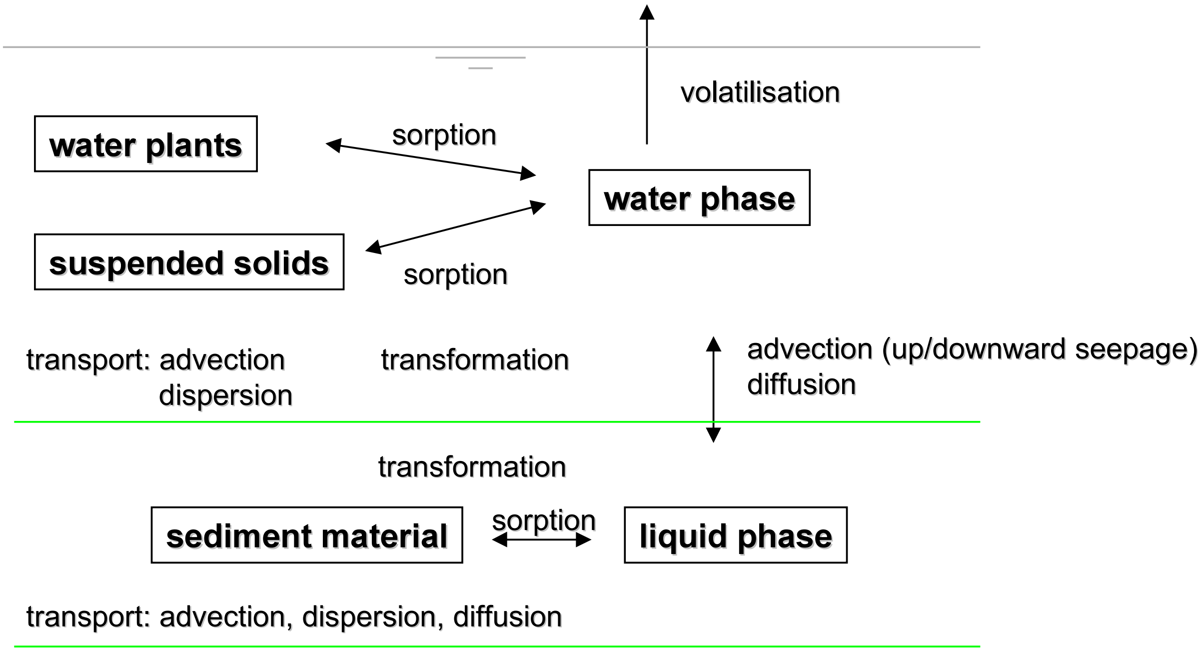


Figure II-2 *Modelled processes in TOXSWA and possible entry routes of pesticides*

II.4.7. Distribution routes for application of non-agricultural pesticides

The distribution module for non-agricultural pesticides follows the general pathways as presented in Figure II-1. The scenarios have already been discussed in the release estimation module. The scenarios for non-agricultural pesticides can deliver four types of output:

1) Local emissions to air and/or water (in kg/d) together with a number of emission days. These emissions are treated with the standard modules for new and existing substances. Sometimes, minor changes to these modules are required (e.g. dilution in surface water).

2) A single dosage for pesticides (in kg/m^2), together with number of applications, interval between applications, and fractions drift to air and to water. These emissions are treated with the specific distribution routes for pesticides (the target area).

3) Concentrations in a specific water body or a specific patch of soil. These concentrations are used directly in the exposure and risk characterisation modules.

4) In one specific scenario (remedial timber treatment in buildings), a dosage on wood is output which is used directly in risk characterisation for a specific RCR (the Relative Toxicity Index) for bats.

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-3 (EC, 1996).

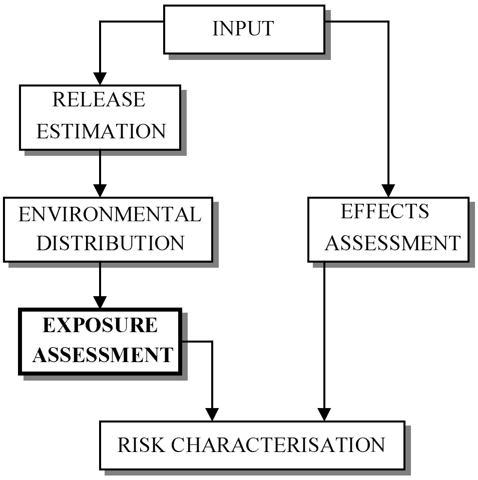


Figure II-17 *System structure.*

Table II-3 *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.

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. Two example food chains are considered (see Figure II-18):

- Water → fish → fish-eating birds or mammals (Romijn *et al*., 1993).
- Soil → earthworm → worm-eating birds or mammals (Romijn *et al.*,1994).

These 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.

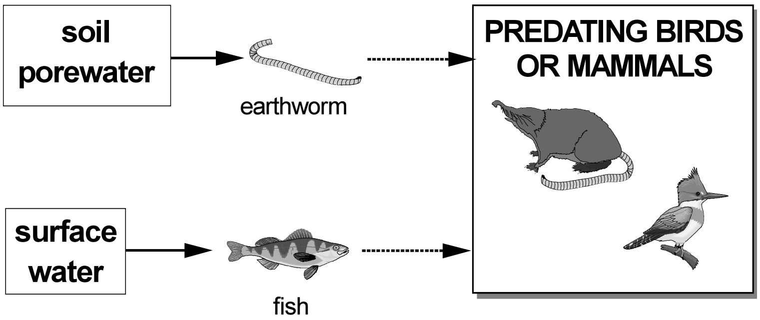


Figure II-18 *Food chains for assessing secondary poisoning.*

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. 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. In the TGD it is proposed to use a scenario where 50% of the diet is derived from the local environment and 50% from the regional environment. This scenario is 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, 1996).

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, 1996). 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.5.1.2. BCF for earthworms

The concentration in earthworms is thought to be proportional to the concentration in the pore water of soil. The hypothesis is that uptake through the solid phase contributes significantly to bioaccumulation for extremely hydrophobic substances only (log *Kow* > 5) (Belfroid, 1994). The experimental data, analysed by Connell and Markwell (1990), are broadly consistent with the transfer of lipophilic substances through a three-phase system, involving soil to pore water, and pore water to organism partitioning. This is thought to be a passive process and is principally dependent on the lipid content of the worm and the properties of the soil type. The worms are assumed to be in equilibrium with the concentration in soil.

No internationally accepted guidelines are available at the moment for deriving BCFs for earthworms. The BCF for earthworms is estimated using a QSAR from Connell and Markwell (1990). These authors derived an empirical equation for the earthworm-pore water partition coefficient through regression on experimental data for pesticides with a log *Kow* ranging from 1.0 to 6.5. As data from experiments conducted under different conditions are included, it should be noted that the sources of variation in this study are substantial.

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-19. 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.

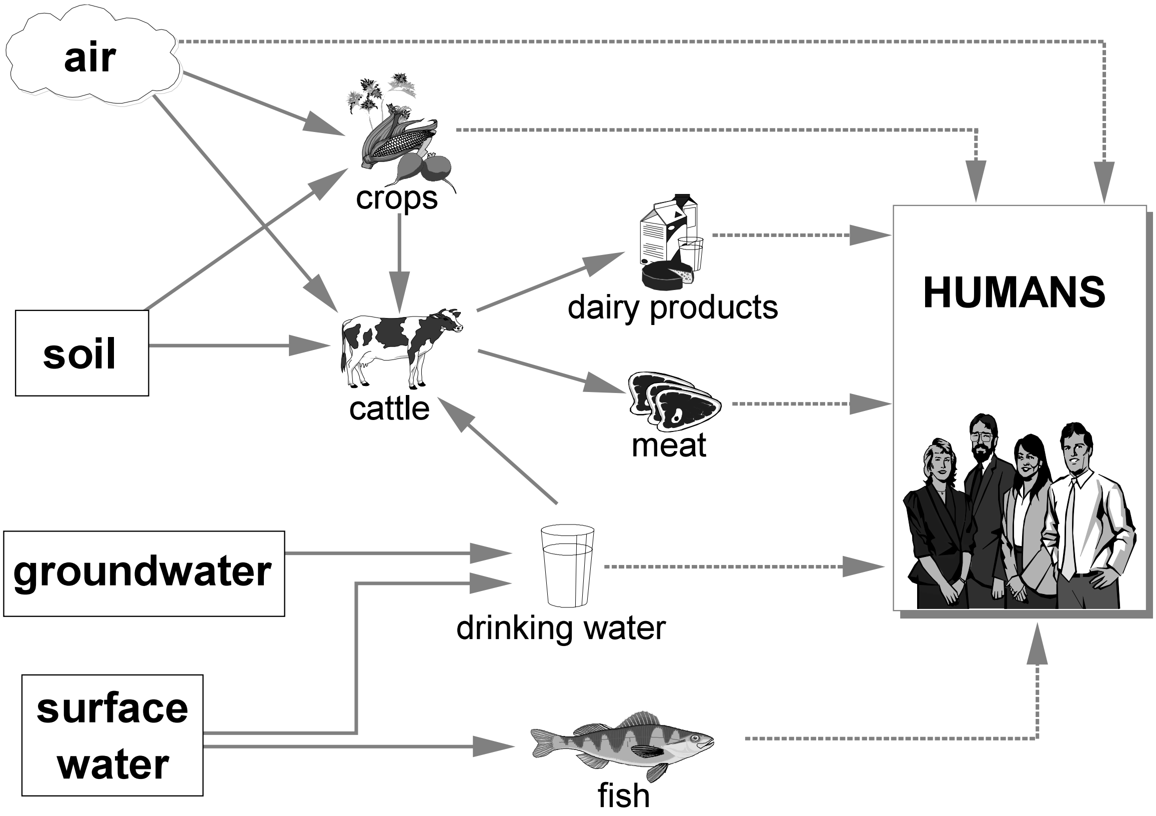


Figure II-19 *Indirect exposure routes for humans through the environment. Solid lines indicate (bio)transfer, broken lines indicate human intake.*

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-4 *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-5 *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-4. 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-4. 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, accounting for the generally lower bioavailability for inhalation.

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.5.1.1 on secondary poisoning. The same BCF estimation routines are used for human exposure.

II.5.2.5. Biotransfer from soil and air to plants

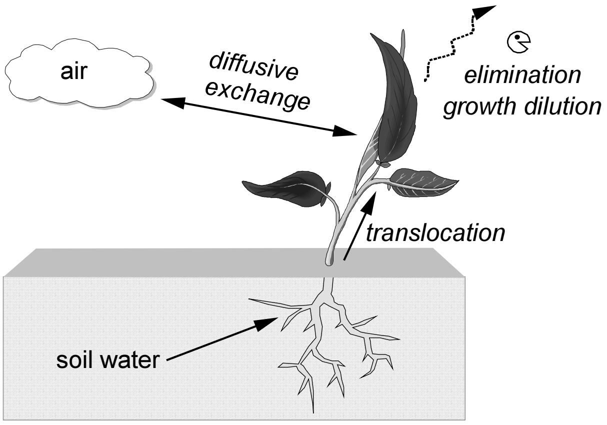


Figure II-20 *Fate processes accounted for in the plant uptake model.*

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:

- There are hundreds of different plant species forming the heterogenous 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. Kow 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

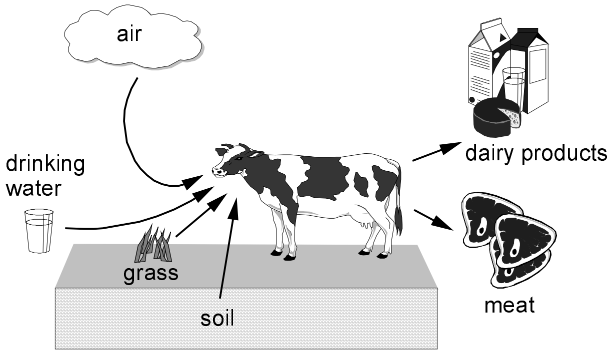


Figure II-21 *Uptake routes for cattle accounted for in the model.*

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 which 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, 1995), THERdbASE, 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.

- Product Registers contain valuable information on the composition of products.
- Specific information on use durations and contact frequencies with regard to consumer products is generally lacking. An estimate of these quantities can be derived from time-budget data. Time budgets comprise information on the behaviour of a population during the day, week, or year. Assuming that certain products are used for one or more recorded tasks, data on how long and how often these tasks are performed provide an estimation of product use durations and contact frequencies. The main disadvantage of time-budget

data is that the task categories are often non-specific, like 'being indoors', 'driving car' or 'cleaning car'. Therefore, a direct link between a time-budget task and the use of certain products might be problematic.
- Product-use data. Little research has been done to reveal actual product use. The directions of the producer give information on the intended use only, not on the way products are handled before or after actual use or on foreseeable misuse. Information can be gained from reports from poisoning centres (e.g. Velvart, 1993; Hofstee *et al.*, 1990) and cases reported in literature. However, these cases generally represent the more extreme misuses of the product and may not be that informative about the normal range of uses.
- Information accompanying exposure assessment programs, such as THERdbASE (prepared at the H. Reid Center of Environmental Studies, Las Vegas) and CONSEXPO (RIVM, the Netherlands).
- Datasets that are gathered to comply with regulations for new and existing chemicals .
- US-EPA reports. The US-EPA regularly calls for research with regard to use and contents of consumer products.
- Open literature. For instance: Risk Analysis, an international journal; Science of the Total Environment; Journal of Exposure Analysis and Environmental Epidemiology; American Industrial Hygiene Association Journal.
- Consumer information leaflets provided by producers.

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.

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 ($AREA_{der}$).

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.

II.5.4. Human exposure at the workplace

II.5.4.1. Introduction

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.

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 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 predominantly to the hands and forearms. Although exposures are normally defined in this way they take no 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.

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.

II.5.4.2. EASE

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. The options for these variables are shown in Table II-6. 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 contained within the UK National Exposure Database for inhalation exposure, and experimental data and expert judgement for dermal exposure. The logic of deriving scenarios and assigning ranges to the scenarios is described in Appendix V.

Table II-6 *Options for variables for exposure assessment in EASE.*

A.	Process physical properties	
	- gas	inhalation
	- liquid, high vapour pressure	inhalation/dermal contact
	- liquid, medium vapour pressure	inhalation/dermal contact
	- liquid, low vapour pressure	inhalation/dermal contact
	- solid, respirable dust	inhalation/dermal contact
	- solid, inhalable dust	inhalation/dermal contact
	- solid, granular	inhalation/dermal contact
	- aerosol	inhalation
B.	Use pattern	
	- closed system	inhalation
	- within a matrix	inhalation
	- non-dispersive (industrial controlled use)	inhalation/dermal contact
	- wide dispersive	inhalation/dermal contact
C.	Pattern of control	
	- full containment	inhalation
	- local exhaust ventilation (LEV)	inhalation
	- segregation	inhalation
	- dilution ventilation	inhalation
	- direct handling	inhalation/dermal contact

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.

II.5.5. Indirect exposure of humans to pesticides

For human exposure to pesticides, the same routes will be followed as described in Section II.5.2. However, groundwater will be retrieved from below target soil (the application area), whereas crops and cows will reside on non-target soil. The annual average concentration in the ditch surrounding target soil will be used for concentrations in drinking water when surface water is considered as source for drinking water, and to calculate the estimated concentration in fish for human consumption. In the situation that there is only release of the substance through an STP, the intake routes for the pesticides will be completely analogous to the routes for other substances.

II.5.6. Exposure of birds and mammals through application of pesticides

To give an indication of the bioaccumulating potential of a substance through food chains, the following food chains will be regarded in USES:

- birds and/or mammals with a diet consisting entirely of fish caught in polluted surface water, or in a ditch surrounding target soil;
- birds and/or mammals with a diet consisting entirely of worms caught in polluted non-target land or target soil;
- in the case of pesticide application: birds and mammals exposed through diet (including crops/insects, fish/worms, and direct ingestion of treated seeds or granules) or drinking water (surface water or spray liquid from crops). The intake routes for mammals and birds in case of pesticide application are summarised in Figure II-3. The predators will catch worms on target soil unless there is no application of the substance on this soil. In that case the predator will be exposed to worms from non-target soil.

Fish-eating predators will consume the same fish as described above for indirect human exposure assessment.

The concentration in earthworms is thought to be proportional to the concentration in porewater. The experimental data, analysed by Connell and Markwell (1990) are broadly consistent with the transfer of lipophilic compounds through a three-phase system involving soil to porewater to organism partitioning. This is thought to be a passive process and is principally dependent on the lipid content of the worm and the properties of the soil type. The equation used is derived by Connell and Markwell (1990) through regression on experimental data and is consistent with the theoretically derived equation for bioconcentration.

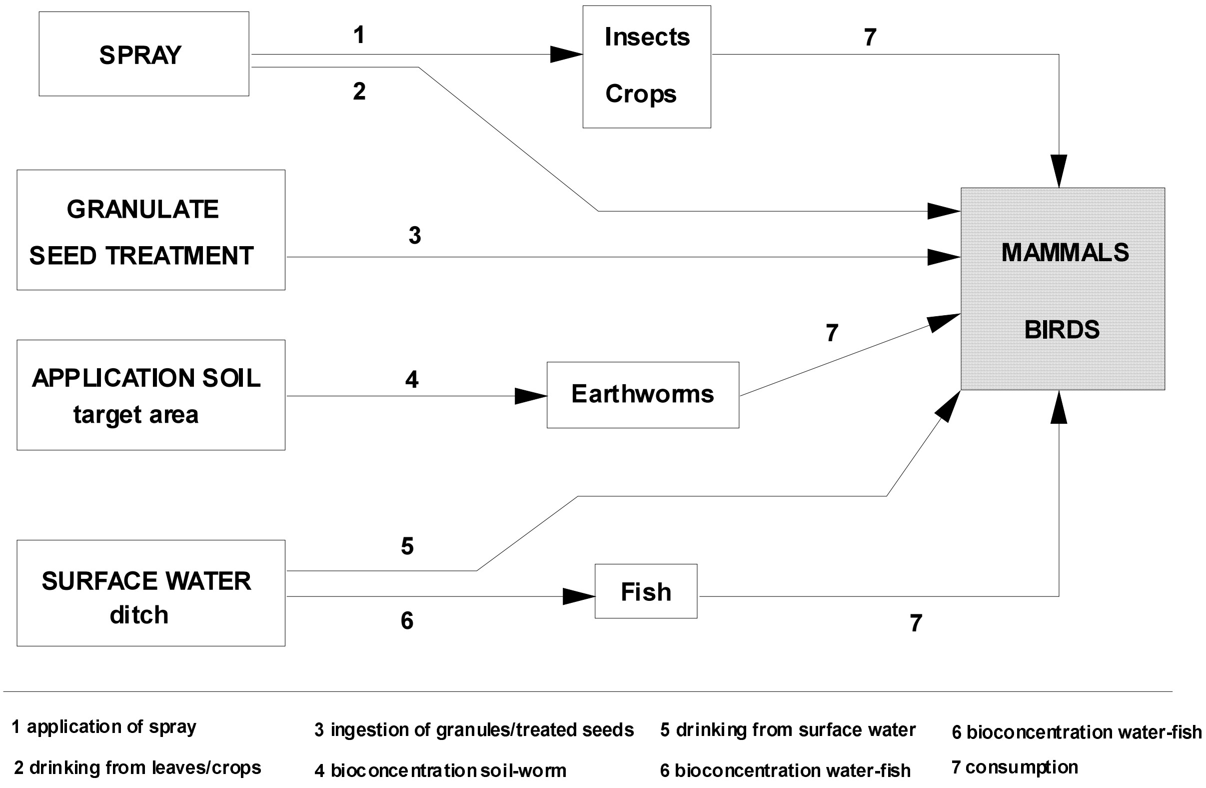


Figure II-3 *Schematic representation of the possible intake routes considered for the exposure of birds and mammals to pesticides.*

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.

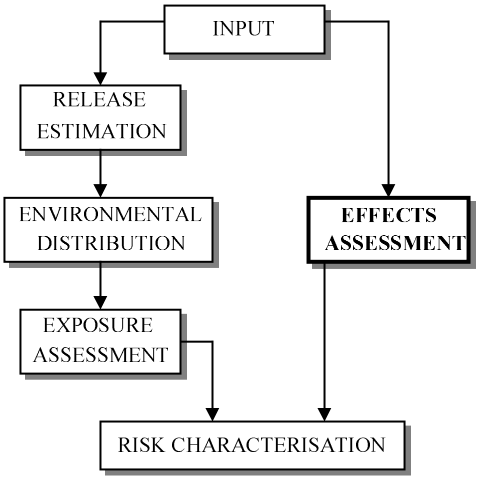


Figure II-22 *System structure.*

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, 1996) 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

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 depends on the most sensitive species; 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-7.

Table II-7 *Assessment factors to derive a PNEC for the water 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)
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.

(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 effects assessment performed with assessment factors can be supported by a statistical extrapolation method (Aldenberg and Slob, 1993) if at least four NOECs are available for different taxonomic groups.

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.

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. At present, only a few internationally accepted test systems exist, such as OECD 209 (inhibition of respiration of activated sludge) and ISO 9509 (inhibition of nitrification). For assessing the toxicity of a substance to micro-organisms in a STP, the effluent concentration is compared to microbial effect data. A PNEC is derived as follows:

- The PNEC is set equal to a NOEC from a test performed with 'specific bacterial populations' like nitrifying bacteria and *P. putida*. An EC50 from this test is divided by an assessment factor of 10.
- A NOEC or EC10 from other test systems like the respiration inhibition test (OECD 209) is divided by an assessment factor of 10. An EC50 from this test is divided by an assessment factor of 100. It should be noted that the effluent concentration is used, while heterotrophic micro-organisms in the aeration tank are probably exposed to a concentration which relates more to the influent concentration. Therefore a higher assessment factor is applied compared with the assessment factor for nitrifying bacteria. For nitrifying bacteria the exposure concentration is more related to the effluent concentration, since nitrification is the last treatment step in an STP.
- The lowest value is selected as the PNEC.

II.6.1.5. Effects assessment for sediment

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 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 the equilibrium method is used in a modified form. In order to take uptake via ingestion of sediment into account, the PEC 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.

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.

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-8.
- 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 in soil is increased by a factor of 10 for compounds with a log $Kow > 5$ in the risk characterisation.

The same assessment factors are used for the terrestrial system (see Table II-8) as for the aquatic system (see Table II-7), 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-8 *Assessment factors to derive a PNEC.*

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
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-8 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.6.2. Effects assessment for man

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. 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 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. Toxicity data for the (sub-)chronic time scale will include tests of 28 and 90 days duration and longer.

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-9 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.

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. However, the potential differences in sensitivity of human studies and animal studies should be taken into account, on a case-by-case basis. A no-observed effect level is always preferred over a lowest-observed effect level. If both an LD50 value and a Discriminating Dose are entered, EUSES chooses the LD50 for the risk characterisation of acute oral exposure.

Table II-9 *Effect-parameters 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

In two distinct cases no quantitative risk characterisation is possible:

1. A threshold for toxicity can be assumed but has not been established for the route of exposure under investigation. Such data gaps may be filled by EUSES by conversion from effect parameters for other routes of exposure, as will be explained in the next section. 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 very often cannot be derived form the toxicological database, EUSES allows the user to flag substances for this property in the output by entering the appropriate EU classification (EC, 1993d) in the input (Table II-10).
2. A threshold cannot be identified in relation to an end-point. This situation applies to substances considered genotoxic or (possibly) carcinogenic to man by a genotoxic mechanism of action. It can also be assumed to apply to sensitising substances. The user can flag substances for these properties in the output by entering the appropriate EU classification in the input (Table II-10).

Table II-10 *Classification flags in EUSES.*

Corrosive (C, R34 or R35)
Irritating to skin (Xi, R38)
Irritating to eyes (Xi, R36)
Risk of serious damage to eyes (Xi, R41)
Irritating to the respiratory system (Xi, R37)
May cause sensitisation by inhalation (Xn, R42)
May cause sensitisation by skin contact (Xi, R43)
May cause cancer (T, R45)
May cause cancer by inhalation (T, R49)
Possible risk of irreversible effects (Xn, R40)

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 differences among routes of exposure with respect to degree and rate of absorption and metabolism. 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.

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.
The following extrapolations are available:

- Dermal effect parameter from an oral value: the extrapolation assumes that the dermal value is the same as the oral value on a mg/kg body weight basis. If oral and dermal absorption rates are known, these can be used to adjust the estimation.
- Inhalatory effect parameter from an oral value: two methods are available and the user will have to choose. In the first method, applicable to the (sub-)chronic N(L)OAEL, the ratio of the inhalatory LC50 to the oral LD50 is used to estimate the inhalatory N(L)OAEL. The second method is 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.

II.6.2.4. Other conversions

NOEC to NOAEL

If a (sub-)chronic N(L)OAEL (in mg/kg body weight/day) for mammals is not available but an N(L)OEC (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}.

Intermittent to continuous exposure

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

$$\boldsymbol{NOAEL_{ihl,continuous}} = \boldsymbol{NOAEL_{ihl,intermittent}} \cdot \frac{x}{24} \cdot \frac{y}{7} \qquad [mg \cdot m^{-3}]$$

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.

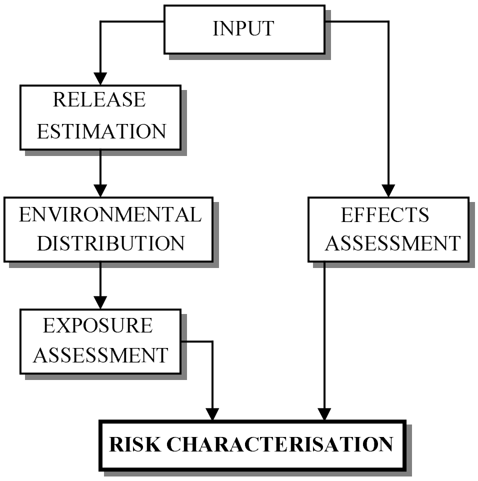


Figure II-23 *System structure.*

II.7.1. 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,
- terrestrial ecosystem,
- sediment-dwelling organisms,
- top predators,
- micro-organisms in sewage treatment plants.

A list of the various PEC/PNEC ratios following from the previous chapters is given in Table II-11. 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, 1996).

Table II-11 *Overview of possible PEC/PNEC ratio's in 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	$PEC_{stp} / PNEC_{micro-organisms}$	
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.

II.7.2. Risk characterisation for man

II.7.2.1. Introduction

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 a chronic LOEC in food, and an exposure value of corresponding time scale and route of exposure. The risk characterisation can be performed for each subpopulation to be protected and for the time scales and route(s) of exposure chosen. The following combinations of subpopulation, time scales and routes of exposure can occur:

- Man exposed via the environment:
  - Time scale: chronic.
  - Routes of exposure: oral and inhalatory combined.
- Consumers:
  - Time scales: acute and (sub)chronic.
  - Routes of exposure: inhalatory, dermal and oral.
- Workers:
  - Time scales: acute and (sub)chronic.
  - Routes of exposure: inhalatory and dermal.

The MOS indicates the degree of risk. This approach, rather than a more rigid extrapolation-factor approach, allows greater freedom for expert judgement and can readily be applied to substances with limited data-bases. Depending on the species for which the effect parameter value is derived (man or experimental animal), the exposure period and frequency, the incidence, type and severity of the effect, the dose-effect and dose-response relationships observed, and the availability of other data on the toxicological profile of a substance, the resulting MOS can be judged to be sufficient or not. In judging the acceptability of the MOS, the MOS should also account for uncertainties resulting from intraspecies variations, i.e. variations in the sensitivity among individuals of one species, uncertainties resulting from interspecies variations, i.e. variations between the species man and the test animal, and uncertainties resulting from differences in the exposure scenario, e.g. short-term versus long-term exposure and continuous versus intermittent exposure. Last, but not least, the MOS should account for the uncertainty in the estimated exposure.

If no quantitative risk characterisation is possible, the user can make this visible in the output of EUSES (see Section II.6.2.2 and Table II-10).

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 exposure parameter, which is the (sub)chronic oral No- or Lowest-Observed-Adverse-Effect Level N(L)OAEL. It is assumed here that man is exposed throughout his or her lifetime. A subchronic N(L)OAEL is only used if no chronic value is available, and such cases need extra attention in the evaluation of the MOS. Additionally, the air concentration to which man is estimated to be exposed can be compared to the (sub)chronic inhalatory N(L)OAEL, if available.

II.7.2.3. Consumers

Table II-12 shows the Margins of Safety which can be calculated for consumers, provided the required effects and exposure results are available. 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. if the MOS in Table II-12 indicates reasons for concern and further refinement of the risk assessment is required. This refinement is outside the scope of EUSES. Additional tools offering uptake models have been incorporated into CONSEXPO 1.10 (Van Veen, 1995).

Table II-12 *Overview of possible Margin Of Safety (MOS) for consumers (for explanation of parameter symbols, see Appendix II).*

Route	**Acute scenario**	**Chronic scenario**
Inhalatory	$LC50_{mammal,inh} / C_{inh}$ $NOAEL_{man,inh,acute} / C_{inh}$	$N(L)OAEL_{mammal,inh,chr} / C_{inh}$ $N(L)OAEL_{man,inh,chr} / C_{inh}$
Dermal	$LD50_{mammal,der} / U_{der,pot}$ $N(L)OAEL_{man,der,acute} / U_{der,pot}$ $N(L)OEC_{man,medium,acute} / C_{der}$	$N(L)OAEL_{mammal,der,chr} / U_{der,pot}$ $N(L)OAEL_{man,der,chr} / U_{der,pot}$ $N(L)OEC_{man,medium} / C_{der}$
Oral	$LD50_{mammal,oral} / I_{oral}$ $DD_{mammal,oral} / I_{oral}$ $N(L)OAEL_{man,oral,acute} / I_{oral}$	$N(L)OAEL_{mammal,oral,chr} / I_{oral}$ $N(L)OAEL_{man,oral,chr} / I_{oral}$ $N(L)OEC_{mammal,food,chr} / C_{oral}$
All routes	$LD50_{mammal,oral} / U_{tot}$ $DD_{mammal,oral} / U_{tot}$ $N(L)OAEL_{man,oral,acute} / U_{tot}$	$N(L)OAEL_{mammal,oral,chr} / U_{tot}$ $N(L)OAEL_{man,oral,chr} / U_{tot}$

II.7.2.4. Workers

Table II-13 shows the Margins of Safety (MOS) which can be calculated for workers, provided the required effects and exposure results are available. RCRs are calculated using chronic effect parameters only, since the output of the EASE model is based on 8-hour time-weighted averages (see Section II.5.4.2) and cannot be considered as an estimate for acute exposures. 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. if the MOS in Table II-13 indicate reasons for concern and further refinement of the risk assessment is required. This refinement is outside the scope of EUSES. Additional uptake models that offer tools for possible refinement have been incorporated into CONSEXPO 1.10 (Van Veen, 1995).

Table II-13 *MOS for workers (for explanation of parameter symbols, see Appendix II)*

Route	Exposure type	Chronic scenario
Inhalatory	exposure to vapour	$N(L)OAEL_{mammal,inh,chr} / C_{inh,worker,vapour}$ $N(L)OAEL_{man,inh,chr} / C_{inh,worker,vapour}$
	exposure to fibre	$N(L)OAEL_{mammal,inh,fibre,chr} / C_{inh,worker,fibre}$ $N(L)OAEL_{man,inh,fibre,chr} / C_{inh,worker,fibre}$
	exposure to non-fibrous dust	$N(L)OAEL_{mammal,inh,chr} / C_{inh,worker,dust}$ $N(L)OAEL_{man,inh,chr} / C_{inh,worker,dust}$
Dermal	all types	$N(L)OAEL_{mammal,der,chr} / U_{der,worker,pot}$ $N(L)OAEL_{man,der,chr} / U_{der,worker,pot}$ $N(L)OEC_{man,medium,chr} \cdot TH_{der,worker} \cdot n_{worker} / W_{der,worker}$

II.7.3. Risk characterisation for pesticides

For pesticides several Risk Characterisation Ratios (RCRs) are constructed to account for different types of application and different exposure timescales. For each species evaluated, a separate RCR is calculated. The species for which a risk characterisation is carried out are birds, mammals, water organisms (fish, daphnids and algae), earthworms, beneficial arthropods, micro-organisms and bats. In addition, a calculation is performed for the bacterial population in an STP. These RCRs are based on the PEC/NEC concept, but, in this case the non-extrapolated toxicity data for single species are used. This yields e.g. PEC/LC50 quotients. PECs will be derived from concentrations on 'target soil' and from the concentration in the ditch surrounding this soil type. In case of release through an STP only (mushroom culture, several scenarios for non-agricultural pesticides), PECs from non-target soil and surface water from the effluent of the STP after dilution will be used.

For pesticides there will also be a calculation of a PEC/PNEC quotient for the ecosystem. This involves extrapolation of toxicity data to a PNEC for the ecosystem as described in Section II.6.1. This PNEC will be compared to the PEC of target soil or ditch water averaged over the exposure time for the most sensitive species (i.e. the species with the lowest NOEC). For agricultural pesticides the extrapolation of toxicity data to derive a PNEC (in the Netherlands, under specific conditions, also called MPC or MTR) may differ in the Netherlands from the approach mentioned in Section II.6.1. The extrapolation factors to be used are laid down in the framework of the Netherlands Pesticide Act and other relevant policy documents. At the beginning of 1998 a project started to harmonise the extrapolation methodology for deriving the PNECs (MPC or MTR) for agricultural pesticides. The results of this project, an unequivocal approach to derive 'specific' PNECs, will however be used in future.

Different hazard indicators can be given in specific situations. In the case of application of granules and treated seeds for instance, an LD50 is calculated in number of particles, as well as a risk characterisation ratio in number of LD50s per m^2. Expert judgement will be unavoidable to interpret these results.

As a lead the following criteria for the exposure through granules or treated seed can be used according to Luttik (1992). When the quotient of the amount of active ingredient in one particle and the LD50, $RCRone\text{-}particle_{bird/mammal}$ is ≥ 1, high risk is assumed for the species of concern. When it is assumed that the complete daily food intake of the species of concern constist of the particles under consideration and the quotient of the amount of active ingredient in the daily food intake and the LD50 of the species of concern, $RCRparticle_{bird/mammal}$ is ≤ 0.001, low risk for birds and mammals is assumed. When a particle resembles natural food it is supposed that the risk for bird and mammals is related to the amount of avialable active ingredient per unit area. High risk is assumed when the quotient of number of available particles per unit area and the LD50 of the species of concern expressed in number of particles, $RCRitem_{bird/mammal}$ is ≥ 10. Low risk is assumed when the quotient is ≤ 0.1.

For the exposure through drinking water from suface water or spray liquids the following criteria can be used. High risk is assumed when the $RCRsurf/spray_{bird/mammal} \geq 0.1$ and low risk is assumed when $RCRsurf_{bird,semi}$, the $RCRspray_{bird/mammal}$ or the $RCRsurf_{mammal} \leq 0.001$. For intermediate results additional steps in the decision scheme should be taken to classify the risc level. For more details see Luttik (1992).

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 Organization 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:

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

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 the TGD (EC, 1996).

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, 1996) 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, 1996). 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 recognized 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 given 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, 1996). 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.
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.

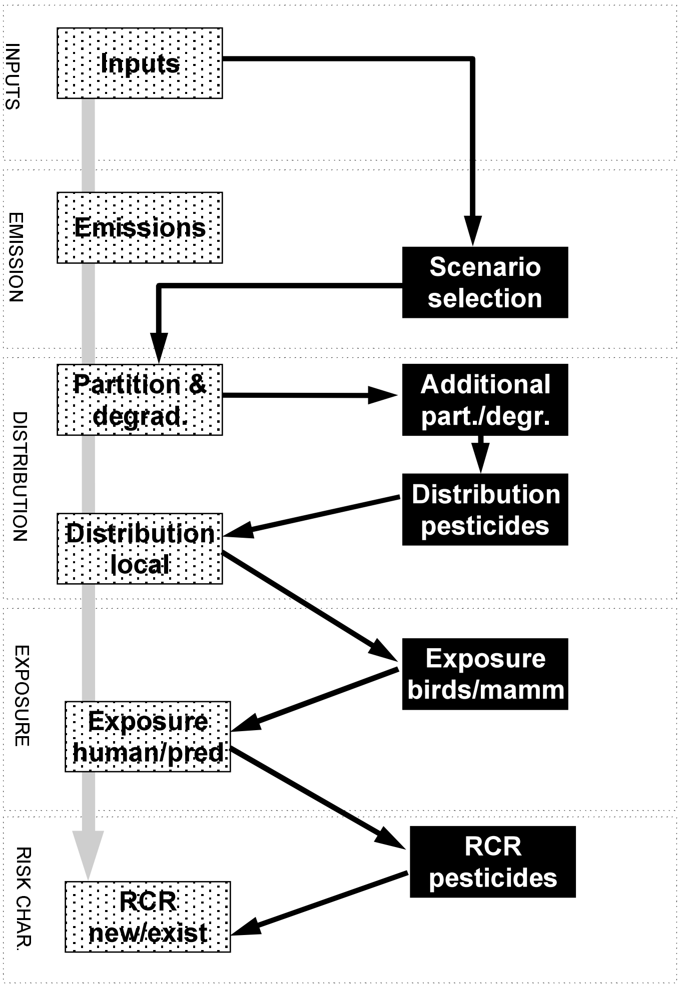
Appendix II contains a list of all the symbols applied in the calculations of USES with explanation, units, defaults, ranges etc.

The equations in this chapter are numbered but, in several cases, the numbering is not continuous. This is caused by changes which were required in this documentation after the draft of March 1996. Since the same equation numbering is also used in the USES on-line help and in the code of the program, the equations that were added received a sub numbering *a*, *b* etc. E.g., equations added between Equation 6 and 7 will be numbered as 6a, 6b etc.

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.

The figure on the right shows the program flow of USES 4.0. The light gray boxes and the large grey arrow indicate the EUSES modules for new and existing substances, the black boxes and arrows indicate the specific pesticide modules described in this chapter. The EUSES modules will also be used to assess the stages of production and formulation of pesticides. Furthermore, these modules will be applied in case pesticides are released through an STP and for exposure of humans via the environment. The modelled humans are exposed through crops grown on a field adjacent to the application site.



III.2.1. Assessment types

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

Assessment

A. Assessment of new and existing substances:

- 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.

Regional model: Choice between “EUSES compatible” and “SimpleBox 2.0”

B. Assessment of plant protection products and biocides

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.

Numbering of tables

The tables for USES 4.0 in Section III.4-III.7 are numbered as follows:

A Tables for agricultural pesticides
B Tables for amenity use scenarios
C Tables for biocides
D Tables for the remainder of the document
S Tables for SimpleBox 2.0

III.2.2. Input data

The following data on substance identification and physico-chemical data need be entered in this module.

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	[-]
SOL	water solubility	[$kg_c.m^{-3}$]
VP	vapour pressure	[Pa]
TEMPboil	boiling point (used for some release estimations and EASE)	[K]
TEMPmelt	melting point (used for solids only and for EASE)	[K]

Experimentally derived chemical properties will usually be measured at a standard temperature which is different from the temperature used in the models of USES. 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). For the local and regional fate models, no temperature correction is carried out as no extrapolation method is specified in the TGD. Nevertheless, for chemicals were considerable differences are expected within this temperature range, entering a more relevant value (measured or extrapolated) is advised (note that in that case care must be taken with the assessment of human exposure at the workplace where a correction of vapour pressure from 25 degrees to the process temperature is always applied).

There are no calculations in this section. No estimation routines for physico-chemical properties are implemented.

III.3. Release estimation

Releases of new and existing substances on all spatial scales are estimated, based on use pattern and substance properties. The tables in Appendix IV provide default release estimates for each category of substance. For release of agricultural pesticides and non-agricultural pesticides see section III.3.6.

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	processing	ind	industrial soil (regional scale only)
4	private use	surf	surface water (regional scale only)
5	recovery	agric	agricultural soil (regional only, no estimation)

Table III-1 *Defaults for emission calculations.*

Parameter	**Symbol**	**Unit**	**Value**
Fraction of EU production volume of substance produced in the region	$Fprodvol_{reg}$	[-]	0.10
Fraction connected to sewer systems	$Fconnect_{stp}$	[-]	0.70

III.3.1. Calculation of the tonnage of substance

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

$$\boldsymbol{TONNAGE = PRODVOL + IMPORT - EXPORT} \qquad (1)$$

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).

$$\boldsymbol{TONNAGE_k = Ftonnage_k \cdot TONNAGE} \qquad (2)$$

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 will be calculated with the full 100% of the production volume and a correction must be performed manually.

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.

$$PRODVOLreg = Fprodvol_{reg} \cdot PRODVOL \tag{3}$$

$$PRODVOLcont = (1 - Fprodvol_{reg}) \cdot PRODVOL \tag{4}$$

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \tag{5}$$

$$TONNAGEcont = (1 - Fprodvol_{reg}) \cdot TONNAGE \tag{6}$$

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 IV

The fractions released in each stage of the life cycle and to every compartment are derived from the tables in Appendix IV. 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 IV, 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.

$$TONNAGEreg_{form} = \frac{1}{Fchem_{form}} \cdot TONNAGEreg \qquad (6a)$$

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 IV			
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 processing in IC=8)	$[kg_c.mol^{-1}]$	S
TEMPboil	boiling point (only for some release estimations)	[K]	S
Output from A tables in Appendix IV			
$F_{i,j}$	fraction of tonnage released during stage *i* to compartment *j*	[-]	O
Output from B tables in Appendix IV			
$Fmainsource_i$	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 (2) and (5). 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 $F_{1,\,water} \cdot PRODVOLcont$
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. processing

$RELEASEcont_{3,j}$:
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: $(1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2j}) \cdot TONNAGEcont$

5. recovery

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

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. processing

$RELEASEreg_{3,j}$:

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: $(1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2j}) \cdot TONNAGEreg$

5. recovery

$RELEASEreg_{5,j}$:

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

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

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 processing (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).

$$Elocal_{i,j} = Fmainsource_i \cdot RELEASEreg_{i,j} \cdot \frac{365}{Temission_i} \qquad j \in \{air, water\} \qquad (7)$$

Input

$RELEASEreg_{i,j}$	release during life-cycle stage *i* to compartment *j*	$[kg_c.d^{-1}]$	O
$Fmainsource_i$	fraction of main local source during life-cycle stage *i*	[-]	O
$Temission_i$	number of days per year for emission in stage *i*	$[d.yr^{-1}]$	O
Output			
$Elocal_{i,j}$	local emission during episode to comp. *j* during stage *i*	$[kg_c.d^{-1}]$	O

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).

$$Ereg_j = \sum_{i=1}^{5} RELEASEreg_{i,j} \qquad j \in \{air, ind\} \qquad (8)$$

$$Ereg_{water} = Fconnect_{stp} \cdot \sum_{i=1}^{5} RELEASEreg_{i,water} \qquad (9)$$

$$Ereg_{direct\text{-}water} = RELEASEreg_{i,surf} + (1 - Fconnect_{stp}) \cdot \sum_{i=1}^{5} RELEASEreg_{i,water} \qquad (10)$$

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.

$$Econt_j = \sum_{i=1}^{5} RELEASEcont_{i,j} \qquad j \in \{air, ind\} \tag{11}$$

$$Econt_{water} = Fconnect_{stp} \cdot \sum_{i=1}^{5} RELEASEcont_{i,water} \tag{12}$$

$$Econt_{direct-water} = RELEASEcont_{i,surf} + (1 - Fconnect_{stp}) \cdot \sum_{i=1}^{5} RELEASEcont_{i,water} \tag{13}$$

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. Emissions of pesticides at application (processing in UC=38/39)

A distinction is made between agricultural pesticides (plant protection products) and non-agricultural pesticides (biocides). The stages of production and formulation of pesticides are treated as for new and existing chemicals, the emissions during the stage of processing (the actual application of the pesticide) are however, treated separately. A large number of application-specific scenarios are presented to account for the different routes the chemical may enter the environment. In contrast with industrial chemicals, the emission module for pesticides does not usually result in emissions to waste water and air from point sources. Instead, emissions take place to a specific area of application directly (the application soil or target area) and the surface water surrounding this area (the ditch or a specific surface-water body). To identify the different compartments for these applications, the parameters are given the subscript '*pest*'. Several parts of the pesticide-emission module require parameters from the distribution module (partition coefficients and degradation rates). Therefore, application of the pesticide emission scenarios which characterise the releases to the environment, is moved to the distribution module. In the emission module, the application scenario must be selected.

III.3.6.1. Plant protection products UC=38

The following scenarios are possible for agricultural pesticides:

1) Application via sprays
    1.1) Field application
    1.2) Application in greenhouse
2) Application via granules and treated seeds (particles)
3) Discharge to an STP (via a settling tank)
4) Amenity use, including several application-specific scenario's:
    4.1) Paved areas:
        a) Direct run-off to surface water
        b) Discharge through rain water flow of a separated sewage system
        c) Discharge through pour over of a mixed sewage system
        d) Discharge through an STP connected to a mixed sewage system.
    4.2) Plantings
        a) drift
    4.3) Railways (not implemented in USES)
    4.4) Water courses
        a) drift
    4.5) Paved dike bodies and slopes
        a) Drift to large surface water
        b) Drift to small surface water
        c) Run-off to large surface water
        d) Run-off to small surface water

III.3.6.2. Biocides UC=39

For biocides, scenarios have been implemented in USES 4.0 for the following product-types of Directive EC/98/8, cross references to USES 3.0 are shown in Appendix IV:

- 1 Human hygiene biocidal products
    - 1.1 Private use
    - 1.2 Industrial use
- 2 Private area and public health area disinfectants and other biocidal products
    - 2.1 Swimming pools
        - Public swimming pools connected to STP (acute and chronic situation)
        - Public and private swimming pools discharging (acute situation)
    - 2.2 Sanitary sector
        - Formulation
        - Private use
    - 2.3 Horticulture(fogging of greenhouses)
    - 2.4 Tiles and surfaces
    - 2.5 Medical sector
        - 2.5.1 Disinfection of rooms, furniture and objects
        - 2.5.2 Disinfection of instruments
            - Washers/disinfectors
            - Baths
        - 2.5.3 Laundry disinfectants
    - 2.8 Disinfectants for sewage and wastewater
- 6 In-can preservatives
    - 6.1 Washing and cleaning fluids, human hygienic products and cosmetics
    - 6.3 Paints and coatings
        - Formulation
        - Industrial use
        - Waste treatment (landfill)
    - 6.4 Fluids used in paper, textile and leather production
        - 6.4.1 Fluids used in paper production
        - 6.4.2 Fluids used in textile production
        - 6.4.3 Fluids used in leather production
- 7 Film preservative
    - 7.1 Paints and coatings (see PT 6.3)
    - 7.2 Plastics (see PT 9.3)
    - 7.3 Glues and adhesives (waste treatment, landfill)
    - 7.4 Paper and cardboard (industrial use)
- 8 Wood preservatives
    - 8.1 Industrial use
        - 8.1.1 Creosote impregnation
        - 8.1.2 Salt impregnation
        - 8.1.3 Drenching and dipping
        - 8.1.4 Curative application: Remedial timber treatment in buildings
    - 8.2 Service life
        - 8.2.1 Leaching from impregnated wood to surface water

- 8.2.2 Leaching from impregnated wood to sandy soil and groundwater
- 8.2.3 Leaching from impregnated wood to soil

8.3 Waste treatment

9 Fibre, leather, rubber and polymerised materials preservatives

9.1 Textile and fabrics

- Biocides present in imported material
- Industrial use
- Waste treatment (landfill)

9.2 Leather and hides (industrial use)

9.4 Paper and cardboard (industrial use)

11 Preservatives for liquid cooling and processing systems

12 Slimicides

13 Metalworking-fluid preservatives

14 Rodenticides (fumigants)

21 Antifouling products

22 Embalming and taxidermist fluids

22.1 Taxidermy

22.2 Embalming

- Industrial use
- Releases in cemetries

Landfill model as used by product-types 6, 7, 8, and 9

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)			
$K_{air-water}$	air-water partition coefficient	[m^3.m^{-3}]	c
$K_{soil-water}$	soil-water partition coefficient	[m^3.m^{-3}]	c
$K_{susp-water}$	suspended matter-water partition coefficient	[m^3.m^{-3}]	c
$K_{sed-water}$	sediment-water partition coefficient	[m^3.m^{-3}]	c

Table III-2 *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
Temperature (12 °C)	TEMP	[K]	285
Constant of Junge equation	CONjunge	[Pa.m]	[a]
Surface area of aerosol particles	$SURF_{aer}$		[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).
[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.

$$\boldsymbol{RHO_{soil} = Fsolid_{soil} \cdot RHOsolid + Fwater_{soil} \cdot RHOwater + Fair_{soil} \cdot RHOair} \qquad (14)$$

$$\boldsymbol{RHO_{sed} = Fsolid_{sed} \cdot RHOsolid + Fwater_{sed} \cdot RHOwater} \qquad (15)$$

$$\boldsymbol{RHO_{susp} = Fsolid_{susp} \cdot RHOsolid + Fwater_{susp} \cdot RHOwater} \qquad (16)$$

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.

$$\boldsymbol{CONV_{soil} = \frac{RHO_{soil}}{Fsolid_{soil} \cdot RHOsolid}} \tag{17}$$

$$\boldsymbol{CONV_{sed} = \frac{RHO_{sed}}{Fsolid_{sed} \cdot RHOsolid}} \tag{18}$$

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_{sed}	wet bulk density of sediment	$[kg_{wwt}.m^{-3}]$	O^c
$Fsolid_{sed}$	volume fraction of solids in sediment	$[m^3.m^{-3}]$	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
$CONV_{sed}$	conversion factor for sediment concentrations: 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).

$$Fass_{aer} = \frac{CONjunge \cdot SURF_{aer}}{VP_L + CONjunge \cdot SURF_{aer}} \tag{19}$$

If *TEMPmelt* <= *TEMP* (substance is liquid):

$$VP_L = VP \tag{20}$$

If *TEMPmelt* > *TEMP* (substance is solid):

$$VP_L = \frac{VP}{e^{6.79\left(1 - \frac{TEMPmelt}{TEMP}\right)}} \tag{21}$$

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:

$$HENRY = \frac{VP \cdot MOLW}{SOL} \tag{22}$$

$$K_{air\text{-}water} = \frac{HENRY}{R \cdot TEMP} \tag{23}$$

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 equation as a general default for non-polar, organic compounds (Sabljic *et al.*, 1995). The QSAR was derived from a range of log *Kow* values from 1 -7.5.

$$Koc = \frac{1.26 \cdot Kow^{0.81}}{1000} \tag{24}$$

Input			
Kow	octanol-water partition coefficient	[-]	S
Output			
Koc	organic carbon-water partition coefficient:	[$m^3.kg^{-1}$]	O

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.

$$Kp_{soil} = Foc_{soil} \cdot Koc \tag{25}$$

$$Kp_{sed} = Foc_{sed} \cdot Koc \tag{26}$$

$$Kp_{susp} = Foc_{susp} \cdot Koc \tag{27}$$

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-3 *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*.

$$Kp_i = Foc_i \cdot Koc \qquad i \in \{RS, PS, A, SLS\} \tag{28}$$

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

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.

$$\boldsymbol{K_{soil-water} = Fair_{soil} \cdot K_{air-water} + Fwater_{soil} + Fsolid_{soil} \cdot Kp_{soil} \cdot RHOsolid} \qquad (29)$$

$$\boldsymbol{K_{susp-water} = Fwater_{susp} + Fsolid_{susp} \cdot Kp_{susp} \cdot RHOsolid} \qquad (30)$$

$$\boldsymbol{K_{sed-water} = Fwater_{sed} + Fsolid_{sed} \cdot Kp_{sed} \cdot RHOsolid} \qquad (31)$$

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
$K_{air-water}$	air-water partition coefficient	$[m^3.m^{-3}]$	O^c
Output			
$K_{soil-water}$	total soil-water partition coefficient	$[m^3.m^{-3}]$	O^c
$K_{susp-water}$	total suspended matter-water partition coefficient	$[m^3.m^{-3}]$	O^c
$K_{sed-water}$	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 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)	
$DT50hydr_{water}$	half-life for hydrolysis in water	[d]
$DT50photo_{water}$	half-life for photolysis in water	[d]
k_{OH}	specific degradation rate constant with OH-radicals	[$m^3.molec^{-1}.d^{-1}$]
Intermediate results 1		
$DT50bio_{stp}$	half-life for biodegradation in STP	[d]
$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]
$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]
Output		
$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]
$kdeg_{air}$	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-4 *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

III.4.2.1. Hydrolysis in water

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.

$$khydr_{water} = \frac{\ln 2}{DT50\,hydr_{water}} \qquad (32)$$

Input			
DT50hydr$_{water}$	half-life for hydrolysis in water	[d]	S
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.

$$kphoto_{water} = \frac{\ln 2}{DT\,50\,photo_{water}} \qquad (33)$$

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:

$$k\deg_{air} = k_{OH} \cdot OHCONC_{air} \qquad (34)$$

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-5 have been derived to extrapolate from the biodegradation screening tests.

Table III-5 *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-5 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:

$$\boldsymbol{k\,\mathrm{deg}_{stp} = kbio_{stp} + kabio_{stp}} \qquad (35)$$

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 first-order rate constants for biodegradation in bulk surface water, based on the results of screening tests for biodegradability.

Table III-6 *rate constants and half-lives for biodegradation in bulk surface water based on results of screening tests on biodegradability.*

Test result	**Rate constant (d^{-1})**	**Half-life (d)**
	$kbio_{water}$	$DT50bio_{water}$
Readily biodegradable	$4.6.10^{-2}$	15
Readily biodegradable, but failing 10-d window	$1.4.10^{-2}$	50
Inherently biodegradable	$4.6.10^{-3}$	150
Not biodegradable	0	∞

Input

	results of screening test on biodegradability		P

Output

$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]	O
$kbio_{water}$	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.

$$k\deg_{water} = khydr_{water} + kphoto_{water} + kbio_{water} \tag{36}$$

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-7 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-7 *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
$>0.1, \leq 1.0$	300	900	3000
$>1.0, \leq 10$	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

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.

$$kbio_{soil} = \frac{\ln 2}{DT50bio_{soil}} \tag{37}$$

$$k\,\deg_{soil} = kbio_{soil} + kabio_{soil} \tag{38}$$

Input			
$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[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 as that for soil is assumed (see Table III-7).

$$kbio_{aer\text{-}sed} = \frac{\ln 2}{DT50bio_{air-sed}} \tag{39}$$

$$k\ deg_{sed} = Faer_{sed} \cdot kbio - aer_{sed} + (1 - Faer_{sed}) \cdot kbio - anaer_{sed} + kabio_{sed} \tag{40}$$

Input			
$DT50bio\text{-}aer_{sed}$	half-life for biodegradation in aerobic sediment	[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 3.0 is used. 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-8 lists the fixed parameters, subdivided into the categories raw sewage, primary sedimentation (9-box only), aerator and solids-liquid separation.

Table III-8 *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-9). 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-9 *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	[-]	O
	$i \in \{air,water,sludge,degr\}$		

EUSES will perform a check wether 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.

$$Clocal_{inf} = \frac{Elocal_{water}}{EFFLUENTlocal_{stp}} \qquad (41)$$

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
Output			
$Clocal_{inf}$	concentration in untreated wastewater	$[kg_c.m^{-3}]$	O

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 49 and 57). 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.

$$EFFLUENTlocal_{stp} = Nlocal \cdot Q_{stp} \qquad (42)$$

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

For calculating the PEC in surface 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.

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:

$$PEC_{stp} = Clocal_{eff} \tag{43}$$

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.

$$PEC_{stp} = Clocal_{inf} \tag{44}$$

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.

$$Estp_{air} = Fstp_{air} \cdot Elocal_{water} \tag{45}$$

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.

$$Estp\text{-}reg_i = Fstp\text{-}reg_i \cdot Ereg_{water} \tag{46}$$

$$Estp\text{-}cont_i = Fstp\text{-}cont_i \cdot Econt_{water}$$

$$i \in \{air, water, sludge/agric\} \tag{47}$$

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 Brandes *et al.* (1996). 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-10 *General parameter settings for the regional and continental scales.*

Parameter		**Symbol**	**Unit**	**Value**
Area of system	region EU	AREA *	[m^2]	$4.0.10^{10}$ $3.56.10^{12}$
Number of inhabitants	region EU	N *	[eq]	20.10^6 [a] 370.10^6 [a]
Fraction connected to sewer systems		$Fconnect_{stp}$	[-]	0.70 [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.

* Different parameter value possible on regional and continental scale.

Table III-10a *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	$Fsolid_{sed}$	[$m_{solid}^3.m_{sed}^{-3}$]	0.2 [a]
Volume fraction of water in sediment	$Fwater_{sed}$	[$m_{water}^3.m_{sed}^{-3}$]	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-11 *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]	0.7 O[c] 6.5 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-12 *Parameter settings for regional and continental surface waters.*

Parameter	**Symbol**	**Unit**	**Value**
Area fraction of water	F_{water} *	[-]	0.03
Water depth	$DEPTH_{water}$ *	[m]	3
Fraction of flow from region larger scale continent	$Fflow_{out}$ *	[-]	0.034 0
Residence time of water region continent	TAU_{water} *	[d]	40 O[c] 166 O[c]
Suspended-solids conc. region continent	$SUSP_{water}$ *	$[kg_{dwt}.m^{-3}]$	0.015 0.025
Concentration of biota	$BIOTA_{water}$	$[kg_{wwt}.m^{-3}]$	0.10

* Different parameter value possible on regional and continental scale.

Table III-13 *Parameter settings for regional and continental 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 water	$SUSPPROD_{water}$	$[kg.d^{-1}]$	0
Suspended solids in STP effluent	$SUSP_{eff}$	$[kg_{dwt}.m^{-3}]$	0.030 [a]
Net sedimentation rate region continent	NETsedrate *	$[m_{sed}.d^{-1}]$	$8.4.10^{-6}$ O[c] $7.5.10^{-6}$ O[c]

[a] Already defined in STP sub-module.
* Different parameter value possible on regional and continental scale.

Table III-14 *Parameter settings for regional and continental soils.*

Parameter	**Symbol**	**Unit**	**Value**
Area fraction of natural soil	$F_{natural}$ *	[-]	0.60
Mixing depth of natural soil	$DEPTH_{natural}$	[m]	0.05
Area fraction of agricultural soil	F_{agric} *	[-]	0.27
Mixing depth of agricultural soil	$DEPTH_{agric}$	[m]	0.2
Area fraction of industrial/urban soil	F_{ind} *	[-]	0.10
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-15 *Mass-transfer coefficients for regional and continental scales.*

Parameter	**Symbol**	**Unit**	**Value**
Air-film partial mass-transfer coefficient (air-water and air-soil interfaces)	$kasl_{air}$ / kaw_{air}	[m.d^{-1}]	120
Water-film partial mass-transfer coefficient (air-water interface)	kaw_{water}	[m.d^{-1}]	1.2
Soil-air partial mass-transfer coefficient (air-soil interface)	$kasl_{soilair}$	[m.d^{-1}]	0.48
Soil water-water film partial-mass transfer coefficient (air-soil interface)	$kasl_{soilwater}$	[m.d^{-1}]	4.8.10^{-5}
Water-film partial mass-transfer coefficient (sediment-water interface)	kws_{water}	[m.d^{-1}]	0.24
Pore water partial mass-transfer coefficient (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.

$$AREA(cont) = AREA(EU) - AREA(reg) \tag{48}$$

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

$$N(cont) = N(EU) - N(reg) \tag{49}$$

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.

$$TAU_{air} = \frac{\sqrt{AREA \cdot \frac{\pi}{4}}}{WINDSPEED} \qquad (50)$$

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.

$$FLOW_{water} = Fflow_{out} \cdot FLOW_{water}(*) + WASTEW + RUNOFF + RAINDIRECT \qquad (51)$$

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.

$$TAU_{water} = \frac{AREA \cdot F_{water} \cdot DEPTH_{water}}{FLOW_{water}} \qquad (52)$$

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:

$$\boldsymbol{RAINDIRECT = RAINRATE \cdot AREA \cdot F_{water}} \tag{53}$$

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:

$$\boldsymbol{RUNOFF = Frunoff_{soil} \cdot (F_{natural} + F_{agric} + F_{ind}) \cdot AREA \cdot RAINRATE} \tag{54}$$

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:

$$\boldsymbol{WASTEW = N \cdot Q_{stp}} \tag{55}$$

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.

$$\begin{gathered}\mathbf{NETsedrate} = \\ [\ SUSPPROD_{water} + SUSP_{water}(*) \cdot Fflow_{out} \cdot FLOW_{water}(*) + \\ SUSP_{eff} \cdot EFFLUENT_{stp} + EROSION \cdot (F_{natural} + F_{agric} + F_{ind}) \cdot \\ AREA \cdot Fsolid_{soil} \cdot RHOsolid - SUSP_{water} \cdot FLOW_{water}\ ] \\ \cdot \frac{1}{Fsolid_{sed} \cdot RHOsolid} \cdot \frac{1}{AREA \cdot F_{water}}\end{gathered} \tag{56}$$

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.

$$EFFLUENT_{stp} = N \cdot Q_{stp} \cdot Fconnect_{stp} \tag{57}$$

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 (BCF) for aquatic biota used in this equation is calculated from Equation (86/87). 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.

$$PECreg_{water} = \frac{PECreg_{water,tot}}{1 + Kp_{susp} \cdot SUSP_{water} + BCF_{biota} \cdot BIOTA_{water}} \tag{58}$$

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.

$$PECreg_{agric,porew} = \frac{PECreg_{agric,porew} \cdot RHO_{soil}}{K_{soil-water}} \tag{58a}$$

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.4.5. 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	[-]	
$K_{air-water}$	air-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{soil-water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	c
$K_{susp-water}$	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	$[kg_c.m^{-3}]$	
$PECreg_{natural}$	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*	$[d^{-1}]$	
	$i \in$ {soil,agric,grassland}		
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	$[kg_c.m^{-3}]$	
$Clocal_{soil}$	local concentration in agric. soil averaged over 30 days	$[kg_c.kg_{wwt}^{-1}]$	
$Clocal_{agric}$	local concentration in agric. soil averaged over 180 days	$[kg_c.kg_{wwt}^{-1}]$	
$Clocal_{grassland}$	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*	[-]	c
	$i \in$ {soil,agric,grassland}		
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)	$[kg_c.m^{-3}]$	
$PEClocal_{sed}$	predicted environmental concentration in sediment	$[kg_c.kg^{-1}]$	
$PEClocal_{soil}$	local PEC in agric. soil (total) averaged over 30 days	$[kg_c.kg^{-1}]$	
$PEClocal_{agric}$	local PEC in agric. soil (total) averaged over 180 days	$[kg_c.kg^{-1}]$	
$PEClocal_{grassland}$	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-16 *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	DILUTION	[-]	10
Soil			
Partial mass transfer coeff. at air side of soil-air interface	$kasl_{air}$	$[m.d^{-1}]$	120 [a]
Partial mass transfer coeff. at soil-air side of soil-air interface	$kasl_{soilair}$	$[m.d^{-1}]$	0.48 [a]
Partial mass transfer coeff. at soil-water side of air-soil interface	$kasl_{soilwater}$	$[m.d^{-1}]$	$4.8.10^{-5}$ [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.

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.

$$Clocal_{air} = \max\left(Elocal_{air}, Estp_{air} \right) \cdot Cstd_{air} \tag{59}$$

$$Clocal_{air,ann} = Clocal_{air} \cdot \frac{Temission}{365} \tag{60}$$

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.

$$PEClocal_{air,ann} = Clocal_{air,ann} + PECregional_{air} \tag{61}$$

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.

$$\boldsymbol{DEPtotal = \left(Elocal_{air} + Estp_{air} \right) \cdot \left(Fass_{aer} \cdot DPstd_{aer} + (1 - Fass_{aer}) \cdot DEPstd_{gas} \right)} \tag{62}$$

$$\boldsymbol{DEPtotal_{ann} = DEPtotal \cdot \frac{Temission}{365}} \tag{63}$$

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

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 wether 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.

$$Clocal_{water} = \frac{Clocal_{eff}}{(1 + Kp_{susp} \cdot SUSP_{water}) \cdot DILUTION} \tag{64}$$

$$Clocal_{water,ann} = Clocal_{water} \cdot \frac{Temission}{365} \tag{65}$$

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	[-]	D/O^c
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

If a more site-specific assessment is appropriate, 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.

$$DILUTION = \frac{EFFLUENTlocal_{stp} + FLOW}{EFFLUENTlocal_{stp}} \tag{66}$$

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	[-]	D/O^c

The concentration on the regional scale is used as background concentration for the local scale. Therefore, these concentrations are summed.

$$PEClocal_{water} = Clocal_{water} + PECreg_{water} \tag{67}$$

$$PEClocal_{water,ann} = Clocal_{water,ann} + PECreg_{water} \tag{68}$$

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
Output			
$PEClocal_{water}$	predicted environmental concentration during episode	$[kg_{c}.m^{-3}]$	O
$PEClocal_{water,ann}$	annual average predicted environmental concentration	$[kg_{c}.m^{-3}]$	O

III.4.5.3. Local concentration in sediment

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).

$$PEClocal_{sed} = \frac{K_{susp-water}}{RHO_{susp}} \cdot PEClocal_{water} \tag{69}$$

Input			
$PEClocal_{water}$	concentration in surface water during emission episode	$[kg_{c}.m^{-3}]$	O
$K_{susp-water}$	suspended matter-water partition coefficient	$[m^{3}.m^{-3}]$	O^{c}
RHO_{susp}	bulk density of suspended matter	$[kg_{wwt}.m^{-3}]$	O^{c}
Output			
$PEClocal_{sed}$	predicted environmental concentration in 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-17).

Table III-17 *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. The soil side of the interface is treated as a pair of parallel resistances (air phase and water phase of soil) (Mackay *et al.*, 1992). The rate constant for volatilisation from soil is given by:

$$\frac{1}{k_{volat\ i}} = \left(\frac{1}{kasl_{air} \cdot K_{air\text{-}water}} + \frac{1}{kasl_{soilair} \cdot K_{air\text{-}water} + kasl_{soilwater}} \right) \cdot K_{soil\text{-}water} \cdot DEPTH_i \quad (70)$$

Input

$kasl_{air}$	partial mass-transfer coeff. at air side of air-soil interface	$[m.d^{-1}]$	D
$kasl_{soilair}$	partial mass-transfer coeff. at soil-air side of air-soil int.	$[m.d^{-1}]$	D
$kasl_{soilwater}$	partial mass-trnsf. coeff. at soil-water side of air-soil int.	$[m.d^{-1}]$	D
$K_{air\text{-}water}$	air-water partition coefficient	$[m^3.m^{-3}]$	O^c
$K_{soil\text{-}water}$	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.

$$k_{leach\ i} = \frac{Finf_{soil} \cdot RAINRATE}{K_{soil\text{-}water} \cdot DEPTH_i} \quad (71)$$

Input

$Finf_{soil}$	fraction of rainwater that infiltrates into soil	[-]	D
RAINRATE	rate of wet precipitation	$[m.d^{-1}]$	D
$K_{soil\text{-}water}$	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.

$$k_i = k_{volat\ i} + k_{leach\ i} + kdeg_{soil} \quad (72)$$

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:

$$D_{air\ i} = \frac{DEPtotal_{ann}}{DEPTH_i \cdot RHO_{soil}} \tag{73}$$

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:

$$Cdep10_i = \frac{D_{air\ i}}{k_i} - \frac{D_{air\ i}}{k_i} \cdot e^{-365 \cdot 10 \cdot k_i} \tag{74}$$

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:

$$Csludge1_i = \frac{C_{sludge} \cdot APPLsludge_i}{DEPTH_i \cdot RHO_{soil}} \tag{75}$$

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.

$$Facc_i = e^{-365 k_i} \tag{76}$$

$$Csludge10_i = Csludge1_i \cdot \left[1 + \sum_{n=1}^{9} Facc_i^{\,n} \right] \tag{77}$$

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.

$$Clocal10_i = Cdep10_i + Csludge10_i \tag{78}$$

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 soil concentration from 0 to *T* days:

$$Clocal_i = \frac{1}{T_i} \cdot \int_0^{T_i} Clocal_i(t)\, dt \tag{79}$$

The analytical solution of this integral is then given by:

$$Clocal_i = \frac{D_{air\,i}}{k_i} + \frac{1}{k_i T_i}\left[Clocal\,10_i - \frac{D_{air\,i}}{k_i} \right] \cdot \left[1 - e^{-k_i T_i} \right] \tag{80}$$

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.

$$PEClocal_i = Clocal_i + PECreg_{natural} \tag{81}$$

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.

$$PEClocal_{i,porew} = \frac{PEClocal_i \cdot RHO_{soil}}{K_{soil-water}} \tag{82}$$

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.

$$Fst-st_i = \frac{Clocal\,10_i}{Cinf_i} \tag{83}$$

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:

$$C\,inf_i = \frac{D_{air\,i}}{k_i} + Csludge1_i \cdot \frac{1}{1-Facc_i} \tag{84}$$

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.

$$PEClocal_{grw} = PEClocal_{agric,porew} \tag{85}$$

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.4.6. Additional parameters for pesticides

III.4.6.1. Additional partition coefficients for pesticides

Input			
Koc	organic carbon-water partition coefficient	$[m^3.kg^{-1}]$	
Kom	organic matter-water partition coefficient	$[m^3.kg^{-1}]$	
Output 1			
RHO_{pest}	wet bulk density of application soil	$[kg_{wwt}.m^{-3}]$	c
$CONV_{pest}$	conversion factors for application soil concentrations	$[kg_{wwt}.kg_{dwt}^{-1}]$	c
Kp_{pest}	solids-water partition coefficient in application soil	$[m^3.kg^{-1}]$	
Output 2			
$K_{pest\text{-}water}$	total soil-water partition coefficient in application soil	$[m^3.m^{-3}]$	c

For direct pesticide application to soils, a separate soil type is defined with the subscript "pest". Also, a specific surface water body is defined as a ditch surrounding this application soil (indicated with the subscript "ditch"). The properties of the soil and ditch are given in Table A-1.

Table A-1 *Default settings for pesticide application soil and ditch water.*

Parameter	**Symbol**	**Unit**	**Value**
Volume fraction of water in application soil	$Fwater_{pest}$	$[m^3.m^{-3}]$	0.2
Volume fraction of water in saturated soil	$Fwater_{satsoil}$	$[m^3.m^{-3}]$	0.4
Volume fraction of solids in application soil	$Fsolid_{pest}$	$[m^3.m^{-3}]$	0.6
Volume fraction of air in application soil	$Fair_{pest}$	$[m^3.m^{-3}]$	0.2
Weight fraction of organic matter in suspended matter ditch	Fom_{ditch}	$[kg.kg^{-1}]$	0.085
Weight fraction of organic matter in application soil	Fom_{pest}	$[kg.kg^{-1}]$	0.05

Bulk densities of the 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.

$$\boldsymbol{RHO_{pest} = Fsolid_{pest} \cdot RHOsolid + Fwater_{pest} \cdot RHOwater + Fair_{pest} \cdot RHOair} \quad \text{(P-1)}$$

$$\boldsymbol{RHO_{satsoil} = Fsolid_{pest} \cdot RHOsolid + Fwater_{satsoil} \cdot RHOwater} \quad \text{(P-2)}$$

Input			
$Fwater_{pest}$	volume fraction of water in application soil	$[m^3.m^{-3}]$	D
$Fwater_{satsoil}$	volume fraction of water in saturated soil	$[m^3.m^{-3}]$	D
$Fsolid_{pest}$	volume fraction of solids in application soil	$[m^3.m^{-3}]$	D
$Fair_{pest}$	volume fraction of air in application soil	$[m^3.m^{-3}]$	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_{pest}	wet bulk density of application soil	$[kg_{wwt}.m^{-3}]$	O^c
$RHO_{satsoil}$	wet bulk density of saturated soil	$[kg_{wwt}.m^{-3}]$	O^c

Conversion wet weight-dry weight

$$CONV_{pest} = \frac{RHO_{pest}}{Fsolid_{pest} \cdot RHOsolid} \tag{P-3}$$

$$CONV_{satsoil} = \frac{RHO_{satsoil}}{Fsolid_{pest} \cdot RHOsolid} \tag{P-4}$$

Input			
RHO_{pest}	wet bulk density of application soil	$[kg_{wwt}.m^{-3}]$	O^c
$RHO_{satsoil}$	wet bulk density of saturated soil	$[kg_{wwt}.m^{-3}]$	O^c
$Fsolid_{pest}$	volume fraction of solids in application soil	$[m^3.m^{-3}]$	D
RHOsolid	density of solid phase	$[kg.m^{-3}]$	D
Output			
$CONV_{pest}$	conversion factors for application soil concentrations	$[kg_{wwt}.kg_{dwt}^{-1}]$	O^c
$CONV_{satsoil}$	conversion factors for saturated soil concentrations	$[kg_{wwt}.kg_{dwt}^{-1}]$	O^c

Solids-water partitioning in the environment

The organic-matter normalised partition coefficient (*Kom*) can be entered directly, or estimated from *Koc*, assuming an organic carbon to organic matter ratio of 1:1.724. It is usually assumed that organic matter contains about 58 w/w % carbon. This figure results from the analysis of alkaline soluble humus compounds (Schultze, 1849). If no *Koc* is available from the data set, it may be estimated from *Kow* (see Section III.4.1.5).

$$Kom = \frac{Koc}{1.724} \tag{P-5}$$

Input			
Koc	organic carbon-water partition coefficient	$[m^3.kg^{-1}]$	O
Output			
Kom	organic matter-water partition coefficient	$[m^3.kg^{-1}]$	O

The solids-water partition coefficient (*Kp*) in the pesticide application soil will normally be available in the data set. If no *Kp* is entered, it can be derived from the normalised partition coefficient (*Kom*) and the fraction of organic matter in the compartment.

$$Kp_{pest} = Fom_{pest} \cdot Kom \tag{P-6}$$

Input			
Fom_{pest}	weight fraction of organic matter in application soil	$[kg.kg^{-1}]$	D
Kom	organic matter-water partition coefficient	$[m^3.kg^{-1}]$	O
Output			
Kp_{pest}	solids-water partition coefficient in application soil	$[m^3.kg^{-1}]$	O

Total compartment-water partitioning

$$K_{pest\text{-}water} = Fair_{pest} \cdot K_{air\text{-}water} + Fwater_{pest} + Fsolid_{pest} \cdot Kp_{pest} \cdot RHOsolid \tag{P-7}$$

Input			
$Fwater_{pest}$	volume fraction of water in application soil	$[m^3.m^{-3}]$	D
$Fsolid_{pest}$	volume fraction of solids in application soil	$[m^3.m^{-3}]$	D
$Fair_{pest}$	volume fraction of air in application soil	$[m^3.m^{-3}]$	D
RHOsolid	density of solid phase	$[kg.m^{-3}]$	D
Kp_{pest}	solids-water partition coefficient in application soil	$[m^3.kg^{-1}]$	O
Output			
$K_{pest\text{-}water}$	total soil-water partition coefficient in application soil	$[m^3.m^{-3}]$	O^c

Notes for pesticide assessment: Environmental distribution

The application of pesticides (processing in UC=38/39) is treated separately in the Sections III.4.7 to III.4.9. For pesticides, several additional paramaters are needed (Section III.4.6), a variety of application scenarios is implemented. Several scenarios from the 'emission' Sections III.4.7 (agricultural pesticides) and III.4.8 (non-agricultural pesticides) make use of the specific distribution submodule for pesticides (Section III.4.9). Other scenarios, however, make use of the local distribution submodules for new and existing substances (Section III.4.3 and III.4.5). To clarify the program flow for pesticide application, the possible outputs from the emission sub modules are specified below.

Treated in the local distribution module for new and existing substances (Sections III.4.3-III.4.5)

$Elocal_{air}$	local emission to air during episode	$[kg_c.d^{-1}]$
$Elocal_{water}$	local emission to waste water during episode	$[kg_c.d^{-1}]$
Temission	number of emission days	[d]

Treated in the pesticide-distribution module (Sections III.4.9)

$DOSE_{pest}$	single dosage for pesticide	$[kg_c.m^{-2}]$
$DOSE_{pest,gh}$	single dosage in case of pesticide in greenhouse	$[kg_c]$
$DOSE_{max}$	apparent maximum dosage (spray & particles)	$[kg_c.m^{-2}]$
N_{appl}	number of applications in one year	[-]
$T_{interval}$	application interval	[d]
N_{lt}	number of application periods per registration period	[-]
$T_{interval\text{-}lt}$	long term interval for application periods	[d]
MIX	mixing with soil	[yes/no]
F_{air}	fraction of dosage emitted to air	[-]
F_{soil}	fraction of dosage that reaches the soil	[-]
F_{drift}	fraction drift related to location and way of application	[-]

Directly used in exposure of birds and mammals for pesticides (Section III.5.5)

$Cwater_{pest\text{-}T}$	average concentration in ditch over *T* days	$[kg_c.m^{-3}]$
$Csoil_{pest\text{-}T}$	average concentration in application soil over *T* days	$[kg_c.kg_{wwt}^{-1}]$

Directly used in pesticide-risk characterisation (Section III.7.3)

$Cwater_{pest\text{-}T}$	average concentration in ditch over *T* days	$[kg_c.m^{-3}]$
$Csoil_{pest\text{-}T}$	average concentration in application soil over *T* days	$[kg_c.kg_{wwt}^{-1}]$
$DOSE_{wood}$	dosage of a.i. per m^2 of wood (scenario timber treatment)	$[kg_c.m^{-2}]$

III.4.7. Application of agricultural pesticides (processing in UC=38)

The following scenarios are possible for agricultural pesticides:

1) Application via sprays
2) Application via granules and treated seeds (particles)
3) Discharge to an STP (via a settling tank)
4) Amenity use (several application-specific scenario's)

General application inputs

-	scenario choice for agricultural pesticides	[-]
-	crop and growing stage choice for agricultural pesticides	[-]
DOSE$_{pest}$	single dosage for pesticide	[kg$_c$.m^{-2}]

Inputs for spray applications

N$_{appl}$	number of applications in one year	[-]
T$_{interval}$	application interval	[d]
N$_{lt}$	number of application periods per registration period	[-]
T$_{interval\text{-}lt}$	long term interval for application periods	[d]
-	choice of crop and growing stage	[-]
-	choice of application	[-]
MIX	mixing with soil	[yes/no]
AMOUNTspray	amount of spray liquid used	[m$_{spray}^{3}$.m^{-2}]
DRAINS	is drainage present?	[yes/no]
T$_{bird}$	test duration for bird toxicity test	[d]
T$_{mammal}$	test duration for mammalian toxicity test	[d]
VP	vapour pressure	[Pa]
kdeg$_{soil}$	rate constant for biodegradation in bulk application soil	[d^{-1}]

Output 1 for spray application

F$_{air}$	fraction of dosage emitted to air	[-]
F$_{soil}$	fraction of dosage that reaches the soil	[-]
F$_{drift}$	fraction drift related to location and way of application	[-]
F$_{int}$	fraction of dosage that is intercepted by crops	[-]

Output 2 for spray application

DOSE$_{max}$	apparent maximum dosage (spray & particles)	[kg$_c$.m^{-2}]

Inputs for particles applications

N$_{appl}$	number of applications in one year	[-]
T$_{interval}$	application interval	[d]
N$_{lt}$	number of application periods per registration period	[-]
T$_{interval\text{-}lt}$	long term interval for application periods	[d]
MIX	mixing with soil	[yes/no]
Cparticle	concentration of pesticide in granules or treated seeds	[kg$_c$.kg$_{particle}^{-1}$]
WEIGHT$_{particle}$	weight of one granule or treated seed	[kg$_{particle}$.particle^{-1}]
DRAINS	is drainage present?	[yes/no]
T$_{bird}$	test duration for bird toxicity test	[d]
T$_{mammal}$	test duration for mammalian toxicity test	[d]
kdeg$_{soil}$	rate constant for biodegradation in bulk soil	[d^{-1}]

Output 1 particles

F$_{soil}$	fraction of dosage that reaches the soil	[-]
F$_{drift}$	fraction drift related to location and way of application	[-]

Output 2 particles

DOSE$_{max}$	apparent maximum dosage (spray & particles)	[kg$_c$.m^{-2}]

Inputs for discharge to STP

N_{appl}	number of applications in one year (per cell of 200 m^2)	[-]
Output via STP		
$Elocal_{water}$	emission to the sewage treatment plant during episode	[$kg_c.d^{-1}$]
Temission	number of days for the emission	[d]

Inputs for amenity use

SPOT	spotwise application (Only amenity use scenario 5)	[yes/no]
Kom	organic matter-water partition coefficient	[$m^3.kg_{om}^{-1}$]
$kdeg_{water}$	rate constant for degradation in surface water	[d^{-1}]
T_{bird}	test duration for bird toxicity test	[d]
T_{mammal}	test duration for mammalian toxicity test	[d]
Intermediate results		
$Cwater_{au}$	water concentration for amenity use scenario	[$kg_c.m^{-3}$]
Output amenity use		
$Cwater_{pest\text{-}0}$	peak concentration in water	[$kg_c.m^{-3}$]
$Cwater_{pest\text{-}T}$	average concentration in water over T days $T \in \{4,7,14,21,28,T_{bird},T_{mammal},365\}$	[$kg_c.m^{-3}$]

III.4.7.1. Fraction of the dosage of a pesticide that reaches the soil

The dosage of pesticides applied via granules and treated seeds reaches the soil completely. In case of sprays, the dosage is partly intercepted by crops. The remainder reaches the soil or the surface water, or disappears into the air. It is assumed that the most regular spraying methods are used. Table A-3 gives an overview of the fraction of the spraying-liquid that is intercepted by crops depending on the crop and growing stage. The true fraction to air as a function of the vapour pressure is given in Table A-2 (the source of these fractions is discussed in more detail in the pesticide air-distribution module in Section III.4.9.2, Table D-3 and Table D-4).

Application via sprays	F_{soil} = table or user input
Application via granules and treated seeds	$F_{soil} = 1$; $F_{air} = 0$
Only release through STP	$F_{soil} = 0$; $F_{air} = 0$
Amenity use	$F_{soil} = 0$; $F_{air} = 0$

Table A-2 *Emission factors to air for field use and greenhouses of pesticides with different vapour pressures (F_{air}).*

Vapour pressure **[Pa]**	**Total emission factor to air for field application** **[-]**	**Total emission factor to air for greenhouse application** **[-]**
$> 10.10^{-3}$	1	0.4
1.10^{-3} - 10.10^{-3}	0.5	0.32
$0.1.10^{-3}$ - 1.10^{-3}	0.2	0.15
$0.01.10^{-3}$ - $0.1.10^{-3}$	0.1[1]	0.08
$\leq 0.01.10^{-3}$	0.01	0.02

[1] Default value is set to 10%, not dependent on vapour pressure

Input

VapDep	vapour pressure dependence of Fair	[yes/no]	P
-	scenario choice for agricultural pesticides	[-]	P
VP	vapour pressure	[Pa]	S

Output

F_{air}	fraction of dosage emitted to air	[-]	O

Table A-3 *Fraction that is intercepted by the crop (F_{int})*

Crop and growing stage	**No interception**	**minimal crop cover**	**average crop cover**	**Full canopy**
Cereals, spring	0	0.25	0.5	0.7
Cereals, winter	0	0.25	0.5	0.7
Field beans	0	0.25	0.4	0.7
Grass / alfalfa	0	0.4	0.6	0.75
Legumes	0	0.25	0.5	0.7
Maize	0	0.25	0.5	0.75
Oil seed rape, spring	0	0.4	0.7	0.75
Oil seed rape, winter	0	0.4	0.7	0.75
Pome / stone fruit, (early)	0	0.2	0.4	0.7
Pome / stone fruit (late)	0	0.2	0.4	0.7
Potatoes	0	0.15	0.5	0.7
Soybeans	0	0.2	0.5	0.75
Sugar beet	0	0.2	0.7	0.75
Vegetables, bulb	0	0.1	0.25	0.4
Vegetables, fruiting	0	0.25	0.5	0.7
Vegetables, leafy	0	0.25	0.4	0.7
Vegetables, root	0	0.25	0.5	0.7
Apples, hand (crop < 50 cm)	0	0.2	0.5	0.7
Apples, hand (crop > 50 cm)	0	0.2	0.5	0.7
Default	0	0.2	0.5	0.7
No drift (incorp/seed trtmt)[1]	0	0	0	0

[1] emission to air is not relevant in this case, $F_{air} = 0$

Input

-	scenario choice for agricultural pesticides	[-]	P
-	choice of crop and growing stage	[-]	P

Output

F_{int}	fraction of dosage intercepted by crops	[-]	O
F_{air}	fraction of dosage emitted to air	[-]	O

$$F_{soil} = (1 - F_{int}) \cdot (1 - F_{air}) \qquad \text{(P-8)}$$

Input			
F_{int}	fraction of dosage intercepted by crops	[-]	O
F_{air}	fraction of dosage emitted to air	[-]	O
Output			
F_{soil}	fraction of dosage that reaches the soil	[-]	O

The apparent maximum dose

The apparent maximum dose is calculated from the part of the dose that reaches the soil (only for sprays and particles). This dosage is used to calculate concentrations in groundwater and the concentration in food for mammals due to spraying.

$$F_{rs} = e^{-k\,deg_{soil} \cdot T_{interval}} \qquad \text{(P-9)}$$

$$DOSE_{max} = F_{soil} \cdot DOSE_{pest} \cdot \frac{1 - F_{rs}^{N_{appl}}}{1 - F_{rs}} \qquad \text{(P-10)}$$

Input			
$DOSE_{pest}$	single dosage	$[kg_c.m^{-2}]$	S
F_{soil}	fraction that reaches the soil	[-]	O
$kdeg_{soil}$	rate constant for biodegradation in bulk soil	$[d^{-1}]$	O
N_{appl}	number of applications in one year	[-]	S
$T_{interval}$	application interval	[d]	S
F_{rs}	fraction of the concentration remaining after time $T_{interval}$	[-]	O^c
Output			
$DOSE_{max}$	apparent maximum dosage	$[kg_c.m^{-2}]$	O

III.4.7.2. Drift to surface water

A part of the applied dosage of a sprayed pesticide reaches the surface water directly. The way in which the pesticide is applied has a great influence on the degree of drift. Emans *et al.* (1992) provides a table with estimations of the degree of drift as a function of method and location of treatment. Table A-4 gives information on the final drift fractions based on recent research and established by the Dutch government. In this table fractions of the original dosages are presented that do not reach the target areas. In this hazard assessment system this means a ditch with a mean depth of 0.25 m.

Application via sprays	F_{drift} = table or user input
Application via granules and treated seeds	$F_{drift} = 0$
Only release through STP	$F_{drift} = 0$

The fraction drift for spray applications is taken from the following table.

Input			
-	choice of application	[-]	P
Output			
F_{drift}	fraction drift related to location and way of application	[-]	O

Table A-4 Fraction drift (F_{drift} [-]) related to location and way of application

1. Indoor applications[1] (excl. greenhouses)	-	storage cells, etc.	0
	-	shower rooms, etc.	0
2. Protected applications			
a. Specific applications	-	overhead irrigation	0
	-	manual pouring	0
	-	soil treatment	0
	-	granule application	0
	-	trickling	0
	-	chicory for silage	0
b. Non-specific applications	-	remaining ways of application in greenhouses (spraying, mist blowing, fogging, smoke generating, etc.: mainly through condensation on glass roof)[2]	0.001
3. Field applications:			
a. Specific applications:	-	manual pouring	0
	-	dipping	0
	-	granule application[3]	0
	-	baiting	0
	-	injecting soil/plant	0
	-	treating plant base	0
	-	smearing	0
	-	brushing	0
	-	spraying with direct incorporation into soil[4]	0.01
	-	seed treatment	0
b. Spot applications:	-	waste dump	0.005
	-	row spraying[5]	0.005
	-	knapsack spraying	0.005
	-	road signs	0.005
c. Non-specific applications:	1.	arboriculture	
	a.	low trees (downward spraying possible)	0.01
	b.	nursery trees	
	-	spindle	0.008
	-	transplanted	0.028
	2.	full field applications	0.01
	3.	small fruit (as full field)	0.01
	4.	fruit	
	-	before May 1, no leaves	0.17
	-	after May 1, leaves	0.07
	5.	ditch slope	0.1
	6.	flower bulbs	0.01
	7.	Greenhouse application	0.001
d. Specific applications:	-	spraying by aircraft	1.0
	-	willow-coppice	1.0
	-	dry ditch bottom	1.0

[1] Whenever no direct exposure of surface water by drift is to be expected from the method of applying, the load through this route is assumed to be 0%.

[2] From research into condensate discharge, it was derived that approximately 0.1% of the plant protection products dosage on the glasshouse roof can load the surface water via condensate. Up to now, it has been impossible to explicate per way of application.

[3] With special synthesis granule broadcasting device.

[4] Spraying with direct incorporation into the soil during application.

[5] This figure is based on the assumption, that during row spraying less drift will occur than during field application, as the distance from nozzle to soil is substantially less during row spraying than during whole field treatments.

The application mentioned under 3 ‘Field applications’ c ‘Non-specific applications’ may be subject to emission reduction proposals by the applicants or prescribed by the authorities. The applicable emission reduction factors vary between 0.14 and 0.90. The remaining part still contributes to the drift. The relevant reduction factors are presented in Table A-5.

Table A-5 *Emission reduction factors for drift ($Fred_{drift}$) to surface waters for applications mentioned under 3c in Table A-4.*

Application	Reduction measure	emission reduction factor $Fred_{drift}$
1b	Driving path + tunnel device	0.90
2	air assistance end nozzles low drift nozzles row or knap-sack sprayer extra crop free zone: - 1 meter - 2 meter	0.53 0.14 0.18 0.50 0.52 0.67
3	air assistance end nozzles low drift nozzles row or knap-sack sprayer extra crop free zone: - 1 meter - 2 meter	0.53 0.14 0.18 0.50 0.52 0.67
4	Driving path + tunnel device Driving path + wind catch: - before May 1, no leaves - after May 1, leaves	0.85 0.70 0.90

REDUCTION = ‘yes’:

$$F_{drift} = F_{drift}(Table\ A - 4) \cdot (1 - Fred_{drift}) \qquad \text{(P-11)}$$

Input

-	choice of application	[-]	P
REDUCTION	reduction measure available	[yes/no]	P
-	choice of reduction measure	[-]	P
$Fred_{drift}$	fraction emission reduction for drift	[-]	O

Output

F_{drift}	fraction drift related to location and way of application	[-]	O

III.4.7.3. Discharge via settling tank on a sewage treatment plant.

In some cases it is possible that a pesticide reaches a sewage treatment plant (STP) via a settling-tank (for example with the culture of mushrooms). In this case the total dosage emitted to the sewage treatment plant is equally spread out over 25 days (Jobsen, 1988 in Emans *et al.* 1992). Thus each day 4% of the total dosage is emitted to the STP. A cell is an areal production unit. It should be noted that no other releases to the environment are taken into account in this scenario.

Table A-6 *Default settings for specific distribution routes for pesticide application.*

Parameter	**Symbol**	**Unit**	**Value**
Emission period for discharge to STP	$Temission_{stp}$	[d]	25
Area of one cell	$AREA_{cell}$	[$m^2.cell^{-1}$]	200
Number of cells	N_{cells}	[cell]	5

Source: Emans *et al.* (1992).

$$DOSE_{cell} = DOSE_{pest} \cdot AREA_{cell} \qquad \text{(P-12)}$$

$$SUMDOSE = N_{cells} \cdot DOSE_{cell} \qquad \text{(P-13)}$$

$$Elocal_{water} = \frac{SUMDOSE}{Temission_{stp}} \qquad \text{(P-14)}$$

$$Temission = Temission_{stp} \cdot N_{appl} \qquad \text{(P-15)}$$

Input

$DOSE_{cell}$	dosage per cell	[$kg_c.cell^{-1}$]	O^c
SUMDOSE	total dosage	[kg_c]	O^c
$DOSE_{pest}$	single dosage of pesticide	[$kg_c.m^{-2}$]	S
$AREA_{cell}$	area of one cell	[$m^2.cell^{-1}$]	D
N_{appl}	number of applications in one year (per cell of 200 m^2)	[-]	S
N_{cells}	number of cells	[cell]	D
$Temission_{stp}$	emission period for discharge to STP	[d]	D

Output

$Elocal_{water}$	emission to waste water during episode	[$kg_c.d^{-1}$]	O
Temission	number of emission days	[d]	O

III.4.7.4. Agricultural pesticides for amenity use

The emission of agricultural pesticides is generally described in the previous section. For specific amenity use a separate emission module has been developed (Kraaij and Verstappen, 1995). The calculation procedures in this report estimate the concentration in the aquatic environment depending on specific amenity uses of pesticides. A distinction has been made in five main scenarios, each split up into several sub-scenarios:

1) paved areas
2) plantings
3) railways (not implemented in USES)
4) water courses
5) paved dike bodies and slopes

For several of these areas the possible entry routes into the environment have been analysed, e.g. leaching, run-off and drift. The separate model descriptions for these application are given below. For more specific information reference is made to the original publication (Kraaij and Verstappen, 1995).

Table B-1 *Default settings.*

Parameter	**Symbol**	**Unit**	**Value**
Concentration suspended solids in the ditch	$SUSP_{water}$	$[kg_{solid} \cdot m_{water}^{-3}]$	0.015

The average concentration in surface water during test periods

The concentration from the application scenario is used to calculate concentrations averaged over the duration of various toxicity tests (Linders and Luttik, 1995). Only removal through degradation (biotic and abiotic) is taken into account and not the removal by volatilisation.

The average concentration is calculated over a period of 4, 7, 14, 21 or 28 days (the duration of the toxicity test) starting from the peak concentration given by the amenity use scenario. The factor $Fdiss_{ditch}$ is used to convert the total concentration in water to the dissolved concentration.

$$Fdiss_{ditch} = \frac{1}{1 + Kp_{susp,pest} \cdot SUSP_{water}} \tag{P-16}$$

$$Cwater_{pest\text{-}0} = Cwater_{au} \cdot Fdiss_{ditch} \tag{P-17}$$

$$Cwater_{pest-T} = Cwater_{pest-0} \cdot \frac{1 - e^{-kdeg_{water,temp} \cdot T}}{kdeg_{water} \cdot T}$$

$$T \in \{4,7,14,21,28,T_{bird},T_{mammal},365\} \tag{P-18}$$

Input			
$Kp_{susp,pest}$	solids-water partition coefficient of susp. matter for pesticides	$[m^3.kg^{-1}]$	S
$SUSP_{water}$	concentration suspended solids in the ditch	$[kg_{solid}.m_{water}^{-3}]$	D
$Fdiss_{ditch}$	fraction of the chemical in the water phase of the ditch	[-]	O^c
$Cwater_{au}$	water concentration for amenity use scenario	$[kg_c.m^{-3}]$	O
$kdeg_{water,temp}$	temperature dependent rate constant for degradation in water	$[d^{-1}]$	O
T_{bird}	test duration for bird toxicity test	[d]	S
T_{mammal}	test duration for mammalian toxicity test	[d]	S
Output			
$Cwater_{pest\text{-}0}$	peak concentration in water	$[kg_c.m^{-3}]$	O
$Cwater_{pest\text{-}T}$	average concentration in water over T days	$[kg_c.m^{-3}]$	O

Amenity use scenarios

1) Paved areas

Four situations are distinguished for application of pesticides on paved areas:

A) Direct run-off to surface water
B) Discharge through rain water overflow of a separated sewer system
C) Discharge through pour over of a mixed sewage system
D) Discharge through an STP connected to a mixed sewage system.

Each of these situations is characterised by a standardised scenario using estimations of several parameters based on expert judgements or available data of the specific sample cities. It concerns discharge coefficients of roofs and pavements, dilution factors width of water courses, surface areas of pavements and roofs, etc. The original method described in Kraaij and Verstappen (1995) gives the possibility to adjust for sorption of the substance. As sorption to pavements is disputable it was decided not to take this into account.

Table B-2 *Default settings scenarios 'paved areas'.*

Parameter	**Symbol**	**Unit**	**Value**
Rain intensity, worst case situation	i_{rain}	[m]	0.007
Discharge coefficient roof	w_{roof}	[-]	0.9
Discharge coefficient pavement	w_{pavem}	[-]	0.8
Dilution factor for stagnant surface water	$DILUTION_{ss}$	[-]	3
Dilution factor for large surface water with low flow	$DILUTION_{ls}$	[-]	10
Fraction treated area	F_{treat}	[-]	0.9

Table B-3 *Defaults for calculating the Predicted Environmental Concentration due to direct run-off.*

Parameter	**Symbol**	**Unit**	**Value**
Model width of paved quay	$WIDTH_{d}$	[m]	4
Width of city water course	$WIDTH_{water\ d}$	[m]	10
Depth of city water course	$DEPTH_{water\ d}$	[m]	1.5

Table B-4 *Default settings for model towns.*

Parameter	**Symbol**	**Unit**	**Value**
Surface of roofs in model town (Lelystad)	$AREAroofs_L$	[m^2]	$1.2.10^6$
Surface of pavements (excl. roofs) in model town (Lelystad)	$AREApavem_L$	[m^2]	$3.0.10^6$
Surface of roofs in model town (Raamsdonk-Dorp)	$AREAroofs_R$	[m^2]	$3.83.10^3$
Surface of pavements (excl. roofs) in model town (Raamsdonk-Dorp)	$AREApavem_R$	[m^2]	$7.77.10^3$
Surface of roofs in model town (Dongemond)	$AREAroofs_D$	[m^2]	$1.82.10^6$
Surface of pavements (excl. roofs) in model town (Dongemond)	$AREApavem_D$	[m^2]	$3.69.10^6$

Table B-5 *Default settings for calculating concentrations in surface water after discharge through a STP connected to a mixed sewage system.*

Parameter	**Symbol**	**Unit**	**Value**
Fraction dry weather in spring campaign	F_{dry}	[-]	0.1
Daily dry weather flow in STP	DWA_{day}	[m^3.d^{-1}]	16,000
Fraction dry weather discharge during storm event	F_{DWA}	[-]	0.1
Fraction of time for dry weather discharge	$Ftime_{DWA}$	[-]	0.33

1-A) Direct run-off to surface water

Direct discharge of pesticides to surface water may take place in urban areas by run-off of paved quays to canals. In the standardised water course (a canal in the city) instantaneous and complete mixing is assumed. Possible dilution by rain water is considered to be negligible.

Model for calculating concentrations in surface water after direct run-off.

$$Cwater_{au} = \frac{DOSE_{pest} \cdot WIDTH_{d} \cdot w_{pavem}}{WIDTH_{water\ d} \cdot DEPTH_{water\ d}} \qquad \text{(P-19)}$$

Input			
$DOSE_{pest}$	single dosage of pesticide	$[kg_c.m^{-2}]$	S
w_{pavem}	discharge coefficient pavement	[-]	D
$WIDTH_d$	model width of paved quay	[m]	D
$WIDTH_{water\ d}$	width of city water course	[m]	D
$DEPTH_{water\ d}$	depth of city water course	[m]	D
Output			
$Cwater_{au}$	water concentration for amenity use scenario	$[kg_c.m^{-3}]$	O

It should be noted that the additional dilution of the water volume in city water by the rain event is not taken into account, because it is small (less than 1% for a rain event of 7 mm).

1-B) Discharge through rain water overflow of a separated sewer system

About 24% of the sewer systems in The Netherlands consist of separate channels for rain water and waste water. As model town, the city of Lelystad is considered representative.

Model for calculating concentrations in surface water after discharge through rain water overflow of a separated sewer system.

$$V_{rain} = i_{rain} \cdot AREAroofs_L \cdot w_{roof} + i_{rain} \cdot AREApavem_L \cdot w_{pavem} \qquad \text{(P-20)}$$

$$AREAtreat_L = F_{treat} \cdot AREApavem_L \qquad \text{(P-21)}$$

$$C_{rainflow} = \frac{DOSE_{pest} \cdot AREAtreat_L \cdot w_{pavem}}{V_{rain}} \qquad \text{(P-22)}$$

$$Cwater_{au} = \frac{C_{rainflow}}{DILUTION_{ss}} \qquad \text{(P-23)}$$

Input			
$DOSE_{pest}$	single dosage of pesticide	$[kg_c.m^{-2}]$	S
V_{rain}	volume of rain flowing into separated sewage system	$[m^3]$	O^c
i_{rain}	rain intensity, worst case situation	[m]	D
$AREAroofs_L$	surface of roofs in model town (Lelystad)	$[m^2]$	D
$AREApavem_L$	surface of pavements (excl. roofs) in model town (Lelystad)	$[m^2]$	D
w_{roof}	discharge coefficient roof	[-]	D
w_{pavem}	discharge coefficient pavement	[-]	D
$AREAtreat_L$	treated area of pavements in model town (Lelystad)	$[m^2]$	O^c
$C_{rainflow}$	concentration in discharged rain water	$[kg_c.m^{-3}]$	O^c
F_{treat}	fraction treated area	[-]	D
$DILUTION_{ss}$	dilution factor for stagnant surface water	[-]	D
Output			
$Cwater_{au}$	water concentration for amenity use scenario	$[kg_c.m^{-3}]$	O

In a separated system the whole volume of rain is directly discharged into surface water. In the receiving surface water instantaneous and complete mixing is assumed.

1-C) Discharge through overflow of a mixed sewage system

The remaining 76% of sewer systems in The Netherlands consist of a mixed system, indicating that rain water and waste water are combined. The town of Raamsdonk-dorp is taken a representative community.

Model for calculating concentrations in surface water after discharge through overflow of a mixed sewage system.

$$V_{rain} = i_{rain} \cdot AREAroofs_R \cdot w_{roof} + i_{rain} \cdot AREApavem_R \cdot w_{pavem} \qquad \text{(P-24)}$$

$$AREAtreat_R = F_{treat} \cdot AREApavem_R \qquad \text{(P-25)}$$

$$C_{rainflow} = \frac{DOSE_{pest} \cdot AREAtreat_R \cdot w_{pavem}}{V_{rain}} \qquad \text{(P-26)}$$

$$Cwater_{au} = \frac{C_{rainflow}}{DILUTION_{ss}} \qquad \text{(P-27)}$$

Input			
$DOSE_{pest}$	single dosage of pesticide	$[kg_c.m^{-2}]$	S
V_{rain}	volume of rain flowing into separated sewage system	$[m^3]$	O
i_{rain}	rain intensity, worst case situation	[m]	D
$AREAroofs_R$	surface of roofs in model town (Raamsdonk-Dorp)	$[m^2]$	D
$AREApavem_R$	surface of pavements (excl. roofs) in model town (Raamsdonk-Dorp)	$[m^2]$	D
w_{roof}	discharge coefficient roof	[-]	D
w_{pavem}	discharge coefficient pavement	[-]	D
F_{treat}	fraction treated area	[-]	D
$AREAtreat_R$	treated area of pavements in model town (Raamsdonk-Dorp)	$[m^2]$	O
$C_{rainflow}$	concentration in discharged rain water	$[kg_c.m^{-3}]$	O
$DILUTION_{ss}$	dilution factor for stagnant surface water	[-]	D
Output			
$Cwater_{au}$	water concentration for amenity use scenario.	$[kg_c.m^{-3}]$	O

1-D) Discharge through an STP connected to a mixed sewage system.

About 76% of the sewer systems is based on a mixed system (see 1-C). In this scenario discharge into the STP is considered. The sewage system of the town of Dongemond is considered representative for this situation. The effluent of the STP is discharged into a bigger canal taking into account a dilution factor of 10. Model for calculating concentrations in surface water after discharge through an STP connected to a mixed sewage system.

$$V_{rain} = i_{rain} \cdot AREAroofs_D \cdot w_{roof} + i_{rain} \cdot AREApavem_D \cdot w_{pavem} \tag{P-28}$$

$$AREAtreat_D = F_{treat} \cdot AREApavem_D \cdot F_{DWA} \tag{P-29}$$

$$C_{rainflow} = \frac{DOSE_{pest} \cdot AREAtreat_D \cdot w_{pavem}}{V_{rain}} \tag{P-30}$$

$$DWA = DWA_{day} \cdot F_{dry} \cdot Ftime_{DWA} \tag{P-31}$$

$$C_{infl} = \frac{C_{rainflow} \cdot V_{rain}}{V_{rain} + DWA_{day}} \tag{P-32}$$

$$Cwater_{au} = C_{infl} \cdot \frac{1 - Fpur_{pest}}{DILUTION_{ls}} \tag{P-33}$$

Input			
$DOSE_{pest}$	single dosage of pesticide	$[kg_c.m^{-2}]$	S
V_{rain}	volume of rain flowing into separated sewage system	$[m^3]$	O
i_{rain}	rain intensity, worst case situation	[m]	D
$AREAroofs_D$	surface of roofs in model area (Dongemond)	$[m^2]$	D
$AREApavem_D$	surface of pavements (excl. roofs) in model area (Dongemond)	$[m^2]$	D
w_{roof}	discharge coefficient roof	[-]	D
w_{pavem}	discharge coefficient pavement	[-]	D
F_{treat}	fraction treated area	[-]	D
F_{dry}	fraction dry weather in spring campaign	[-]	D
$AREAtreat_D$	treated area of pavements in model area (Dongemond)	$[m^2]$	O
$C_{rainflow}$	concentration in discharged rain water	$[kg_c.m^{-3}]$	O
DWA_{day}	daily dry weather flow of STP	$[m^3.d^{-1}]$	D
F_{DWA}	fraction dry weather discharge during storm event	[-]	D
$Ftime_{DWA}$	fraction of time for dry weather discharge	[d]	D
DWA	dry weather flow in model area	$[m^3.d^{-1}]$	O
C_{infl}	influent concentration STP	$[kg_c.m^{-3}]$	O
$Fpur_{pest}$	purification factor STP	[-]	S
$DILUTION_{ls}$	dilution factor for large surface water with low flow	[-]	D
Output			
$Cwater_{au}$	water concentration for amenity use scenario	$[kg_c.m^{-3}]$	O

2 Plantings

For public plantings three cases of surface water contamination can be considered:

A) drift
B) run-off (not implemented)
C) leaching (not implemented).

The emission routes B) and C) are not yet implemented because the expected concentrations related to these routes are considered negligible compared to drift input.

Table B-6 *Default settings for calculating concentrations in surface water in plantings.*

Parameter	**Symbol**	**Unit**	**Value**
Fraction treated area	$Ftreat_p$	[-]	0.5
Fraction drift	$Fdrift_p$	[-]	0.01
Depth of city water course	$DEPTH_{water\ p}$	[m]	0.25

2-A) Drift in plantings

Plantings in the amenity use sector are including bare terrains, parks, sport field, lawns, etc. It is assumed that instantaneous and complete mixing takes place in the receiving surface water bodies.

Model for calculating concentrations in surface water after drift in plantings.

$$Cwater_{au} = \frac{DOSE_{pest} \cdot Ftreat_p \cdot Fdrift_p}{DEPTH_{water\ p}} \tag{P-34}$$

Input			
$DOSE_{pest}$	single dosage of pesticide	$[kg_c.m^{-2}]$	S
$Ftreat_p$	fraction treated area	[-]	D
$Fdrift_p$	fraction drift	[-]	D
$DEPTH_{water\ p}$	depth of city water course	[m]	D
Output			
$Cwater_{au}$	water concentration for amenity use scenario	$[kg_c.m^{-3}]$	O

4 Water courses

The term water courses in this respect is reserved for:

- water containing water courses and ponds
- ditch bottoms of temporary dry water courses
- ditch slopes.

For the contamination of surface water after application of pesticides to water courses again the distinction in the three routes is assumed:

A) drift
B) run-off (not implemented)
C) leaching (not implemented).

The same considerations are valid for not taking into account the routes B) and C) as accounted for in plantings. The amount of contamination is considered to be negligible compared to drift.

Table B-7 *Default settings for calculating concentrations in surface water after leaching from water courses.*

Parameter	Symbol	Unit	Value
Depth of city water course	$DEPTH_{water\ w}$	[m]	0.25
Fraction drift	$Fdrift_w$	[-]	0.1

4-A) Drift and direct application to water courses

This scenario is used for spray drift occurring during treatment of ditch slopes but can also be used for direct application to water. Direct application to water bodies occurs in the case of excessive plant growth to ensure sufficient water flow capacity.

If direct application to water course is "yes" then $Fdrift_w = 1$

$$Cwater_{au} = \frac{DOSE_{pest} \cdot Fdrift_w}{DEPTH_{water\ w}} \qquad \text{(P-35)}$$

Input

-	direct application to water course?	[yes/no]	P
$DOSE_{pest}$	single dosage of pesticide	[$kg_c.m^{-2}$]	S
$Fdrift_w$	fraction drift	[-]	D
$DEPTH_{water\ w}$	depth of city water course	[m]	D

Output

$Cwater_{au}$	water concentration for amenity use scenario	[$kg_c.m^{-3}$]	O

5 Paved dike bodies and slopes.

Concerning the application of pesticides to paved dike bodies and slopes a distinction is made for large flowing waters and small ditches. The difference is considered by a different depth. As contaminating processes only drift and run-off are taken into account.

A) Drift to large surface water
B) Drift to small surface water
C) Run-off to large surface water
D) Run-off to small surface water

Table B-8 *Default settings for scenarios 'paved dike bodies and slopes'.*

Parameter	**Symbol**	**Unit**	**Value**
General			
Fraction surface application - if spotwise application (SPOT = yes) - if full application (SPOT = no)	$Ftreat_s$	[-]	 0.1 1
Fraction drift	$Fdrift_s$	[-]	0.1
Width of paved dike or slope	$WIDTH_s$	[m]	4
Scenario 5-A			
Depth of city water course	$DEPTH_{water\ s1}$	[m]	2
Scenario 5-B			
Depth of small water course	$DEPTH_{water\ s2}$	[m]	0.25
Scenario 5-C			
Width of receiving surface water (large river)	$WIDTH_{water\ s3}$	[m]	10
Depth of water (large river)	$DEPTH_{water\ s3}$	[m]	2
Scenario 5-D			
Width of receiving surface water (small river)	$WIDTH_{water\ s4}$	[m]	2
Depth of water (small river)	$DEPTH_{water\ s4}$	[m]	0.25

5-A) Drift to large surface water

Model for calculating concentrations in large surface water after drift.

$$Cwater_{au} = \frac{DOSE_{pest} \cdot Fdrift_{s} \cdot Ftreat_{s}}{DEPTH_{water\ s1}} \tag{P-36}$$

Input			
$DOSE_{pest}$	single dosage of pesticide	$[kg_c.m^{-2}]$	S
SPOT	spotwise application	[yes/no]	P
$Ftreat_s$	fraction surface application	[-]	O
$Fdrift_s$	fraction drift	[-]	D
$DEPTH_{water\ s1}$	depth of city water course	[m]	D
Output			
$Cwater_{au}$	water concentration for amenity use scenario	$[kg_c.m^{-3}]$	O

5-B) Drift to small surface water

Model for calculating concentrations in small surface water after drift.

$$Cwater_{au} = \frac{DOSE_{pest} \cdot Fdrift_{s} \cdot Ftreat_{s}}{DEPTH_{water\ s2}} \tag{P-37}$$

Input			
$DOSE_{pest}$	single dosage of pesticide	$[kg_c.m^{-2}]$	S
SPOT	spotwise application	[yes/no]	P
$Ftreat_s$	fraction surface application	[-]	O
$Fdrift_s$	fraction drift	[-]	D
$DEPTH_{water\ s2}$	depth of small water course	[m]	D
Output			
$Cwater_{au}$	water concentration for amenity use scenario	$[kg_c.m^{-3}]$	O

5-C) Run-off to large surface waters

Model for calculating concentrations in large surface water.

$$Cwater_{au} = \frac{DOSE_{pest} \cdot Ftreat_{s} \cdot WIDTH_{s}}{WIDTH_{water\ s3} \cdot DEPTH_{water\ s3}} \qquad \text{(P-38)}$$

Input			
$DOSE_{pest}$	single dosage of pesticide	$[kg_c.m^{-2}]$	S
SPOT	spotwise application	[yes/no]	P
$Ftreat_s$	fraction treated area	[-]	O
$WIDTH_s$	width of paved dike or slope	[m]	D
$WIDTH_{water\ s3}$	width of receiving surface water (large river)	[m]	D
$DEPTH_{water\ s3}$	depth of water (large river)	[m]	D
Output			
$Cwater_{au}$	water concentration for amenity use scenario	$[kg_c.m^{-3}]$	O

5-D) Run-off to small surface waters

Model for calculating concentrations in small surface water.

$$Cwater_{au} = \frac{DOSE_{pest} \cdot Ftreat_{s} \cdot WIDTH_{s}}{WIDTH_{water\ s4} \cdot DEPTH_{water\ s4}} \qquad \text{(P-39)}$$

Input			
$DOSE_{pest}$	single dosage of pesticide	$[kg_c.m^{-2}]$	S
SPOT	spotwise application	[yes/no]	P
$Ftreat_s$	fraction treated area	[-]	O
$WIDTH_s$	width of paved dike or slope	[m]	D
$WIDTH_{water\ s4}$	width of receiving surface water (small river)	[m]	D
$DEPTH_{water\ s4}$	depth of water (small river)	[m]	D
Output			
$Cwater_{au}$	water concentration for amenity use scenario	$[kg_c.m^{-3}]$	O

III.4.8. Non-agricultural pesticides (biocidesUC=39)

There is no general input-output table for this sub module due to the diversity of the possible inputs and outputs.

The scenarios that have been implemented are already mentioned in Section III.3.6.

Table C-1 *General defaults.*

Parameter	**Symbol**	**Unit**	**Value**
Concentration of suspended matter in surface water	$SUSP_{water}$	$[kg_{dwt}.m^{-3}]$	0.015 [a]

[a] Already defined in regional distribution sub module.

Product-type1: Human hygiene biocidal products

III.4.8.1. Private use of human hygiene biocidal products

Model for calculating concentrations in the municipal STP and surface water of biocides used in products like deodorants, antiperspirants, anti-dandruff shampoos, skin antiseptics, antimicrobial soaps and products to combat acne. It is possible to perform the calculations on A) the annual tonnage of the substance in the EU or in the region (if known), and B) the average consumption per inhabitant or C) the average consumption per application. For the average consumptions the average amounts may be entered by volume or by weight. The content may be entered as weight per volume or as weight per weight. The scenarios based on average consumption should be carried out for every product in which the specific biocide is applied.

A) Annual tonnage

$$\boldsymbol{TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE} \qquad \text{(P-40)}$$

$$\boldsymbol{Elocal_{water} = TONNAGEreg \cdot Fmainsource_4 \cdot F_{4,water} \cdot \frac{365}{Temission_4}} \qquad \text{(P-41)}$$

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
$Fmainsource_4$	fraction of the main source (local STP)	[-]	D
$F_{4,water}$	fraction released to wastewater	[-]	D
$Temission_4$	number of emission days	[d]	D
Output			
$Elocal_{water}$	local emission to waste water during episode	[kg$_c$.d^{-1}]	O

Table C-2 *Default settings for calculating concentrations in the STP and surface water of compounds used in human hygiene products, based on annual tonnage*

Parameter	**Symbol**	**Unit**	**Value**
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1
Fraction of the main source (local STP)	$Fmainsource_4$	[-]	0.002
Fraction released to wastewater	$F_{4,water}$	[-]	1
Number of emission days	$Temission_4$	[d]	365

B) Average consumption per inhabitant

B1) Consumption by volume and content by weight per volume

$$\boldsymbol{Elocal_{water} = Nlocal \cdot F_{4,water} \cdot Vform_{inh} \cdot Cform_{volume} \cdot Fpenetr} \qquad \text{(P-42)}$$

B2) Consumption by volume and content by weight per weight

$$\boldsymbol{Elocal_{water} = Nlocal \cdot F_{4,water} \cdot Vform_{inh} \cdot RHOform \cdot Cform_{weight} \cdot Fpenetr} \qquad \text{(P-43)}$$

B3) Consumption by weight and content by weight per weight

$$Elocal_{water} = Nlocal \cdot F_{4,water} \cdot Qform_{inh} / RHOform \cdot Cform_{volume} \cdot Fpenetr \qquad \text{(P-44)}$$

B4) Consumption by weight and content by weight per volume

$$Elocal_{water} = Nlocal \cdot F_{4,water} \cdot Qform_{inh} \cdot Cform_{weight} \cdot Fpenetr \qquad \text{(P-45)}$$

C) Average consumption per application

C1) Consumption by volume and content by weight per volume

$$Elocal_{water} = Nlocal \cdot Nappl \cdot Finh \cdot F_{4,water} \cdot Vform_{appl} \cdot Cform_{volume} \cdot Fpenetr \qquad \text{(P-46)}$$

C2) Consumption by volume and content by weight per weight

$$Elocal_{water} = Nlocal \cdot Nappl \cdot Finh \cdot F_{4,water} \cdot Vform_{appl} \cdot RHOform \cdot Cform_{weight} \cdot Fpenetr \qquad \text{(P-47)}$$

C3) Consumption by weight and content by weight per weight

$$Elocal_{water} = Nlocal \cdot Nappl \cdot Finh \cdot F_{4,water} \cdot Qform_{appl} / RHOform \cdot Cform_{volume} \cdot Fpenetr \qquad \text{(P-48)}$$

C4) Consumption by weight and content by weight per volume

$$Elocal_{water} = Nlocal \cdot Nappl \cdot Finh \cdot F_{4,water} \cdot Qform_{appl} \cdot Cform_{weight} \cdot Fpenetr \qquad \text{(P-49)}$$

Input			
Nlocal	number of inhabitants feeding one STP	[eq]	D
$F_{4,water}$	fraction released to wastewater	[-]	D
$Cform_{volume}$	active substance in product	[$kg_c.m^{-3}$]	S
$Cform_{weight}$	active substance in product	[$kg.kg^{-1}$]	S
-	type of product	[-]	P
$Vform_{inh}$	consumption per inhabitant	[$l.d^{-1}$]	O
$Qform_{inh}$	consumption per inhabitant	[$kg.d^{-1}$]	O
$Vform_{appl}$	consumption per application	[l]	O
$Qform_{appl}$	consumption per application	[kg]	O
Nappl	number of applications	[-]	O
Finh	fradtion of inhabitants using the product	[-]	O
Fpenetr	penetration factor of disinfectant	[-]	D
RHOform	specific density of product	[$kg.m^{-3}$]	D
Output			
$Elocal_{water}$	local emission to waste water during episode	[$kg_c.d^{-1}$]	O

Table C-3 *Default settings for calculating concentrations in the STP and surface water of compounds used in human hygiene products, based on average consumption*

Parameter	**Symbol**	**Unit**	**Value**
Number of inhabitants feeding one STP	Nlocal	[eq]	10,000[a]
Fraction released to wastewater	$F_{4,water}$	[-]	1
Average consumption per inhabitant per day	$Vform_{inh}$ / $Qform_{inh}$	[$m^3.d^{-1}$] /[$kg.d^{-1}$]	
- anti-dandruff shampoo			-
- anti-perspirants/deodorants, aerosol			-
- anti-perspirants/deodorants, stick/roll-on			-
- creams			-
- mouth wash			-
Average consumption per inhabitant per day	$Vform_{appl}$ / $Qform_{appl}$	[$10^{-3}m^3$] /[kg]	
- anti-dandruff shampoo			0.0120[b]
- anti-perspirants/deodorants, aerosol			0.0030[b]
- anti-perspirant/deodorants, stick/roll-on			0.0005[b]
- creams			0.0008[e]
- mouth wash			0.0100
Number of applications per day	Nappl	[d^{-1}]	
- anti-dandruff shampoo			0.71[c]
- anti-perspirants/deodorants, aerosol			2.00[d]
- anti-perspirant/deodorants, stick/roll-on			1.00[b]
- creams			2.00[e]
- mouth wash			3.00
Fraction of inhabitants using the product	Finh	[-]	
- anti-dandruff shampoo			0.10
- anti-perspirants/deodorants, aerosol			0.20
- anti-perspirant/deodorants, stick/roll-on			0.80
- creams			0.10
- mouth wash			0.05
Penetration factor of disinfectant	Fpenetr	[-]	0.5
Specific density of product	RHOform	[$kg.m^{-3}$]	1,000

[a] already defined in the sewage treatment distribution sub module
[b] TGD (EC, 1996a)
[c] TGD: 2-7 times per week; default 5 times per week = 0.71 times per day
[d] TGD: 1-3 times per day
[e] Data from the TGD for facial cream: 1-2 times per day

III.4.8.2. Industrial use of human hygiene biocidal products

Model for calculating concentrations in the municipal STP and surface water of biocides used in products like skin antiseptics, antimicrobial soaps and products for health care personnel handwash. It is possible to perform the calculations on A) the annual tonnage of the substance in the EU or in the region (if known), and B) the average consumption per inhabitant or C) the average consumption per application. For the average consumptions the average amounts may be entered by volume or by weight.The content may be entered as weight per volume or as weight per weight.

A) Annual tonnage

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \qquad \text{(P-50)}$$

$$Elocal_{water} = TONNAGEreg \cdot Fmainsource_3 \cdot F_{3,water} \cdot \frac{365}{Temission_3} \qquad \text{(P-51)}$$

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
$Fmainsource_3$	fraction of the main source (local STP)	[-]	D
$F_{3,water}$	fraction released to wastewater	[-]	D
$Temission_3$	number of emission days	[d]	D
Output			
$Elocal_{water}$	local emission to waste water during episode	[kg$_c$.d^{-1}]	O

Table C-4 *Default settings for calculating concentrations in the STP and surface water of compounds used in industrial use of human hygiene products, based on annual tonnage*

Parameter	Symbol	Unit	Value
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1
Fraction of the main source (local STP)	$Fmainsource_3$	[-]	0.007
Fraction released to wastewater	$F_{3,water}$	[-]	1
Number of emission days	$Temission_3$	[d]	365

B) Average consumption per bed

$$Elocal_{water} = Nbeds_{pres} \cdot Qsubst_{pres\_bed} \cdot F_{3,water} \qquad \text{(P-52)}$$

$$Elocal_{water} = Nbeds_{occup} / Foccup \cdot Qsubst_{pres\_bed} \cdot F_{3,water} \qquad \text{(P-53)}$$

C) Consumption per application

$$Elocal_{water} = Nbeds_{pres} \cdot Foccup \cdot Qsubst_{occup\_bed} \cdot F_{3,water} \qquad \text{(P-54)}$$

$$Elocal_{water} = Nbeds_{occup} \cdot Qsubst_{occup\_bed} \cdot F_{3,water} \qquad \text{(P-55)}$$

Input

$Nbeds_{pres}$	number of beds in model hospital	[-]	D
Foccup	occupancy rate	[-]	D
$Nbeds_{occup}$	number of occupied beds in model hospital	[-]	D
$F_{3,water}$	fraction released to wastewater	[-]	D
-	specification of type of active ingredient used	[-]	P
$Qsubst_{pres\_bed}$	consumption of active ingredient per bed	[kg.d^{-1}]	O
-	specification of type of active ingredient used	[-]	P
$Qsubst_{occup\_bed}$	consumption of active ingredient per occupied bed	[kg.d^{-1}]	O

Output

$Elocal_{water}$	local emission to waste water during episode	[kg$_c$.d^{-1}]	O

Table C-5 *Default settings for calculating concentrations in the STP and surface water of compounds used in industrial use of human hygiene products, based on average consumption*

Parameter	**Symbol**	**Unit**	**Value**
Number of beds in model hospital	$Nbeds_{pres}$	[-]	400
Occupancy rate	Foccup	[-]	0.75
Number of occupied beds in hospital	$Nbeds_{occup}$	[-]	300
Consumption of active ingredient per bed	$Qsubst_{pres\_bed}$	[kg.d^{-1}]	
- alcohols			$1.5.10^{-2}$
- quarternairy ammonium compounds			$4.0.\ 10^{-6}$
- guanides			$1.5.\ 10^{-5}$
- compounds splitting off oxygen			$3.8.\ 10^{-5}$
- compounds splitting off halogen			$1.0.\ 10^{-4}$
- others			$3.8.\ 10^{-5}$
Consumption of active ingredient per bed	$Qsubst_{pres\_bed}$	[kg.d^{-1}]	
- alcohols			$2.0.10^{-2}$
- quarternairy ammonium compounds			$5.0.\ 10^{-6}$
- guanides			$2.0.\ 10^{-5}$
- compounds splitting off oxygen			$5.0.\ 10^{-5}$
- compounds splitting off halogen			$1.3.\ 10^{-4}$
- others			$5.0.\ 10^{-5}$
Fraction released to waste water	$F_{3,water}$	[-]	1

Product-type2: Private area and public health area disinfectants and other biocidal products

Swimming pools

III.4.8.3. Discharge of swimming water by public swimming pools in the sewage system (acute and chronic)

Model for calculating concentrations in the municipal STP and surface water of compounds/metabolites/reaction products used or formed in swimming water. The user must specify whether the discharge is 'acute' (the whole pool is emptied completely in the STP) or 'chronic' (a fixed amount of water per visitor is discharged).

'acute' situation (the 1 in the formula is one day of the emission episode)

$$\boldsymbol{Elocal_{water}} = \frac{\boldsymbol{AREA_{swimw} \cdot DEPTH_{swimw} \cdot C_{swimw}}}{\mathbf{1}} \qquad \text{(P-56)}$$

'chronic' situation (the 1 in the formula is one day of the emission episode)

$$\boldsymbol{Elocal_{water}} = \frac{\boldsymbol{N_{visit} \cdot Q_{repl} \cdot C_{swimw}}}{\mathbf{1}} \qquad \text{(P-57)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{swimw,ac}$ $Temission_{swimw,chr}$	[d] [d]	2 300

Input

$AREA_{swimw}$	water surface	[m^2]	D
$DEPTH_{swimw}$	average depth of water	[m]	D
N_{visit}	number of visitors per day	[-]	D
C_{swimw}	concentration in swimming water	[$kg_c.m^{-3}$]	S
Q_{repl}	water replaced per visitor	[m^3]	D
$Temission_{swimw,ac}$	number of emission days 'acute'	[d]	D
$Temission_{swimw,chr}$	number of emission days 'acute'	[d]	D

Output

$Elocal_{water}$	local emission to waste water during episode	[$kg_c.d^{-1}$]	O
Temission	number of emission days	[d]	O

Table C-6 *Default settings for calculating concentrations in the STP and surface water of compounds, metabolites and reaction products used or formed in swimming water.*

Parameter	**Symbol**	**Unit**	**Value**
Water surface	$AREA_{swimw}$	[m^2]	440
Average depth of water	$DEPTH_{swimw}$	[m]	1.8
Number of visitors per day	N_{visit}	[-]	400
Water replaced per visitor	Q_{repl}	[m^3]	0.05

Note 1 USES 4.0 was not designed to assess degradation and/or reaction products. If a substance like chloroform has to be assessed the concentration of chloroform in the swimming water should be entered at C_{swimw} together with the toxicity data and all the other parameters for chloroform.

Note 2 Volatilisation of compounds/degradation and or reaction products is not taken into consideration, because it is assumed that the concentration of the compounds in the waste water of the swimming pools will be low. Therefore, the role of volatilisation will be of minor importance.

III.4.8.4. Acute discharge of swimming water by public and private swimming pools into the surface water

Model for calculating concentrations in the surface water for compounds used or formed in swimming water for 'acute' situations (at release of the whole pool capacity).

If *POOLTYPE* = 'public':

$$Cwater_{pest\text{-}1\,appl} = \frac{C_{swimw}}{DILUTION_{public}} \qquad \text{(P-58)}$$

If *POOLTYPE* = 'private':

$$Cwater_{pest\text{-}1\,appl} = \frac{C_{swimw}}{DILUTION_{private}} \qquad \text{(P-59)}$$

The concentration in surface water during the required time periods is calculated using the same equations as described in Section III.4.9.3. The peak concentration is converted into a dosage as required by SLOOT.BOX model.

$$DOSE_{pest} = Cwater_{pest\text{-}1\,appl} \cdot DEPTH_{ditch} \qquad \text{(P-60)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
F_{drift}	-	[-]	1
$T_{interval}$	-	[d]	1
N_{appl}	-	[-]	1

Input			
POOLTYPE	type of swimming pool	[public/private]	P
C_{swimw}	concentration in swimming water	$[kg_c.m^{-3}]$	S
$DILUTION_{public}$	dilution factor of receiving surface water public pools	[-]	D
$DILUTION_{private}$	dilution factor of receiving surface water private pools	[-]	D
$DEPTH_{ditch}$	depth of ditch	[m]	D
$Cwater_{pest\text{-}1\ appl}$	peak concentration in surface water	$[kg_c.m^{-3}]$	O^c
Output			
$DOSE_{pest}$	single dosage of pesticide	$[kg_c.m^{-2}]$	O
F_{drift}	fraction of dosage to surface water	[-]	O^c
$T_{interval}$	application interval	[d]	O^c
N_{appl}	number of applications in one year	[-]	O^c

Table C-7 *Default settings for dilution factor of receiving surface water.*

Parameter	**Symbol**	**Unit**	**Value**
Dilution factor for public swimming pools	$DILUTION_{public}$	[-]	4
Dilution factor for private swimming pools	$DILUTION_{private}$	[-]	2
Depth of ditch	$DEPTH_{ditch}$	[m]	0.30 [a]

[a] already defined in distribution module for pesticides.

Sanitary sector

III.4.8.5. Formulation of washing powders and liquid cleaning products

Model calculations for the stage of formulation of washing powders and liquid cleaning products are based on the annual tonnage applied. The default values for the emission factors are derived from the emission scenario document for industrial categories 5 and 6 in the TGD. Table C-9 presents the default values for the establishment of the size of the point source, which are based on the generic B-tables of the TGD and EUSES for industrial categories 5 and 6.

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \tag{P-61}$$

$$Elocal_{water} = TONNAGEreg \cdot Fmainsource_2 \cdot F_{2,water} \cdot \frac{365}{Temission_2} \tag{P-62}$$

$$Elocal_{air} = TONNAGEreg \cdot Fmainsource_2 \cdot F_{2,air} \cdot \frac{365}{Temission_2} \tag{P-63}$$

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
HPVC	code to specify whether a substance is a HPVC or not	[yes/no]	P
$Fmainsource_2$	fraction of the main source (local STP)	[-]	O
$Temission_2$	number of emission days	[d]	O
$F_{2,water}$	fraction released to wastewater	[-]	D
$F_{2,air}$	fraction released to air	[-]	D
Output			
$Elocal_{water}$	local emission to waste water during episode	[$kg_c.d^{-1}$]	O
$Elocal_{air}$	local emission to waste water during episode	[$kg_c.d^{-1}$]	O

Table C-8 *Default settings for calculating concentrations in the STP and surface water of compounds used in human hygiene products*

Parameter	**Symbol**	**Unit**	**Value**
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1
Fraction of the main source	$Fmainsource_4$	[-]	Table C-9
Fraction released to wastewater	$F_{2,water}$	[-]	0.0009
Fraction released to air	$F_{2,air}$	[-]	0.00002
Number of emission days	$Temission_4$	[d]	Table C-9

Table C-9 *Fraction of the main source, $Fmainsource_2$ [-], and the number of emission days, $Temission_2$ [d], for the formulation stage of general purpose and lavatory cleaners based on the corrected regional tonnage, $TONNAGEreg_{form}$ [tonnes .yr^{-1}], of the biocide*

TONNAGEreg	$Fmainsource_2$	$Temission_2$
HPVC = yes		
< 3500	1	300
3500-10,000	0.8	300
10,000-25,000	0.7	300
25,000-50,000	0.6	300
> 50,000	0.4	300
HPVC = no		
< 100	1	2 · Fmainsource · TONNAGEreg
100-500	0.6	Fmainsource · TONNAGEreg
500-1000	0.6	0.5 · Fmainsource · TONNAGEreg
> 1000	0.4	300

* HPVC is the code to specify if the substance is a so-called high production volume chemical

III.4.8.6. Private use of sanitary disinfectants

Parameters/variables for 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 Netherlands, received by a large STP. In USES 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

$$TONNAGEreg = TONNAGEreg \cdot Fprodvol_{reg} \qquad \text{(P-64)}$$

$$Elocal_{water} = TONNAGEreg \cdot Fmainsource_4 \cdot F_{4,water} \cdot \frac{365}{Temission_4} \qquad \text{(P-65)}$$

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
$Fprodvol_{reg}$ fwater	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

$Elocal_{water}$	local emission to wastewater	$[kg_c.d^{-1}]$	O
Temission	number of emission days	[d]	O

Table C-10 *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

$$Elocal_{water} = Nlocal \cdot Vfrom \cdot Cform \cdot Fpenetr \cdot F_{4,water} \qquad \text{(P-66)}$$

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			
$Elocal_{water}$	Emission rate to waste water	[kg.d^{-1}]	O

Table C-11 *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

Horticulture

III.4.8.7. Disinfectants used in horticulture, disinfection of greenhouses in agriculture

In the rather simple model for disinfection of greenhouses the input for the biocide has to be specified as the amount for a single application.

$$Elocal_{air} = \frac{Q_{subst} \cdot (1 - F_{ret}) \cdot (1 - F_{disin})}{1} \qquad \text{(P-67)}$$

(the 1 in the formula is one day of the emission episode)

input

Q_{subst}	amount of active ingredient used	[kg]	S
F_{ret}	fraction of retention in goods	[-]	D
F_{disin}	fraction of disintegration	[-]	D
$Temission_{fogging}$	number of emission days for fogging	[d]	D
Output			
$Elocal_{air}$	local emission to air during episode	[kg.d^{-1}]	O
Temission	number of emission days		

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{fogging}$	[d]	1

Table C-12 *Default settings for calculating releases to air from disinfection of greenhouses in agriculture through fogging*

Parameter	Symbol	Unit	Value
Fraction of retention in goods	F_{ret}	[-]	0.02
Fraction of disintegration	F_{disin}	[-]	0.001

Tiles and surfaces

III.4.8.8. Products used for disinfection of tiles and surfaces

In Annex V to Directive 98/8/EC (EC, 1998) product type 2 is described as "Products used for the disinfection of air, surfaces, materials, equipment and furniture which are not used for direct food or feed contact in private, public and industrial areas, including hospitals, as well as products used as algaecides". For tiles an surfaces we can think of small-scale application at home. It is unclear at this moment if a biocidal product for this purpose is specifically notified for private application on one hand and for industrial use on the other.

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \qquad \text{(P-68)}$$

$$Elocal_{water} = TONNAGEreg \cdot Fmainsource_4 \cdot F_{4,water} \cdot \frac{365}{Temission_4} \qquad \text{(P-69)}$$

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
$Fmainsource_4$	fraction of the main source (local STP)	[-]	D
$F_{4,water}$	fraction released to wastewater	[-]	D
$Temission_4$	number of emission days	[d]	D

Output

$Elocal_{water}$	local emission to waste water during episode	[kg$_c$.d^{-1}]	O

Table C-13 *Default settings for calculating concentrations in the STP and surface water of compounds used disinfection of tiles and surfaces*

Parameter	Symbol	Unit	Value
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1
Fraction of the main source (local STP)	$Fmainsource_4$	[-]	0.002
Fraction released to wastewater	$F_{4,water}$	[-]	1
Number of emission days	$Temission_4$	[d]	365

Medical sector

III.4.8.9. 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

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \qquad \text{(P-70)}$$

$$Elocal_{water} = TONNAGEreg \cdot Fhospital \cdot F_{3,water} \cdot \frac{365}{Temission_3} \qquad \text{(P-71)}$$

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$_{water}$	local emission to waste water during episode	[kg$_c$.d^{-1}]	O

Table C-14 *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	$F_{4,water}$	[-]	0.75
Number of emission days	Temission$_4$	[d]	260

B) Amount of solution used

Sanitary purposes

$$Elocal_{water} = Vcons_{san} \cdot Cproc_{san} \cdot Fsan \qquad \text{(P-72)}$$

Brushes

$$Elocal_{water} = Vcons_{obj} \cdot Cproc_{obj} \cdot Fobj \qquad \text{(P-73)}$$

Sanitary purposes and brushes

$$Elocal_{water} = Vcons_{san} \cdot Cproc_{san} \cdot Fsan + Vcons_{obj} \cdot Cproc_{obj} \cdot Fobj \qquad \text{(P-74)}$$

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	$[m^3d^{-1}]$	D
Output			
$Elocal_{water}$	emission rate to waste water	$[kg.d^{-1}]$	O

Table C-15 *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:

$$TONNAGEreg = 956 \cdot Cproc_{san} \qquad \text{sanitary purposes}$$

$$TONNAGEreg = 1560 \cdot Cproc_{obj} \qquad \text{brushes}$$

$$TONNAGEreg = 956 \cdot Cproc_{san} + 1560 \cdot Cproc_{obj} \qquad \text{sanitary purposes and brushes}$$

III.4.8.10. Disinfection of instruments

Disinfection of instruments like endoscopes – called scopes in most cases – should be done in automated washers/disinfectors (BSG, 1998). The majority of the hospitals with endoscopy units performing several thousands procedures per year use these washers nowadays (Van Gossum et al., 1989). There are two types: 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:

$$Cproc_{carry\_over} = \frac{Cproc}{(1 + Fcarry\_over)^{Tint_{repl}}} \qquad \text{(P-75)}$$

Concentration at day of replacement including conversion:

$$Cproc_{repl} = Cproc_{carry\_over} \cdot e^{-kdeg_{disinf} \cdot Tint_{repl}} \qquad \text{(P-76)}$$

$$Elocal_{water} = Nmax_{mach} \cdot Vproc \cdot Cproc_{repl} \qquad \text{(P-77)}$$

Washers or disinfector, once through

$$Elocal_{water} = Nmax_{mach} \cdot Vproc \cdot Cproc \qquad \text{(P-78)}$$

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			
$Elocal_{water}$	emission rate to waste water	[kg.d^{-1}]	O

Table C-16 *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

$$Tint_{repl} = INT(1/Temission_3 + 0.5) \qquad \text{(P-79)}$$

$$Elocal_{water} = \frac{Qsubst}{Temission_3} \cdot e^{-kdeg_{disinf} \cdot Tint_{repl}} \quad \text{(P-80)}$$

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			
$Elocal_{water}$	emission rate to waste water	[kg.d^{-1}]	O

Table C-17 *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

III.4.8.11. 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

$$Elocal_{water} = Nmach \cdot Qmat \cdot Vform_{kg} \cdot Cform \cdot (1 - Fred) \quad \text{(P-81)}$$

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			
$Elocal_{water}$	emission rate to waste water	[kg.d^{-1}]	O

Table C-18 *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 wahing tube	Qmat	[kg.d^{-1}]	8,000
Concentration reduction in washing process	Fred	[-]	0

Washing machines

$$Elocal_{water} = Nbatch \cdot Qmat \cdot Vform_{kg} \cdot Cform \cdot (1 - Fred) \qquad \text{(P-82)}$$

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			
$Elocal_{water}$	emission rate to waste water	[kg.d^{-1}]	O

Table C-19 *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 wahing tube	Qmat	[kg.d^{-1}]	8,000
Concentration reduction in washing process	Fred	[-]	0

III.4.8.12. Disinfectants for sewage and waste water

$$Clocal_{water} = Clocal_{eff} / DILUTION \qquad \text{(P-83)}$$

Input			
$Clocal_{eff}$	working concentration of the active substance in effluent	[kg.m^{-3}]	S
DILUTION	dilution factor for receiving surface water	[-]	D
Output			
$Clocal_{water}$	concentration in receiving surface water	[kg.m^{-3}]	O

Table C-20 *Default settings for calculating concentrations in surface water of disinfectants used for sewage and wastewater treatment*

Parameter	Symbol	Unit	Value
Dilution factor for receiving surface water	DILUTION	[-]	10

Product type 6: In-can preservatives

III.4.8.13. Washing and cleaning fluids, human hygienic products and cosmetics

Model for calculating concentrations in the municipal STP and surface water of biocides used in products like washing and cleaning fluids as well in deodorants, antiperspirants, shampoos, soaps and similar products. The products will be released to wastewater at the stage of private use or in the case of washing and cleaning fluids for professional use at the stage of industrial use (processing). For diffuse releases from households the standard STP is regarded as the point source for the releases.

It is possible to perform the calculations on A) the annual tonnage of the substance in the EU or in the region (if known), and B) the average consumption per inhabitant or C) the average consumption per application. For the average consumptions the average amounts may be entered by volume or by weight.The content may be entered as weight per volume or as weight per weight. The scenarios based on average consumption should be carried out for every product in which the specific biocide is applied. The data for average consumption are derived from Bremmer and Van Veen (2000) and from the the emission scenario document for industrial categories 5 (Personal/domestic) and 6 (Public domain) in the TGD (EC, 1996). The defaults fraction of inhabitants using the product have been generated by expert judgement

A) Annual tonnage

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \qquad \text{(P-84)}$$

$$Elocal_{water} = TONNAGEreg \cdot Fmainsource_4 \cdot F_{4,water} \cdot \frac{365}{Temission_4} \qquad \text{(P-85)}$$

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
$Fmainsource_4$	fraction of the main source (local STP)	[-]	D
$F_{4,water}$	fraction released to wastewater	[-]	D
$Temission_4$	number of emission days	[d]	D

Output

$Elocal_{water}$	local emission to waste water during episode	[kg$_c$.d^{-1}]	O

Table C-21 *Default settings for calculating concentrations in the STP and surface water of compounds used in human hygiene products and cosmetics*

Parameter	**Symbol**	**Unit**	**Value**
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1
Fraction of the main source (local STP)	$Fmainsource_4$	[-]	0.002
Fraction released to wastewater	$F_{4,water}$	[-]	1
Number of emission days	$Temission_4$	[d]	365

B) Average consumption per inhabitant

B1) Consumption by volume and content by weight per volume

$$\boldsymbol{Elocal_{water} = Nlocal \cdot F_{4,water} \cdot Vform_{inh} \cdot Cform_{volume} \cdot Finh} \tag{P-86}$$

B2) Consumption by volume and content by weight per weight

$$\boldsymbol{Elocal_{water} = Nlocal \cdot F_{4,water} \cdot Vform_{inh} \cdot RHOform \cdot Cform_{weight} \cdot Finh} \tag{P-87}$$

B3) Consumption by weight and content by weight per weight

$$\boldsymbol{Elocal_{water} = Nlocal \cdot F_{4,water} \cdot Qform_{inh} / RHOform \cdot Cform_{volume} \cdot Finh} \tag{P-88}$$

B4) Consumption by weight and content by weight per volume

$$\boldsymbol{Elocal_{water} = Nlocal \cdot F_{4,water} \cdot Qform_{inh} \cdot Cform_{weight} \cdot Finh} \tag{P-89}$$

C) Average consumption per application

C1) Consumption by volume and content by weight per volume

$$\boldsymbol{Elocal_{water} = Nlocal \cdot Nappl \cdot Finh \cdot F_{4,water} \cdot Vform_{appl} \cdot Cform_{volume} \cdot Finh} \tag{P-90}$$

C2) Consumption by volume and content by weight per weight

$$\boldsymbol{Elocal_{water} = Nlocal \cdot Nappl \cdot Finh \cdot F_{4,water} \cdot Vform_{appl} \cdot RHOform \cdot Cform_{weight} \cdot Finh} \tag{P-91}$$

C3) Consumption by weight and content by weight per weight

$$\boldsymbol{Elocal_{water} = Nlocal \cdot Nappl \cdot Finh \cdot F_{4,water} \cdot Qform_{appl} / RHOform \cdot Cform_{volume} \cdot Finh} \tag{P-92}$$

C4) Consumption by weight and content by weight per volume

$$\boldsymbol{Elocal_{water} = Nlocal \cdot Nappl \cdot Finh \cdot F_{4,water} \cdot Qform_{appl} \cdot Cform_{weight} \cdot Finh} \tag{P-93}$$

Input			
Nlocal	number of inhabitants feeding one STP	[eq]	D
$F_{4,water}$	fraction released to wastewater	[-]	D
$Cform_{volume}$	active substance in product	[$kg_c.m^{-3}$]	S
$Cform_{weight}$	active substance in product	[$kg.kg^{-1}$]	S
-	type of product	[-]	P
$Vform_{inh}$	consumption per inhabitant	[$l.d^{-1}$]	O
$Qform_{inh}$	consumption per inhabitant	[$kg.d^{-1}$]	O
$Vform_{appl}$	consumption per application	[l]	O
$Qform_{appl}$	consumption per application	[kg]	O
Nappl	number of applications	[d^{-1}]	O
Finh	fraction of inhabitants using the product	[-]	O
Fpenetr	penetration factor of disinfectant	[-]	D
RHOform	specific density of product	[$kg.m^{-3}$]	D
Output			
$Elocal_{water}$	local emission to waste water during episode	[$kg_c.d^{-1}$]	O

Table C-22 *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	[eq]	10,000[a]
Fraction released to wastewater	$F_{4,water}$	[-]	1
Penetration factor of disinfectant	Fpenetr	[-]	0.5
Specific density of product	RHOform	[kg.m^{-3}]	1,000

[a] already defined in the sewage treatment distribution sub module

Table C-23 *Pick-list for average consumptions per inhabitant per day, $Vform_{inh}$ [$10^{-3}m^3.d^{-1}$] &$Qform_{inh}$ [kg.d^{-1}], per application, $Vform_{appl}$ [.$10^{-3}m^3$] & $Qform_{appl}$ [kg], number of applications, Nappl [d^{-1}], and the fraction of inhabitants using the product, Finh [-].*

Product	**$Vform_{inh}$** **$Qform_{inh}$**	**$Vform_{appl}$** **$Qform_{appl}$**	**Nappl**	**Finh**
Fabric washing				
- washing liquids	0.004			
- auxilliary products	0.0006			
- fabric sinsing products	0.007			
Washing-up liquid				
- hand wah	0.007			
- machine wash	0.0016			
Cosmetics				
- hair conditioner (cream rinse)		0.014	0.2	0.3
- hair conditioner		0.0027	0.75	0.3
- hair gel		0.0029	1	0.2
Permanent wash fluid				
- curling fluid		0.08	0.01	0.1
- fixing fluid		0.0	0.01	0.1
- eye shadow		0.00001	2	0.3
- mascara		0.000025	1	0.2
- eye liner		0.000005	1	0.1
- lipstick, lip oinment		0.0001	4	0.3
Human hygiene products				
- toilet soaps	0.0016			
-shampoo	0.0023			
-shower products		0.005	0.9	0.95
-bath products		0.017	0.2	0.15

Anti-perspirants/deodorants				
- aerosol		0.003	2	0.2
- stick, roll-on		0.0005	1	0.8
Creams				
- general creams		0.001	1.5	0.2
- facial creams		0.0008	2	0.1
- body lotion		0.0075	1.5	0.2
- hand cream		0.0003	2	0.5
Suntan products				
- creams		0.008	2	0.4
- lotions		0.010	2	0.4

III.4.8.14. Paints and coatings

In-can preservatives serve another goal than film preservatives in paints and coatings but the emission pattern will be exactly the same. However, in-can preservatives will only be added to water-based coating products whereas film preservatives may be added to solvent based coating products as well. The stages of the life cycle of interest are the life cycle stages 2 (formulation), 3 (industrial use) and 4 (private use), service life, and life cycle stages 5a (waste treatment), and 5b (recycling). Service life has not been investigated; so, no specific attention is given to this stage in this report. Recycling may be a potential stage for some painted articles (e.g. steel or aluminium) but has not been investigated yet.

Formulation

The TGD includes an emission scenario document for industrial category 14 (Paints, lacquers and varnishes industry). This emission scenario document gives emission factors for several types of industrial paint formulations. The general scenario approach of EUSES can be applied.

$$\boldsymbol{TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE} \qquad \text{(P-94)}$$

$$\boldsymbol{Elocal_{water} = TONNAGEreg \cdot Fmainsource_{2} \cdot F_{2,water} \cdot \frac{365}{Temission_{2}}} \qquad \text{(P-95)}$$

$$\boldsymbol{Elocal_{air} = TONNAGEreg \cdot Fmainsource_{2} \cdot F_{2,air} \cdot \frac{365}{Temission_{2}}} \qquad \text{(P-96)}$$

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
-	type of application/product	[-]	P
VP	vapour pressure	[Pa]	S
SOL	water solubility	[kg.m^{-3}]	S
$F_{2,water}$	fraction released to wastewater	[-]	O
$F_{2,air}$	fraction released to air	[-]	O
HPVC	high production volume chemical	[yes/no]	P
$Fmainsource_2$	fraction of the main local source	[-]	O
$Temission_2$	number of emission days	[d]	O

Output

$Elocal_{water}$	local emission to waste water	[kg$_c$.d^{-1}]	O
$Elocal_{air}$	local emission to waste water	[kg$_c$.d^{-1}]	O

Volatile substances are defined as having a vapour pressure >10 Pa at 23 °C and a water-soluble substances as having a water solubility >1000 mg.l^{-1}.

Table C-24 *Default settings for calculating concentrations in the STP and surface water of compounds used in human hygiene products*

Parameter	Symbol	Unit	Value
Code for high production volume chemical	HPVC	[yes/no]	no
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1

Table C-25 *Emission factors to air $F_{2,air}$ and (waste)water $F_{2,water}$ for the formulation of some types of paint and coating products that are likely to contain in –can preservatives. I = volatile, II =non-volatile & water soluble and II = non-volatile and & non-water soluble*

Type of product/application	I		II		III	
	$F_{2,air}$	$F_{2,water}$	$F_{2,air}$	$F_{2,water}$	$F_{2,air}$	$F_{2,water}$
Furniture	0.010	0.010	0	0.010	0	0.010
Wood lacquer	0.010	0.020	0	0.020	0	0.020
Coil coating	0.010	0	0	0.010	0	0.010
Can coatings general	0.030	0	0	0	0	0
2 piece can external enamel	0.015	0	0	0	0	0
OEM car manufacturing	0.030	0	0	0	0	0
Car refinish	0.030	0	0	0	0	0

The size of the point source for emission estimations at the local scale can be dervied from the B-tables for industrial category 14 of the TGD (EC, 1996). The regional tonnage of the biocide, TONNAGEreg, has to be corrected for the calculation of the fraction of the main source and the number of emission days by deviding it with the concentration of the substance in the formulation $Fchem_{form}$. The resulting tonnage, $TONNAGEreg_{form}$, can be considered as the tonnage formulated in the Netherlands.

Table C-26 *Fraction of the main source, Fmainsource$_2$ [-], and the number of emission days, Temission$_2$ [d], for the formulation stage of paints and coatings with in-can preservatives based on the corrected regional tonnage, TONNAGEreg$_{form}$ [tonnes .yr^{-1}], of the biocide*

TONNAGEreg	**Fmainsource$_2$**	**Temission$_2$**
HPVC* = yes		
< 3500	1	300
3500-10,000	0.8	300
10,000-25,000	0.7	300
25,000-50,000	0.6	300
> 50,000	0.4	300
HPVC* = no		
< 100	1	2 · Fmainsource · TONNAGEreg
100-500	0.6	Fmainsource · TONNAGEreg
500-1000	0.6	0.5 · Fmainsource · TONNAGEreg
> 1000	0.4	300

* HPVC is the code to specify if the substance is a so-called high production volume chemical

Industrial use

Industrial paint application may be carried out by professionals at a relatively small scale and in industries at a variable scale (from small to very large). Paints may be applied, for example, by brush, rollers or spraying. Emissions will vary depending on the way of application and – especially at techniques such as spraying – the abatement techniques applied. As paint application is not a typical biocide application no emission scenarios have been developed specifically. For emission estimation the scenarios for new and existing substances may be applied. In the TGD (EC, 1996) an emission scenario document is found for industrial category 14 (Paints, lacquers and varnishes industry). The emission factors for the relevant paint types are determined analogous to the stage of formulation as are the fraction of the main source and number of emission days.

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \qquad \text{(P-97)}$$

$$Elocal_{water} = TONNAGEreg \cdot Fmainsource_3 \cdot F_{3,water} \cdot \frac{365}{Temission_3} \qquad \text{(P-98)}$$

$$Elocal_{air} = TONNAGEreg \cdot Fmainsource_3 \cdot F_{3,air} \cdot \frac{365}{Temission_3} \qquad \text{(P-99)}$$

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
$Fmainsource_3$	fraction of the main source	[-]	O
$Temission_3$	number of emission days	[d]	O
-	type of product/application	[-]	P
$F_{3,water}$	fraction released to wastewater	[-]	O
$F_{3,air}$	fraction released to air	[-]	O
Output			
$Elocal_{water}$	local emission to waste water	[kg$_c$.d^{-1}]	O
$Elocal_{air}$	local emission to air	[kg$_c$.d^{-1}]	O

Volatile substances are defined as having a vapour pressure >10 Pa at 23 °C and a water-soluble substances as having a water solubility >1000 mg.l^{-1}.

Table C-27 *Default settings for calculating concentrations in the STP and surface water of compounds used in human hygiene products*

Parameter	**Symbol**	**Unit**	**Value**
Fraction for the region	$Fprodvol_{reg}$	[-]	0.1

Table C-28 *Emission factors to air $F_{3,air}$ and (waste)water $F_{3,water}$ for the application of some types of paint and coating products that are likely to contain in –can preservatives. I = volatile, II =non-volatile & water soluble and II = non-volatile and & non-water soluble*

Type of product/application	**I**		**II**		**III**	
	$F_{3,air}$	$F_{3,water}$	$F_{3,air}$	$F_{3,water}$	$F_{3,air}$	$F_{3,water}$
Furniture	0.970	0.010	0	0.030	0	0.030
Wood lacquer	0.920	0.050	0	0.050	0	0.050
Coil coating	0.010	0.010	0	0.010	0	0.010
Can coatings general	0.940	0	0	0	0	0
2 piece can external enamel	0.965	0	0	0	0	0
OEM car manufacturing	0.970	0	0	0	0	0
Car refinish	0.970	0	0	0	0	0.010

* assuming treatment of flue gasses (0.98 if no treatment)

Table C-29 *Fraction of the main source, Fmainsource$_3$ [-], and the number of emission days, Temission$_3$ [d], for the industrial use of paints and coatings with in-can preservatives based on the corrected regional tonnage, TONNAGEreg$_{form}$ [tonnes .yr^{-1}], of the biocide*

TONNAGEreg	**Fmainsource$_3$**	**Temission$_3$**
< 10	0.90	$20 \cdot Fmainsource_3 \cdot TONNAGEreg_{form}$
10-50	0.60	$6.66 \cdot Fmainsource_3 \cdot TONNAGEreg_{form}$
50-300	0.30	$3.33 \cdot Fmainsource_3 \cdot TONNAGEreg_{form}$
300-5,000	0.15	300
5,000-25,000	0.10	300
>25,000	0.05	300

Waste treatment

Required defaults for the input data for the emission scenario of the model landfill.

$$\boldsymbol{Qsubst\_reg_i = Qreg\_prod_i \cdot Fsubst\_prod_i \cdot Fpres\_prod_i \cdot Fpenetr_i \cdot (1 - Fdiff_i - Fdeg_i)} \quad \text{(P-100)}$$

$$\boldsymbol{Csubst\_landf_0 = \sum_{i=1}^{n} \frac{(Qsubst\_reg_i * Flandf_i)}{(Qwaste\_reg * Flandf_{total})}} \quad \text{(P-101)}$$

Input			
$Fsubst\_prod_i$	fraction of biocide (by weight) in the product	[-]	D
$Qreg\_prod_i$	quantity of product i in the region	[kg.d^{-1}]	D
$Fpres\_prod_i$	fraction of product with a biocid added	[-]	D
$Fpenetr_i$	penetration factor	[-]	D
$Fdiff_i$	fraction lost due to diffuse releases	[-]	D
$Fdeg_i$	fraction lost due to degradation	[-]	D
$Flandf_i$	fraction of product waste landfilled	[-]	D
$Flandf_{total}$	fraction of (total) waste landfilled	[-]	D
Qwaste_reg	total quantity of waste in the region	[kg.d^{-1}]	D
$Qsubst\_reg_i$	quantity of biocide in total waste in the region	[kg.d^{-1}]	O^c
Output			
$Csubst\_landf_i$	ìnitial concentration of biocide in landfilled waste	[kg.kg^{-1}]	O

Table C-30 *Default settings for calculating concentrations in the STP and surface water of compounds used in human hygiene products*

Parameter	**Symbol**	**Unit**	**Value**
Fraction of preservative (by weight) in product before application	$Fsubst\_prod_i$	[-]	0.02
Quantity of product i in the region	$Qreg\_prod_u$	[kg.d-1]	575.10^3
Fraction of product with a preservative added	$Fpres\_prod_i$	[-]	0.8
Penetration factor	$Fpenetr_i$	[-]	0.25
Fraction lost due to diffuse releases	$Fdiff_i$	[-]	0.25
Fraction lost due to degradation	$Fdeg_i$	[-]	0
Fraction of product waste landfilled	$Flandf_i$	[-]	0.75
Fraction of total waste landfilled	$Flandf_{total}$	[-]	0.6
Total quantity of waste in the region	$Qwaste_{reg}$	[kg.d^{-1}]	$32.5.10^6$

Fluids used in paper, textile and leather production

III.4.8.15. Fluids used in paper production

The emission scenarios in the emission scenario document on paper coating and finishing (Tissier and Migné, 2001a) comprise life cycle stages 3 ("processing", industrial use) and 5 (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.

Releases from drying sections after size-pressing, industrial use

$$Qsubst = Vform \cdot Cform \tag{P-102}$$

$$Elocal_{air} = Qpaper \cdot Qsubst \cdot Fevap \cdot (1 - Fdecomp) \tag{P-103}$$

Input

Vform	quantity of product with preservative applied per kg of paper	[m^3.kg^{-1}]	S
Cform	concentration fo active substance in the biocidal product	[kg.m^{-3}]	S
Qsubst	quantity of active substance applied per kg of paper	[kg.kg^{-1}]	S/O
-	type of paper produced	[-]	P
Qpaper	quantity of coated paper produced per day	[kg.d^{-1}]	O
VP	vapour pressure	[Pa]	S
Fevap	fraction evaporated	[-]	O

Output

$Elocal_{air}$	local emission of active substance to air	[kg$_c$.d^{-1}]	O

Table C-31 *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 carboard			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
Fraction decomposed during drying	Fdecomp	[-]	0

Releases from "broke", industrial use

$$Qsubst = Vform \cdot Cform \qquad \text{(P-104)}$$

$$Elocal_{water} = Qpaper \cdot Qsubst \cdot Fbroke \cdot (1 - Ffix) \cdot (1 - Fclosure) \qquad \text{(P-105)}$$

Input

Vform	quantity of product with preservative applied per kg of paper	[m^3.kg^{-1}]	S
Cform	concentration fo active substance in the biocidal product	[kg.m^{-3}]	S
Qsubst	quantity of active substance applied per kg of paper	[kg.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			
$Elocal_{water}$	local emission of active substance to waste water	[kg$_c$.d^{-1}]	O

Table C-32 *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	Fclosure	[-]	
- news print			0.75
- printing and writing paper			0.55
- printing and cardboard for packaging			0.95
- paper for sanitary and domestic use (tissue paper)			0.55
- special and industrial paper (all types)			0.55
Cardboard			
- flat carboard			0.95
- corrugated cardboard			0.95
Fraction of coated broke produced compared to overall production	Fbroke	[-]	0.2
Fixation fraction	Ffix	[-]	0

Paper recylcing

$$\boldsymbol{TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE} \tag{P-106}$$

$$\boldsymbol{Elocal_{water} = TONNAGEreg \cdot Frec \cdot Fmainsource_5 \cdot Fdeink \cdot (1 - Fprelim) \cdot (1 - Fdecomp) \cdot \frac{365}{Nwdays}} \tag{P-107}$$

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
$Fmainsource_5$	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 deinking	[-]	D
Fdecomp	fraction decomposed during deinking	[-]	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			
$Elocal_{water}$	local emission of active substance to waste water	$[kg_c.d^{-1}]$	O

Table C-33 *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	$Fmainsource_5$	[-]	0.1
Fraction of recycled paper	Frec	[-]	
- 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 carboard			0.92
- corrugated cardboard			0.90
Fraction of preservatives released at deinking	Fdeink	[-]	1
Fraction decomposed during deinking	Fdecomp	[-]	0
Fraction removed from wastewater during preliminary on-site treatment	Fprelim	[-]	
- easy soluble[1]			0.1
- poorly soluble			0.8
Number of working days	Nwdays	[d]	320

[1)] Easy soluble substances are defined as having a water solubility >1000 mg.l^{-1}.

III.4.8.16. Fluids used in textile production

The stage of waste treatment is connected directly to the industrial use of products with the biocide assessed (as an in-can preservative); this is caused by the fact that it is expected that almost the whole amount of the biocide will be emitted into the wastewater (default for fixation fraction is zero).

Tissier, Chesnais and Migné (2001) do not mention the use of in-can preservatives in fluids for textile production. This is not surprising as most aqueous fluids used will not have organic chemicals in them. One of the exceptions is the use of detergents but the application of in-can preservatives in this kind of products belongs to product type 6.2. However, no specific emission scenario is presented in that section III.4.8.11. Therefore, a simple scenario is presented here. The scenario assumes that an average amount of fluid per unit of mass of product can be established in some way. It should be noted that the user's instructions only have to contain the prescription of the in-can preservative in the product (fluid); it will not have to prescribe the quantity of product in textile processing.

$$\boldsymbol{Qsubst_i = Vform_i \cdot Cform_i} \qquad \text{(P-108)}$$

$$\boldsymbol{Elocal\_water_i = Qfibres \cdot Qsubst_i \cdot (1 - Ffix)} \qquad \text{(P-109)}$$

$$\boldsymbol{Elocal_{water} = \sum Elocal\_water_i} \qquad \text{(P-110)}$$

Input

$Vform_i$	quantity of fluid applied per kg of fibres / fabric for treatment step *i*	$[m^3.kg^{-1}]$	S
$Cform_i$	concentration fo active substance in the biocidal product for treatment step *i*	$[kg.m^{-3}]$	S
$Qsubst_i$	quantity of active substance applied per kg of fibres for treatment step *i*	$[kg.kg^{-1}]$	S/O
-	type of fibre produced	[-]	P
Qfibres	quantity of fibres / fabrics treated per day	$[kg.d^{-1}]$	O
Ffix	fixation fraction	[-]	D
$Elocal\_water_i$	local emission of active substance to waste water for treatment step *i*	$[kg_c.d^{-1}]$	O

Output

$Elocal_{water}$	local emission of active substance to waste water	$[kg_c.d^{-1}]$	O

Table C-34 *Default settings for calculating release to water from fluids with in-can preservatives used in textile production*

Parameter	**Symbol**	**Unit**	**Value**
Quantity of fibres treated per day	Qfibres	$[kg.d^{-1}]$	
- cotton spinning			7,000
- wool preparation			1,000
- wool spinning			2500
- silk, synthetic			1,000
- sewing knit			4,000
- cotton weaving			2,000
- wool weaving			1,000
- silk weaving			100
- other weaving			1500
- textile ennobling			6500
- house and furnish fabric			500
- other textile goods			200
- cords. filets			3,000
- non woven			4,000
- mail fabrics			2,000
Fixation fraction	Ffix	[-]	0

III.4.8.17. Fluids used in leather production

The scheme of the life cycle stages is presented below. The stage of waste treatment connected directly to the industrial use of products with the biocide assessed (as an in-can preservative); this is caused by the fact that it is expected that almost the whole amount of the biocide will be emitted into the wastewater (default for fixation fraction is zero).

Tissier and Chesnais (2001) do not mention the use of in-can preservatives in fluids for leather production either. It is not likely that fluids with in-can preservatives will be used at all. However, as for textile production an emission scenario is presented.

$$\boldsymbol{Qsubst_i = Vform_i \cdot Cform_i} \qquad \text{(P-111)}$$

$$\boldsymbol{Elocal\_water_i = Qleather \cdot Qsubst_i \cdot \left(1 - Ffix\right)} \qquad \text{(P-112)}$$

$$\boldsymbol{Elocal_{water} = \sum Elocal\_water_i} \qquad \text{(P-113)}$$

Input			
$Vform_i$	quantity of fluid applied per kg of leather for treatment step *i*	$[m^3.kg^{-1}]$	S
$Cform_i$	concentration fo active substance in the biocidal product for treatment step *i*	$[kg.m^{-3}]$	S
-	processing step	[-]	P
$Qsubst_i$	quantity of active substance applied per kg of leather for treatment step *i*	$[kg.kg^{-1}]$	S/O
Qleather	quantity of leather treated per day	$[kg.d^{-1}]$	D
Ffix	fixation fraction	[-]	D
$Elocal\_water_i$	local emission of active substance to waste water for treatment step *i*	$[kg_c.d^{-1}]$	O
Output			
$Elocal_{water}$	local emission of active substance to waste water	$[kg_c.d^{-1}]$	O

Table C-35 *Default settings for calculating releases from fluids with in-can preservatives used in leather production*

Parameter	**Symbol**	**Unit**	**Value**
Quantity of treated raw hides per day	Qleather	[kg.d^{-1}]	15,000
Quantity of active substance per kg of fibres process step - curing (salting) - soaking - pickling - tanning (large hides) - tanning (small hides) - fininshing	Qsubst$_i$	[kg.kg^{-1}]	 0.005 0.005 0.005 0.003 0.005 0.003
Fixation fraction	Ffix	[-]	0

Product type 7: Film preservatives

III.4.8.18. Film presevatives in paints and coatings

Product types 6 and 7 overlap for paints and coatings. Therefore, the same emission scenarios as presented for paint and coating can be used. For the stage of waste treatment the default value for the fraction of product with preservative added is then: Fpres_prod$_i$ = 0.6.

III.4.8.19. Film preservatives for plastics

Plastics are polymerised materials and therefore overlaps with product type 9. This topic will be discussed into more detail in the description of the release models for product type 9.

III.4.8.20. Film preservatives in glues and adhesives

Glues and adhesives are produced in a variety of types and for a variety of purposes. Large amounts are used for short-term applications and/or dry conditions (no microbial attack), for example cardboard packaging materials. In those adhesive products no or little preservatives will be used. For long term applications and/or moist conditions preservatives are required, for example plywood for outdoors use. Emissions may occur at application of the adhesives (life cycle stage 3), private use (life cycle stage 4), service life of the product with the adhesive, waste treatment (life cycle stage 5a) and recycling (life cycle stage 5b). Only the waste treatment stage has been covered by an emission scenario.

<u>Waste treatment</u>

$$\boldsymbol{Qsubst\_reg_i = Qreg\_prod_i \cdot Fsubst\_prod_i \cdot Fpres\_prod_i \cdot Fpenetr_i \cdot (1 - Fdiff_i - Fdeg_i)} \quad \text{(P-114)}$$

$$Csubst\_landf_0 = \sum_{i=1}^{n} \frac{(Qsubst\_reg_i * Flandf_i)}{(Qwaste\_reg * Flandf_{total})} \qquad \text{(P-115)}$$

Input

-	type of adhesive landfilled	[-]	P
$Fsubst\_prod_i$	fraction of biocide (by weight) in the product	[-]	O
$Qreg\_prod_i$	quantity of product i in the region	$[kg.d^{-1}]$	O
$Fpres\_prod_i$	fraction of product with a biocid added	[-]	O
$Fpenetr_i$	penetration factor	[-]	O
$Fdiff_i$	fraction lost due to diffuse releases	[-]	O
$Fdeg_i$	fraction lost due to degradation	[-]	O
$Flandf_i$	fraction of product waste landfilled	[-]	O
$Flandf_{total}$	fraction of (total) waste landfilled	[-]	O
Qwaste_reg	total quantity of waste in the region	$[kg.d^{-1}]$	D
$Qsubst\_reg_i$	quantity of biocide in total waste in the region	$[kg.d^{-1}]$	O^c

Output

$Csubst\_landf_i$	initial concentration of biocide in landfilled waste	$[kg.kg^{-1}]$	O

Table C-36 *Default settings for the input parameters of the model for preservatives applied in adhesives (I = water based adhesives, II = dispersion adhesives) at landfilling*

Parameter	**Symbol**	**Unit**	**Value** I	II
Fraction of preservative (by weight) in product before application	$Fsubst\_prod_i$	[-]	0.003	0.003
Quantity of product i in the region	$Qreg\_prod_u$	[kg.d-1]	68.10^3	164.10^3
Fraction of product with a preservative added	$Fpres\_prod_i$	[-]	0.80	0.80
Penetration factor	$Fpenetr_i$	[-]	0.25	0.25
Fraction lost due to diffuse releases	$Fdiff_i$	[-]	0.15	0.40
Fraction lost due to degradation	$Fdeg_i$	[-]	0	0
Fraction of product waste landfilled	$Flandf_i$	[-]	0.26	0.54
Total quantity of waste in the region	$Qwaste_{reg}$	[-]	$32.5.10^6$	
Fraction of total waste landfilled	$Flandf_{total}$	[-]	0.60	0.60

III.4.8.21. Film preservatives paper and carboard

It is questionable whether film preservatives are used for paper (and cardboard). However it seems possible that coatings on paper have to be preserved. Anyway, the emission scenarios presented for product type 6.4: fluids used in paper production, provide a possibility for the evaluation of this product type. Only the scenarios for calculating the releases from the drying sections after size-pressing and coating and the emission scenario for calculating the releases from “broke” are different for the calculation of the quantity of active substance (active ingredient) per amount of paper. Therefore, new scenarios are presented below which replace them respectively.

Releases from drying sections after size pressing and coating, industrial use

$$Qsubst = Qform \cdot Cform_{solid} \qquad \text{(P-116)}$$

$$Qsubst = Vform \cdot Cform_{liquid} \qquad \text{(P-117)}$$

$$Elocal_{air} = Qpaper \cdot Qsubst \cdot Fevap \cdot (1 - Fdecomp) \qquad \text{(P-118)}$$

Input			
Qform	quantity of product with preservative applied per kg of paper	$[kg.kg^{-1}]$	S
Vform	volume of product with preservative applied per kg of paper	$[m^3.kg^{-1}]$	S
$Cform_{solid}$	concentration fo active substance in the biocidal product	$[kg.kg^{-1}]$	S
$Cform_{liquid}$	concentration fo active substance in the biocidal product	$[kg.m^{-3}]$	S
Qsubst	quantity of active substance applied per kg of paper	$[kg.kg^{-1}]$	S/O
-	type of paper produced	[-]	P
Qpaper	quantity of coated paper produced per day	$[kg.d^{-1}]$	O
VP	vapour pressure	[Pa]	S
Fevap	fraction evaporated	[-]	O
Fdecomp	fraction decomposing during drying	[-]	D
Output			
$Elocal_{air}$	local emission of active substance to air for one treatment	$[kg_c.d^{-1}]$	O

Table C-37 *Default settings for calculating release to air from the drying sections after size-pressing and coating for film preservatives used 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 carboard			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
Fraction decomposed during drying	Fdecomp	[-]	0

Releases from “broke”, industrial use

$$Qsubst = Qform \cdot Cform_{solid} \qquad \text{(P-119)}$$

$$Qsubst = Vform \cdot Cform_{liquid} \qquad \text{(P-120)}$$

$$Elocal_{water} = Qpaper \cdot Qsubst \cdot Fbroke \cdot (1 - Ffix) \cdot (1 - Fclosure) \qquad \text{(P-121)}$$

Input			
Qform	quantity of product with preservative applied per kg of paper	[kg.kg^{-1}]	S
Vform	volume of product with preservative applied per kg of paper	[m^3.kg^{-1}]	S
$Cform_{solid}$	concentration fo active substance in the biocidal product	[kg.kg^{-1}]	S
$Cform_{liquid}$	concentration fo active substance in the biocidal product	[kg.m^{-3}]	S
Qsubst	quantity of active substance applied per kg of paper	[kg.kg^{-1}]	S/O
Fbroke	fraction of coated broke produced compared to overall production	[-]	D
Ffix	fixation fraction	[-]	D
-	type of paper produced	[-]	P
Qpaper	quantity of coated paper produced per day	[kg.d^{-1}]	O
Fclosure	degree of closure of the water system	[-]	O
Output			
$Elocal_{water}$	local emission of active substance to waste water	[kg$_c$.d^{-1}]	O

Table C-38 *Default settings for calculating release to waste water of biocidal compounds from "broke" for film preservatives used in paper production*

Parameter	**Symbol**	**Unit**	**Value**
Degree of closure of the water system	Fclosure	[-]	
- news print			0.75
- printing and writing paper			0.55
- printing and cardboard for packaging			0.95
- paper for sanitary and domestic use (tissue paper)			0.55
- special and industrial paper (all types)			0.55
Cardboard			
- flat carboard			0.95
- corrugated cardboard			0.95
Fraction of coated broke produced compared to overall production	Fbroke	[-]	0.2
Fixation fraction	Ffix	[-]	0

Paper recylcing

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \qquad \text{(P-122)}$$

$$Elocal_{water} = TONNAGEreg \cdot Frec \cdot Fmainsource_5 \cdot Fdeink \cdot (1 - Fprelim) \cdot (1 - Fdecomp) \cdot \frac{365}{Nwdays} \qquad \text{(P-123)}$$

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$_5$	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 deinking	[-]	D
Fdecomp	fraction decomposed during deinking	[-]	D
-	degree of solubilty	[-]	P
Fprelim	fraction removed from waste water during preliminary on-site treatment	[-]	O
Nwdays	number of working days	[d]	D
Output			
Elocal$_{water}$	local emission of active substance to waste water	[kg$_c$.d^{-1}]	O

Table C-39 *Default settings for calculating releases of film preservatives used in paper production from paper recycling*

Parameter	**Symbol**	**Unit**	**Value**
Fraction for the region	Fprovol$_{reg}$	[-]	0.1
Fraction of the main source	Fmainsource$_5$	[-]	0.1
Fraction of recycled paper	Frec	[-]	0.5
- news print			0.58
- printing and writing paper			0.11
- printing and cardboard for packaging			0.46
- paper for sanitary and domestic use (tissue paper)			0.46
- special and industrial paper (all types)			0.55
Cardboard			
- flat carboard			0.92
- corrugated cardboard			0.90
Fraction of preservatives released at deinking	Fdeink	[-]	1
Fraction decomposed during deinking	Fdecomp	[-]	0
Fraction removed from wastewater during preliminary on-site treatment	Fprelim	[-]	
- easy soluble[1]			0.1
- poorly soluble			0.8
Number of working days	Nwdays	[d]	320

1) Easy soluble substances are defined as having a water solubility >1000 mg.l^{-1}.

Product type 8: Wood preservatives and wood protectors

Industrial use

III.4.8.22. Scenario for creosote impregnation

Parameters/variables and default values for creosote impregnation.

$$Elocal_{water} = Q_{mater,creos} \cdot Q_{creos} \cdot F_{creos} \cdot F_{ws,creos} \cdot F_{w,creos} \qquad \text{(P-124)}$$

$$Elocal_{air} = Q_{mater,creos} \cdot Q_{creos} \cdot F_{creos} \cdot F_{a,creos} \qquad \text{(P-125)}$$

$$F_{s,creos} = 1 - F_{w,creos} \qquad \text{(P-126)}$$

$$DOSE_{pest} = D_{wood,creos} \cdot Q_{creos} \cdot F_{creos} \cdot F_{ws,creos} \cdot F_{s,creos} \qquad \text{(P-127)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{creos}$	[d]	250
F_{soil}	-	[d]	1*
$T_{interval}$	$T_{interval,creos}$	[d]	70
N_{appl}	$N_{appl,creos}$	[-]	5
MIX	-	[yes/no]	no

* This fraction to soil is set to one since this is the fraction of the calculated dose. In *$DOSE_{pest}$*, the fraction of the total release directed to soil is already accounted for by $F_{ws,creos}$ x $F_{s,creos}$.

Input

$Q_{mater,creos}$	quantity of wood impregnated	$[m^3.d^{-1}]$	S
Q_{creos}	quantity of creosote per m^3 wood	$[kg.m^{-3}]$	S
F_{creos}	fraction of substance in creosote	[-]	S
VP	vapour pressure	[Pa]	S
SOL	water solubility	$[kg_c.m^{-3}]$	S
$F_{ws,creos}$	fraction released to water/soil	[-]	O
$F_{w,creos}$	fraction to waste water	[-]	S
$F_{a,creos}$	fraction released to air	[-]	O
$F_{s,creos}$	fraction released to soil	[-]	O^c
$D_{wood,creos}$	storage density of treated wood per m^2	$[m^3.m^{-2}]$	S
$Temission_{creos}$	number of emission days for creosote impregnation	[d]	D
$T_{interval,creos}$	application interval for creosote impregnation	[d]	D
$N_{appl,creos}$	number of applications in one year for creosote impregnation	[-]	D

Output

$Elocal_{water}$	local emission to waste water during episode	$[kg_c.d^{-1}]$	O
$Elocal_{air}$	local emission to air during episode	$[kg_c.d^{-1}]$	O
Temission	number of emission days	[d]	O
$DOSE_{pest}$	dosage for pesticide	$[kg_c.m^{-2}]$	O
F_{soil}	fraction of dosage that reaches the soil	[-]	O^c
MIX	mixing with soil	[yes/no]	O^c
$T_{interval}$	application interval	[d]	O
N_{appl}	number of applications in one year	[-]	O

Table C-40 *Default settings for creosote impregnation.*

Parameter	**Symbol**	**Unit**	**Value**
Quantity of wood impregnated	$Q_{mater,creos}$	$[m^3.d^{-1}]$	50
Quantity of creosote per m^3 wood	Q_{creos}	$[kg.m^{-3}]$	80
Fraction of substance in creosote	F_{creos}	[-]	0.05
Fraction released to water/soil *Solubility in water* $[mg.m^{-3}]$ <0.25 0.25 - 1 1 - 50 50-100 ≥ 100	$F_{ws,creos}$	[-]	 0.0001 0.0015 0.003 0.015 0.03
Fraction to waste water	$F_{w,creos}$	[-]	0.99
Fraction released to air *Vapour pressure at 20 °C [Pa]* <0.005 0.005 - 0.05 0.05 - 0.5 0.5 - 1.25 1.25 - 2.5 2.5 – 15 ≥ 15	$F_{a,creos}$	[-]	 0.0005 0.005 0.01 0.05 0.1 0.2 0.25
Storage density treated wood per m^2	$D_{wood,creos}$	$[m^3.m^{-2}]$	0.76

III.4.8.23. Scenario for salt impregnation

Parameters/variables and default values for salt impregnation

$$\boldsymbol{Elocal_{water} = Q_{mater,salt} \cdot Q_{salt} \cdot F_{ws,salt} \cdot F_{w,salt}} \tag{P-128}$$

$$\boldsymbol{F_{s,salt} = 1 - F_{w,salt}} \tag{P-129}$$

$$\boldsymbol{DOSE_{pest} = D_{wood,salt} \cdot Q_{salt} \cdot F_{ws,salt} \cdot F_{s,salt}} \tag{P-130}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{salt}$	[d]	250
F_{soil}	-	[-]	1*
$T_{interval}$	$T_{interval,salt}$	[d]	36
N_{appl}	$N_{events,salt}$	[-]	10
MIX	-	[yes/no]	no

* This fraction to soil is set to one since this is the fraction of the calculated dose. In $DOSE_{pest}$, the fraction of the total release directed to soil is already accounted for by $F_{ws,salt}$ x $F_{s,salt}$.

Input			
$Q_{mater,salt}$	quantity of wood impregnated	$[m^3.d^{-1}]$	S
Q_{salt}	quantity of salt per m^3 wood	$[kg.m^{-3}]$	S
$F_{ws,salt}$	fraction released to water/soil	[-]	S
$F_{w,salt}$	fraction released to waste water	[-]	S
$F_{s,salt}$	fraction released to soil	[-]	O^c
$D_{wood,salt}$	storage density of treated wood per m^2	$[m^3.m^{-2}]$	S
$Temission_{salt}$	number of emission days for salt impregnation	[d]	D
$T_{interval,salt}$	application interval for salt impregnation	[d]	D
$N_{appl,salt}$	number of applications in one year for salt impregnation	[-]	D
Output			
$Elocal_{water}$	local emission to waste water during episode	$[kg_c.d^{-1}]$	O
Temission	number of emission days	[d]	O
$DOSE_{pest}$	dosage for pesticide	$[kg_c.m^{-2}]$	O
F_{soil}	fraction of dosage that reaches the soil	[-]	O^c
MIX	mixing with soil	[yes/no]	O^c
$T_{interval}$	application interval	[d]	O
N_{appl}	number of applications in one year	[-]	O

Table C-41 *Default settings for salt impregnation.*

Parameter	**Symbol**	**Unit**	**Value**
Quantity of wood impregnated	$Q_{mater,salt}$	$[m^3.d^{-1}]$	50
Quantity of salt per m^3 wood	Q_{salt}	$[kg.m^{-3}]$	2
Fraction released to water/soil	$F_{ws,salt}$	[-]	0.0001
Fraction to waste water	$F_{w,salt}$	[-]	0.99
Storage density treated wood per m^2	$D_{wood,salt}$	$[m^3.m^{-2}]$	0.76

III.4.8.24. Drenching and dipping

Parameters/variables and default values for drenching and dipping

$$Elocal_{water} = Q_{mater,drench} \cdot Q_{ai,drench} \cdot F_{ws,drench} \cdot \left(F_{w,drench} - F_{a,drench} \right) \qquad \text{(P-131)}$$

$$Elocal_{air} = Q_{mater,drench} \cdot Q_{ai,drench} \cdot F_{a,drench} \qquad \text{(P-132)}$$

$$F_{s,drench} = 1 - F_{w,drench} \qquad \text{(P-133)}$$

$$DOSE_{pest} = D_{wood,drench} \cdot Q_{ai,drench} \cdot F_{ws,drench} \cdot F_{s,drench} \qquad \text{(P-134)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{drench}$	[d]	50
F_{soil}	-	[-]	1*
$T_{interval}$	$T_{interval,drench}$	[d]	35
N_{appl}	$N_{appl,drench}$	[-]	10
MIX	-	[yes/no]	no

* This fraction to soil is set to one since this is the fraction of the calculated dose. In $DOSE_{pest}$, the fraction of the total release directed to soil is already accounted for by $F_{ws,drench}$ x $F_{s,drench}$.

Input			
$Q_{mater,drench}$	quantity of wood impregnated	$[m^3.d^{-1}]$	S
$Q_{ai,drench}$	quantity of a.i. per m^3 wood	$[kg.m^{-3}]$	S
$F_{ws,drench}$	fraction released to water/soil	[-]	S
$F_{w,drench}$	fraction released to waste water	[-]	S
$F_{s,drench}$	fraction released to soil	[-]	O^c
$D_{wood,drench}$	storage density of treated wood per m^2	$[m^3.m^{-2}]$	S
VP	vapour pressure	[Pa]	S
$F_{a,drench}$	fraction released to air	[-]	O
$Temission_{drench}$	number of emission days for drenching	[d]	D
$T_{interval,drench}$	application interval for drenching	[d]	D
$N_{appl,drench}$	number of applications in one year for drenching	[-]	D
Output			
$Elocal_{water}$	local emission to waste water during episode	$[kg_c.d^{-1}]$	O
$Elocal_{air}$	local emission to air during episode	$[kg_c.d^{-1}]$	O
Temission	number of emission days	[d]	O
$DOSE_{pest}$	dosage for pesticide	$[kg_c.m^{-2}]$	O
F_{soil}	fraction of dosage that reaches the soil	[-]	O^c
MIX	mixing with soil	[yes/no]	O^c
$T_{interval}$	application interval	[d]	O
N_{appl}	number of applications in one year	[-]	O

Table C-42 *Default settings for drenching and dipping.*

Parameter	**Symbol**	**Unit**	**Value**
Quantity of wood impregnated	$Q_{mater,drench}$	[$m^3.d^{-1}$]	2
Quantity of creosote per m^3 wood	$Q_{ai,drench}$	[$kg.m^{-3}$]	1
Fraction released to water/soil	$F_{ws,drench}$	[-]	0.0005
Fraction to waste water	$F_{w,drench}$	[-]	0.9
Fraction released to air *Vapour pressure at 20 °C [Pa]* <0.005 0.005 - 0.05 0.05 - 0.5 0.5 - 1.25 1.25 - 2.5 ≥ 2.5 *When "organic solvent" = "no"*	$F_{a,drench}$	[-]	 0.001 0.01 0.02 0.075 0.15 0.25 0
Storage density treated wood per m^2	$D_{wood,drench}$	[$m^3.m^{-2}$]	0.76

III.4.8.25. Remedial timber treatment in buildings

Parameters/variables and default values for remedial timber treatments in buildings. The calculated dose is used in a specific risk-characterisation ratio: the Relative Toxicity Index (RTI) for bats. The active ingredient can be applied either in a solid or liquid formulation.

$$DOSE_{wood} = APPL_{solid} \cdot F_{ai,remed} \qquad \text{(P-135)}$$

or:

$$DOSE_{wood} = APPL_{fluid} \cdot RHO_{form} \cdot F_{ai,remed} \qquad \text{(P-136)}$$

Input

$F_{ai,remed}$	fraction of a.i. in formulation	[-]	S
$APPL_{solid}$	solid application rate of formulation	[$kg_{form}.m^{-2}$]	S
or:			
$APPL_{fluid}$	fluid application rate of formulation	[$m_{form}^3.m^{-2}$]	S
RHO_{form}	density of formulation	[$kg_{form}.m^{-3}$]	S

Output

$DOSE_{wood}$	dosage of a.i. per m^2 wood	[$kg_c.m^{-2}$]	O

Service life

III.4.8.26. Leaching from impregnated wood to surface water

Model for calculating concentrations in surface water for compounds used for impregnating wood.

$$AREA_{leach} = 2 \cdot N_{pole} \cdot DIAM_{pole} \cdot \pi \cdot DEPTH_{wway} \tag{P-137}$$

In general, the experimentally determined compound-flux will decrease in time. The function of the lixiviation time and the flux can be described as follows:

$$FLUX(t) = e^{b} \cdot t^{a} \tag{P-138}$$

The concentration in the waterway as a function of time is given by:

If t ≤ TAU_{wway} and ($-1 < a < 0$)

$$C_{wway}(t) = \frac{AREA_{leach} \cdot e^{b}}{DEPTH_{wway} \cdot WIDTH_{wway} \cdot (a+1)} \cdot t^{a+1} \tag{P-139}$$

if t > TAU_{wway} and ($-2 < a < 0$ and $a \neq -1$)

$$C_{wway}(t) = \frac{AREA_{leach} \cdot e^{b}}{DEPTH_{wway} \cdot WIDTH_{wway} \cdot (a+1)} \cdot [t^{a+1} - (t - TAU_{wway})^{a+1}] \tag{P-140}$$

The maximum concentration is reached at t = TAU_{ditch}, the average concentration over an interval T is calculated started from t = TAU_{ditch}:

$$Cwater_{pest\text{-}T} = Fdiss_{ditch} \cdot \frac{1}{T} \cdot \int_{TAU_{ditch}}^{TAU_{ditch}+T} C_{wway}(t)\, dt \tag{P-141}$$

This integral can be solved analytically and yields the following equations:

$$Fdiss_{ditch} = \frac{1}{1 + Kp_{susp,pest} \cdot SUSP_{water}} \tag{P-142}$$

$$Cwater_{pest\text{-}T} = \frac{AREA_{leach} \cdot e^{b}}{DEPTH_{wway} \cdot WIDTH_{wway} \cdot (a+1)} \cdot$$

$$Fdiss_{ditch} \cdot \frac{\left(T + TAU_{wway}\right)^{a+2} - T^{a+2} - TAU_{wway}^{a+2}}{(a+2) \cdot T} \qquad \text{(P-143)}$$

$$T \in \{1,4,7,14,21,28,T_{bird},T_{mammal},365\}$$

$$Cwater_{pest\text{-}0} = Cwater_{pest\text{-}1} \qquad \text{(P-144)}$$

In case curve fitting is not possible C_{wway} can be estimated as follows:

$$Cwater_{pest,eq} = \frac{AREA_{leach} \cdot FLUX_{avg}}{DEPTH_{wway} \cdot \frac{WIDTH_{wway}}{TAU_{wway}}} \qquad \text{(P-145)}$$

$$Cwater_{pest\text{-}T} = \frac{Cwater_{pest,eq}}{1 + Kp_{susp,pest} \cdot SUSP_{water}} \quad T \in \{0,4,7,14,21,28,T_{bird},T_{mammal},365\} \qquad \text{(P-146)}$$

Input			
$DEPTH_{wway}$	waterway depth	[m]	D
$WIDTH_{wway}$	waterway width	[m]	D
TAU_{wway}	residence time of waterway water	[d]	D
$DIAM_{pole}$	diameter of poles	[m]	D
N_{pole}	number of poles per meter (both sides)	[m^{-1}]	D
$AREA_{leach}$	leaching surface of impreg. wood per meter model waterway	[$m^{2}.m^{-1}$]	O^{c}
$Cwater_{pest,eq}$	equilibrium concentration in waterway	[$kg_{c}.m^{-3}$]	O^{c}
$Kp_{susp,pest}$	solids-water partition coefficient in susp. matter for pesticides	[$m^{3}.kg^{-1}$]	O
$SUSP_{water}$	concentration suspended matter	[$kg.m^{-3}$]	D
T_{bird}	test duration for bird toxicity test	[d]	S
T_{mammal}	test duration for mammalian toxicity test	[d]	S
a	regression constant a (curve fitting)	[-]	S
e^{b}	regression constant e^{b} (curve fitting)	[-]	S
or:			
$FLUX_{avg}$	mean flux of compound over a certain period	[$kg_{c}.m^{-2}.d^{-1}$]	S
Output			
$Cwater_{pest\text{-}0}$	peak concentration in water	[$kg_{c}.m^{-3}$]	O
$Cwater_{pest\text{-}T}$	average concentration in water over *T* days *T* in $\{4,7,14,21,28,T_{bird},T_{mammal},365\}$	[$kg_{c}.m^{-3}$]	O

Table C-43 *Default settings for leaching from impregnated wood.*

Parameter	**Symbol**	**Unit**	**Value**
Waterway depth	$DEPTH_{wway}$	[m]	1.5
Waterway width	$WIDTH_{wway}$	[m]	5
Residence time of waterway water	TAU_{wway}	[d]	20
Diameter of poles	$DIAM_{pole}$	[m]	0.1
Number of poles per meter (both sides)	N_{pole}	[m^{-1}]	5

III.4.8.27. Leaching from impregnated wood to ground water

Leaching area [m^2]

$$AREA_{leach} = 2 \cdot DEPTH_{pole} \cdot \pi \cdot RAD_{pole} \tag{P-147}$$

Amount of leached substance over 1 year

$$Q_{pole} = 365 \cdot AREA_{leach} \cdot FLUX_{comp} \tag{P-148}$$

Soil volume around pole [m^3]

$$V_{soil} = DEPTH_{pole} \cdot \left[\pi \cdot RAD_{soil}^2 - \pi \cdot RAD_{pole}^2 \right] \tag{P-149}$$

Fraction influenced soil per ha [-]

$$F_{influence} = \frac{200}{10000} \cdot \left[\pi \cdot RAD_{soil}^2 - \pi \cdot RAD_{pole}^2 \right] \tag{P-150}$$

Soil mass around pole [kg$_{dwt}$]

$$M_{soil} = V_{soil} \cdot \frac{RHO_{satsoil}}{CONV_{satsoil}} \tag{P-151}$$

Pore water volume around pole [m^3]

$$V_{pore} = V_{soil} \cdot Fwater_{satsoil} \tag{P-152}$$

Concentration of leached substance in soil pore water [kg$_c$.m^{-3}]

$$C_{porew} = \frac{Q_{pole}}{V_{pore} + M_{soil} \cdot Kp_{pest}} \tag{P-153}$$

Concentration in groundwater for drinking water [kg$_c$.m^{-3}]

$$Cgrw_{pest} = C_{porew} \cdot F_{influence} \tag{P-154}$$

Concentration of leached substance in soil [$kg_c.kg_{wwt}^{-1}$]

$$Csoil_{pest\text{-}0} = \frac{C_{porew} \cdot Kp_{pest}}{CONV_{satsoil}} \qquad \text{(P-155)}$$

Input			
$FLUX_{comp}$	mean flux of compound	[$kg_c.m^{-2}.d^{-1}$]	S
$AREA_{leach}$	leaching area	[m^2]	O^c
$DEPTH_{pole}$	part of pole in saturated zone	[m]	D
RAD_{pole}	radius of pole	[m]	D
Q_{pole}	amount of substance leached over 1 year	[kg_c]	O^c
V_{soil}	volume of soil around pole	[m^3]	O^c
RAD_{soil}	radius of soil area	[m]	D
$F_{influence}$	fraction influenced area per ha	[-]	O^c
M_{soil}	soil mass around pole	[kg_{dwt}]	O^c
$RHO_{satsoil}$	bulk density of saturated soil	[$kg_{wwt}.m^{-3}$]	O^c
$CONV_{soil}$	conversion factor wet weight-dry weight soil	[$kg_{wwt}.kg_{dwt}^{-1}$]	O^c
V_{pore}	pore water volume around pole	[m^3]	O^c
$Fwater_{satsoil}$	volume fraction water in saturated soil	[$m^3.m^{-3}$]	D
Kp_{pest}	solids-water partition coefficient in application soil	[$m^3.kg_{dwt}^{-1}$]	O
C_{porew}	concentration of leached substance in porewater	[$kg_c.m^{-3}$]	O
Output			
$Csoil_{pest\text{-}0}$	peak concentration in soil	[$kg_c.kg_{wwt}^{-1}$]	O
$Cgrw_{pest}$	concentration in ground water	[$kg_c.m^{-3}$]	O

Table C-44 *Default settings for calculating ground water concentrations for compounds used for impregnating wood.*

Parameter	**Symbol**	**Unit**	**Value**
Fraction water in saturated soil	$Fwater_{satsoil}$	[$m^3.m^{-3}$]	0.4
Part of pole in saturated zone	$DEPTH_{pole}$	[m]	0.1
Radius of pole	RAD_{pole}	[m]	0.05
Radius of soil area	RAD_{soil}	[m]	0.1

III.4.8.28. Leaching from impregnated wood to soil

Leaching area [m^2]

$$AREA_{fence} = HEIGHT_{fence} \cdot LENGTH_{fence} \tag{P-156}$$

Amount of leached substance over 1 year [kg$_c$]

$$Q_{fence} = T_{rain} \cdot AREA_{fence} \cdot FLUX_{fence} \tag{P-157}$$

Soil volume beneath fence [m^3]

$$V_{soil} = DEPTH_{fence} \cdot WIDTH_{fence} \cdot LENGTH_{fence} \tag{P-158}$$

Soil mass beneath fence [kg$_{dwt}$]

$$M_{soil} = V_{soil} \cdot \frac{RHO_{pest}}{CONV_{pest}} \tag{P-159}$$

Pore water volume beneath fence [m^3]

$$V_{pore} = V_{soil} \cdot Fwater_{pest} \tag{P-160}$$

Concentration of leached substance in soil pore water [kg$_c$.m^{-3}]

$$C_{porew} = \frac{Q_{fence}}{V_{pore} + M_{soil} \cdot Kp_{pest}} \tag{P-161}$$

Concentration of leached substance in soil [kg$_c$.kg$_{wwt}^{-1}$]

$$Csoil_{pest\text{-}0} = \frac{C_{porew} \cdot Kp_{pest}}{CONV_{pest}} \tag{P-162}$$

Input			
$DEPTH_{fence}$	depth of soil layer	[m]	D
$WIDTH_{fence}$	width of soil layer	[m]	D
$HEIGHT_{fence}$	height of the fence	[m]	D
$LENGTH_{fence}$	length of fence	[m]	D
T_{rain}	number of days with leaching	[d]	D
$FLUX_{fence}$	mean flux of compound over 1 year	$[kg_c.m^{-2}.d^{-1}]$	S
V_{soil}	volume of soil around fence	$[m^3]$	O^c
M_{soil}	soil mass around fence	$[kg_{dwt}]$	O^c
RHO_{pest}	bulk density of application soil	$[kg.m^{-3}]$	O^c
$CONV_{pest}$	conversion factor wet weight-dry weight soil	$[kg_{wwt}.kg_{dwt}^{-1}]$	O^c
$AREA_{fence}$	leaching surface of impregnated fence per m length	$[m^2]$	O^c
Q_{fence}	quantity leached per m length of fence	$[kg_c]$	O^c
$Fwater_{pest}$	volume fraction water in application soil	$[m^3.m^{-3}]$	D
V_{pore}	pore water volume around fence	$[m^3]$	O^c
Kp_{pest}	solids-water partition coefficient in application soil	$[m^3.kg_{dwt}^{-1}]$	O
Output			
$Csoil_{pest-0}$	peak concentration in soil	$[kg_c.kg_{wwt}^{-1}]$	O
C_{porew}	concentration in porewater of soil	$[kg_c.m^{-3}]$	O

Table C-45 *Default settings for leaching from impregnated wood to soil.*

Parameter	**Symbol**	**Unit**	**Value**
Depth of soil layer	$DEPTH_{fence}$	[m]	0.05
Width of soil layer	$WIDTH_{fence}$	[m]	0.025
Number of days with leaching	T_{rain}	[d]	35
Length of the fence	$LENGTH_{fence}$	[m]	1
Height of the fence	$HEIGHT_{fence}$	[m]	2

Waste treatment

III.4.8.29. Wood preservatives at landfilling

Waste treatment, impregnated wood

$$\boldsymbol{Qsubst\_reg_i = Qsubst\_prep_i \cdot Fsubst \cdot Fpenetr_i \cdot (1 - Fdiff_i)} \qquad \text{(P-163)}$$

Waste treatment, surface protection

$$\boldsymbol{Qsubst\_reg_i = Qreg\_prod_i \cdot Fsubst\_prod_i \cdot Fpenetr_i \cdot (1 - Fdiff_i)} \qquad \text{(P-164)}$$

$$\boldsymbol{Csubst\_landf_0 = \sum_{i=1}^{n} \frac{(Qsubst\_reg_i * Flandf_i)}{(Qwaste\_reg * Flandf_{total})}} \qquad \text{(P-165)}$$

Input			
-	type of biocide/preservative	[-]	P
$Qsubst\_prep_i$	quantity of biocide for application in preparation *i* in total waste	[kg.d^{-1}]	O
Fsubst	fraction of component in wood preservative	[-]	O
$Fsubst\_prod_i$	fraction of biocide in the product (by weight) before application	[-]	D
$Qreg\_prod_i$	quantity of product i in the region	[kg.d^{-1}]	D
$Fpenetr_i$	penetration factor	[-]	D
$Fdiff_i$	fraction lost due to diffuse releases	[-]	D
$Flandf_i$	fraction of product waste landfilled	[-]	D
$Flandf_{total}$	fraction of (total) waste landfilled	[-]	D
Qwaste_reg	total quantity of waste in the region	[kg.d^{-1}]	D
$Qsubst\_reg_i$	quantity of biocide in total waste in the region	[kg.d^{-1}]	O^c
Output			
$Csubst\_landf_0$	initial concentration of biocide in landfilled waste	[kg.kg^{-1}]	O

Table C-46 *Default settings for the input parameters of the model for wood preservatives at landfilling*

Parameter	**Symbol**	**Unit**	**Value**
Quantity of biocide for application in preparation i in total waste - salts - coal tar - others	$Qsubst\_prep_i$	[kg.d^{-1}]	 4,400 7,500 5,500
Quantity of product i in the region	$Qreg\_prod_i$	[kg.d^{-1}]	12,329
Fraction of component in wood preservative - salts - coal tar - others	Fsubst	[-]	 0.35 0.050 0.80
Fraction of preservative (by weight) in product before application	$Fsubst\_prod_i$	[-]	0.1
Penetration factor - impregnated material - surface treatment	$Fpenetr_i$	[-]	 0.25 0.40
Fraction lost due to diffuse releases	$Fdiff_i$	[-]	0
Total quantity of waste in the region	Qwaste-reg	[kg.d^{-1}]	$32.5.10^6$
Fraction of total waste landfilled	$Flandf_{total}$	[-]	0.60

Table C-47 *Default settings for the input parameters of the model for wood preservatives in products for general-use surface protection at landfilling*

Parameter	**Symbol**	**Unit**	**Value**
Quantity of biocide for application in preparation i in total waste	$Qsubst\_prep_i$	[kg.d^{-1}]	12,300
Fraction of component in wood preservative	Fsubst	[-]	0.1
Penetration factor	$Fpenetr_i$	[-]	0.4
Fraction lost due to diffuse releases	$Fdiff_i$	[-]	0
Fraction of product waste landfilled	$Flandf_i$	[-]	0.6
Fraction of total waste landfilled	$Flandf_{total}$	[-]	0.6

Product type 9: Fibre, leather, rubber and polymerised materials preservatives

III.4.8.30. Textile and fabrics preservatives

Textile production, imported material

$$\boldsymbol{Eimport_{water} = Qfibres \cdot Cmat} \tag{P-166}$$

$$\boldsymbol{Elocal_{water} = Eimport_{water}} \tag{P-167}$$

Input			
-	type of imported fibre treated	[-]	P
Qfibres	quantity of fibres / fabrics treated per day	[kg.d^{-1}]	O
-	type of material imported	[-]	P
Cmat	estimated content of active substance present in imported material	[kg.kg^{-1}]	O
$Eimport_{water}$	local emission of active substance to waste water due to imported material	[kg.d^{-1}]	O
Output			
$Elocal_{water}$	local emission of active substance to waste water due to imported material	[kg.d^{-1}]	O

Table C-48 *Default settings for the input parameters of the model for calculating the releases of the biocide that is present in imported material*

Parameter	**Symbol**	**Unit**	**Value**
Quantity of fibres / fabrics treated per day	Qfibres	[kg.d^{-1}]	Table C-34
Estimated content of active substance present in imported material - wool - cotton	Cmat	[kg.kg^{-1}]	 0.01.10^{-6} 0.004.10^{-6}

Textile production

$$\boldsymbol{Elocal\_water_i = Qfibres \cdot Qsubst_i \cdot (1 - Ffix)} \tag{P-168}$$

$$\boldsymbol{Elocal_{water} = Eimport_{water} + \sum_{i=1}^{m} Elocal\_water_i} \tag{P-169}$$

Input

-	type of fibre treated	[-]	P
Qfibres	quantity of fibres / fabrics treated per day	$[kg.d^{-1}]$	O
$Qsubst_i$	quantity of active substance applied per kg of fibres / fabrics for treatment $step_i$	$[kg.kg^{-1}]$	S
Ffix	fixation fraction	[-]	S/D
$Eimport_{water}$	local emission of active substance to waste water due to imported material	$[kg.d^{-1}]$	O
$Elocal\_water_i$	local emission of active substance to waste water for one treatment step	$[kg.d^{-1}]$	O

Output

$Elocal_{water}$	total emission of active substance to waste water	$[kg.d^{-1}]$	O

Table C-49 *Default settings for the input parameters of the model for calculating the releases of the biocide from the different application steps in textile production*

Parameter	**Symbol**	**Unit**	**Value**
Quantity of fibres / fabrics treated per day	Qfibres	$[kg.d^{-1}]$	Table C-34
Fixation fraction	Ffix	[-]	0.7

Service life

$$\boldsymbol{RELEASEreg_{i,service,j} = Fprodvol_{reg} \cdot F_{service,j} \cdot Qsubst\_tot_k \cdot \sum_{y=1}^{Tservice_k} \left(1 - F_{service,j}\right)^{y-1} \cdot \frac{365}{Temission_{service}}} \qquad \text{(P-170)}$$

$$\boldsymbol{RELEASEreg_{service,j} = \sum_{k=1}^{m} RELEASEreg_{k,service,j}} \qquad \text{(P-171)}$$

$$\boldsymbol{Elocal_{service,j} = Fmainsource_{service} \cdot RELEASEreg_{service,j}} \qquad \text{(P-172)}$$

Input

$Qsubst\_tot_k$	annual input of the substance in article k	$[kg.d^{-1}]$	S
$Fprodvol_{reg}$	fraction of the region	[-]	D
-	type of article	[-]	P
$Tservice_k$	service life of article *k*	[d]	O
$F_{service,j}$	average (over one year) fraction of mass released in one day during service life to compartment *j*	[-]	D
$Temission_{service}$	emission duration per year	[d]	D
$Fmainsource_{service}$	fraction of the main source	[-]	D

Output

$RELEASEreg_{k,service,j}$	regional release for the stage of service life to compartment *j* for biocide for product *k*	$[kg.d^{-1}]$	O
$RELEASEreg_{service,j}$	total regional release for the stage of service life to compartment *j* for biocide for all *m* products with the biocide	$[kg.d^{-1}]$	O
$Elocal_{service,j}$	total local emission for the stage of service life to compartment *j* from all products	$[kg.d^{-1}]$	O

Table C-50 *Default settings for the input parameters of the model for calculating the releases from articles during their service life*

Parameter	**Symbol**	**Unit**	**Value**
Fraction of the region	$Fprodvol_{reg}$	[-]	0.1
Emission duration per year	$Temission_{service}$	$[d.yr^{-1}]$	365
Fraction of the mainsource$_{service}$	$Fmainsoure_{service}$	[-]	0.002
Service life for article $_k$	$Tservice_k$	[d]	
- clothes on contact with skin			365
- ohter clothes and bed linen			1278
- bedding (mattress)			4380
- carpets			3650
- wall-to-wall carpet			6205
- sunblind			4015
- tents			4380
- awning			730

III.4.8.31. Leather and hides preservatives

$$Qsubst_i = Vform_i \cdot Cform_i \qquad \text{(P-173)}$$

$$Elocal\_water_i = Qleather \cdot Qsubst_i \cdot (1 - Ffix) \qquad \text{(P-174)}$$

$$Elocal_{water} = \sum_{i=1}^{n} Elocal\_water_i \qquad \text{(P-175)}$$

Input

$Vform_i$	quantity of fluid applied per kg of leather for treatment step *i*	$[kg.kg^{-1}]$	S
$Cform_i$	concentration fo active substance in the biocidal product for treatment step *i*	$[kg.m^{-3}]$	S
-	process step	[-]	P
$Qsubst_i$	quantity of active substance applied per kg of leather for	$[kg.kg^{-1}]$	O
Qleather	quantity of leather treated per day treatment step *i*	$[kg.d^{-1}]$	D
Ffix	fixation fraction	[-]	D
$Elocal\_water_i$	local emission of active substance to waste water for treatment step *i*	$[kg_c.d^{-1}]$	O

Output

$Elocal_{water}$	local emission of active substance to waste water	$[kg_c.d^{-1}]$	O

Table C-51 *Default settings for calculating releases from biocides used as preservatives in the leather industry*

Parameter	**Symbol**	**Unit**	**Value**
Quantity of treated raw hides per day	Qleather	[kg.d^{-1}]	15,000
Quantity of active substance per kg of fibres	Qsubst$_i$	[kg.kg^{-1}]	
process step			
- curing (salting)			0.005
- soaking			0.005
- pickling			0.005
- tanning (large hides)			0.003
- tanning (small hides)			0.005
- fininshing			0.03
Fixation fraction	Ffix	[-]	0

III.4.8.32. Paper and cardboard preservatives

Releases from drying sections after size-pressing and coating

$$Qsubst = Vform \cdot Cform \qquad \text{(P-176)}$$

$$Elocal_{air} = Qpaper \cdot Qsubst \cdot Fevap \cdot (1 - Fdecomp) \qquad \text{(P-177)}$$

Input

Vform	quantity of product with preservative applied per kg of paper	[m^3.kg^{-1}]	S
Cform	concentration fo active substance in the biocidal product	[kg.m^{-3}]	S
Qsubst	quantity of active substance applied per kg of paper	[kg.kg^{-1}]	S
-	type of paper produced	[-]	P
Qpaper	quantity of coated paper produced per day	[kg.d^{-1}]	O
VP	vapour pressure	[Pa]	P
Fevap	fraction evaporated	[-]	O
Fdecomp	decomposition rate during drying	[-]	D
Output			
Elocal$_{air}$	local emission of active substance to air for one treatment	[kg$_c$.d^{-1}]	O

Table C-52 *Default settings for calculating release to air of biocidal compounds from the drying sections after size-pressing and coating in paper production for paper and cardboard preservatives*

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 carboard			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
Fraction decomposed during drying	Fdecomp	[-]	0

Releases from "broke"

$$Qsubst = Vform \cdot Cform \tag{P-178}$$

$$Elocal_{water} = Qpaper \cdot Qsubst \cdot Fbroke \cdot (1 - Ffix) \cdot (1 - Fclosure) \tag{P-179}$$

Input

Vform	quantity of product with preservative applied per kg of paper	[m^3.kg^{-1}]	S
Cform	concentration fo active substance in the biocidal product	[kg.m^{-3}]	S
Qsubst	quantity of active substance applied per kg of paper	[kg.kg^{-1}]	S
-	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
-	type of paper produced	[-]	P
Fclosure	degree of closure of the water system	[-]	O

Output

$Elocal_{water}$	local emission of active substance to waste water	[kg$_c$.d^{-1}]	O

Table C-53 *Default settings for calculating release to waste water of paper and cardboard preservatives from "broke" in paper production*

Parameter	**Symbol**	**Unit**	**Value**
Degree of closure of the water system	Fclosure	[-]	
- news print			0.75
- printing and writing paper			0.55
- printing and cardboard for packaging			0.95
- paper for sanitary and domestic use (tissue paper)			0.55
- special and industrial paper (all types)			0.55
Cardboard			
- flat carboard			0.95
- corrugated cardboard			0.95
Fraction of coated broke produced compared to overall production	Fbroke	[-]	0.2
Fixation fraction	Ffix	[-]	0

Paper recylcing

$$TONNAGEreg = Fprodvol_{reg} \cdot TONNAGE \tag{P-180}$$

$$\begin{gathered} Elocal_{water} = TONNAGEreg \cdot Frec \cdot Fmainsource_5 \cdot Fdeink \cdot \\ (1 - Fprelim) \cdot (1 - Fdecomp) \cdot \frac{365}{Nwdays} \end{gathered} \tag{P-181}$$

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$_5$	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 deinking	[-]	D
Fdecomp	fraction decomposed during deinking	[-]	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$_{water}$	local emission of active substance to waste water	[kg$_c$.d^{-1}]	O

Table C-54 *Default settings for calculating releases of biocidal compounds used as paper and cardboard preservatives from recycling*

Parameter	Symbol	Unit	Value
Fraction for the region	$Fprovol_{reg}$	[-]	0.1
Fraction of the main source	$Fmainsource_5$	[-]	0.1
Fraction of recycled paper	Frec	[-]	0.5
- news print			0.58
- printing and writing paper			0.11
- printing and cardboard for packaging			0.46
- paper for sanitary and domestic use (tissue paper)			0.46
- special and industrial paper (all types)			0.55
Cardboard			
- flat carboard			0.92
- corrugated cardboard			0.90
Fraction of preservatives released at deinking	Fdeink	[-]	1
Fraction decomposed during deinking	Fdecomp	[-]	0
Fraction removed from wastewater during preliminary on-site treatment	Fprelim	[-]	
- easy soluble[1]			0.1
- poorly soluble			0.8
Number of working days	Nwdays	[d]	320

[1] Easy soluble substances are defined as having a water solubility >1000 mg.l^{-1}.

Product type 11: Preservatives for liquid-cooling and processing systems

III.4.8.33. Biocides in process and cooling-water installations

Model for process and cooling-water installations. Since the release can be characterised as continuous, the concentration over each test period is set equal to the peak concentration.

$$Cwater_{pest\text{-}0} = \frac{C_{ai,cooling}}{(1 + Kp_{susp,pest} \cdot SUSP_{water}) \cdot DILUTION_{cooling}} \qquad \text{(P-182)}$$

$$Cwater_{pest\text{-}T} = Cwater_{pest\text{-}0} \quad T \in \{4,7,14,21,28,T_{bird},T_{mammal},365\} \qquad \text{(P-183)}$$

Only if *COOLTYPE* = 'open':

$$DOSE_{pest} = Q_{circ} \cdot C_{ai,cooling} \cdot \frac{F_{depos}}{AREA_{soil,cooling}} \qquad \text{(P-184)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
F_{soil}	-	[d]	1
$T_{interval}$	$T_{interval,cooling}$	[d]	1
N_{appl}	$N_{appl,cooling}$	[-]	300
MIX	-	[yes/no]	no

Input

COOLTYPE	type of cooling water system (open circulation/contin. flow)	[open/cont.]	P
$DILUTION_{cooling}$	dilution factor in receiving surface water	[-]	D
$C_{ai,cooling}$	concentration of a.i. in cooling water	[$kg_c.m^{-3}$]	S
$Kp_{susp,pest}$	solids-water partition coefficient in susp. matter for pesticides	[$m^3.kg^{-1}$]	O
$SUSP_{water}$	concentration suspended matter	[$kg.m^{-3}$]	D
T_{bird}	test duration for bird toxicity test	[d]	S
T_{mammal}	test duration for mammalian toxicity test	[d]	S

only open circulation systems:

Q_{circ}	quantity of water in circulation	[$m^3.d^{-1}$]	S
F_{depos}	fraction of water lost due to spray and wind drift	[-]	S
$AREA_{soil,cooling}$	soil surface where deposition occurs	[m^2]	S
$T_{interval,cooling}$	time period between two emission events	[d]	D
$N_{appl,cooling}$	number of applications in one year	[-]	D
$Cwater_{pest\text{-}0}$	peak concentration of chemical in surface water	[$kg_c.m^{-3}$]	O

Output

$Cwater_{pest\text{-}T}$	average concentration in surface water over *T* days	[$kg_c.m^{-3}$]	O

only open circulation systems:

$DOSE_{pest}$	dosage for one event	[$kg_c.m^{-2}$]	O
F_{soil}	fraction of dosage that reaches the soil	[-]	O^c
MIX	mixing with soil	[yes/no]	O^c
$T_{interval}$	application interval	[d]	O
N_{appl}	number of applications in one year	[-]	O

Table C-55 *Default settings of the model for biocides in process and cooling-water installations.*

Parameter	**Symbol**	**Unit**	**Value**
Dilution factor of receiving surface water	$DILUTION_{cooling}$	[-]	3
Concentration of a.i. in cooling water (0.5 mg/l)	$C_{ai,cooling}$	[$kg_c.m^{-3}$]	0.0005
Quantity of water in circulation	Q_{circ}	[$m^3.d^{-1}$]	10,000
Fraction of water lost due to spray and wind drift	F_{depos}	[-]	0.00025
Soil surface where deposition occurs	$AREA_{soil,cooling}$	[m^2]	100

Product type 12: Slimicides

III.4.8.34. Slimicides

Release of slimicide in paper mills not taking degradation into account

$$Qsubst = Qform_{uins} \cdot Cform \,/\, RHOform \tag{P-185}$$

A) based on amount of active ingredient per unit of mass of dry paper

$$Cinf = Qsubst \,/\, Vww \tag{P-186}$$

B) based on amount of active ingredient per unit of volume of process water

$$Cinf = Qsubst \cdot Fww1 \cdot (1 - Fww2) \tag{P-187}$$

C) based on concentration of process water prescribed

$$Cinf = Cproc \cdot Fww1 \cdot (1 - Fww2) \tag{P-188}$$

$$Elocal_{water} = EFFLUENT_{stp} \cdot Cinf \tag{P-189}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_3$	[d]	300
Nlocal	$Nlocal_3$	[eq]	25,000
DILUTION	$DILUTION_3$	[-]	10

Input			
Qform_uins	amount of biocide prescribed in user's instructions for one tonne of dry paper or per m^3 process water	[kg.kg^{-1}]	S
Cform	content of active ingredient in biocidal product	[kg$_c$.m^{-3}]	S
RHOform	specific density of biocide formulation	[kg.m^{-3}]	S
Vww	amount of waste water per kilogram of dry paper	[m^3.kg^{-1}]	D
APPL	treatment of both long and short circulation with slimicide	[yes/no]	P
Fww1	fraction of the total waste water flow coming from the short circulation of the wire part	[-]	O
CONN	connection to pulp mill	[yes/no]	P
Fww2	fraction dilution of waste water with waste water from pulping	[-]	O
Cproc	concentration of process water prescribed in the user's intructions	[kg.m^{-3}]	S
Qsubst	amount of active ingredient per kilogram of dry paper	[kg$_c$.kg^{-1}]	O
Cinf	theoretical concentration of active ingredient in effluent from paper mill (influent waste water treatment plant)	[kg.m^{-3}]	O
EFFLUENTlocal$_{stp}$	effluent discharge of STP for paper plant	[m^3.d^{-1}]	D
Temission$_3$	number of emission days	[d]	D
Nlocal$_3$	capacity of local STP of paper plant	[eq]	D
DILUTION$_3$	dilution factor for receiving surface water	[-]	D
Output			
Nlocal	capacity of the local STP	[eq]	O
Temission	number of emission days	[d]	O
DILUTION	dilution factor	[-]	O
Elocal$_{water}$	local emission to waste water during episode	[kg.d^{-1}]	O

Table C-56 *Default settings for calculating the daily release to the STP excluding biodegradation*

Parameter	**Symbol**	**Unit**	**Value**
Specific density of biocide formulation	RHOform	[kg.m^{-3}]	1,000
Amount of waste water per kilogram of dry paper	Vww	[m^3]	0.015
Treatment of both long and short circulation with slimicide	APPL	[yes/no]	yes
Fraction of the total waste water flow coming from the short circulation of the wire part APPL = yes APPL = no	Fww1	[-]	 1 0.6
Connection of pulp mill	CONN	[yes/no]	no
Fraction dilution of waste water with waste water from pulping CONN = yes CONN = no	Fww2	[-]	 0 0.5
Effluent discharge of STP for paper plant	EFLLUENTlocal$_{stp}$	[m^3.d^{-1}]	5,000

Release of slimicides in paper mills taking degradation into account

Calculating rate constants

$$khydr_{acid} = ln\ 2 \ /\ DT50hydr_{acid} \quad \text{(P-190)}$$

$$khydr_{water} = ln\ 2 \ /\ DT50hydr_{water} \quad \text{(P-191)}$$

$$khydr_{alkal} = ln\ 2 \ /\ DT50hydr_{alkal} \quad \text{(P-192)}$$

$$kphototot_{water} = ln\ 2 \ /\ DT50photo_{water} \quad \text{(P-193)}$$

$$kphoto_{water} = kphototot_{water} - khydr_{water} \quad \text{(P-194)}$$

$$kbiotot_{stp} = ln\ 2 \ /\ DT50bio_{stp} \quad \text{(P-195)}$$

I) Biodegradation test 12 hours light/12 hours dark

$$kbiotot_{water} = ln\ 2 \ /\ DT50bioI_{water} \quad \text{(P-196)}$$

$$kbioh_{water} = kbiotot_{water} - kphoto_{water} \quad \text{(P-197)}$$

$$kbio_{water} = kbioh_{water} - khydr_{water} \quad \text{(P-198)}$$

II) Biodegradation test in dark

$$kbioh_{water} = ln\ 2 \ /\ DT50bioII_{water} \quad \text{(P-199)}$$

$$kbio_{water} = kbioh_{water} - khydr_{water} \quad \text{(P-200)}$$

$$kbiotot_{water} = kbioh_{water} + kphoto_{water} \quad \text{(P-201)}$$

Input			
$DT50hydr_{acid}$	half-life time for hydrolysis in acid circumstances	[d]	S
$DT50hydr_{water}$	half-life time for hydrolysis in neutral circumstances	[d]	S
$DT50hydr_{alkal}$	half-life time for hydrolysis in alkaline circumstances	[d]	S
$DT50bio_{water}$	half-life time for biodegradation in water	[d]	S
$DT50bio_{stp}$	half-life time for for biodegradation in activated sludge	[d]	S
$DT50photo_{water}$	half-lifte time for photolysis in water	[d]	S
TESTTYPE	type of biodegradation test	[dark/light-dark]	P
$DT50bioI_{water}$	half-life for biodegradation in water from biodegradation test 12 hours light/12 hours dark	[d]	S
$DT50bioII_{water}$	half-life for biodegradation in water from biodegradation test in the dark	[d]	S
$kbiotot_{water}$	rate constant for biodegradation in water including hydrolysis and photolysis	[d^{-1}]	O
$kbioh_{water}$	rate constant for biodegradation in water including hydrolysis	[d^{-1}]	O
$khydr_{water}$	rate constant for degradation due to hydrolysis at neutral ($pH \approx 7$) conditions	[d^{-1}]	O
$kphoto_{water}$	rate constant for photolysis	[d^{-1}]	O
Output			
$khydr_{acid}$	rate constant for degradation due to hydrolysis at acid ($pH \approx 5$) conditions	[d^{-1}]	O
$khydr_{alkal}$	rate constant for degradation due to hydrolysis at alkaline ($pH \approx 8$) conditions	[d^{-1}]	O
$kbio_{water}$	rate constant for biodegradation in water	[d^{-1}]	O
$kbiotot_{stp}$	rate constant for biodegradation in STPs including hydrolysis	[d^{-1}]	O
$kphototot_{water}$	rate constant for photolysis including hydrolysis	[d^{-1}]	O

Table C-57 *Default settings for calculating the daily release to the STP including biodegradation, calculating rate constants*

Parameter	**Symbol**	**Unit**	**Value**
Type of biodegradation test	TESTTYPE	[dark/dark-light]	dark
Half-life time for biodegradation in activated sludge	$DT50bio_{stp}$	[d]	$DT50bio_{water}$ / 2

Calculating PECs

concentrations after primary settling

$$Cacid = Cinf \cdot e^{-\{(kbio_{water} + khydr_{acid})\cdot Tpr + kbiotot_{water}\cdot Tps)\}} \tag{P-202}$$

$$Cneutr = Cinf \cdot e^{-kbiotot_{water}\cdot (Tpr + Tps)} \tag{P-203}$$

$$Calkal = Cinf \cdot e^{-\{(kbio_{water} + khydr_{alkal})\cdot Tpr + kbiotot_{water}\cdot Tps)\}} \tag{P-204}$$

concentrations after secondary settling

$$Cacid_{AS} = Cacid \cdot e^{-(kbiotot_{stp}\cdot Tas + kbiotot_{water}\cdot Tss)} \tag{P-205}$$

$$Cneutr_{AS} = Cneutr \cdot e^{-(kbiotot_{stp}\cdot Tas + kbiotot_{water}\cdot Tss)} \tag{P-206}$$

$$Cneutr_{AS} = Cneutr \cdot e^{-(kbiotot_{stp}\cdot Tas + kbiotot_{water}\cdot Tss)} \tag{P-207}$$

concentrations after chemical/mechanical treatment

$$Cacid_{CM} = Cacid \cdot e^{-kbiotot_{water}\cdot Tcm} \tag{P-208}$$

$$Cneutr_{CM} = Cneutr \cdot e^{-kbiotot_{water}\cdot Tcm} \tag{P-209}$$

$$Calkal_{CM} = Calkal \cdot e^{-kbiotot_{water})\cdot Tcm} \tag{P-210}$$

concentrations after long-term biological treatment

$$Cacid_{BT} = Cacid \cdot e^{-Tbt\cdot (kbiotot_{water} + 0.5kphoto_{water})} \tag{P-211}$$

$$Cneutr_{BT} = Cneutr \cdot e^{-Tbt\cdot (kbiotot_{water} + 0.5kphoto_{water})} \tag{P-212}$$

$$Calkal_{BT} = Calkal \cdot e^{-Tbt\cdot (kbiotot_{water} + 0.5kphoto_{water})} \tag{P-213}$$

PEC in aeration tank at activated slugde treatment

$$PEC_{AS\ stp\_acid} = Cacid \cdot e^{-0.5\cdot kbiotot_{stp}\cdot Tas} \tag{P-214}$$

$$PEC_{AS\ stp\_neutr} = Cneutr \cdot e^{-0.5\cdot kbiotot_{stp}\cdot Tas} \tag{P-215}$$

$$PEC_{AS\ stp\_alkal} = Calkal \cdot e^{-0.5\cdot kbiotot_{stp}\cdot Tas} \tag{P-216}$$

PEC in aeration basin at long-term biological treatment

$$PEC_{BT\ stp\_acid} = Cacid \cdot e^{-0.5\cdot Tbt\cdot (kbiotot_{water} + 0.5kphoto_{water})} \tag{P-217}$$

$$PEC_{BT\ stp\_neutr} = Cneutr \cdot e^{-0.5\cdot Tbt\cdot (kbiotot_{water} + 0.5kphoto_{water})} \tag{P-218}$$

$$PEC_{BT\ stp\_alkal} = Calkal \cdot e^{-0.5\cdot Tbt\cdot (kbiotot_{water} + 0.5kphoto_{water})} \tag{P-219}$$

PEC in receiving surface water after activated sludge treatment

$$PEClocal_{AS\_water\_acid} = Cacid_{AS} \cdot DILUTION \qquad \text{(P-220)}$$

$$PEClocal_{AS\_water\_neutr} = Cneutr_{AS} \cdot DILUTION \qquad \text{(P-221)}$$

$$PEClocal_{AS\_water\_alkal} = Calkal_{AS} \cdot DILUTION \qquad \text{(P-222)}$$

PEC in receiving surface water after chemical/mechanical treatment

$$PEClocal_{CM\_water\_acid} = Cacid_{CM} \cdot DILUTION \qquad \text{(P-223)}$$

$$PEClocal_{CM\_water\_neutr} = Cneutr_{CM} \cdot DILUTION \qquad \text{(P-224)}$$

$$PEClocal_{CM\_water\_alkal} = Calkal_{CM} \cdot DILUTION \qquad \text{(P-225)}$$

PEC in receiving surface water after long-term biological treatment

$$PEClocal_{BT\_water\_acid} = Cacid_{BT} \cdot DILUTION \qquad \text{(P-226)}$$

$$PEClocal_{BT\_water\_neutr} = Cneutr_{BT} \cdot DILUTION \qquad \text{(P-227)}$$

$$PEClocal_{BT\_water\_alkal} = Calkal_{BT} \cdot DILUTION \qquad \text{(P-228)}$$

Input

Cinf	theoretical concentration of active ingredient	[kg.m^{-3}]	O
Tpr	retention time for paper making process	[d]	D
Tps	retention time for primary settling	[d]	D
Tas	retention time for the activated sludge unit	[d]	D
Tss	retention time for secondary settling	[d]	D
Tmc	retention time for chemical/mechanical treatment	[d]	D
Tbt	retention time for long-term biological treatment	[d]	D
DILUTION	dilution factor at discharge to surface water	[-]	D
Cacid	concentration after primary settling for acid process conditions	[kg.m^{-3}]	O
Cneutr	concentration after primary settling for neutral process conditions	[kg.m^{-3}]	O
Calkal	concentration after primary settling for alkaline process conditions	[kg.m^{-3}]	O
$Cacid_{AS}$	concentration after secondary settling for acid process conditions	[kg.m^{-3}]	O
$Cneutr_{AS}$	concentration after secondary settling for neutral process conditions	[kg.m^{-3}]	O
$Calkal_{AS}$	concentration after secondary settling for alkaline process conditions	[kg.m^{-3}]	O
$Cacid_{CM}$	concentration after chemical/mechanical treatment for acid process conditions	[kg.m^{-3}]	O
$Cneutr_{CM}$	concentration after chemical/mechanical treatment for neutral process conditions	[kg.m^{-3}]	O
$Calkal_{CM}$	concentration after chemical/mechanical treatment for alkaline process conditions	[kg.m^{-3}]	O
$Cacid_{BT}$	concentration after long-term biological treatment for acid process conditions	[kg.m^{-3}]	O
$Cneutr_{BT}$	concentration after long-term biological treatment for neutral process conditions	[kg.m^{-3}]	O
$Calkal_{BT}$	concentration after long-term biological treatment for alkaline process conditions	[kg.m^{-3}]	O

Output

PEC_{ASstp_acid}	predicted environmental concentration for assessment of micro-organisms in STP with activated sludge for acid conditions at the paper making process	[kg.m^{-3}]	O
PEC_{ASstp_neutr}	predicted environmental concentration for assessment of micro-organisms in STP with activated sludge for neutral conditions at the paper making process	[kg.m^{-3}]	O
PEC_{ASstp_alkal}	predicted environmental concentration for assessment of micro-organisms in STP with activated sludge for alkaline conditions at the paper making process	[kg.m^{-3}]	O
PEC_{BTstp_acid}	predicted environmental concentration for assessment of micro-organisms in STP with a long-term biological treatment for acid conditions at the paper making process	[kg.m^{-3}]	O
PEC_{BTstp_neutr}	predicted environmental concentration for assessment of micro-organisms in STP with a long-term biological treatment for neutral conditions at the paper making process	[kg.m^{-3}]	O
PEC_{BTstp_alkal}	predicted environmental concentration for assessment of micro-organisms in STP with a long-term biological treatment for alkaline conditions at the paper making process	[kg.m^{-3}]	O
$PEClocal_{AS\_water\_acid}$	predicted Environmental Concentration in receiving surface water after activated sludge treatment for acid process conditions at paper making	[kg.m^{-3}]	O
$PEClocal_{AS\_water\_alkal}$	predicted Environmental Concentration in receiving surface water after activated sludge treatment for alkaline process conditions at paper making	[kg.m^{-3}]	O
$PEClocal_{AS\_water\_neutr}$	predicted Environmental Concentration in receiving surface water after activated sludge treatment for neutral process	[kg.m^{-3}]	O

	conditions at paper making		
$PEClocal_{CM\_water\_acid}$	predicted Environmental Concentration in receiving surface water after chemical/mechanical treatment for acid process conditions at paper making	[kg.m^{-3}]	O
$PEClocal_{CM\_water\_alkal}$	predicted Environmental Concentration in receiving surface water after chemical/mechanical treatment for alkaline process conditions at paper making	[kg.m^{-3}]	O
$PEClocal_{CM\_water\_neutr}$	predicted Environmental Concentration in receiving surface water after chemical/mecanical treatment for neutral process conditions at paper making	[kg.m^{-3}]	O
$PEClocal_{BT\_water\_acid}$	predicted Environmental Concentration in receiving surface water after long-term biological treatment for acid process conditions at paper making	[kg.m^{-3}]	O
$PEClocal_{BT\_water\_alkal}$	predicted Environmental Concentration in receiving surface water afte long-term biological treatment for alkaline process conditions at paper making	[kg.m^{-3}]	O
$PEClocal_{BT\_water\_neutr}$	predicted Environmental Concentration in receiving surface water after long-term biological treatment for neutral process conditions at paper making	[kg.m^{-3}]	O

Product type 13: Metal working-fluid preservatives

III.4.8.35. Preservatives in metal industry

Parameters/variables and default values for water based metalworking fluids.

$$Elocal_{water} = Q_{pres} \cdot F_{suppl} \cdot F_{ai,pres} \qquad \text{(P-229)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{pres}$	[d]	300

Input

Q_{pres}	system capacity	[kg]$^{1)}$	S
F_{suppl}	fraction of fluid supplemented per day	[d^{-1}]	S
-	type of metalworking fluid	[-]	P
$F_{ai,pres}$	fraction of active ingredient in (diluted) fluid	[-]	O
$Temission_{pres}$	number of emission days for preservative	[d]	D

Output

$Elocal_{water}$	local emission to waste water during episode	[kg$_c$.d^{-1}]	O
Temission	number of emission days	[d]	O

1) Amount of metalworking fluid in system of machinery used

Table C-58 *Default settings of the model for preservatives in metal industry.*

Parameter	**Symbol**	**Unit**	**Value**
System capacity	Q_{pres}	[kg]	100
Fraction of fluid supplemented per day	F_{suppl}	[d^{-1}]	0.035
Fraction of active ingredient in (diluted) fluid:	$F_{a.i.,pres}$	[-]	
- emulsions			0.0005
- dispersions			0.00025
- synthetics			0.0002
- semi-synthetics			0.00035
- unknown			0.0005

Product type 14: Rodenticides

III.4.8.36. Household products used for fogging

The risk assessment of pesticides used in private gardens and as rodenticides on dump sites already incorporated in USES 4.0. The evaluation method used is the same as for pesticides used in agriculture (application via sprays, field application). In addition, a method for household products used for fogging or fumigation has been developed.

Model for calculating release to the air for compounds used for fumigation of buildings, silos, etc.

(the one in the formula is one day of the emission episode)

$$Elocal_{air} = \frac{Q_{subst} \cdot (1 - F_{ret}) \cdot (1 - F_{disin})}{1} \qquad \text{(P-230)}$$

Parameters required for distribution modules	**Defaults for this scenario**	**Unit**	**Value**
Temission	$Temission_{fogging}$	[d]	1

Input

Q_{subst}	amount used	[kg]	S
F_{ret}	fraction of retention in goods	[-]	D
F_{disin}	fraction of disintegration	[-]	D
$Temission_{fogging}$	number of emission days for fogging	[d]	D

Output

$Elocal_{air}$	local emission to air during episode	[$kg_c.d^{-1}$]	O
Temission	number of emission days	[d]	O

Table C-59 *Default settings of the model for household products used for fogging.*

Parameter	**Symbol**	**Unit**	**Value**
Fraction of retention in goods	F_{ret}	[-]	0.02
Fraction of disintegration	F_{disin}	[-]	0.001

Product type 21: Antifouling products

III.4.8.37. Antifoulings

Model for calculating concentrations in surface water for compounds used as antifoulings.

$$AREA_{ship} = (1 + F_{water\text{-}ship}) \cdot AREA_{deck} \tag{P-231}$$

$$V_{basin} = N_{ship} \cdot AREA_{ship} \cdot DEPTH_{basin} \tag{P-232}$$

$$AREA_{anti} = AREAlitre_{anti} \cdot V_{anti} \cdot N_{ship} \cdot F_{ship} \cdot F_{s\text{-}ns} \tag{P-233}$$

$$k_{advec,basin} = \frac{ln\,2}{DT50_{advec,ba\,sin}} \tag{P-234}$$

$$k_{basin} = \frac{kdeg_{water}}{1 + Kp_{susp.\,pest} \cdot SUSP_{water}} + k_{advec,basin} \tag{P-235}$$

$$Cwater_{pest,eq} = \frac{AREA_{anti} \cdot FLUX_{anti}}{V_{basin} \cdot k_{basin}} \tag{P-236}$$

$$Cwater_{pest\text{-}T} = \frac{Cwater_{pest,eq}}{1 + Kp_{susp,pest} \cdot SUSP_{water}} \quad T \in \{0,4,7,14,21,28,T_{bird},T_{mammal},365\}$$

(P-237)

Input

N_{ship}	number of yachts in yacht-basin	[-]	D
$AREA_{deck}$	mean ship deck area	[m^2]	D
$F_{water\text{-}ship}$	ratio water/ship in yacht-basin	[-]	D
-	specification of season for fraction of ships in water	[-]	P
F_{ship}	fraction ships in water	[-]	O
V_{anti}	liters paint per yacht	[m^3]	S
$AREAlitre_{anti}$	cover of antifouling paint	[m^2.m^{-3}]	S
$DEPTH_{basin}$	depth of yacht-basin	[m]	D
$F_{s\text{-}ns}$	fraction ships in yacht-basin	[-]	D
$FLUX_{anti}$	mean flux of compound	[kg$_c$.m^{-2}.d^{-1}]	S
$Kp_{susp,pest}$	solids-water partition coefficient in susp. matter for pesticides	[m^3.kg^{-1}]	O
$SUSP_{water}$	concentration suspended matter	[kg.m^{-3}]	D
$kdeg_{water}$	degradation rate in surface water	[d^{-1}]	O
$DT50_{advec,basin}$	advection half-life time in basin	[d]	D
$AREA_{ship}$	necessary harbour area per yacht	[m^2]	O^c
V_{basin}	amount of water in yacht-basin	[m^3]	O^c
$AREA_{anti}$	antifouling surface per yacht-basin	[m^2]	O^c
$k_{advec,basin}$	rate constant for advection	[d^{-1}]	O^c
k_{basin}	overall rate constant for removal from basin	[d^{-1}]	O^c
T_{bird}	test duration for bird toxicity test	[d]	S
T_{mammal}	test duration for mammalian toxicity test	[d]	S

Output

$Cwater_{pest\text{-}0}$	peak concentration in water	[kg$_c$.m^{-3}]	O
$Cwater_{pest\text{-}T}$	average concentration in water over T days $T \in \{4,7,14,21,28,T_{bird},T_{mammal},365\}$	[kg$_c$.m^{-3}]	O

Table C-60 *Default settings for calculating concentrations in surface water for compounds used as antifoulings.*

Parameter	Symbol	Unit	Value
Number of yachts in yacht-basin	N_{ship}	[-]	250
Mean ship deck area	$AREA_{deck}$	[m^2]	10
Ratio water/ship in yacht-basin	$F_{water\text{-}ship}$	[-]	3
Fraction ships in water - Whole year - Summer - Winter	F_{ship}	[-]	 0.5 * 1.0 0.25
Litres paint per yacht	V_{anti}	[m^3]	0.002
Cover of antifouling paint	$AREAlitre_{anti}$	[m^2.m^{-3}]	2500
Depth of yacht-basin	$DEPTH_{basin}$	[m]	2.5
Fraction ships in yacht-basin	$F_{s\text{-}ns}$	[-]	0.71
Mean flux of compound	$FLUX_{anti}$	[kg$_c$.m^{-2}.d^{-1}]	2.5.10^{-5}
Advection time in basin (d^{-1})	$DT50_{advec,basin}$	[d]	50

* The whole-year value is used as default, the user is able to make a selection.

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.

III.4.8.38. biocides used in taxidermy

Model for calculating release to water for compounds used in taxidermist fluids.

$$Elocal\_water_i = Qskin \cdot Qsubst \cdot (1 - Ffix) \qquad \text{(P-238)}$$

$$Elocal_{water} = \sum_i Elocal\_water_i \qquad \text{(P-239)}$$

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			
$Elocal_{water}$	local emission of active substance to waste water for all treatment steps	[kg$_c$.d^{-1}]	O

Table C-61 *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

III.4.8.39. Biocides used in the embalming process

Model for calculating release to water for compounds used in the embalming process.

$$\begin{aligned} Elocal_{water} = {} & Vform_{arterial} \cdot RHOform \cdot Cform_{arterial} \cdot (1 - Fret_{arterial}) + \\ & Vform_{cavity} \cdot RHOform \cdot Cform_{cavity} \cdot (1 - Fret_{cavity}) \end{aligned} \qquad \text{(P-240)}$$

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
$Vform_{cavity}$	volume of solution applied per embalmed corpse for cavity treatment	[m^3]	O
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	[-]	S/O
$Fret_{cavity}$	retention rate of cavity fluid	[-]	S/O
Output			
$Elocal_{water}$	local emission of active substance to waste water	[$kg.d^{-1}$]	O

Table C-62 *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
- fromaldehyde 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
- fromaldehyde 22%			0.9
Long-term			
- formaldehyde 4%			0.8
- formaldehyde 22%			0.9
Specific mass of solution	RHOform	[kg.m^{-3}]	1,000

III.4.8.40. Biocides releases in cemeteries

Model for calculating release in cemeteries of compounds used in the embalming process.

$$\begin{aligned}\mathit{Elocal}_{soil} = [&\mathit{Vform}_{arterial} \cdot \mathit{RHOform} \cdot \mathit{Cform}_{arterial} \cdot (1 - \mathit{Fret}_{arterial})\\ &+ \mathit{Vform}_{cavity} \cdot \mathit{RHOform} \cdot \mathit{Cform}_{cavity} \cdot (1 - \mathit{Fret}_{cavity})] \cdot\\ &(1 - \mathit{Freact}) \cdot \mathit{Ncorpse}\end{aligned} \qquad \text{(P-241)}$$

$$\begin{aligned}\mathit{Csoil\_av}_{cem} = \mathit{Elocal}_{soil} \,/\, (&\mathit{LENGTHcem} \cdot \mathit{WIDTHcem} \cdot \mathit{DEPTHmix}_{cem\text{-}soil}\\ &\cdot \mathit{RHOsoil} \cdot \mathit{krem}_{soil})\end{aligned} \qquad \text{(P-242)}$$

$$\mathit{Cporew\_av}_{cem} = \mathit{Csoil\_av}_{cem} \cdot \mathit{RHOsoil} \,/\, K_{soil\text{-}water} \qquad \text{(P-243)}$$

Input			
-	type of preservation and type of biocide applied	[-]	P
$\mathrm{Vform}_{arterial}$	volume of solution applied per embalmed corpse for arterial injection	$[m^3]$	O
Vform_{cavity}	volume of solution applied per embalmed corpse for cavity treatment	$[m^3]$	O
RHOform	specific mass of solution	$[kg.m^{-3}]$	D
$\mathrm{Cform}_{arterial}$	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
$\mathrm{Fret}_{arterial}$	retention rate of arterial fluid	[-]	S/O
Fret_{cavity}	retention rate of cavity fluid	[-]	S/O
Freact	factor for reaction with body	[-]	S/D
Ncorpse	number of embalmed corpses burried per day	[-]	D
LENGTHcem	length of cemetery	[m]	D
WIDTHcem	widht of cemetery	[m]	D
$\mathrm{DEPTHmix}_{cem\text{-}soil}$	mixing depth of soil	[m]	D
RHOsoil	bulk density of soil	$[kg.m^{-3}]$	D
$K_{soil\text{-}water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	O^c
krem_{soil}	first order rate constant for removal in soil	$[d^{-1}]$	O
Elocal_{soil}	daily average input of active substance to the cemetery	$[kg.d^{-1}]$	O
$\mathrm{Csoil\_av}_{cem}$	average concentration in soil	$[kg.kg_{wwt}^{-1}]$	O
Output			
$\mathrm{Cporew\_av}_{cem}$	average concentration in soil porewater	$[kg.m^{-3}]$	O

Table C-63 *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	$\text{Vform}_{\text{arterial}}$ / $\text{Vform}_{\text{cavity}}$	[m^3]	
Short-term			
- formaldehyde 4%			0.0060
- fromaldehyde 22%			0.0005
Long-term			
- formaldehyde 4%			0.0100
- formaldehyde 22%			0.0005
Retention rate of both arterial injection fluid and cavity treatment fluid	$\text{Fret}_{\text{arterial}}$ / $\text{Fret}_{\text{cavity}}$	[-]	
Short-term			
- formaldehyde 4%			0.9
- fromaldehyde 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	$\text{DEPTHmix}_{\text{cem-soil}}$	[m]	0.5
Bulk density of soil	RHOsoil	[$kg.m^{-3}$]	1,700
Specific mass of solution	RHOform	[$kg.m^{-3}$]	1,000

Waste treatment, landfill model

III.4.8.41. Waste treatment, landfill model

Model for calculating releases from a sanitary landfill.

$$\begin{aligned} \boldsymbol{Vlandf} &= \boldsymbol{AREAlandf \cdot DEPTHwaste - 4\pi \cdot DEPTHwaste^{2} \cdot} \\ &\quad \boldsymbol{\sqrt{\frac{AREAlandf}{\pi}} + 5\,{}^{1}\!/_{3}\,\pi \cdot DEPTHwaste^{3}} \end{aligned} \tag{P-244}$$

$$\boldsymbol{Qwaste_{landf} = Vlandf \cdot RHOwaste/\,Tutil} \tag{P-245}$$

Amount of percolating water in various sections of the landfill and the entire landfill, for the situation that percolating water is discharged without treatment

$$\boldsymbol{Vwater_{dump} = AREAlandf \cdot WS_{bare}/\,Tutil} \tag{P-246}$$

$$\boldsymbol{Vwater_{veg} = AREAlandf \cdot WS_{veg}/\,Tutil} \tag{P-247}$$

$$\boldsymbol{Vwater_{final} = AREAlandf \cdot WS_{final}/\,Tutil} \tag{P-248}$$

$$\boldsymbol{Vwater_{open} = AREAlandf \cdot RAINRATE/\,Tutil} \tag{P-249}$$

$$\begin{aligned} \boldsymbol{Vwater\_percol_{i}} &= \boldsymbol{Vwater_{dump} + (i - 1) \cdot \left[i - 1 - INT \frac{i-1}{Tfinal\_top} \right] \cdot Tfinal\_top \cdot} \\ &\quad \boldsymbol{Vwater_{verg} + (Tutil - 1) \cdot Vwater_{open} + \left(INT \frac{i-1}{Tfinal\_top} \right) \cdot} \\ &\quad \boldsymbol{Tfinal\_top \cdot Vwater_{final} + i \cdot Vwater_{produced} \left[for\ i = 1 \ldots Tutil \right]} \\ &= \boldsymbol{Tutil \cdot Vwater_{final} + Tutil \cdot Vwater_{produced} \left[for\ i > Tutil \right]} \end{aligned} \tag{P-250}$$

Removal rates for the various sections of the landfill and the entire landfill

Degradation

$$\boldsymbol{kdeg_{waste\_subst} = kdeg_{soil}} \tag{P-251}$$

Leaching

$$\boldsymbol{kleach_{bare} = WS_{bare}/\left(K_{soil-water} \cdot DEPTHwaste\right)} \tag{P-252}$$

$$\boldsymbol{kleach_{veg} = WS_{veg}/\left(K_{soil-water} \cdot DEPTHwaste\right)} \tag{P-253}$$

$$\boldsymbol{kleach_{final} = WS_{final}/\left(K_{soil-water} \cdot DEPTHwaste\right)} \tag{P-254}$$

Volatilisation

$$\frac{1}{kvolat_{water}} = \left(\frac{1}{kasl_{air} \cdot K_{soil-water}} + \frac{1}{kasl_{soilair} \cdot K_{air-water} + kasl_{soilwater}} \right) \cdot K_{soil-water} \cdot DEPTHwaste \qquad \text{(P-255)}$$

Overall removal rates

$$krem_{bare} = kdeg_{waste\text{-}subst} + kleach_{bare} + kvolat_{waste} \qquad \text{(P-256)}$$

$$krem_{veg} = kdeg_{waste\text{-}subst} + kleach_{veg} + kvolat_{waste} \qquad \text{(P-257)}$$

$$krem_{final} = kdeg_{waste\text{-}subst} + kleach_{final} + kvolat_{waste} \qquad \text{(P-258)}$$

Concentration in waste at the beginning of a year *i* in a sector of the landfill

$$\begin{aligned} Csubst\_landf_i &= Csubst\_landf_{i-1} \cdot e^{-krem_{bare} \cdot i} \ [for\ i = 1] \\ &= Csubst\_landf_{i-1} \cdot e^{-krem_{veg} \cdot i} \ [for\ i = 2 \ldots Tutil] \\ &= Csubst\_landf_{i-1} \cdot e^{-krem_{final} \cdot i} \ [for\ i > Tutil] \end{aligned} \qquad \text{(P-259)}$$

Amount removed from waste in a sector in year *i*

$$Qrem\_sec_i = Csubst\_landf_{i-1} - Csubst\_landf_i \cdot Qwaste_{landf} \qquad \text{(P-260)}$$

Amount of substance leached in a sector and the entire landfill in year *i*

$$\begin{aligned} Qleach\_sec_i &= kleach_{bare} / krem_{bare} \cdot Qrem\_sec_i [for\ i = 1] \\ &= kleach_{veg} / krem_{veg} \cdot Qrem\_sec_i \ [for\ i = 2 \ldots Tutil] \\ &= kleach_{final} / krem_{final} \cdot Qrem\_sec_i \ [for\ i > Tutil] \end{aligned} \qquad \text{(P-261)}$$

$$Qleach\_landf_i = \sum_{j-i}^{i} Qleach\_sec_i \qquad \text{(P-262)}$$

Amount of substance volatilised in a sector and the entire landfill in year *i*

$$\begin{aligned} Qvolat\_sec_i &= kvolat_{waste} / krem_{bare} \cdot Qrem\_sec_i [for\ i = 1] \\ &= kvolat_{waste} / krem_{veg} \cdot Qrem\_sec_i \ [for\ i = 2 \ldots Tutil] \\ &= kvolat_{waste} / krem_{final} \cdot Qrem\_sec_i \ [for\ i > Tutil] \end{aligned} \qquad \text{(P-263)}$$

$$Qvolat\_landf_i = \sum_{j-i}^{i} Qvolat\_sec_i \qquad \text{(P-264)}$$

Amount of gas produced in the entire landfill in year *i* for the situation that landfill gas is not burnt

$$\begin{aligned} Vgas\_landf_i &= \sum_{i=1}^{Tutil} \sum_{j=1}^{i} Fgas_{formation} \cdot Vgas_{orgC} \cdot Qwaste_{landf} \cdot Corg_{landf} \cdot \\ &\quad kdeg_{waste\_orgC} \cdot e^{-kdeg_{waste\_orgC} \cdot i} \ [for\ i = 1 \ldots Tutil] \\ &= \sum_{i=Tutil+1}^{Tutil+5} \sum_{j=1}^{Tutil} Fgas_{formation} \cdot Vgas_{orgC} \cdot Qwaste_{landf} \cdot Corg_{landf} \cdot \\ &\quad kdeg_{waste\_orgC} \cdot e^{-kdeg_{waste\_orgC} \cdot i} \ [for\ i > Tutil] \end{aligned} \qquad \text{(P-265)}$$

End calculations: all calculations for i = 1…Tutil+5

$$Qsubst\_STP_i = \left(1 - Fleach_{subsoil}\right) \cdot Qleach\_landf_i \tag{P-266}$$

$$Qsubst\_soil_i = Fleach_{subsoil} \cdot Qleach\_landf_i \tag{P-267}$$

$$Qsubst\_air_i = Fvolat \cdot Qvolat\_landf_i \tag{P-268}$$

$$Qsubst\_perc_i = Qleach\_landf_i \,/\, Vwater\_percol_i \tag{P-269}$$

$$Qsubst\_gas_i = Qvolat\_landf_i \,/\, Vgas\_landf_i \tag{P-270}$$

Input

AREAlandf	bottom surface of the landfill	[m^2]	D
DEPTHwaste	total height of waste dumped	[m]	D
RHOwaste	density of waste	[kg. m^{-3}]	D
Tutil	utilisation period	[d]	D
Vlandf	total volume of landfill	[m^3]	O^c
Qwaste$_{landf}$	mass of waste dumped daily	[kg.d^{-1}]	O^c
RAINRATE	wet precipitation	[m.d^{-1}]	D
WS$_{bare}$	precipitation surplus in sector with a surface without vegetation	[m.d^{-1}]	D
WS$_{veg}$	precipitation surplus in sector with a surface with vegetation	[m.d^{-1}]	D
WS$_{final}$	precipitation surplus in sector with a surface with top seal	[m.d^{-1}]	D
Vwater$_{produced}$	water produced in waste sector	[m^3.d^{-1}]	D
Vwater$_{dump}$	amount of percolating water in section where dumping takes	[m^3.d^{-1}]	O^c
Vwater$_{veg}$	amount of percolating water in a section where dumping has taken place in one of the previous years during the utilitsation period	[m^3.d^{-1}]	O^c
Vwater$_{final}$	amount of percolating water in section where dumping has taken place after closure of the landfill and application of final seal	[m^3.d^{-1}]	O^c
Vwater$_{open}$	amount of water in section where dumping stil has to take palce in future year	[m^3.d^{-1}]	O^c
Vwater_percol$_i$	amount of percolating water for year i = 1…Tutil +5 in the entire landfill	[m^3.d^{-1}]	O^c
Fgas$_{formation}$	factor of (gas) formation	[-]	D
Vgas$_{orgC}$	volume of landfill gas produced from organic carbon	[m^3.kg]	D
-	type of waste, inorganic or domestic	[inorg/domestic]	P
Corg$_{landf}$	content of biodegradable organic carbon in waste	[kg.kg^{-1}]	D
kdeg$_{waste\_orgC}$	rate constant for biodegradation of organic carbon inwaste	[d^{-1}]	D
kdeg$_{soil}$	rate constant for degradation in bulk soil	[d^{-1}]	O
Vgas_landf$_i$	total amount of gas produced in year i in the entire landfill for i = 1…Tutil+5	[m^3.d^{-1}]	O^c
kdeg$_{waste\text{-}subst}$	rate constant for degradation of substance in waste	[d^{-1}]	O^c
K$_{soil\text{-}water}$	soil-water partition coefficient	[m^3.m^{-3}]	O^c
K$_{air\text{-}water}$	air-water partition coefficient	[m^3.m^{-3}]	O^c
kasl$_{air}$	partial mass transfer coefficient at air side of air–soil interface	[m.d^{-1}]	D
kasl$_{soil\text{-}air}$	partial mass transfer coefficient at soil-air side of air-soil interface	[m.d^{-1}]	D
kasl$_{soil\text{-}water}$	partial mass transfer coefficient at soil-water side of soil-water interface	[m.d^{-1}]	D
kleach$_{bare}$	rate constant for leaching of substance in sector with a surface without vegetation	[d^{-1}]	O^c
kleach$_{veg}$	rate constant for leaching of substance in sector with a surface with vegetation	[d^{-1}]	O^c
kleach$_{final}$	rate constant for leaching of substance in sector with a surface with top seal	[d^{-1}]	O^c
kvolat$_{waste}$	rate constant for volatilisation of substance without vegetation	[d^{-1}]	O^c
krem$_{bare}$	overall removal rate constant in sector with a surface without vegetation	[d^{-1}]	O^c
krem$_{veg}$	overall removal rate constant in sector with a surface with vegetation	[d^{-1}]	O^c
krem$_{final}$	overall removal rate constant in sector with a surface with top seal	[d^{-1}]	O^c
Csubst_landf$_i$	concentration in waste at beginning of year i in a sector for i = 1..Tutil+5	[kg.kg^{-1}]	O^c
Qrem_sec$_i$	amount removed from waste in a sector in year i for i = 1…Tutil+5	[kg.d^{-1}]	O^c
Qleach_sec$_i$	amount of substance leached from a sector in year i for	[kg.d^{-1}]	O^c

	i = 1…Tutil+5		
Qleach_landf$_i$	total amount of substance leached from landfill in year i for i = 1…Tutil+5	[kg.d^{-1}]	O^c
Qvolat_sec$_i$	amount of substance volatilised from a sector in year i for i = 1…Tutil+5	[kg.d^{-1}]	O^c
Qvolat_landf$_i$	total amount of substance volatilised from landfill in year i for i = 1…Tutil+5	[kg.d^{-1}]	O^c
Fleach$_{subsoil}$	fraction of substance leached and penetrating into the subsoil	[-]	D
Fvolat	fraction of substance volatilised and escaping into the air	[-]	D
Csubst_landf$_0$	initial concentration of substance in landfilled waste	[kg.kg^{-1}]	O
Output			
Elocal$_{water}$	local emission of active substance to waste water	[kg.d^{-1}]	O
Qsubst_STP$_i$	amount of substance leached per day in year i and transported to the STP for i = 1…Tuitl+5	[kg]	O
Qsubst_soil$_i$	amount of substance leached per day in year i and penetrated into the subsoil for i = 1…Tuitl+5	[kg]	O
Qsubst_air$_i$	amount of substance volatilised per day in year i and escaped to the air for i = 1…Tuitl+5	[kg]	O
Csubst_perc$_i$	concentration of substance in percolating water in year i for i = 1…Tuitl+5	[kg.m^{-3}]	O
Qsubst_gas$_i$	concentration of substance in landfill gas in year i and transported to the STP for i = 1…Tuitl+5	[kg.m^{-3}]	O

Table C-64 *Default settings of the model for calculating the release of biocides from landfills.*

Parameter	**Symbol**	**Unit**	**Value**
Bottom surface of the landfill	AREAlandf	[m^2]	300,000
Total height of waste dumped	DEPTHwaste	[m]	20
Density of waste	RHOwaste	[kg. m^{-3}]	1,000
Utilisation period	Tutil	[d]	5,475
Period of installation of final top seal	Tfinal_top	[d]	1,825
Wet precipitation	RAINRATE	[m.d^{-1}]	0.0022
Precipitation surplus in sector with a surface without vegetation	WS$_{bare}$	[m.d^{-1}]	0.0012
Precipitation surplus in sector with a surface with vegetation	WS$_{veg}$	[m.d^{-1}]	0.0008
Precipitation surplus in sector with a surface with top seal	WS$_{final}$	[m.d^{-1}]	0.0001
Water produced in waste sector	Vwater$_{produced}$	[m^3.d^{-1}]	0
Factor of (gas) formation	Fgas$_{formation}$	[-]	0.58
Volume of landfill gas produced from organic carbon	Vgas$_{oprgC}$	[m^3.kg]	1.87
Content of biodegradable organic carbon in inorganic waste	Corg$_{landf}$	[kg.kg^{-1}]	0.050
Content of biodegradable organic carbon in domestic waste	Corg$_{landf}$	[kg.kg^{-1}]	0.112
Rate constant for biodegradation of organic carbon inwaste	kdeg$_{waste\_orgC}$	[d^{-1}]	2.57.10^{-4}
Partial mass transfer coefficient at air side of air–soil interface	kasl$_{air}$	[m.d^{-1}]	1.39.10^{-3}
Partial mass transfer coefficient at soil-air side of air-soil	kasl$_{soil-air}$	[m.d^{-1}]	5.56.10^{-6}

interface			
Partial mass transfer coefficient at soil-water side of soil-water interface	$kasl_{soil-water}$	$[m.d^{-1}]$	$5.56.10^{-6}$
Fraction of substance leached and penetrating into the subsoil	$Fleach_{subsoil}$	[-]	0.05
Fraction of substance volatilised and escaping into the air	Fvolat	[-]	0.15

III.4.9. Local distribution routes for pesticide application

Input application of pesticide			
$DOSE_{pest}$	single dosage for pesticide	$[kg_{c}.m^{-2}]$	
$DOSE_{pest,gh}$	single dosage in case of pesticide in greenhouse	$[kg_{c}]$	
$DOSE_{max}$	apparent maximum dosage	$[kg_{c}.m^{-2}]$	
N_{appl}	number of applications in one year	[-]	
$T_{interval}$	application interval	[d]	
N_{lt}	number of application periods per registration period	[-]	
$T_{interval\text{-}lt}$	long term interval for application periods	[d]	
MIX	mixing with soil	[yes/no]	
F_{soil}	fraction of dosage that reaches the soil	[-]	
F_{drift}	fraction drift related to location and way of application	[-]	
DRAINS	is drainage present?	[yes/no]	
Input other			
T_{bird}	test duration for bird toxicity test	[d]	
T_{mammal}	test duration for mammalian toxicity test	[d]	
$kdeg_{soil}$	rate constant for degradation in bulk soil	$[d^{-1}]$	
$DT50bio_{soil}$	half life for biodegradation in soil	[d]	
$kdeg_{water}$	first order rate constant for degradation in surface water	$[d^{-1}]$	
$Csoil_{std,pest\text{-}1}$	standard concentration in plough layer after one year	$[kg_{c}.kg^{-1}/kg_{c}.m^{-2}]$	c
RHO_{pest}	bulk density of application soil	$[kg.m^{-3}]$	c
$CONV_{sed}$	conversion factor for sediment concentrations: wwt to dwt	$[kg_{wwt}.kg_{dwt}^{-1}]$	c
F_{bound}	fraction of bound residues at end of metabolism study	[-]	
Output soil			
$Csoil_{pest\text{-}0}$	peak concentration in soil after N applications	$[kg_{c}.kg_{wwt}^{-1}]$	
$Csoil_{pest\text{-}10}$	peak concentration in plough layer after 10 years	$[kg_{wwt}.m^{-3}]$	
$Csoil_{pest\text{-}11}$	peak concentration in plough layer after 11 years	$[kg_{wwt}.m^{-3}]$	
$Csoil_{pest\text{-}12}$	peak concentration in plough layer after 12 years	$[kg_{wwt}.m^{-3}]$	
$Csoil_{pest\text{-}28}$	average concentration in soil over 28 days	$[kg_{c}.kg_{wwt}^{-1}]$	
$Csoil_{pest\text{-}Tbird}$	average concentration in soil over T_{bird} days	$[kg_{c}.kg_{wwt}^{-1}]$	
$Csoil_{pest\text{-}Tmammal}$	average concentration in soil over T_{mammal} days	$[kg_{c}.kg_{wwt}^{-1}]$	
$Csoil_{pest\text{-}lt}$	concentration in soil after $(N_{lt} + 2)$ years	$[kg_{c}.kg_{wwt}^{-1}]$	
Output water			
$Cwater_{pest\text{-}0}$	peak concentration after the N applications (dissolved)	$[kg_{c}.m^{-3}]$	
$Cwater_{pest\text{-}4}$	average concentration in the ditch over 4 days (dissolved)	$[kg_{c}.m^{-3}]$	
$Cwater_{pest\text{-}21}$	average concentration in the ditch over 21 days (dissolved)	$[kg_{c}.m^{-3}]$	
$Cwater_{pest\text{-}28}$	average concentration in the ditch over 28 days (dissolved)	$[kg_{c}.m^{-3}]$	
$Cwater_{pest\text{-}Tbird}$	average concentration in the ditch over T_{bird} days (dissolved)	$[kg_{c}.m^{-3}]$	
$Cwater_{pest\text{-}Tmammal}$	average concentration in the ditch over T_{mammal} days (dissolved)	$[kg_{c}.m^{-3}]$	
C_{river}	average concentration in a river for human exposure	$[kg_{c}.m^{-3}]$	
Output sediment			
$Csed_{pest\text{-}7}$	average concentration in sediment over 7 days	$[kg_{c}.kg_{wwt}^{-1}]$	
$Csed_{pest\text{-}14}$	average concentration in sediment over 14 days	$[kg_{c}.kg_{wwt}^{-1}]$	
$Csed_{pest\text{-}28}$	average concentration in sediment over 28 days	$[kg_{c}.kg_{wwt}^{-1}]$	
$Csed_{pest\text{-}lt}$	concentration after $(N_{lt} + 2)$ years of applications	$[kg_{c}.kg_{wwt}^{-1}]$	
Output groundwater			
$Cgrw_{pest}$	concentration in ground water used in drinking water	$[kg_{c}.m^{-3}]$	
Output air			
$Clocal_{air}$	local concentration in air during episode	$[kg_{c}.m^{-3}]$	
$Clocal_{air,ann}$	annual average local concentration in air	$[kg_{c}.m^{-3}]$	
$DEPtotal_{ann}$	annual average total deposition flux	$[kg_{c}.m^{-2}.d^{-1}]$	

Table D-1 *Default settings for pesticide application.*

Parameter	Symbol	Unit	Value
Long term application interval	$T_{interval\text{-}lt}$	[d]	365
Number of application per registration period	N_{lt}	[-]	9

III.4.9.1. Pesticide application soil (target area)

Concentration of pesticide after one application

Granules, treated seeds and the dosage applied via spray can all be mixed with the soil. If mixed with the soil the dosage of pesticide is assumed to be distributed homogeneously over the top 20 cm of soil. If not mixed, a distribution over the top 5 cm is assumed for calculations. With these assumptions the concentration after one application can be calculated. The concentration after one application is given by:

if MIX = "yes" then $DEPTH_{pest}$ = 0.2 m else $DEPTH_{pest}$ = 0.05 m

$$Csoil_{pest\text{-}1\,appl} = \frac{F_{soil} \cdot DOSE_{pest}}{DEPTH_{pest} \cdot RHO_{pest}} \qquad \text{(P-271)}$$

For biocides, use the parameters for industrial soil instead of application soil:

$$Csoil_{pest\text{-}1\,appl} = \frac{F_{soil} \cdot DOSE_{pest}}{DEPTH_{ind} \cdot RHO_{soil}} \qquad \text{(P-272)}$$

Input			
$DOSE_{pest}$	dosage	$[kg_c.m^{-2}]$	S
MIX	mixing with soil	[yes/no]	P
$DEPTH_{pest}$	mixing depth of application soil	[m]	O
$DEPTH_{ind}$	mixing depth of industrial soil	[m]	D
F_{soil}	fraction of dosage that reaches the soil	[-]	O
RHO_{pest}	bulk density of application soil	$[kg.m^{-3}]$	O^c
RHO_{soil}	bulk density of soil	$[kg.m^{-3}]$	O^c
Output			
$Csoil_{pest\text{-}1\,appl}$	concentration in soil after one application	$[kg_c.kg_{wwt}^{-1}]$	O

PECs for soil, application per growing season

It is possible that application of granules or spray is repeated during the season. If this is the case, the maximum concentration, reached during the season, should be calculated. Assuming only first order biodegradation this concentration can be calculated as the concentration after one application plus the remaining contributions from earlier applications. The result depends on the half-life for biodegradation, the application frequency, and the interval between two applications.

The initial Predicted Environmental Concentration is set at this maximum concentration during the season. This PEC is considered to be equal to the concentration on day 0 ($Clocal_{pest\text{-}0}$), which is used in several models. For each toxicity test a Predicted Environmental Concentration (PEC) is calculated as the average concentration over a period, equal to the test duration in ecotoxicity tests with relevant organisms following the last application of the chemical (again assuming first order biodegradation).

$$F_{rs} = e^{-kdeg_{soil} \cdot T_{interval}} \qquad \text{(P-273)}$$

$$\begin{aligned} Csoil_{pest\text{-}0} &= Csoil_{pest\text{-}1\,appl} + Csoil_{pest\text{-}1\,appl} \cdot F_{rs} + \\ &\quad Csoil_{pest\text{-}1\,appl} \cdot F_{rs}^{2} + \ldots + Csoil_{pest\text{-}1\,appl} \cdot F_{rs}^{(N_{appl}-1)} \\ &= Csoil_{pest\text{-}1\,appl} \cdot \frac{1 - F_{rs}^{N_{appl}}}{1 - F_{rs}} \end{aligned} \qquad \text{(P-274)}$$

$$\begin{aligned} Csoil_{pest\text{-}T} &= \frac{1}{T} \cdot \int_{0}^{T} Csoil_{pest\text{-}0} \cdot e^{-kdeg_{soil} \cdot t} \cdot dt \\ &= Csoil_{pest\text{-}0} \cdot \frac{1 - e^{-kdeg_{soil} \cdot t}}{kdeg_{soil} \cdot T} \qquad T \in \{28, T_{bird}, T_{mammal}\} \end{aligned} \qquad \text{(P-275)}$$

Input			
$Csoil_{pest\text{-}1\,appl}$	concentration in soil after one application	$[kg_c.kg_{wwt}^{-1}]$	O
$kdeg_{soil}$	rate constant for degradation in soil	$[d^{-1}]$	O
N_{appl}	number of applications in one year	[-]	S
F_{rs}	fraction of the concentration remaining after time $T_{interval}$	[-]	O^c
$T_{interval}$	application interval	[d]	S
T_{bird}	test duration for bird toxicity test	[d]	S
T_{mammal}	test duration for mammalian toxicity test	[d]	S
Output			
$Csoil_{pest\text{-}0}$	peak concentration in soil after N applications	$[kg_c.kg_{wwt}^{-1}]$	O
$Csoil_{pest\text{-}T}$	average in soil concentration over T days	$[kg_c.kg_{wwt}^{-1}]$	O

PECs for soil, long-term application

The PEC after long-term application is set at the concentration after the last application in the tenth year. This PEC is considered to be equal to the soil concentration at year 10 ($Csoil_{pest\text{-}0,lt}$). After the tenth year the resulting concentration, $Csoil_{pest\text{-}lt}$, is compared to the PNEC.

$$\boldsymbol{Csoil_{pest-1} = Csoil_{std,pest-1} \cdot DOSE_{max}} \qquad \text{(P-276)}$$

$$\boldsymbol{F_{lt} = \frac{Csoil_{pest-1}}{Csoil_{pest-0}}} \qquad \text{(P-277)}$$

Peak concentration at last application:

$$\begin{aligned} \boldsymbol{Csoil_{pest\text{-}0,lt}} &= \boldsymbol{Csoil_{pest\text{-}0} + Csoil_{pest\text{-}0} \cdot F_{lt} +} \\ &\quad \boldsymbol{Csoil_{pest\text{-}0} \cdot F_{lt}^{2} + \ldots + Csoil_{pest\text{-}0} \cdot F_{lt}^{(N_{lt}-1)}} \qquad \text{(P-278)} \\ &= \boldsymbol{Csoil_{pest\text{-}0} \cdot \frac{1 - F_{lt}^{N_{lt}}}{1 - F_{lt}}} \end{aligned}$$

Concentration 2 years after last application:

$$\boldsymbol{Csoil_{pest\text{-}lt} = Csoil_{pest\text{-}0,lt} \cdot F_{lt}^{2}} \qquad \text{(P-279)}$$

Input			
$DOSE_{max}$	apparent maximum dosage	$[kg_c.m^2]$	S
$Csoil_{std,pest\text{-}1}$	standard concentration in plough layer after one year, read from PEARL tables	$[kg_c.kg^{-1}/kg_c.m^{-2}]$	S
$DEPTH_{pest}$	mixing depth of application soil	[m]	O
RHO_{pest}	wet bulk density of application soil	$[kg_{wwt}.m^3]$	O^c
N_{lt}	number of application periods per registration period	[-]	S
$T_{interval\text{-}lt}$	long term interval for application periods	[d]	S
F_{lt}	fraction of the concentration remaining after time $T_{interval,lt}$	[-]	O^c
$Csoil_{pest\text{-}1}$	concentration in plough layer after 1 year	$[kg_c.kg_{wwt}^{-1}]$	O^c
$Csoil_{pest\text{-}0}$	peak concentration in plough layer after 1 year	$[kg_c.kg_{wwt}^{-1}]$	O^c
$Csoil_{pest\text{-}0,lt}$	peak concentration in soil after N_{lt} years	$[kg_c.kg_{wwt}^{-1}]$	O^c
Output			
$Csoil_{pest\text{-}lt}$	concentration in soil after (N_{lt} + 2) years	$[kg_c.kg_{wwt}^{-1}]$	O

For the final risk assessment the concentration in the top soil layer has to be increased with a release of the total amount of bound residues in that layer. The amount released is estimated to be 5% of the bound residues.

$$\boldsymbol{Cres\_bound_{pest-1} = F_{bound} \cdot Csoil_{pest-0}} \qquad \text{(P-280)}$$

Input

F_{bound}	fraction of bound residues at end of metabolism study	[-]	S
$Csoil_{pest-0}$	peak concentration in plough layer after 1 year	$[kg_{wwt}.m^{-3}]$	O^c

Output

$Cres\_bound_{pest-1}$	concentration of bound residues after 1 year	$[kg_{wwt}.m^{-3}]$	O

Thus it is assumed that the amount of bound residues does not increase after the last measurement in the soil metabolism study. Though if there are clear indications that the maximum level of bound residues is not reached an estimated maximum level should be used instead. In addtion it is assumed that 5% of the total concentration is released every year.

$$\boldsymbol{Csoil_{pest-10} = 0.05 \cdot Cres\_bound_{pest-1} \cdot 0.95^{N_{lt}} + Csoil_{pest-0}} \qquad \text{(P-281)}$$

Input

N_{lt}	number of application periods per registration period	[-]	S
$Csoil_{pest-0}$	peak concentration in plough layer after 1 year	$[kg_{wwt}.m^{-3}]$	O^c
$Cres\_bound_{pest-1}$	concentration of bound residues after 1 year	$[kg_{wwt}.m^{-3}]$	O^c

Output

$Csoil_{pest-10}$	peak concentration in plough layer after 10 years	$[kg_{wwt}.m^{-3}]$	O

In the following two years there will be an additional load because of the release of bound residues still present in the plough layer.

$$\boldsymbol{Csoil_{pest-11} = 0.05 \cdot Cres\_bound_{pest-1} \cdot 0.95^{N_{lt}}} \qquad \text{(P-282)}$$

$$\boldsymbol{Csoil_{pest-12} = 0.05 \cdot Cres\_bound_{pest-1} \cdot 0.95^{N_{lt}+1}} \qquad \text{(P-283)}$$

Input

N_{lt}	number of application periods per registration period	[-]	S
$Cres\_bound_{pest-1}$	concentration of bound residues after 1 year	$[kg_{wwt}.m^{-3}]$	O^c

Output

$Csoil_{pest-11}$	peak concentration in plough layer after 11 years	$[kg_{wwt}.m^{-3}]$	O
$Csoil_{pest-12}$	peak concentration in plough layer after 12 years	$[kg_{wwt}.m^{-3}]$	O

III.4.9.2. Local short term atmospheric distribution of agricultural pesticides

Atmospheric emissions of pesticides after application can result from treated agricultural fields and greenhouses, both of which have different properties with respect to the local atmospheric distribution. An agricultural field can be regarded as a field, a greenhouse can be seen as a source with emission in the eddy of a building. For the two source types different methods for calculating the atmospheric downwind concentrations exist. The concentration downwind from a field is calculated with a Dutch version of the American PAL-model (Hanna *et al.*, 1982; Petersen, 1978). The method for the calculation of the concentration as a result of emission by a greenhouse is based on the building influence model (Vereniging Lucht, 1986). Atmospheric emission, dispersion and deposition of pesticides on small spatial and temporal scales are described in further detail in the following sections.

Table D-2 *Default settings for atmospheric distribution of agricultural pesticides.*

Parameter	**Symbol**	**Unit**	**Value**
One hour averaged concentration 10 m. downwind of the field with a standard emission strength	$Cstd_{field, air, 1h}$	$[kg_c.m^{-3}]$	$1.28.10^{-4}$
Coefficient depending on building type	K	[-]	0.2
Area of a standard greenhouse standing perpendicular to the wind direction	A	$[m^2]$	350
Windspeed at the roof top (3 m/s)	u	$[m.d^{-1}]$	$2.6.10^5$
Dry deposition velocity (1.10^{-3} m/s)	$DEPRATE_{dry}$	$[m.d^{-1}]$	86.4
One-hour averaged precipitation intensity	P_{1h}	$[m.d^{-1}]$	0.060
24-hour averaged precipitation intensity	P_{24h}	$[m.d^{-1}]$	0.015

Atmospheric emissions of pesticides

The atmospheric emission of a pesticide from an agricultural field or a greenhouse is estimated from its application density and its emission factor (the fraction of the applied dose that emits to the air). The emission factor on its turn depends on the pesticide's properties, the application technique employed and type of agriculture (field use or greenhouse use). For USES a set of generalised total emission factors, based on these elements, were defined.

These generalised total emission factors and the initial one and 24 hour averaged source strengths corresponding to an application density of 1 $kg.m^{-2}.appl.^{-1}$ for field use and 1 $kg.appl.^{-1}$ for greenhouse use, are presented in Table D-3 and Table D-4, respectively. The total emission factors have been derived from MJP-G (1996), the initial first hour averaged source strengths are calculated assuming that 30% of the total emission occurs in the first hour after application. For the calculation of the initial 24 hour averaged source strength it is assumed that 90% of the total emission occurs during the first day after application, which can be considered as a realistic worst case scenario.

Table D-3 *Emission factors and source strengths for field use of pesticides with different vapour pressures.*

Vapour pressure **[mPa]**	**Total emission factor** **[-]**	**1 hour averaged source strength** **$Estd_{field,air,1h}$ [$kg_c.m^{-2}.d^{-1}$]**	**24 hour averaged source strength** **$Estd_{field,air,24h}$ [$kg_c.m^{-2}.d^{-1}$)]**
> 10	1	7.2	0.9
1 - 10	0.5	3.6	0.45
0.1 - 1	0.2	1.44	0.18
0.01 - 0.1	0.1	0.72	0.09
< 0.01	0.01	0.072	0.009

Table D-4 *Emission factors and source strengths for use of pesticides with different vapour pressures in greenhouses.*

Vapour pressure **[mPa]**	**Total emission factor** **[-]**	**1 hour averaged source strength** **$Estd_{greenhouse,air,1h}$ [$kg_c.d^{-1}$]**	**24 hour averaged source strength** **$Estd_{greenhouse,air,24h}$ [$kg_c.d^{-1}$]**
> 10	0.4	2.880	0.360
1 - 10	0.32	2.304	0.288
0.1 - 1	0.15	1.080	0.135
0.01 - 0.1	0.08	0.576	0.072
< 0.01	0.02	0.144	0.018

Input			
VP	vapour pressure	[Pa]	S
Output			
$Estd_{field, air, 1h}$	standard 1 hour emission strength of the field	[$kg_c.m^{-2}.d^{-1}$]	O
$Estd_{field, air, 24h}$	standard 24 hour emission strength of the field	[$kg_c.m^{-2}.d^{-1}$]	O
$Estd_{greenhouse,air,1h}$	standard 1 hour emission strength of the greenhouse	[$kg_c.d^{-1}$]	O
$Estd_{greenhouse,air,24h}$	standard 24 hour emission strength of the greenhouse	[$kg_c.d^{-1}$]	O

The source strength in the tables is given for a standard dosage of 1 kg/m^2 for field use and 1 kg for greenhouse use (the 1 in the equations below). This standard value is recalculated using the actual dosage.

$$E_{field,air,1h} = \frac{Estd_{field,air,1h}}{1} \cdot DOSE_{pest} \tag{P-284}$$

$$E_{field,air,24h} = \frac{Estd_{field,air,24h}}{1} \cdot DOSE_{pest} \tag{P-285}$$

$$E_{greenhouse,air,1h} = \frac{Estd_{greenhouse,air,1h}}{1} \cdot DOSE_{pest,gh} \tag{P-286}$$

$$E_{greenhouse,air,24h} = \frac{Estd_{greenhouse,air,24h}}{1} \cdot DOSE_{pest,gh} \tag{P-287}$$

Input			
$DOSE_{pest}$	single dosage of pesticide	[$kg_c.m^{-2}$]	S
$DOSE_{pest,gh}$	single dosage of pesticide in greenhouse	[kg_c]	S
$Estd_{field, air, 1h}$	standard 1 hour emission strength of the field	[$kg_c.m^{-2}.d^{-1}$]	O
$Estd_{field, air, 24h}$	standard 24 hour emission strength of the field	[$kg_c.m^{-2}.d^{-1}$]	O
$Estd_{greenhouse,air,1h}$	standard 1 hour emission strength of the greenhouse	[$kg_c.d^{-1}$]	O
$Estd_{greenhouse,air,24h}$	standard 24 hour emission strength of the greenhouse	[$kg_c.d^{-1}$]	O
Output			
$E_{field,air,1h}$	1 hour emission strength of the field	[$kg_c.m^{-2}.d^{-1}$]	O
$E_{field,air,24h}$	24 hour emission strength of the field	[$kg_c.m^{-2}.d^{-1}$]	O
$E_{greenhouse,air,1h}$	1 hour emission strength of the greenhouse	[$kg_c.d^{-1}$]	O
$E_{greenhouse,air,24h}$	24 hour emission strength of the greenhouse	[$kg_c.d^{-1}$]	O

Concentration downwind from an agricultural field

The method presented here for the calculation of the concentration downwind of a field is based on the PALNAT-model. PALNAT is a version of the EPA PAL-model (Hanna *et al.*, 1982; Petersen, 1978) adapted to Dutch circumstances. The PAL-model calculates the concentration in the air for point, area and line sources based on a short term gaussian steady-state algorithm. The concentration in the air is calculated as a one hour averaged concentration at 10 meters downwind of the field.

The calculation of this concentration as a result of the emission from an agricultural field is based on a standard scenario. This standard scenario involves the meteorological conditions, emission height and size of the field. The standard scenario is as follows:

- field: 1 ha (100x100 meter),
- windspeed: 3 $m.s^{-1}$ (at 10 meter height),
- wind direction: constant,
- stability class: 5 (= Pasquill class D),
- mixing height: 500 m,
- roughness length z_0: 0.1 meter (agricultural land),
- emission height: 0 m,
- receptor point: 10 meters downwind,
- emission strength: 1 $kg.m^{-2}.d^{-1}$.

Given this scenario, a simple general formula has been derived from the gaussian plume model PALNAT for calculating the concentration 10 meters downwind of the field. The standard concentration is valid for a source strength of 1 $kg.m^{-2}.d^{-1}$ (the 1 in the equation below). Using the standard (E)USES units this formula is:

$$C_{field,air,1h} = \frac{E_{field,air,1h}}{1} \cdot Cstd_{field,air,1h} \qquad \text{(P-288)}$$

Input

$E_{field,air,1h}$	1 hour emission strength of the field	$[kg_c.m^{-2}.d^{-1}]$	O
$Cstd_{field,air,1h}$	1 hour averaged concentration at 10 meters downwind of field with a standard source strength	$[kg_c.m^{-3}]$	D

Output

$C_{field,air,1h}$	1 hour averaged conc. at 10 meters downwind of field	$[kg_c.m^{-3}]$	O

When it is assumed that the wind direction and windspeed remain constant during 24 hours (worst case situation) then the 24-hour averaged concentration is the same as the one hour averaged concentration, because the dispersion coefficients in PALNAT do not depend on the averaging time. If the dispersion coefficients are assumed to depend on the average time, such as done in the Dutch National model, a larger averaging time leads to greater dispersion coefficients and therefore to smaller concentrations.

Concentration downwind from a greenhouse

Concentrations resulting from emissions from a greenhouse are influenced by the turbulence around the greenhouse. The building influence model (Vereniging Lucht, 1986) is designed for calculating the concentration of a gaseous substance in the lee side eddy of a building. The model calculates the concentration in a lee side eddy assuming that the concentration is homogeneously distributed in the eddy. The method presented here for the calculation of the concentrations downwind from a greenhouse is based on this model.

In the proposed method a standard greenhouse is used for the calculation of the concentration in the lee side eddy. The size of the standard greenhouse is 100 by 100 meters with a height of 3.5 meters. This standard greenhouse was also used in similar projects (Baas and Huygen, 1991) and will be used in future projects for the Ministry of Housing, Spatial Planning and the Environment (Baas, 1996). The lee side eddy of the standard greenhouse stretches out to about 25 meters downwind from the building (Baas and Huygen, 1992). The coefficient K can vary between 0.2 (the wind direction has an angle of 45° to the front of the building) and 1.0 (the wind direction is perpendicular to the front of the building). Under realistic worst case conditions K is 0.2, corresponding to a wind direction of 45°. The windspeed is the same as for the field, i.e. 3 $m.s^{-1}$.

It is further assumed that the emission of pesticides takes place through the windows in the roof of the greenhouse. This means that the emission directly enters the lee eddy. The formula, adapted from the building influence model, for calculating the one hour averaged concentration in the lee side eddy, using standard units, is:

$$\boldsymbol{Cstd_{greenhouse,air,1h} = \frac{1}{K \cdot A \cdot u}} \qquad \text{(P-289)}$$

Input

K	coefficient dependent on wind direction to front of greenh.	[-]	D
A	area of standard greenhouse perpendicular to wind direction	[m^2]	D
u	windspeed at the roof top	[$m.d^{-1}$]	D
Output			
$Cstd_{greenhouse,air,1h}$	1 hour averaged concentration in the lee side eddy of the greenhouse with a standard source strength	[$kg_c.m^{-3}$]	O

For other source strengths the previous formula must be converted. The standard concentration is valid for a source strength of 1 $kg.d^{-1}$ (the 1 in the equation below). As in the case of concentrations downwind of a field, the one hour averaged and the 24 averaged concentrations are the same because the dispersion parameters in the building influence model do not depend on the averaging time.

$$C_{greenhouse,air,1h} = \frac{E_{greenhouse,air,1h}}{1} \cdot Cstd_{greenhouse,air,1h} \qquad \text{(P-290)}$$

Input

$E_{greenhouse,air,1h}$	1 hour emission strength of greenhouse through the roof	$[kg_c.d^{-1}]$	O
$Cstd_{greenhouse,air,1h}$	1 hour averaged concentration in the lee side eddy of the greenhouse with a standard source strength	$[kg_c.m^{-3}]$	O

Output

$C_{greenhouse,air,1h}$	1 hour averaged conc. in the lee side eddy of the greenhouse	$[kg_c.m^{-3}]$	O

Atmospheric deposition of pesticides

The calculation method for atmospheric deposition presented here is restricted to deposition as a result of the emissions *after* application (thus excluding droplet drift). As the spatial and temporal scales considered here are too small for formation of secondary aerosols, the method described here is restricted to atmospheric deposition of gases only. Atmospheric deposition consists of dry and wet deposition. At a low dry deposition velocity, the total deposition flux is mainly determined by wet deposition, which depends on the Henry-coefficient. At a higher dry deposition velocity the total deposition is dominated by dry deposition, in which the Henry coefficient is unimportant. Therefore, dry and wet deposition will be discussed separately. In this paragraph general formulas will be described for both wet and dry deposition near a standard field and a standard greenhouse.

Dry deposition

The dry deposition flux of gaseous substances is proportional to the dry deposition velocity. For the method to be used in USES, an average dry deposition velocity of 0.01 $cm.s^{-1}$ is proposed (Noordijk and De Leeuw, 1991). In EUSES (EC, 1996b) the aerosol deposition velocity is $1.0 \cdot 10^{-3}$ $m.s^{-1}$ instead of this value of $1.0 \cdot 10^{-4}$ $m.s^{-1}$. Therefore, currently the value $1.0.10^{-3}$ $m.s^{-1}$ is chosen. It appears that on a local scale, concentrations in air of gaseous chemicals are not influenced by the value of the dry deposition velocity, because of the small contribution of removal by deposition to the mass balance on a local scale.

When the deposition velocity is known, the dry deposition flux can easily be calculated by multiplying the gaseous concentration in the air with the deposition velocity. The one hour averaged deposition flux of a substance downwind of the field or on the lee side of the building at a standard source strength with a dry deposition velocity of $1.0 \cdot 10^{-3}$ $m.s^{-1}$ is:

$$\boldsymbol{DEPstd}_{gas\text{-}dry,field,1h} = \boldsymbol{DEPRATE}_{dry} \cdot \boldsymbol{Cstd}_{field,air,1h} \qquad \text{(P-291)}$$

$$\boldsymbol{DEPstd}_{gas\text{-}dry,greenhouse,1h} = \boldsymbol{DEPRATE}_{dry} \cdot \boldsymbol{Cstd}_{greenhouse,air,1h} \qquad \text{(P-292)}$$

Input			
$Cstd_{field,air,1h}$	1 hour averaged concentration at 10 meters downwind of the field with a standard source strength	$[kg.m^{-3}]$	D
$Cstd_{greenhouse,air,1h}$	1 hour averaged concentration in the lee side eddy of the greenhouse with a standard source strength	$[kg.m^{-3}]$	D
$DEPRATE_{dry}$	dry deposition velocity	$[m.d^{-1}]$	D
Output			
$DEPstd_{gas\text{-}dry,field,1h}$	standard one hour averaged deposition flux density downwind of the field with a standard source strength	$[kg.m^{-2}.d^{-1}]$	O
$DEPstd_{gas\text{-}dry,greenhouse,1h}$	standard one hour averaged deposition flux density in the lee-side eddy of the greenhouse with a standard source strength	$[kg.m^{-2}.d^{-1}]$	O

For other source strengths, the dry deposition for the field or the greenhouse must be converted. The standard deposition is valid for a source strength of 1 kg.m^{-2}.d^{-1} in field use or 1 kg.d^{-1} in a greenhouse (the 1 in the equation below).

$$\boldsymbol{DEP}_{\textit{gas-dry,field,}1h} = \frac{\boldsymbol{E}_{\textit{field,air,}1h}}{\mathbf{1}} \cdot \boldsymbol{DEPstd}_{\textit{gas-dry,field,}1h} \qquad \text{(P-293)}$$

$$\boldsymbol{DEP}_{\textit{gas-dry,greenhouse,}1h} = \frac{\boldsymbol{E}_{\textit{greenhouse,air,}1h}}{\mathbf{1}} \cdot \boldsymbol{DEPstd}_{\textit{gas-dry,greenhouse,}1h} \qquad \text{(P-294)}$$

Input			
$E_{\text{field, air, 1h}}$	1 hour emission strength of the field	[kg$_c$.m^{-2}.d^{-1}]	O
$E_{\text{greenhouse, air, 1h}}$	1 hour emission strength of greenhouse through the roof	[kg$_c$.d^{-1}]	O
$\text{DEPstd}_{\text{gas-dry, field, 1h}}$	standard one hour averaged deposition flux density downwind of the field with a standard source strength	[kg$_c$.m^{-2}.d^{-1}]	O
$\text{DEPstd}_{\text{gas-dry, greenhouse,1h}}$	standard one hour averaged deposition flux density in the lee-side eddy of the greenhouse with a standard source strength	[kg$_c$.m^{-2}.d^{-1}]	O
Output			
$\text{DEP}_{\text{gas-dry, field, 1h}}$	1 hour averaged deposition flux density of the field	[kg$_c$.m^{-2}.d^{-1}]	O
$\text{DEP}_{\text{gas-dry, greenhouse, 1h}}$	1 hour averaged deposition flux density of the greenhouse	[kg$_c$.m^{-2}.d^{-1}]	O

With the same assumptions as mentioned in the previous paragraphs, the 24 hour averaged dry deposition flux density is equal to the one hour averaged deposition flux density.

Wet deposition

The wet deposition flux of a substance depends on its solubility (Henry-coefficient) in rain and the precipitation intensity. For a substance that is highly soluble, wet deposition is more important than for a substance that is poorly soluble. For both the one hour and 24 hour averaged deposition flux it is assumed that the concentration in the atmosphere remains constant. This is a reasonable assumption because it is assumed that the emission remains also constant in that time and the distance to the source is very small.

The one hour averaged precipitation intensity, P_{1h}, is set to $6.94 \cdot 10^{-7}$ m.s^{-1}. For the 24 hour averaged deposition flux the precipitation intensity, P_{24h}, is set to $1.74 \cdot 10^{-7}$ m.s^{-1}. Both rain intensities are based on generalised Dutch conditions (Esser, 1993). These values correspond to 2.5 mm in one hour and 15 mm in 24 hour respectively. For both averaging periods it is assumed that the precipitation is homogeneously distributed over the whole period.

The one and 24 hour averaged standard wet deposition flux of a substance downwind of the field or on the lee side of the building is obtained by using a standard source strength in the next formulas. For the actual source strength the wet deposition flux is:

$$DEP_{gas\text{-}wet,\,field,1h} = P_{1h} \cdot \frac{1}{K_{air\text{-}water}} \cdot Cstd_{field,air,1h} \cdot E_{field,air,1h} \qquad \text{(P-295)}$$

$$DEP_{gas\text{-}wet,\,field,24} = P_{24h} \cdot \frac{1}{K_{air\text{-}water}} \cdot Cstd_{field,air,1h} \cdot E_{field,air,24h} \qquad \text{(P-296)}$$

$$DEP_{gas\text{-}wet,greenhouse,1h} = P_{1h} \cdot \frac{1}{K_{air\text{-}water}} \cdot Cstd_{greenhouse,air,1h} \cdot E_{greenhouse,air,1h} \qquad \text{(P-297)}$$

$$DEP_{gas\text{-}wet,greenhouse,24h} = P_{24h} \cdot \frac{1}{K_{air\text{-}water}} \cdot Cstd_{greenhouse,air,1h} \cdot E_{greenhouse,air,24h} \qquad \text{(P-298)}$$

Input			
P_{1h}	1 hour averaged precipitation intensity	[m.d^{-1}]	D
P_{24h}	24 hours averaged precipitation intensity	[m.d^{-1}]	D
$K_{air\text{-}water}$	air-water partition coefficient	[-]	O^c
$Cstd_{field,air,1h}$	standard air concentration 10 meters downwind of the field	[kg$_c$.m^3]	D
$Cstd_{greenhouse,air,1h}$	standard air concentration in the lee side eddy of greenhouse	[kg$_c$.m^3]	O
$E_{field,air,1h}$	1 hour emission strength of the field	[kg$_c$.m^{-2}.d^{-1}]	O
$E_{greenhouse,air,1h}$	1 hour emission strength of greenhouse through the roof	[kg$_c$.d^{-1}]	O
$E_{field,air,24h}$	24 hour emission strength of the field	[kg$_c$.m^{-2}.d^{-1}]	O
$E_{greenhouse,air,24h}$	24 hour emission strength of greenhouse through the roof	[kg$_c$.d^{-1}]	O
Output			
$DEP_{gas\text{-}wet,field,1h}$	1 hour averaged wet deposition flux downwind of field	[kg$_c$.m^{-2}.d^{-1}]	O
$DEP_{gas\text{-}wet,field,24h}$	24 hours averaged wet deposition flux downwind of field	[kg$_c$.m^{-2}.d^{-1}]	O
$DEP_{gas\text{-}wet,greenhouse,1h}$	1 hour averaged wet dep. flux downwind of greenhouse	[kg$_c$.m^{-2}.d^{-1}]	O
$DEP_{gas\text{-}wet,greenhouse,24h}$	24 hours averaged wet dep. flux downwind of greenhouse	[kg$_c$.m^{-2}.d^{-1}]	O

For the total deposition flux near a standard field or a standard greenhouse the dry deposition flux calculated in the previous paragraph and the wet deposition flux calculated in this paragraph should be summed.

$$DEP_{total,\,field,\,1h} = DEP_{gas\text{-}dry,\,field,\,1h} + DEP_{gas\text{-}wet,\,field,\,1h} \tag{P-299}$$

$$DEP_{total,\,field,\,24h} = DEP_{gas\text{-}dry,\,field,\,24h} + DEP_{gas\text{-}wet,\,field,\,24h} \tag{P-300}$$

$$DEP_{total,\,greenhouse,\,1h} = DEP_{gas\text{-}dry,\,greenhouse,\,1h} + DEP_{gas\text{-}wet,\,greenhouse,\,1h} \tag{P-301}$$

$$DEP_{total,\,greenhouse,\,24h} = DEP_{gas\text{-}dry,\,greenhouse,\,24h} + DEP_{gas\text{-}wet,\,greenhouse,\,24h} \tag{P-302}$$

Input			
$DEP_{gas-wet,field,1h}$	1 hour averaged wet deposition flux downwind of field	$[kg_{c}.m^{-2}.d^{-1}]$	O
$DEP_{gas-wet,field,24h}$	1 hours averaged wet deposition flux downwind of field	$[kg_{c}.m^{-2}.d^{-1}]$	O
$DEP_{gas-wet,greenhouse,1h}$	1 hour averaged wet dep. flux downwind of greenhouse	$[kg_{c}.m^{-2}.d^{-1}]$	O
$DEP_{gas-wet,greenhouse,24h}$	24 hours averaged wet dep. flux downwind of greenhouse	$[kg_{c}.m^{-2}.d^{-1}]$	O
$DEP_{gas-dry,field,1h}$	1 hour averaged dry deposition flux downwind of field	$[kg_{c}.m^{-2}.d^{-1}]$	O
$DEP_{gas-dry,field,24h}$	24 hours averaged dry deposition flux downwind of field	$[kg_{c}.m^{-2}.d^{-1}]$	O
$DEP_{gas-dry,greenhouse,1h}$	1 hour averaged dry deposition flux downwind of greenhouse	$[kg_{c}.m^{-2}.d^{-1}]$	O
$DEP_{gas-dry,greenhouse,24h}$	24 hours averaged dry dep. flux downwind of greenhouse	$[kg_{c}.m^{-2}.d^{-1}]$	O
Output			
$DEP_{total,field,1h}$	1 hour averaged total deposition flux downwind of field	$[kg_{c}.m^{-2}.d^{-1}]$	O
$DEP_{total,field,24h}$	24 hours averaged total deposition flux downwind of field	$[kg_{c}.m^{-2}.d^{-1}]$	O
$DEP_{total,greenhouse,1h}$	1 hour averaged total dep. flux downwind of greenhouse	$[kg_{c}.m^{-2}.d^{-1}]$	O
$DEP_{total,greenhouse,24h}$	24 hours averaged total dep. flux downwind of greenhouse	$[kg_{c}.m^{-2}.d^{-1}]$	O

Concentrations and deposition fluxes for further calculations

The local air concentrations and deposition rates replace the air distribution module for new and existing substances (Section III.4.5.1). The deposition rates are used to calculate concentrations in non-application soil.

For amenity use applications and granules:

$$Clocal_{air} = Clocal_{air,ann} = DEPtotal = DEPtotal_{ann} = 0$$

If spray application is on fields:

$$\boldsymbol{Clocal_{air} = C_{field,\,air,\,1h}} \tag{P-303}$$

$$\boldsymbol{DEPtotal = DEP_{total,field,24h}} \tag{P-304}$$

If spray application is in greenhouses:

$$\boldsymbol{Clocal_{air} = C_{greenhouse,air,1h}} \tag{P-305}$$

$$\boldsymbol{DEPtotal = DEP_{total,greenhouse,24h}} \tag{P-306}$$

Annual averages:

$$\boldsymbol{Clocal_{air,ann} = Clocal_{air} \cdot \frac{N_{appl}}{365}} \tag{P-307}$$

$$\boldsymbol{DEPtotal_{ann} = DEPtotal \cdot \frac{N_{appl}}{365}} \tag{P-308}$$

Input			
N_{appl}	number of applications in one year	[-]	S
$C_{field,air,1h}$	1 hour averaged conc. at 10 meters downwind of field	$[kg_c.m^{-3}]$	O
$C_{greenhouse,air,1h}$	1 hour averaged conc. in the lee side eddy of the greenhouse	$[kg_c.m^{-3}]$	O
$DEP_{total,field,24h}$	24 hours averaged total deposition flux downwind of field	$[kg_c.m^{-2}.d^{-1}]$	O
$DEP_{total,greenhouse,24h}$	24 hours averaged total dep. flux downwind of greenhouse	$[kg_c.m^{-2}.d^{-1}]$	O
Output			
$Clocal_{air}$	local concentration in air during episode	$[kg_c.m^{-3}]$	O
$Clocal_{air,ann}$	annual average local concentration in air	$[kg_c.m^{-3}]$	O
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.4.9.3. Ditch surrounding the application soil

Table D-5 *Default settings for specific distribution routes for pesticide application.*

Parameter	**Symbol**	**Unit**	**Value**
Default temperature of water compartment	TEMPwater	[°C]	10 or 12
Temperature of water compartment under test conditions	$TEMPwater_{test}$	[°C]	20
Depth of ditch	$DEPTH_{ditch}$	[m]	0.30
Concentration suspended solids in the ditch	$SUSP_{water}$	$[kg_{solid}.m_{water}^{-3}]$	0.015
Fraction organic matter in suspended matter of ditch	$Fom_{susp,pest}$	$[kg.kg^{-1}]$	0.50
Weight fraction of organic carbon in susp. solids for pesticides	$Foc_{susp,pest}$	$[kg_{oc}.kg_{solid}^{-1}]$	0.294
Dilution factor for drainage water reaching surface water	$DILUTION_{drai}$	[-]	10
Dilution factor ditch to surface water (river)	$DILUTION_{ditch}$	[-]	10
Total concentration resulting from a standard input of 1.10^{-6} kg/m^{-2} at the water surface	$Cwater_{pest\text{-}standard}$	$[kg_c.m^{-3}]$	$4.76.10^{-6}$
Width of the water surface in ditch	$WIDTH_{ditch}$	[m]	1
Cross sectional area of water layer in ditch	$AREA_{ditch}$	[m^2]	0.21

Short term concentration in surface water as a result of drift

A pesticide specific weight fraction of organic carbon in suspended solids is used. The fraction mentioned in Table III-2 (Page III-19) should not be used.

$$Kp_{susp,pest} = Foc_{susp,pest} \cdot Koc \qquad \text{(P-309)}$$

Or in case the fraction of organic matter is used:

$$Kp_{susp,pest} = Fom_{susp,pest} \cdot Kom \qquad \text{(P-310)}$$

Input			
$Foc_{susp,ditch}$	weight fraction of organic carbon in susp. solids for pesticides	$[kg.kg^{-1}]$	D
Koc	organic carbon-water partition coefficient	$[m^3.kg^{-1}]$	O
$Fom_{susp,ditch}$	weight fraction of organic matter in susp. solids for pesticides	$[kg.kg^{-1}]$	D
Kom	organic matter partition coefficient	$[m^3.kg^{-1}]$	O
Output			
$Kp_{susp,pest}$	solids-water partition coefficient in susp. matter for pesticides	$[m^3.kg^{-1}]$	O

The Equations P-309 and P-310 are related with each other according to Equation P-5, where Kom=Koc/1.724.

The first step is the calculation of the concentration in surface water directly after one application as a result of drift.

$$\boldsymbol{Cwater_{pest-standard} = DOSE_{standard} \cdot \frac{WIDTH_{ditch}}{AREA_{ditch}}} \quad \text{(P-311)}$$

$$\boldsymbol{Cwater_{pest-1appl} = \frac{F_{drift} \cdot DOSE_{pest} / DOSE_{standard} \cdot Cwater_{pest-standard}}{1 + SUSP_{water} \cdot Kp_{susp,pest}}} \quad \text{(P-312)}$$

Input			
$DOSE_{standard}$	standard dosage of pesticide = 1 mg.m^{-2}	[kg.m^{-2}]	D
$WIDTH_{ditch}$	width of the water surface in ditch	[m]	D
$AREA_{ditch}$	cross section of water layer in ditch	[m^2]	D
$Cwater_{pest-standard}$	total concentration of 4.76 mg.m^{-3} (dissolved plus sorbed to susp.matter) resulting from a standard input or dose of 1 mg.m^{-2} at the water surface	[kg$_c$.m^{-3}]	D
F_{drift}	Fraction drift related to location and way of application	[-]	O
$DOSE_{pest}$	single dosage of pesticide	[kg$_c$.m^{-2}]	S
$SUSP_{water}$	Concentration suspended solids in the ditch =0.015 kg.m^{-3}	[kg$_{solid}$.m$_{water}$$^{-3}$]	D
$Kp_{susp,pest}$	solids-water partition coefficient in suspended matter	[m^3.kg^{-1}]	O
Output			
$Cwater_{pest-1appl}$	concentration in water in the ditch after one application	[kg$_c$.m^{-3}]	O

In case of single applications the $Cwater_{pest-1appl}$ in autumn equals $Cwater_{pest-1appl}$ in spring.

Concentrations in surface water according to TOXSWA

For compounds with Kom <10000 l kg^{-1} the time weighted averaged concentrations in surface water over periods equalling the duration of toxicity test periods are determined using the standard tables that have been generated by TOXSWA. To derive the time weighted average exposure concentration with the aid of these tables, it is necessary to calculate the total rate constant for removal in the ditch k_{ditch} (dissipation rate). The removal in the ditch (k_{ditch}) is calculated from the transformation rate for the pesticide in water ($kdeg_{water}$) and the volatilisation rate coefficient k_{volat}. For compounds with a Kom >10000 l.kg^{-1} calculations with the TOXSWA model are required. In that case USES 4.0 starts the TOXSWA model (if available). The TOXSWA tables have been derived using a Kom of 1000 l.kg^{-1}. In USES 4.0 the denominator of Equation P-312 accounts for a correction of the concentration in water according to the TOXSWA tables based on the actual Kom-value. Another small difference occurs because the Freundlich adsorption with a 1/n value of 0.9 is used in the TOXSWA model, while USES 4.0 calculates with a linear adsorption in Equation P-312 (4.76 versus 4.73 mg.m^{-3}).

Temperature corrections

The temperature correction is already incorporated in the results of TOXSWA. In TOXSWA several parameters are corrected for the difference between the temperature as defined in the standard scenario and the default value. These parameters include: DT50 in the water and the sediment, saturated vapour pressure and water solubility. For using the standard tables of TOXSWA, which are incorporated in USES 4.0, the removal in the ditch (k_{ditch}) must be corrected for a temperature of 10°C. When the actual TOXSWA model is used by USES 4.0 (Kom >10000 l kg^{-1}) the removal in the ditch (k_{ditch}) must be determined at 20°C, because the TOXSWA model itself corrects for the temperature.

First order rate constant for dissipation from the ditch

For the removal in the ditch the temperature corrections are carried out according to the Arrhenius and Van ’t Hoff equations, as described in e.g. Van den Berg and Boesten (1998).

$$DT50_{water,temp} = DT50_{water} \cdot e^{(0.08(TEMPwater_{test} - TEMPwater))} \qquad \text{(P-313)}$$

$$kdeg_{water} = \frac{\ln 2}{DT50_{water}} \qquad \text{(P-314)}$$

$$kdeg_{water,temp} = \frac{\ln 2}{DT50_{water,temp}} \qquad \text{(P-315)}$$

First order rate constant for volatilisation in ditch

Volatilisation from surface water can be described with the two film resistance model of Liss and Slater (1974). In this model the main water body is assumed to be well mixed, with a thin layer on the surface in which there is a concentration gradient. The air above is assumed to be well mixed (i.e. the background level is assumed to be low), and a thin layer, in contact with the surface, contains another concentration gradient. At the interface between these two layers the ratio of concentrations across it (air to water) is assumed to equal the Henry's law constant. Transfer through these films is by straightforward molecular diffusion. The molecules are assumed to diffuse through the layers at a rate dependent on the phase exchange coefficients found in the equations rather than vaporise directly from solution along with the water vapour.

The only difference between this calculation and the calculation used in SimpleBox is in the choice of the kaw_{air} and kaw_{water}. Here, these two are estimated on the basis of the molecular weight, while in SimpleBox constant values are assumed. The molecular weights of H_2O and CO_2 are used in the formulas and are 0.018 [kg.mol^{-1}] and 0.044 [kg.mol^{-1}] respectively.

Volatilisation model according to Liss and Slater:

$$kaw\text{ - }pest_{water} = 4.8 \cdot \sqrt{\frac{0.044}{MOLW}} \qquad \text{(P-316)}$$

$$kaw\text{ - }pest_{air} = 720 \cdot \sqrt{\frac{0.018}{MOLW}} \qquad \text{(P-317)}$$

$K_{air\text{-}water}$ is calculated according to Equation 23 (section III.4.1.4.) and is corrected for the temperature (20°C to 10°C) according to Equation P-318 as is done in TOXSWA. In TOXSWA a default value of 27,000 J.mol^{-1} for the enthalpy of dissolution is used. The default value for the enthalpy of vapourisation is assumed to be 95,000 J.mol^{-1} within TOXSWA

$$K_{air-water,temp} = \frac{e^{\frac{\Delta H_{0\ vap}}{R}\cdot\left(\frac{1}{TEMP_{vap}} - \frac{1}{TEMP_{TOXSWA}}\right)}}{e^{\frac{\Delta H_{0\ sol}}{R}\cdot\left(\frac{1}{TEMP_{sol}} - \frac{1}{TEMP_{TOXSWA}}\right)}} \cdot K_{air-water} \qquad \text{(P-318)}$$

$$VOLAT_{ditch} = \frac{1}{\frac{1}{kaw\text{-}pest_{water}} + \frac{1}{kaw\text{-}pest_{air} \cdot K_{air\text{-}water,temp}}} \qquad \text{(P-319)}$$

The ditch dependent volatilisation rate coefficient depends on the ditch properties. It is calculated according to:

$$k_{volat} = VOLAT_{ditch} \cdot \frac{WIDTH_{ditch}}{AREA_{ditch}} \qquad \text{(P-320)}$$

Input			
TEMPwater	default temperature of water compartment (10˚C or 12˚C)	[°C]	P
$TEMPwater_{test}$	temperature of water compartment under test conditions	[°C]	D
$DT50_{water}$	half-life time for degradation in water (under test conditions)	[d]	S
$DT50_{water,temp}$	half-life time for degradation in water corrected for the temperature	[d]	O
MOLW	molecular weight of the substance	$[kg_c.mol^{-1}]$	S
$K_{air\text{-}water}$	air-water partition coefficient or dimensionless Henry Coefficient	[-]	O^c
R	gas constant	$[J.mol^{-1}.K^{-1}]$	D
$\Delta H_{0\ vap}$	enthalpy of vapourisation	$[J.mol^{-1}]$	D
$\Delta H_{0\ sol}$	enthalpy of dissolution	$[J.mol^{-1}]$	D
$TEMP_{vap}$	temperature at which vapour pressure was measured	[K]	D/S
$TEMP_{sol}$	temperature at which solubility was measured	[K]	D/S
$TEMP_{TOXSWA}$	environmental temperature for TOXSWA	[K]	D
$K_{air\text{-}water,temp}$	temperature corrected air-water partition coefficient	[-]	O
$WIDTH_{ditch}$	width of the water surface in ditch	[m]	D
$AREA_{ditch}$	cross section of water layer in ditch	$[m^2]$	D
$VOLAT_{ditch}$	overall mass transfer coefficient for volatilisation referenced to water	$[m_{water}.d^{-1}]$	O
$kaw\text{-}pest_{water}$	partial mass transfer coefficient at the water-side of the air-water interface	$[m.d^{-1}]$	O
$kaw\text{-}pest_{air}$	partial mass transfer coefficient at the air-side of the air-water interface	$[m.d^{-1}]$	O
Output			
$kdeg_{water}$	rate constant for degradation in water	$[d^{-1}]$	O
$kdeg_{water,temp}$	temperature dependent rate constant for degradation in water	$[d^{-1}]$	O
k_{volat}	first order rate constant for volatilisation in ditch	$[d^{-1}]$	O

First order rate constant for removal in the ditch

$$k_{ditch} = kdeg_{water} + k_{volat} \qquad \text{(P-321)}$$

$$k_{ditch,temp} = kdeg_{water,temp} + k_{volat} \qquad \text{(P-322)}$$

Input			
$kdeg_{water}$	rate constant for degradation in water	$[d^{-1}]$	O
$kdeg_{water,temp}$	temperature dependent rate constant for degradation in water	$[d^{-1}]$	O
k_{volat}	first order rate constant for volatilisation in ditch	$[d^{-1}]$	O
Output			
k_{ditch}	total rate constant for removal in the ditch	$[d^{-1}]$	O
$k_{ditch,temp}$	temperature dependent total rate constant for removal in the ditch	$[d^{-1}]$	O

The TOXSWA tables

To estimate the concentration in surface water, the ditch, the model TOXSWA was used for a standardised situation in the Netherlands for specified DT50-values. The tables in Appendix VIII are generated by TOXSWA and give the concentrations in the ditch after 0, 4, 14, 21 and 28 days for a specific combination of the application period (spring or autumn), application frequency ($N = 2, 3, 4, \geq 5$) and application interval ($t = 7$ or 10 days). As the tables are derived for specific values of the DT50, the actual $DT50_{water,temp}$ of a substance is used to linearly interpolate between the appropriate values of the DT50 for which a value in the table is available.
Separate estimations have to be done for the spring and autumn period. Exposure concentrations are determined with the aid of standard tables generated for compounds with Kom <10000 $l.kg^{-1}$. For compounds with Kom >10000 $l.kg^{-1}$ calculations are required using the TOXSWA model.

For **spring** applications the concentration has to be derived from the table in Appendix VIII. There are concentrations for the acute exposure, and for the four periods of $Cwater_{pest-T,spring}$, where $T \in \{4, 14, 21, 28\}$.
Only for the interval periods of 7 and 10 days tables are presented in USES 4.0. The concentration is thus a function of the chosen interval, the averaged concentration of interest (4, 14, 21, or 28 days), the number of applications and the overall removal rate constant k_{ditch}.

In **autumn**, the residence time of water in the ditch is three days, because of the high flow velocity. Therefore, for acute exposure concentrations cumulating effects of concentrations do not occur. The $Cwater_{pest-T,autumn}$ is taken from the metamodel table for $T \in \{4, 14, 21, 28\}$ of Appendix VIII. Again, for acute exposure repeated application has no influence. Given the fixed intervals of 7 and 10 days, for T = 4 days repeated application does not change the maximum concentration over a 4 day period.

For establishing the risk characterisation for birds and mammals the following assumptions have been made:

$$Cwater_{pest-T,Season} = \frac{(PEC_{T,TOXSWA} \cdot FACTOR) \cdot Cwater_{pest-1appl}}{Cwater_{pest-std,TOXSWA}} \quad \text{(P-323)}$$

$$\begin{aligned}
Cwater_{pest-Tbird,Season} &= Cwater_{pest-0,Season} && when\ T_{bird} < 4 \\
Cwater_{pest-Tbird,Season} &= Cwater_{pest-4,Season} && when\ 4 \leq T_{bird} < 14 \\
Cwater_{pest-Tbird,Season} &= Cwater_{pest-14,Season} && when\ 14 \leq T_{bird} < 21 \\
Cwater_{pest-Tbird,Season} &= Cwater_{pest-21,Season} && when\ 21 \leq T_{bird} < 28 \\
Cwater_{pest-Tbird,Season} &= Cwater_{pest-28,Season} && when\ T_{bird} \geq 28 \quad \text{(P-324)}
\end{aligned}$$

$$\begin{aligned}
Cwater_{pest-Tmammal,Season} &= Cwater_{pest-0,Season} && when\ T_{mammal} < 4 \\
Cwater_{pest-Tmammal,Season} &= Cwater_{pest-4,Season} && when\ 4 \leq T_{mammal} < 14
\end{aligned}$$

$$\boldsymbol{Cwater_{pest-Tmammal,Season} = Cwater_{pest-14,Season} \quad when\ 14 \leq T_{mammal} < 21}$$
$$\boldsymbol{Cwater_{pest-Tmammal,Season} = Cwater_{pest-21,Season} \quad when\ 21 \leq T_{mammal} < 28}$$
$$\boldsymbol{Cwater_{pest-Tmammal,Season} = Cwater_{pest-28,Season} \quad when\ T_{mammal} \geq 28} \qquad \text{(P-325)}$$

Input

Season	choice of season (spring/autumn)	spring/autumn	P
$Cwater_{pest\text{-}1appl}$	total concentration in ditch after one application	$[kg_c.m^{-3}]$	O
$PEC_{T,TOXSWA}$	see Toxswa tables in Appendix VIII	$[\mu.l^{-1}]$	P
FACTOR	correction factor of 1.10^{-6}	$[kg.m^{-3}]$	D
$Cwater_{pest\text{-}std,TOXSWA}$	$=EC_0$ or $4.732.10^{-6}$	$[kg_c.m^{-3}]$	D
$Cwater_{pest\text{-}T,Season}$	concentration in ditch over *T* days in spring/autumn	$[kg_c.m^{-3}]$	
N_{appl}	number of applications in one season	[-]	S
$T_{interval}$	application interval	[d]	S
$FAC_{t,N,T,season}$	correction factor for repeated applications in spring/autumn	[-]	O
T_{bird}	test duration for bird toxicity test	[d]	S
T_{mammal}	test duration for mammalian toxicity test	[d]	S

Output

$Cwater_{pest\text{-}Tbird,Season}$	concentration in ditch over T_{bird} days in spring/autumn	$[kg_c.m^{-3}]$	O
$Cwater_{pest\text{-}Tmammal,Season}$	concentration in ditch over T_{mammal} days in spring/autumn	$[kg_c.m^{-3}]$	O

The average concentration in surface water during one year as a result of drift

For indirect exposure the average concentration over the whole year is calculated. A scenario of first-order removal combined with a constant emission flux is proposed. The average emission over the year is calculated on a volume basis. The effects of sedimentation and resuspension are considered equal. Furthermore the upstream water is assumed to be polluted as well. Thus no refreshment of the water by advection occurs. The total first-order rate constant $k_{ditch\text{-}365}$ is calculated from the remaining processes. This scenario results in a constant concentration in the ditch to which the contribution of drainage is added, if applicable.

$$Fdiss_{ditch} = \frac{1}{1 + SUSP_{water} \cdot Kp_{susp,pest}} \tag{P-326}$$

$$DEPTH_{ditch,pest} = \frac{AREA_{ditch}}{WIDTH_{ditch}} \tag{P-327}$$

$$E_{avg} = \frac{N_{appl} \cdot F_{drift} \cdot DOSE_{pest}}{DEPTH_{ditch,pest} \cdot 365} \tag{P-328}$$

$$k_{ditch\text{-}365} = (kdeg_{water,temp} + k_{volat,temp}) \cdot Fdiss_{ditch} \tag{P-329}$$

$$Cwater_{drift\text{-}365} = \frac{E_{avg}}{k_{ditch\text{-}365}} \tag{P-330}$$

Input			
$Fdiss_{ditch}$	fraction of the chemical in the water phase of the ditch	[-]	O
$SUSP_{water}$	concentration suspended solids in the ditch	[$kg_{solid}.m_{water}^{-3}$]	D
$Kp_{susp,pest}$	solids-water partition coefficient in suspended matter	[$m^3.kg^{-1}$]	O
$DEPTH_{ditch,pest}$	depth of ditch	[m]	O
$AREA_{ditch}$	cross section of water layer in ditch	[m^2]	D
$WIDTH_{ditch}$	width of the water surface in ditch	[m]	D
N_{appl}	number of applications in one year	[-]	S
F_{drift}	fraction drift related to location and way of application	[-]	O
$DOSE_{pest}$	single dosage of pesticide	[$kg_c.m^{-2}$]	S
E_{avg}	average emission during the year	[$kg_c.d^{-1}.m^{-3}$]	O^c
$k_{ditch\text{-}365}$	total rate constant for removal in the ditch during one year	[d^{-1}]	O
$kdeg_{water,temp}$	temperature dependent rate constant for degradation in water	[d^{-1}]	O
$k_{volat,temp}$	temperature dependent first order rate constant for volatilisation in ditch	[d^{-1}]	O
Output			
$Cwater_{drift\text{-}365}$	annual average concentration in ditch as result of drift	[$kg_c.m^{-3}$]	O

Average concentration in surface water during one year as a result of drainage.

After the pesticide has reached the shallow groundwater via leaching, there are two possibilities:

- Drains are present.
- Drains are not present.

In case there are no drains, it is assumed that all the pesticide is transported to the groundwater. In case there are drains, it is assumed that 40% of the pesticide is transported to the ground water and that 60% is drained to the surface water. The concentration of the pesticide in the drains (C_{drai}) is assumed to be equal to the concentration in the shallow ground water (from PEARL), but will decrease after the dilution by surface water.

When $DRAINS$ = "no" then $C_{drai} = 0$. Only when $DRAINS$ = "yes" :

$$C_{drai} = C_{shallow\ grw} \qquad \text{(P-331)}$$

$$Cwater_{drai\text{-}365} = \frac{C_{drai}}{DILUTION_{drai}} \qquad \text{(P-332)}$$

Input			
DRAINS	drains are present	[yes/no]	P
C_{drai}	concentration in drainage water	[$kg_c.m^{-3}$]	O
$DILUTION_{drai}$	dilution factor for drainage water reaching the surface water	[-]	D
$C_{shallow\ grw}$	concentration in shallow ground water	[$kg_c.m^{-3}$]	O
Output			
$Cwater_{drai\text{-}365}$	annual average concentration in ditch as result of drainage	[$kg_c.m^{-3}$]	O

Total average concentration in surface water during one year

This total average concentration during the year is calculated by simply adding the contributions of drainage and drift.

Contamination of surface water by atmospheric deposition is not yet taken into account.

$$Cwater_{pest\text{-}365} = (Cwater_{drift\text{-}365} + Cwater_{drai\text{-}365}) \cdot Fdiss_{ditch} \tag{P-333}$$

Input

$Cwater_{drift\text{-}365}$	annual average concentration in ditch as result of drift	[$kg_c.m^{-3}$]	O
$Cwater_{drai\text{-}365}$	annual average concentration in ditch as result of drainage	[$kg_c.m^{-3}$]	O
$Fdiss_{ditch}$	fraction of the chemical in the water phase of the ditch	[-]	O^c

Output

$Cwater_{pest\text{-}365}$	annual average concentration in ditch	[$kg_c.m^{-3}$]	O

The concentration in surface water to be used for human exposure

The concentration in drinking water abstracted from surface water is calculated using the total annual average concentration in the ditch, applying default factors for dilution or if available measured concentrations. The total annual average concentration is calculated with the concentration in the ditch as a result of drift (Equation P-330) plus the concentration in the ditch as a result of drainage (Equation P-332). The calculated total annual average concentration in surface water is also used for estimating the concentration in fish for human consumption.

$$C_{river} = \frac{Cwater_{pest\text{-}365}}{DILUTION_{ditch}} \tag{P-334}$$

Input

$Cwater_{pest\text{-}365}$	annual average concentration in ditch	[$kg_c.m^{-3}$]	O
$DILUTION_{ditch}$	dilution factor ditch to surface water (river)	[-]	D

Output

C_{river}	average concentration in surface water (river) for human exposure	[$kg_c.m^{-3}$]	O

III.4.9.4. Concentration in water sediment after maximum application period

The distribution of the substance between water and sediment is determined by the sediment-water partitioning coefficient, which is estimated from the solids-water partition coefficient in suspended solids for pesticides ($Kp_{susp,pest}$).

$$Cwater_{pest-7,Season} = \frac{7-4}{21-4} \cdot Cwater_{pest-4,Season} + \frac{21-7}{21-4} \cdot Cwater_{pest-21,Season} \qquad \text{(P-335)}$$

$$Csed_{pest-T,Season} = \frac{Kp_{susp,pest} \cdot Cwater_{pest-T,Season}}{CONV_{sed}} \qquad T \in \{0,7,28\} \qquad \text{(P-336)}$$

Input

$Kp_{susp,pest}$	solids-water partition coefficient in susp. solids for pesticides	$[m^3.kg^{-1}]$	S/O
$Cwater_{pest-T,Season}$	concentration in ditch over *T* days in spring/autumn	$[kg_c.m^{-3}]$	O
$CONV_{sed}$	conversion factor for sediment concentrations: wwt to dwt	$[kg_{wwt}.kg_{dwt}^{-1}]$	O^c
Output			
$Csed_{pest-T,Season}$	average concentration in sediment over *T* days in spring/autumn	$[kg_c.kg_{wwt}^{-1}]$	O

The Predicted Environmental Concentration (PEC) in water sediment after long term application is set at the concentration after the last application in the tenth year. This PEC is considered to be equal to the concentration at year 10 ($Csed_{pest-0,lt,w}$). After the tenth year the resulting concentration, $Csed_{pest-LT,w}$, is compared with the PNEC for sediment dwelling organisms.

$$F_{lts} = e^{-kdeg_{sed} \cdot T_{interval-lt}} \qquad \text{(P-337)}$$

Peak concentration in sediment at last application:

$$Csed_{pest-0,lt} = Csed_{pest-0} + Csed_{pest-0} \cdot F_{lts} + Csed_{pest-0} \cdot F_{lts}^{2} + \ldots + Csed_{pest-0} \cdot F_{lts}^{(N_{lt}-1)}$$

$$= Csed_{pest-0} \cdot \frac{1 - F_{lts}^{N_{lt}}}{1 - F_{lts}} \qquad \text{(P-338)}$$

Concentration 2 years after last application:

$$Csed_{pest-lt} = Csed_{pest-0,lt} \cdot F_{lts}^{2} \qquad \text{(P-339)}$$

Input

F_{lts}	fraction of the concentration remaining after time $T_{interval-lt}$	[-]	O^c
$kdeg_{sed}$	first order rate of biodegradation in sediment	$[d^{-1}]$	S
N_{lt}	number of application periods per registration period	[-]	S
$T_{interval-lt}$	long term interval between application periods	[d]	S
$Csed_{pest-0,lt}$	peak concentration after N_{lt} applications (PEC)	$[kg_c.kg_{sed}^{-1}]$	O^c
Output			
$Csed_{pest-lt}$	concentration after (N_{lt} + 2) years of applications	$[kg_c.kg_{wwt}^{-1}]$	O

III.4.9.5. Concentration in shallow groundwater

$$C_{shallow\ grw} = Cstd_{shallow\ grw} \cdot DOSE_{max} \qquad \text{(P-340)}$$

Input			
$DOSE_{max}$	apparent maximum dose	$[kg_c.m^{-2}]$	O
$Cstd_{shallow\ grw}$	standard concentration in upper groundwater	$[(kg_c.m^{-3})/(kg_c.m^{-2})]$	O
Output			
$C_{shallow\ grw}$	concentration in shallow ground water	$[kg_c.m^{-3}]$	O

For this calculation, the results from the PEARL tables are required (see Appendix VII). The PEARL programm is required for substances with an Henry coefficient > 0.0237 $Pa.m^3.mol^{-1}$ or a Kair-water $>1.10^{-5}$ and under the condition of mixing with soil (MIX = yes). Whenever the DT50 ≥ 200 days or when the Kom > 200 $l.kg^{-1}$ and the DT50 ≥ 185 days the PEARL model is also used.

For the spring and autumn situation, the PEARL-tables are giving the resulting concentration in the upper groundwater for the standard scenario and specified combinations of the DT50 and the Kom. The actual DT50 and Kom of the active substance under consideration are used to interpolate in the table according to a logarithmic calculation method. In the table, the four surrounding combinations of DT50 and Kom determine the value of the concentration for the combination of the substance. Therefore, the result is a concentration in the upper groundwater for a spring and/or an autumn application.

Input			
Kom	organic matter-water partition coefficient	$[m^3.kg^{-1}]$	O
$DT50bio_{soil}$	half life for biodegradation in soil	[d]	O
Output			
$Cstd_{shallow\ grw}$	standard concentration in shallow groundwater	$[(kg_c.m^{-3})/(kg_c.m^{-2})]$	O

III.4.9.6. Leaching to deeper groundwater used for drinking water

As already described there are two possibilities after the pesticide has reached the shallow groundwater:

- Drains are present.
- Drains are not present.

If there are drains it is assumed that only 40% of the net precipitation will leach to the deeper groundwater. If there are no drains 100% of the net precipitation will leach to the deeper groundwater. However, the presence or absence of drains is assumed to have no effect on the initial concentration in deeper groundwater which is taken to be the same as in the shallow groundwater.

Transformation in the saturated zone is dependent on the transformation rate coefficient. It is assumed that the transformation rate coefficient equals the hydrolysis rate coefficient and that the process will take place following first order kinetics. Dilution in the deeper groundwater is not taken into account.

A transformation period of four years is assumed in the calculation of the concentration in groundwater.

$$Cgrw_{pest} = C_{shallow\ grw} \cdot e^{-khydr_{water} \cdot 4 \cdot 365} \qquad \text{(P-341)}$$

Input			
$C_{shallow\ grw}$	concentration in shallow ground water	$[kg_c.m^{-3}]$	O
$khydr_{water}$	first-order rate constant for hydrolysis	$[d^{-1}]$	O
Output			
$Cgrw_{pest}$	concentration in ground water used in drinking water	$[kg_c.m^{-3}]$	O

III.4.9.7. Application of pesticides used for seed treatment

For calculating the initial PEC after the use of pesticides for seed treatment, it is assumed that the active substance is homogeneously divided in a spherically range of influence around a single seed. The default radius of the range of influence is 5 cm. The actual range of influence around a single seed is dependent on the diffusion velocity of a substance, where the diffusion velocity again is dependent on the properties of the substance and soil. It is further assumed that the pesticide used for seed treatment is completely released in the soil.

The calculation method for pesticides used for seed treatment can be divided in two parts (Figure III-1):
Scenario A. seeds sown on soil surface.
Scenario B. seeds sown at a depth of 5 cm or more below soil surface.

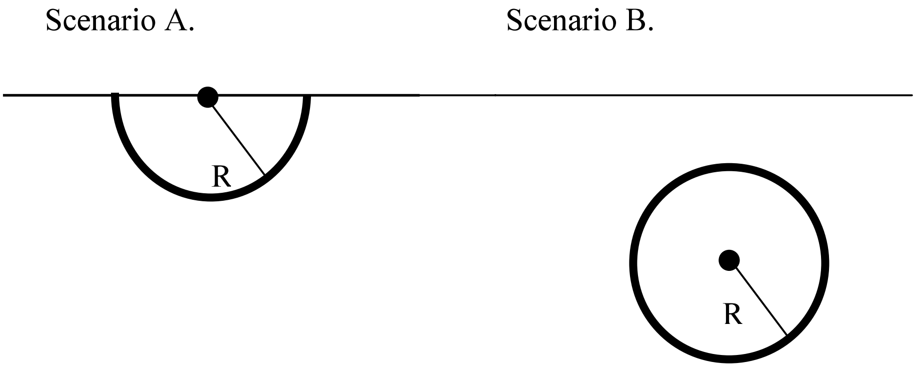


Figure III-1 *Two calculation methods for pesticides used for seed treatment*

The shape of the range of influence is half a sphere of seed sown on the soil surface. The shape of the range of influence is a complete sphere of seed sown below the soil surface (at a default depth of 5 cm). For calculating the total radius, the radius of the range of influence is added to the radius of a single seed.

Table D-6 *Default settings for seed treatment*

Parameter	**Symbol**	**Unit**	**Value**
radius range of influence seed	$RADparticle_{influence}$	[m]	0.05
maximum volume soil of range of influence seed	$Vsoil_{max\ particle}$	$[m^3.m^{-2}]$	0.05
dry bulk density of soil	RHO_{soil}	$[kg_{dwt}.m^{-3}]$	1500

Seed can be mixed with soil or seed can be on the soil surface:

if MIX_{soil}="yes" then CONSTANTsphere = 1 else CONSTANTsphere = 0.5

$$Vsoil_{influence\_particle} = CONSTANTsphere \cdot 4/3 \cdot \pi \cdot RADparticle^3_{influence\_total} \qquad \text{(P-342)}$$

$$RADparticle_{influence\_total} = RADparticle + RADparticle_{influence} \qquad \text{(P-343)}$$

input			
MIX_{soil}	mixing of seed with soil	[yes/no]	P
RADparticle	radius seed	[m]	S
$RADparticle_{influence}$	radius range of influence seed	[m]	D
output			
CONSTANTsphere	constant belonging to a sphere or half a sphere	[-]	O
$RADparticle_{influence\_total}$	total radius range of influence seed	[m]	O
$Vsoil_{influence,particle}$	volume soil in range of influence seed	$[m^3]$	O

The total volume soil of the range of influence on a hectare soil is limited to a maximum of 500 m^3/ha (=0.05 $m^3.m^{-2}$) and is calculated according:

$$Vsoil_{total\_particle} = min\ (Nparticle_{area} \cdot Vsoil_{influence\_particle}, Vsoil_{max\_partickle}) \tag{P-344}$$

The applied dosage of treated seed is divided by the mass of soil within the range of influence of seed. The result is the initial Predicted Environmental Concentration in soil. This PEC is considered to be equal to the concentration on day 0 ($Csoil_{pest-0}$):

$$Csoil_{pest-0} = \frac{DOSE_{pest\_particle}}{RHO_{pest} \cdot Vsoil_{total\_particle}} \tag{P-345}$$

$$Dose_{pest-particle} = Cparticle \cdot Nparticle_{area} \cdot WEIGHTparticle \tag{P-346}$$

$$WEIGHT_{particle} = \frac{1}{Nparticle_{weight}} \tag{P-347}$$

input			
$Nparticle_{area}$	number of seed per m^2	$[m^{-2}]$	S
$Vsoil_{influence\_particle}$	volume soil of range of influence seed	$[m^3]$	O
$Vsoil_{max\_particle}$	maximum volume soil of range of influence seed	$[m^3.m^{-2}]$	D
$DOSE_{pest\_particle}$	dosage pesticide for seed treatment	$[kg_c.m^{-2}]$	S
RHO_{pest}	dry bulk density of application soil	$[kg_{dwt}.m^{-3}]$	D
Cparticle	concentration of pesticide in granules or treated seed	$[kg_c.kg_{particle}^{-1}]$	S/O
WEIGHTparticle	weight of one granule or treated seed	$[kg_{particle}.particle^{-1}]$	S/O
$Nparticle_{weight}$	number of granules or seed per kg	$[kg_{particle}^{-1}]$	S/O
$Nparticle_{area}$	number of granules or seed per m^2	$[m^{-2}]$	S/O
Output			
$Vsoil_{total\_particle}$	total volume soil of range of influence seed	$[m^3.m^{-2}]$	O
$Csoil_{pest-0}$	peak concentration in soil after application	$[kg_c.kg_{soil}^{-1}]$	O

III.4.10. Regional, continental and global environmental distribution

Steady-state exposure concentrations at the regional, continental, and optionally, global scales are calculated for all environmental compartments using a nested version of the multi-media fate model SimpleBox (Van de Meent, 1993; see also Section 2.4.4). In contrast to the version of SimpleBox included in EUSES, the version included in USES 2.0 (the full SimpleBox 2.0) includes the following extra options as described in detail by Brandes *et al.* (1996):

- three global scales,
- sea-water compartment,
- temperature dependence of parameters,
- chemical-specific soil depth (not described in this document),

In the USES 2.0 defaults section, a choice is possible between an "EUSES compatible" calculation (as described in the TGD) or a full Simplebox 2.0 calculation.

Spatial scale	**Compartments**	**Symbol specification**
Regional	Air Fresh water Fresh water sediment Sea water Sea water sediment Agricultural soil Natural soil Industrial soil	air [R] water 1 [R] sed 1 [R] water 2 [R] sed 2 [R] agric [R] natural [R] ind [R]
Continental	Air Fresh water Fresh water sediment Sea water Sea water sediment Agricultural soil Natural soil Industrial soil	air [C] water 1 [C] sed 1 [C] water 2 [C] sed 2 [C] agric [C] natural [C] ind [C]
Moderate	Air Sea water Sea water sediment Soil	air [M] water [M] sed [M] soil [M]
Arctic	Air Sea water Sea water sediment Soil	air [A] water [A] sed [A] soil [A]
Tropic	Air Sea water Sea water sediment Soil	air [T] water [T] sed [T] soil [T]

Input: regional emissions			
$Ereg_j$	direct emission to compartment *j* (annual average flux) $j \in$ {direct-water,natural,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,natural,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: global emissions			
$E[M,A,T]_j$	direct emission to compartment *j* (annual average flux) $j \in$ {water,soil,air}	$[kg_c.d^{-1}]$	
Input: chemical properties			
$Fass_{aer}$	fraction of chemical associated with aerosol particles	[-]	
$K_{air\text{-}water}$	air-water partition coefficient	[-]	c
SOL	water solubility option	$[kg_c.m^{-3}]$	
VP	vapour pressure option	[Pa]	
$K_{soil\text{-}water}$	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	$[m^3.kg_{solids}^{-1}]$	
$kdeg_{air}$	first-order rate constant for degradation in air	$[d^{-1}]$	
$kdeg_{water}$	first-order rate constant for degradation in bulk water	$[d^{-1}]$	
$kdeg_{soil}$	first-order rate constant for degradation in bulk soil	$[d^{-1}]$	
$kdeg_{sed}$	first-order rate constant for degradation in bulk sediment	$[d^{-1}]$	
Output: continental concentrations			
$PECcont_{water\ 1,tot}$	continental PEC in surface water (total)	$[kg_c.m^{-3}]$	c
$PECcont_{water\ 2,tot}$	continental PEC in sea water (total)	$[kg_c.m^{-3}]$	c
$PECcont_{water\ 1}$	continental PEC in surface water (dissolved)	$[kg_c.m^{-3}]$	c
$PECcont_{water\ 2}$	continental PEC in sea 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
$PECcont_{sed\ 1}$	continental PEC in fresh water sediment (total)	$[kg_c.kg_{wwt}^{-1}]$	c
$PECcont_{sed\ 2}$	continental PEC in sea water sediment (total)	$[kg_c.kg_{wwt}^{-1}]$	c
Output: regional concentrations			
$PECreg_{water\ 1,tot}$	regional PEC in surface water (total)	$[kg_c.m^{-3}]$	
$PECreg_{water\ 2,tot}$	regional PEC in sea water (total)	$[kg_c.m^{-3}]$	
$PECreg_{water\ 1}$	regional PEC in surface water (dissolved)	$[kg_c.m^{-3}]$	
$PECreg_{water\ 2}$	regional PEC in sea 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)	$[kg_c.kg_{wwt}^{-1}]$	
$PECreg_{sed\ 1}$	regional PEC in fresh water sediment (total)	$[kg_c.kg_{wwt}^{-1}]$	
$PECreg_{sed\ 2}$	regional PEC in sea water sediment (total)	$[kg_c.kg_{wwt}^{-1}]$	
Output: Global concentrations			
$PEC[M,A,T]_{water,tot}$	global PEC in water (total) on scale [M,A,T]	$[kg_c.m^{-3}]$	c
$PEC[M,A,T]_{water}$	global PEC in water (dissolved) on scale [M,A,T]	$[kg_c.m^{-3}]$	c
$PEC[M,A,T]_{air}$	global PEC in air (total) on scale [M,A,T]	$[kg_c.m^{-3}]$	c
$PEC[M,A,T]_{soil}$	global PEC in soil (total) on scale [M,A,T]	$[kg_c.kg_{wwt}^{-1}]$	c

III.4.10.1. General system definition

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.

The parameter indications R-EU and C-EU are used to indicate the EU-region excluding sea water and the EU-continent, excluding sea water but including the regional scale. The area of C-EU thus is the entire land area of the EU Member States. The area of the continental system in SimpleBox, however, will include an amount of sea water and excludes the area dedicated to the region.

Table S-2 *General parameter settings for the regional and continental scales.*

Parameter		**Symbol**	**Unit**	**Value**
Area of system	R-EU C-EU M A T	$AREA_{[S]}$	[m^2]	$4.0.10^{10}$ $3.56.10^{12}$ $3.89.10^{13}$ $2.55.10^{13}$ $8.93.10^{13}$
Number of inhabitants	R C-EU	$N_{[S]}$	[eq]	20.10^6 [a] 370.10^6 [a]
Fraction of direct emissions to sea water	R C	$Femiss_{water\ 2\ [S]}$	[-]	0 0
Fraction connected to sewer systems	R C	$Fconnect_{stp\ [S]}$	[-]	0.70 [b]
Fraction of STP effluent discharged to sea water	R C	$Fstp_{water\ 2\ [S]}$	[-]	0.1 0.1
Per-capita water use	R C	$Q_{stp\ [S]}$	[$m^3.d^{-1}$]	0.20 [a]

[a] Already defined in STP sub-module.
[b] Already defined in emission module.

III.4.10.2. Fractions of direct and indirect releases to sea water

A fraction of the emissions to water is directed to sea water. Only the equations for the regional scale are shown below, but the same formulas are used for the continental scale.

Fraction of direct emissions to sea water

$$Ereg_{direct\text{-}water\ 1} = Ereg_{direct\text{-}water} \cdot (1 - Femiss_{water\ 2\ [R]}) \tag{S-1}$$

$$Ereg_{direct\text{-}water\ 2} = Ereg_{direct\text{-}water} \cdot Femiss_{water\ 2\ [R]} \tag{S-2}$$

Input			
$Ereg_{direct\text{-}water}$	direct regional emission to water (annual average)	$[kg_c.d^{-1}]$	O
$Femiss_{water\ 2\ [R]}$	fraction of direct-water emissions to sea water on [R]	[-]	D
Output			
$Ereg_{direct\text{-}water\ 1}$	direct regional emission to surface water (annual average)	$[kg_c.d^{-1}]$	O
$Ereg_{direct\text{-}water\ 2}$	direct regional emission to sea water (annual average)	$[kg_c.d^{-1}]$	O

Fraction of the emissions from the STP released to sea water

$$Estp\text{-}reg_{water\ 1} = (1 - Fstp_{water\ 2}) \cdot Estp\text{-}reg_{water} \tag{S-3}$$

$$Estp\text{-}reg_{water\ 2} = Fstp_{water\ 2} \cdot Estp\text{-}reg_{water} \tag{S-4}$$

Input			
$Estp\text{-}reg_{water}$	regional emission to water from STP (annual average)	$[kg_c.d^{-1}]$	O
$Fstp_{water\ 2\ [R]}$	fraction of STP-effluent discharge to sea water on [R]	[-]	D
Output			
$Estp\text{-}reg_{water\ 1}$	regional emission to surface water from STP (ann. average)	$[kg_c.d^{-1}]$	O
$Estp\text{-}reg_{water\ 2}$	regional emission to sea water from STP (ann. average)	$[kg_c.d^{-1}]$	O

The following three sections describe the temperature dependence of physico-chemical properties, partition coefficients and degradation rates. By default, these equations are bypassed according to the assessment procedures described in the TGD (EC, 1996). Nevertheless, when the global spatial scales are used in the assessment, the temperature-dependent equations are advised.

III.4.10.3. Temperature dependence of physico-chemical properties

By default, this option is not used and this section and the next one are skipped. In that case, the following parameters are taken from the partitioning sub module (Section III.4.1):

$Fass_{aer}$	fraction of chemical associated with aerosol particles	[-]	O
$K_{air\text{-}water}$	air-water partition coefficient	[-]	O^c

Table S-3 *General parameter settings for the regional and continental scales.*

Parameter		**Symbol**	**Unit**	**Value**
Environmental temperature	R C M A T	$TEMP_{[S]}$	[K]	285 285 285 263 298
Enthalpy of vaporisation		$H_{0\ vapour}$	$[kJ.mol^{-1}]$	50
Enthalpy of solution		$H_{0\ solution}$	$[kJ.mol^{-1}]$	10
Temperature at which vapour pressure was measured		$TEMP_{VP}$	[K]	298
Temperature at which solubility was measured		$TEMP_{SOL}$	[K]	298

$$VP_{(S)} = VP \cdot e^{\frac{H_{0\,vapour}}{R} \cdot \left(\frac{1}{TEMP_{VP}} - \frac{1}{TEMP_{[S]}} \right)} \tag{S-5}$$

$$SOL_{(S)} = SOL \cdot e^{\frac{H_{0\,solution}}{R} \cdot \left(\frac{1}{TEMP_{SOL}} - \frac{1}{TEMP_{[S]}} \right)} \tag{S-6}$$

Input			
SOL	water solubility	[$kg_c.m^{-3}$]	S
VP	vapour pressure	[Pa]	S
$H_{0\ vapour}$	enthalpy of vaporisation	[$J.mol^{-1}$]	D
$H_{0\ solution}$	enthalpy of solution	[$J.mol^{-1}$]	D
$TEMP_{VP}$	temperature at which vapour pressure was measured	[K]	D
$TEMP_{SOL}$	temperature at which solubility was measured	[K]	D
$TEMP_{[S]}$	environmental temperature on scale [S]	[K]	D
R	gas constant	[$Pa.m^3.mol^{-1}.K^{-1}$]	D
Output			
$SOL_{[S]}$	water solubility on scale [S]	[$kg_c.m^{-3}$]	O
$VP_{[S]}$	vapour pressure on scale [S]	[Pa]	O

III.4.10.4. Partition coefficients

It should be noted that USES 2.0 applies a different estimation routine for the organic carbon-water partition coefficient (*Koc*) than SimpleBox 2.0.

Fraction associated with aerosol

$$Fass_{aer\,[S]} = \frac{CONjunge \cdot SURF_{aer}}{VP_{L\,[S]} + CONjunge \cdot SURF_{aer}} \qquad \text{(S-7)}$$

If *TEMPmelt* <= *TEMP* (substance is liquid):

$$VP_{L\,[S]} = VP_{[S]} \qquad \text{(S-8)}$$

If *TEMPmelt* > *TEMP* (substance is solid):

$$VP_{L\,[S]} = \frac{VP_{[S]}}{e^{6.79\left(1 - \frac{TEMPmelt}{TEMP_{[S]}}\right)}} \qquad \text{(S-9)}$$

Input			
CONjunge	constant of Junge equation	[Pa.m]	D
$SURF_{aer}$	surface area of aerosol particles	$[m^2.m^{-3}]$	D
$VP_{[S]}$	vapour pressure on scale [S]	[Pa]	O
$TEMP_{[S]}$	environmental temperature on scale [S]	[K]	D
TEMPmelt	melting point of substance	[K]	S
Output			
$VP_{L\,[S]}$	sub-cooled liquid vapour pressure on scale [S]	[Pa]	O
$Fass_{aer\,[S]}$	fraction of chemical associated with aerosol particles on [S]	[-]	O

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-water}* (also known as the 'dimensionless' Henry's Law constant) can be estimated from the ratio of the vapour pressure to the water solubility:

$$HENRY_{[S]} = \frac{VP_{[S]} \cdot MOLW}{SOL_{[S]}} \qquad \text{(S-10)}$$

$$K_{air\text{-}water\ [S]} = \frac{HENRY_{[S]}}{R \cdot TEMP_{[S]}} \qquad \text{(S-11)}$$

Input			
$VP_{[S]}$	vapour pressure on scale [S]	[Pa]	O
MOLW	molecular weight	[$kg_c.mol^{-1}$]	S
$SOL_{[S]}$	water solubility on scale [S]	[$kg_c.m^{-3}$]	O
R	gas constant	[$Pa.m^3.mol^{-1}.K^{-1}$]	D^c
$TEMP_{[S]}$	environmental temperature on scale [S]	[K]	D
Output			
$HENRY_{[S]}$	Henry's law constant on scale [S]	[$Pa.m^3.mol^{-1}$]	O
$K_{air\text{-}water\ [S]}$	air-water partition coefficient on scale [S]	[-]	O^c

Soil-water partitioning

The soil-water partitioning coefficients are calculated analogous to equation 29 in section III.4.1.8 but differ at the different scales because the air-water partition coefficient is temperature dependent. note that the inclusion of the air phase in soil in this equation differs from the original SimpleBox 2.0 equations.

$$K_{soil\text{-}water\ [S]} = Fair_{soil} \cdot K_{air\text{-}water\ [S]} + Fwater_{soil} + Fsolid_{soil} \cdot Kp_{soil} \cdot RHOsolid \qquad \text{(S-11a)}$$

III.4.10.5. Temperature dependence of degradation

Degradation rates are scaled by assuming that the degradation rates double with every 10 degrees increase in temperature. It should be noted that the derivation of degradation rates differs from that in the original SimpleBox 2.0 (see Sections III.4.2.5-III.4.2.7).

$$kdeg_{air\ [S]} = kdeg_{air} \tag{S-12}$$

$$kdeg_{water\ i\ [S]} = kdeg_{water} \cdot \left(1.072^{TEMP_{[S]}-TEMP} \right) \quad i \in \{1,2\} \tag{S-13}$$

$$kdeg_{sed\ i\ [S]} = kdeg_{sed} \cdot \left(1.072^{TEMP_{[S]}-TEMP} \right) \quad i \in \{1,2\} \tag{S-14}$$

$$kdeg_{soil\ [S]} = kdeg_{soil} \cdot \left(1.072^{TEMP_{[S]}-TEMP} \right) \tag{S-15}$$

Input			
$kdeg_{air}$	first-order rate constant for degradation in air	[d^{-1}]	O
$kdeg_{water}$	rate constant for degradation in bulk water	[d^{-1}]	O
$kdeg_{sed}$	rate constant for degradation in bulk sediment	[d^{-1}]	O
$kdeg_{soil}$	rate constant for degradation in bulk soil	[d^{-1}]	O
TEMP	environmental temperature (relevant for degradation rates)	[K]	D
$TEMP_{[S]}$	environmental temperature on scale [S]	[K]	D
Output			
$kdeg_{air\ [S]}$	rate constant for degradation in air on scale [S]	[d^{-1}]	O
$kdeg_{water\ i\ [S]}$	rate constant for degradation in bulk water on scale [S]	[d^{-1}]	O
$kdeg_{sed\ i\ [S]}$	rate constant for degradation in bulk sediment on scale [S]	[d^{-1}]	O
$kdeg_{soil\ [S]}$	rate constant for degradation in bulk soil on scale [S]	[d^{-1}]	O

III.4.10.6. Definition of the environmental compartments

The following tables specify the default settings for the regional, continental and global 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 S-4 *Parameter settings for regional and continental surface waters.*

Parameter	**Symbol**	**Unit**	**Value**
Area fraction of water R-EU C-EU M A T	$F_{water\ 1\ [R,C]}$ $F_{water\ [M,A,T]}$	[-]	0.03 0.03 0.5 0.6 0.7
Area fraction of sea water R C	$F_{water\ 2\ [R,C]}$	[-]	0.5 0.5
Water depth of fresh water R C	$DEPTH_{water\ 1\ [R,C]}$	[m]	3 3
Water depth of seawater R C M A T	$DEPTH_{water\ 2\ [R,C]}$ $DEPTH_{water\ [M,A,T]]}$		25 200 1000 1000 1000
Residence time of water R C	$TAU_{water\ [R,C]}$	[d]	40 O^c 166 O^c
Fraction of flow from water 1 [C] to: - water 1 [R] - water 2 [R] - water 2 [C]	 $Fflow_{water\ 1\ [C]-water\ 1\ [R]}$ $Fflow_{water\ 1\ [C]-water\ 2\ [R]}$ $Fflow_{water\ 1\ [C]-water\ 2\ [C]}$	 [-]	 0.0391 0.01 0.951
Suspended-solids conc. fresh water R C	$SUSP_{water\ 1\ [S]}$	$[kg_{dwt}.m^{-3}]$	0.015 0.025
Suspended-solids conc. sea water R C M A T	$SUSP_{water\ 2\ [R,C]}$ $SUSP_{water\ [M,A,T]}$	$[kg_{dwt}.m^{-3}]$	0.005 0.005 0.005 0.005 0.005
Concentration of biota	$BIOTA_{water}$	$[kg_{wwt}.m^{-3}]$	0.001

Table S-5 *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	R C	$TAU_{air\ [R,C]}$	[d]	0.7 6.5	O^{c} O^{c}
Aerosol-deposition velocity		$DEPRATE_{aer}$	$[m.d^{-1}]$	86.4	
Aerosol-collection efficiency		$COLLEFF_{aer}$	[-]	2.10^{5}	
Average daily precipitation	R C M A T	$RAINRATE_{[S]}$	$[m.d^{-1}]$	$1.92.10^{-3}$ $1.92.10^{-3}$ $1.92.10^{-3}$ $6.85.10^{-4}$ $3.56.10^{-3}$	

[a] Already defined in STP sub-module.

Table S-6 *Parameter settings for regional and continental 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 water		$SUSPPROD_{water\ 1\ [R,C]}$ $SUSPPROD_{water\ 2\ [R,C]}$ $SUSPPROD_{water\ [M,A,T]}$	$[kg_{dwt}.m^{-2}.yr^{-1}]$	0.01 [a] 0.001 0.001	
Suspended solids in STP effluent	R C	$SUSP_{eff\ [R,C]}$	$[kg_{dwt}.m^{-3}]$	0.030 [b] 0.040	
Net sedimentation rate	R C	$NETsedrate_{[S]}$	$[m_{sed}.d^{-1}]$	$8.4.10^{-6}$ $7.5.10^{-6}$	O^{c} O^{c}

[a] This parameter is subsequently used on a $kg.d^{-1}$ basis by scaling with the number of days in a year and the area of water in the respective systems.

[b] Already defined in STP sub-module.

Table S-7 *Parameter settings for regional and continental soils.*

Parameter	**Symbol**	**Unit**	**Value**
Area fraction of natural soil	$F_{\mathrm{natural}\ [R,C\text{-}EU\}}$	[-]	0.60
Mixing depth of natural soil	$DEPTH_{\mathrm{natural}}$	[m]	0.05
Area fraction of agricultural soil	$F_{\mathrm{agric}\ [R,C\text{-}EU]}$	[-]	0.27
Mixing depth of agricultural soil	$DEPTH_{\mathrm{agric}}$	[m]	0.2
Area fraction of industrial/urban soil	$F_{\mathrm{ind}\ [R,C\text{-}EU]}$	[-]	0.10
Mixing depth of industrial/urban soil	$DEPTH_{\mathrm{ind}}$	[m]	0.05
Mixing depth of soil at global scales	$DEPTH_{\mathrm{soil}\ [M,A,T]}$	[m]	0.05
Fraction of rainwater infiltrating soil	$Finf_{\mathrm{soil}\ [S]}$	[-]	0.25
Fraction of rainwater run-off from soil	$Frunoff_{\mathrm{soil}\ [S]}$	[-]	0.25
Soil-erosion rate	$EROSION_{[S]}$	[m.d^{-1}]	8.2.10^{-8} *

* Different parameter value possible on regional and continental scale.

Optionally, a chemical-specific soil depth can be calculated. This procedure is described in detail in Brandes *et al.* (1996).

Table S-8 *Mass-transfer coefficients for regional and continental scales.*

Parameter	**Symbol**	**Unit**	**Value**
Air-film partial mass-transfer coefficient (air-water and air-soil interfaces)	$kasl_{air}$ / kaw_{air}	[m.d^{-1}]	120
Water-film partial mass-transfer coefficient (air-water interface)	kaw_{water}	[m.d^{-1}]	1.2
Soil-air partial mass-transfer coefficient (air-soil interface)	$kasl_{soilair}$	[m.d^{-1}]	0.48
Soil water-water film partial-mass transfer coefficient (air-soil interface)	$kasl_{soilwater}$	[m.d^{-1}]	4.8.10^{-5}
Water-film partial mass-transfer coefficient (sediment-water interface)	kws_{water}	[m.d^{-1}]	0.24
Pore water partial mass-transfer coefficient (sediment-water interface)	kws_{sed}	[m.d^{-1}]	2.4.10^{-3}

III.4.10.7. Area and population of the regional and continental system

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. The area and population of the continental system are derived from the value for the total EU and the regional definition. Furthermore, since the area fractions are given excluding sea water, they must be recalculated to total-system fractions.

$$Fscaling_{[C]} = 1 + \frac{F_{water\ 2\ [C]}}{1 - F_{water\ 2\ [C]}} \tag{S-16}$$

$$Fscaling_{[R]} = 1 + \frac{F_{water\ 2\ [R]}}{1 - F_{water\ 2\ [R]}} \tag{S-17}$$

$$AREA_{[R]} = AREA_{[R\text{-}EU]} \cdot Fscaling_{[R]} \tag{S-18}$$

$$AREA_{[C]} = \left(AREA_{[C\text{-}EU]} - AREA_{[R\text{-}EU]} \right) \cdot Fscaling_{[C]} \tag{S-19}$$

$$F_{water\,1\ [R]} = \frac{F_{water\,1\ [R\text{-}EU]}}{Fscaling_{[R]}} \tag{S-20}$$

$$F_{water\,1\ [C]} = \frac{F_{water\,1\ [C\text{-}EU]}}{Fscaling_{[C]}} \tag{S-21}$$

Input			
$Fscaling_{[R,C]}$	scaling factor for including water 2 in system area [R,C]	[-]	O^c
$AREA_{[C\text{-}EU]}$	area of continental EU (excl. sea water)	[m^2]	D
$AREA_{[R\text{-}EU]}$	area of regional system (excl. sea water)	[m^2]	D
$F_{water\ 2\ [C]}$	fraction sea water of continental system	[-]	D
$F_{water\ 2\ [R]}$	fraction sea water of regional system	[-]	D
Output			
$AREA_{[C]}$	area of continental system	[m^2]	O^c
$AREA_{[R]}$	area of regional system	[m^2]	O^c
$F_{water\ 1\ [C\text{-}EU]}$	fraction water of continental EU (excl. sea water)	[-]	O^c
$F_{water\ 1\ [R\text{-}EU]}$	fraction water of regional system (excl. sea water)	[-]	O^c

$$N_{[C]} = N_{[C\text{-}EU]} - N_{[R]} \qquad \text{(S-22)}$$

Input			
$N_{[C\text{-}EU]}$	number of inhabitants of EU	[eq]	D
$N_{[R]}$	number of inhabitants of region	[eq]	D
Output			
$N_{[C]}$	number of inhabitants of continental system	[eq]	O^c

$$F_{i\,[R,C]} = \frac{F_{i\,[R,C\text{-}EU]}}{Fscaling_{[R,C]}} \qquad i \in \{natural, agric, ind\} \qquad \text{(S-23)}$$

Input			
$Fscaling_{[R,C]}$	scaling factor for including water 2 in system area [R,C]	[-]	O
$F_{natural\,[R,C\text{-}EU]}$	area fraction of natural soil on scale [R,C] excl. sea water	[-]	D
$F_{agric\,[R,C\text{-}EU]}$	area fraction of agric. soil on scale [R,C] excl. sea water	[-]	D
$F_{ind\,[R,C\text{-}EU]}$	area fraction of industrial soil on scale [R,C]	[-]	D
Output			
$F_{natural\,[R,C]}$	area fraction of natural soil on scale [R,C]	[-]	O^c
$F_{agric\,[R,C]}$	area fraction of agricultural soil on scale [R,C]	[-]	O^c
$F_{ind\,[R,C]}$	area fraction of industrial soil on scale [R,C]	[-]	O^c

$$F_{soil\,[M,A,T]} = 1 - F_{water\,[M,A,T]} \qquad \text{(S-24)}$$

Input			
$F_{water\,[M,A,T]}$	area fraction of sea water on global scales [M,A,T]	[-]	D
Output			
$F_{soil\,[M,A,T]}$	area fraction of soil on global scales [M,A,T]	[-]	O^c

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.

III.4.10.8. Residence time in air

The residence time of air in the system is given by the area of the system and the wind speed.

$$TAU_{air\,[S]} = \frac{\sqrt{AREA_{[S]} \cdot \frac{\pi}{4}}}{WINDSPEED} \qquad \text{(S-25)}$$

Input

AREA	area of the system on scale [S]	[m^2]	D
WINDSPEED	wind speed	[m.d^{-1}]	D
Output			
TAU$_{air}$	residence time of air on scale [S]	[d]	O^c

III.4.10.9. Residence time in water

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. The total water flow through the system is caused by inflow of water from the other spatial scales, wastewater production (only [R] and [C]), run-off from soil, and direct rainfall into water. Only the equation for water 1 on the regional scale is shown, the other water compartments are calculated analogous.

$$TAU_{water\,1\,[R]} = \frac{AREA_{[R]} \cdot F_{water\,1\,[R]} \cdot DEPTH_{water\,1\,[R]}}{FLOW_{water\,1\,[R]}} \qquad \text{(S-26)}$$

Input

AREA$_{[R]}$	area of system on scale [R]	[m^2]	D
F$_{water\ 1\ [R]}$	area fraction of water 1 on scale [R]	[-]	D
DEPTH$_{water\ 1\ [R]}$	water depth on scale [R]	[m]	D
FLOW$_{water\ 1\ [R]}$	total water flow through system on scale [R]	[m^3.d^{-1}]	O^c
Output			
TAU$_{water\ 1\ [R]}$	residence time of water on scale [R]	[d]	O^c

III.4.10.10. 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. Only the equation for the regional scale is shown:

$$\begin{aligned}
& \boldsymbol{NETsedrate_{[R]}} = \\
& \boldsymbol{[\ SUSPPROD_{water\,1\,[R]} + SUSP_{water\,[C]} \cdot Fflow_{water\,1\,[C]\,-\,water\,1\,[R]} \cdot FLOW_{water\,1\,[C]}} + \\
& \boldsymbol{SUSP_{eff} \cdot EFFLUENT_{stp\,[R]} + EROSION_{[R]} \cdot (\ F_{natural\,[R]} + F_{agric\,[R]} + F_{ind\,[R]}\ )} \cdot \qquad \text{(S-27)} \\
& \boldsymbol{AREA_{[R]} \cdot Fsolid_{soil} \cdot RHOsolid - SUSP_{water\,1\,[R]} \cdot FLOW_{water\,1\,[R]}\ ]} \\
& \cdot \frac{\mathbf{1}}{\boldsymbol{Fsolid_{sed} \cdot RHOsolid}} \cdot \frac{\mathbf{1}}{\boldsymbol{AREA_{[R]} \cdot F_{water\,1\,[R]}}}
\end{aligned}$$

Input			
$SUSPPROD_{water\,1\,[R]}$	(biogenic) production of susp. solids in water on scale [R]	$[kg_{dwt}.d^{-1}]$	D
$FLOW_{water\,[R]}$	total water flow through system on scale [R]	$[m^3.d^{-1}]$	O^c
$FLOW_{water\,[C]}$	total water flow through system on scale [C]	$[m^3.d^{-1}]$	O^c
$Fflow_{water\,1\,[C]-water\,1\,[R]}$	fraction of water flow from scale [C] to scale [R]	[-]	D
$SUSP_{water\,[R]}$	suspended-solids concentration in water on scale [R]	$[kg_{dwt}.m^{-3}]$	D
$SUSP_{water\,[C]}$	suspended-solids concentration in water on scale [C]	$[kg_{dwt}.m^{-3}]$	D
$SUSP_{eff}$	suspended solids concentration in STP effluent	$[kg_{dwt}.m^{-3}]$	D
$EFFLUENT_{stp\,[R]}$	effluent of STP	$[m^3.d^{-1}]$	O^c
$EROSION_{[R]}$	soil-erosion rate	$[m.d^{-1}]$	D
$F_{natural\,[R]}$	area fraction of natural soil	[-]	D
$F_{agric\,[R]}$	area fraction of agricultural soil	[-]	D
$F_{ind\,[R]}$	area fraction of industrial/urban soil	[-]	D
$F_{water\,1\,[R]}$	area fraction of water	[-]	D
$AREA_{[R]}$	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			
$NETsedrate_{[R]}$	net sedimentation rate on scale [R]	$[m.d^{-1}]$	O^c

III.4.10.11. Regional and continental effluent discharges

The effluent discharge from regional and continental STPs depends on the fraction connected to treatment plants.

$$\boldsymbol{EFFLUENT_{stp\,[R,C]} = N_{[R,C]} \cdot Q_{stp\,[R,C]} \cdot Fconnect_{stp\,[R,C]}} \qquad \text{(S-28)}$$

Input			
$N_{[R,C]}$	number of inhabitants of system on scale [R,C]	[eq]	D
$Q_{stp\,[R,C]}$	per-capita sewage flow on scale [R,C]	$[m^3.eq^{-1}.d^{-1}]$	D
$Fconnect_{stp\,[R,C]}$	fraction connected to sewer systems on scale [R,C]	[-]	D
Output			
$EFFLUENT_{stp\,[R,C]}$	effluent of STP on scale [R,C]	$[m^3.d^{-1}]$	O^c

III.4.10.12. 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.

The BCF for aquatic biota is calculated from the Equations (86) and (87). It should be noted that this estimated BCF is always used in this equation. Measured BCF for fish are not used since these can not be assumed as representative for all aquatic biota. The total concentration is converted as follows (only regional water 1 shown, other water compartments are converted analogous):

$$\boldsymbol{PECreg_{water\,1} = \frac{PECreg_{water\,1,tot}}{1 + Kp_{susp} \cdot SUSP_{water1\,[R]} + BCF_{biota} \cdot BIO_{water}}} \qquad \text{(S-29)}$$

Input			
$PECreg_{water\,1,tot}$	regional concentration in surface water (total)	$[kg_c.m^{-3}]$	O
Kp_{susp}	solids-water partition coefficient of suspended matter	$[m^3.kg_{solids}^{-1}]$	O
$SUSP_{water\,1\,[R]}$	concentration of suspended matter in water 1 of region	$[kg_{dwt}.m^{-3}]$	D
BCF_{biota}	bioconcentration factor for aquatic biota	$[m^3.kg_{wwt}^{-1}]$	O
BIO_{water}	concentration of aquatic biota in regional system	$[kg_{wwt}.m^{-3}]$	D
Output			
$PECreg_{water\,1}$	regional PEC in surface water	$[kg_c.m^{-3}]$	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.

EUSES Section III.5.1 must not be used for assessing exposure of organisms to pesticides after application (processing in UC=38/39). Instead, Section III.5.5 applies. For indirect exposure of humans via the environment, the EUSES section must be used (Section III.5.2).

III.5.1. Secondary poisoning

For the assessment of secondary poisoning, two example food chains are modelled: water→fish→predator and 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	[-]	
$K_{soil\text{-}water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	c
Input: environmental properties			
RHO_{soil}	bulk density of soil	$[kg_{wwt}.m^{-3}]$	c
$PEClocal_{water,ann}$	annual average local PEC in surface water (dissolved)	$[kg_c.m^{-3}]$	
$PEClocal_{agric}$	local PEC in agricultural soil	$[kg_c.m^{-3}]$	
$PECreg_{water}$	regional PEC in surface water (dissolved)	$[kg_c.m^{-3}]$	
$PECreg_{agric}$	regional PEC in agricultural soil	$[kg_c.kg_{wwt}^{-1}]$	
Intermediate results			
$K_{worm\text{-}porew}$	worm-pore water partition coefficient	$[m^3.kg_{worm\ wwt}^{-1}]$	
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	$[kg_c.kg_{wwt}^{-1}]$	
$PEC_{oral,worm}$	local 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:

$$\log BCF_{fish} = 0.85 \cdot \log Kow - 0.70 - 3 \tag{86}$$

if log *Kow* > 6 then:

$$\log BCF_{fish} = -0.20 \cdot (\log Kow)^2 + 2.74 \cdot \log Kow - 4.72 - 3 \tag{87}$$

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 fish-eating predators

The exposure level for fish-eating predators is calculated as the average of the local and regional concentration in fish.

$$PEC_{oral,fish} = BCF_{fish} \cdot \frac{PEClocal_{water,ann} + PECreg_{water}}{2} \tag{88}$$

Input			
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
Output			
$PEC_{oral,fish}$	concentration in fish for secondary poisoning	$[kg_c.kg_{wwt}^{-1}]$	O

III.5.1.3. Bioconcentration factor for earthworms

The BCF for worm is estimated using a QSAR from Connell and Markwell (1990). They derived an empirical equation for the worm-pore water partitioning through regression on experimental data for pesticides with a log *Kow* ranging from 1.0 to 6.5 (outside this range the minimum or maximum *Kow* is used). The factor 0.16 is in the equation to correct the estimate to earthworm wet weight.

$$\boldsymbol{K_{worm\text{-}porew} = \frac{0.25 \cdot Kow \cdot 0.16}{1000}} \qquad (89)$$

$$\boldsymbol{BCF_{worm} = K_{worm\text{-}porew} \cdot \frac{RHO_{soil}}{K_{soil\text{-}water}}} \qquad (90)$$

Input			
Kow	octanol-water partition coefficient	$[m^3.m^{-3}]$	S
RHO_{soil}	bulk density of soil	$[kg_{wwt}.m^{-3}]$	O^c
$K_{soil\text{-}water}$	soil-water partition coefficient	$[m^3.m^{-3}]$	O^c
Output			
$K_{worm\text{-}porew}$	worm-pore water partition coefficient	$[m^3.kg_{wwt}^{-1}]$	O
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 and the average of regional and local concentrations in agricultural soil.

$$\boldsymbol{PEC_{oral,worm} = BCF_{worm} \cdot \frac{PEClocal_{agric} + PECreg_{agric}}{2}} \qquad (91)$$

Input			
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
Output			
$PEC_{oral,worm}$	local 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:

$$C_{fish} = BCF_{fish} \cdot C_{water} \tag{92}$$

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-20.

Table III-20 *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.

$$K_{plant-water} = Fwater_{plant} + Flipid_{plant} \cdot Kow^{b} \qquad (93)$$

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:

$$C_{root} = \frac{K_{plant\text{-}water} \cdot C_{agric,porew}}{RHO_{plant}} \qquad (94)$$

Input			
$K_{plant\text{-}water}$	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).

$$TSCF = 0.784 \cdot \exp\left[\frac{-(\log Kow - 1.78)^2}{2.44}\right] \qquad (95)$$

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:

$$K_{leaf\text{-}air} = Fair_{plant} + \frac{K_{plant\text{-}water}}{K_{air\text{-}water}} \tag{96}$$

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:

$$kelim_{plant} = kmetab_{plant} + kphoto_{plant} \tag{97}$$

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:

$$ALPHA = \frac{AREA_{plant} \cdot g_{plant}}{K_{leaf\text{-}air} \cdot V_{leaf}} + kelim_{plant} + kgrowth_{plant} \tag{98}$$

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.

$$BETA_{agric} = C_{agric,porew} \cdot TSCF \cdot \frac{Qtransp}{V_{leaf}} + (1 - Fass_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}} \qquad (99)$$

$$BETA_{grass} = C_{grassland,porew} \cdot TSCF \cdot \frac{Qtransp}{V_{leaf}} + \qquad (100)$$
$$(1 - Fass_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}$$

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).

$$C_{leaf} = \frac{BETA_{agric}}{ALPHA} \cdot \frac{1}{RHO_{plant}} \qquad (101)$$

$$C_{grass} = \frac{BETA_{grass}}{ALPHA} \cdot \frac{1}{RHO_{plant}} \qquad (102)$$

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.

$$Fleaf_{porew} = \frac{C_{agric,porew} \cdot TSCF \cdot \dfrac{Qtransp}{V_{leaf}}}{BETA_{agric}} \tag{103}$$

$$Fleaf_{air} = \frac{(1 - Fass_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \dfrac{AREA_{plant}}{V_{leaf}}}{BETA_{agric}} \tag{104}$$

$$Fgrass_{porew} = \frac{C_{grassland,porew} \cdot TSCF \cdot \dfrac{Qtransp}{V_{leaf}}}{BETA_{grass}} \tag{105}$$

$$Fgrass_{air} = \frac{(1 - Fass_{aer}) \cdot C_{air} \cdot g_{plant} \cdot \dfrac{AREA_{plant}}{V_{leaf}}}{BETA_{grass}} \tag{106}$$

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-21 *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).

$$BAF_{meat} = 10^{-7.6 + \log Kow} \tag{107}$$

$$BAF_{milk} = 10^{-8.1 + \log Kow} \tag{108}$$

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:

$$IC_{grass} = ICdwt_{grass} \cdot CONV_{grass} \tag{109}$$

$$IC_{soil} = ICdwt_{soil} \cdot CONV_{soil} \tag{110}$$

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:

$$C_{milk} = BAF_{milk} \cdot \sum C_i \cdot IC_i \quad i \in \{grass, grassland \setminus soil, air, drw\} \tag{111}$$

$$C_{meat} = BAF_{meat} \cdot \sum C_i \cdot IC_i \quad i \in \{grass, grassland \setminus soil, air, drw\} \tag{112}$$

The contribution of each exposure medium to the intake of cattle can be calculated as:

$$Fcattle_i = \frac{C_i \cdot IC_i}{\sum C_i \cdot IC_i} \quad i \in \{grass, grassland \setminus soil, air, drw\} \tag{113}$$

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-22 *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).

$$F_{pur} = max\ (Fsys1_{pur}\ , Fsys2_{pur}\ ) \qquad (114)$$

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

$$C_{drw} = \max\left(C_{water} \cdot F_{pur}, C_{grw}\right) \tag{115}$$

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.

$$DOSE_j = \frac{C_j \cdot IH_j}{BW} \qquad j \in \{drw, fish, leaf, root, meat, milk\} \tag{116}$$

$$DOSE_{air} = \frac{F_{resp} \cdot C_{air} \cdot IH_{air}}{BW} \cdot \frac{BIO_{inh}}{BIO_{oral}} \tag{117}$$

The total dose can now be calculated as the sum of the dose for each medium:

$$DOSE_{tot} = \sum_i DOSE_i \qquad i \in \{air, drw, fish, leaf, root, meat, milk\} \tag{118}$$

The contribution of each intake medium to the total dose is calculated as:

$$Fdose_i = \frac{DOSE_i}{\sum_i DOSE_i} \tag{119}$$

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}	bioavailability for oral intake	[-]	D
BIO_{inh}	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-23, 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-23 *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-^{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 comp. 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-24 *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).

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:

$$C_{inh} = \frac{Q_{prod} \cdot Fc_{prod}}{V_{room}} \tag{120}$$

The air concentration C_{inh} results in an inhalatory intake of:

$$I_{inh} = \frac{F_{resp} \cdot C_{inh} \cdot IH_{air} \cdot T_{contact}}{BW} \cdot n \tag{121}$$

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-25 *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:

$$C_{der} = \frac{C_{prod}}{D} = \frac{RHO_{prod} \cdot Fc_{prod}}{D} = \frac{Q_{prod} \cdot Fc_{prod}}{V_{prod} \cdot D} \tag{122}$$

The total amount to which the skin is exposed is then given by (two options, depending on format of available data):

$$A_{der} = C_{der} \cdot V_{appl} = C_{der} \cdot TH_{der} \cdot AREA_{der} \tag{123}$$

The potential uptake per kilogram body weight per day is derived as:

$$U_{der,pot} = \frac{A_{der} \cdot n}{BW} \tag{124}$$

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.

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 (122) 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

$$A_{der} = W_{der} \cdot AREA_{der} = C_{der} \cdot TH_{der} \cdot AREA_{der} \tag{125}$$

where $C_{der} \cdot TH_{der}$ is equal to weight per unit of area:

$$W_{der} = C_{der} \cdot TH_{der} \tag{126}$$

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:

$$A_{migr,der} = A_{der} \cdot Fc_{migr} \cdot T_{contact} \tag{127}$$

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:

$$U_{der,pot} = \frac{A_{migr,der} \cdot n}{BW} \tag{128}$$

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

$$C_{oral} = \frac{C_{prod}}{D} = \frac{RHO_{prod} \cdot Fc_{prod}}{D} = \frac{Q_{prod} \cdot Fc_{prod}}{V_{prod} \cdot D} \qquad (129)$$

and the intake is then given by

$$I_{oral} = \frac{F_{oral} \cdot V_{appl} \cdot C_{oral} \cdot n}{BW} \qquad (130)$$

If an undiluted product is swallowed, $D = 1$.

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:

$$C_{oral} = \frac{AREA_{art} \cdot TH_{art} \cdot C_{art} \cdot Fc_{migr} \cdot T_{contact}}{V_{prod}} \qquad (131)$$

Oral intake is given by:

$$I_{oral} = \frac{V_{appl} \cdot C_{oral} \cdot n}{BW} \qquad (132)$$

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 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:

$$C_{route,ann} = \frac{\int_0^{365} C_{route}(t)\, dt}{365} \qquad route \in \{inh, der, oral\} \qquad (133)$$

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:

$$C_{route,ann} = C_{route} \cdot n \cdot T_{contact} \qquad route \in \{inh, der, oral\} \qquad (134)$$

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 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.

$$U_{tot} = I_{inh} \cdot BIO_{inh} + U_{der,pot} \cdot BIO_{der} + I_{oral} \cdot BIO_{oral} \qquad (135)$$

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}	bioavailability for oral intake	[-]	D
BIO_{inh}	bioavailability for inhalation	[-]	D
BIO_{der}	bioavailability for dermal uptake	[-]	D
Output			
U_{tot}	total uptake for one product via different routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O

III.5.4. Workplace exposure

Exposure of workers is estimated by means of the model EASE, implemented in EUSES. The user needs to provide answers on the questions presented by this model (see decision trees in Appendix V). 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 V)	
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	

Inhalatory worker exposure

Input			
-	specific questions on exposure (see decision trees in Appendix V)		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-26 *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}

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.

$$C_{inh,worker,vapour} = \frac{273}{TEMPwork} \cdot MOLW \cdot 10^{-6} \cdot C1_{inh,worker,vapour} \cdot \frac{1000}{22.4} \qquad (172)$$

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

Dermal worker exposure

Input

-	specific questions on exposure (see decision trees in Appendix V)		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 is 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:

$$U_{der,worker,pot} = W_{der,worker} \cdot \frac{AREA_{der,worker}}{BW} \tag{136}$$

Input

$AREA_{der,worker}$	area of contact between substance and skin	[m^2]	S
BW	body weight	[kg]	D
$W_{der,worker}$	dermal weight of substance on skin of workers	[$kg.m^{-2}.d^{-1}$]	O

Output

$U_{der,pot,worker}$	potential dermal uptake for workers	[$kg.kg_{bw}^{-1}.d^{-1}$]	O

III.5.5. Intake for animals due to pesticide application

Input

$DOSE_{pest}$	single dosage for pesticide	$[kg_c.m^{-2}]$
$Cwater_{pest\text{-}Tbird}$	mean concentration in water over T_{bird} days	$[kg_c.m^{-3}]$
$Cwater_{pest\text{-}Tmammal}$	mean concentration in water over T_{mammal} days	$[kg_c.m^{-3}]$
$Csoil_{pest\text{-}Tbird}$	mean concentration in soil over T_{bird} days	$[kg_c.kg_{soil}^{-1}]$
$Csoil_{pest\text{-}Tmammal}$	mean concentration in soil over T_{mammal} days	$[kg_c.kg_{soil}^{-1}]$
BCF_{fish}	bioconcentration factor for fish	$[m_{water}^{3}.kg_{wet\ fish}^{-1}]$
$K_{worm\text{-}porew}$	worm-porewater partition coefficient	$[m^3.kg_{wwt}^{-1}]$
RHO_{pest}	wet bulk density of application soil	$[kg.m^{-3}]$
$K_{pest\text{-}water}$	total application soil-water partition coefficient	$[m^3.m^{-3}]$
$DT50_{food}$	DT50 in food (spray only)	[d]

Output

Spray only:

$Cfood_{bird\text{-}5}$	mean concentration in birds food over 5 days	$[kg_c.kg_{food}^{-1}]$
$Cfood_{mammal\text{-}5}$	mean concentration in mammal food over 5 days	$[kg_c.kg_{food}^{-1}]$
$Cfood_{Tbird}$	mean concentration in food over T_{bird} days	$[kg_c.kg_{food}^{-1}]$
$Cfood_{Tmammal}$	mean concentration in food over T_{mammal} days	$[kg_c.kg_{food}^{-1}]$
C_{spray}	concentration in water on leaves and crops	$[kg_c.m_{water}^{-3}]$

General output

$C_{fish\text{-}Tbird}$	mean concentration in fish for birds	$[kg_c.kg_{wet\ fish}^{-1}]$
$C_{fish\text{-}Tmammal}$	mean conc. in fish for mammals	$[kg_c.kg_{wet\ fish}^{-1}]$
$C_{worm\text{-}Tbird}$	mean concentration in earthworms for birds	$[kg_c.kg_{wet\ worm}^{-1}]$
$C_{worm\text{-}Tmammal}$	mean conc. in earthworms for mammals	$[kg_c.kg_{wet\ worm}^{-1}]$

If UC = 38 or 39 calculate this exposure sub-module for pesticides.

EUSES Section III.5.1 must not be used for assessing exposure of organisms to pesticides after application (processing in UC=38/39). Instead, Section III.5.5 applies. For indirect exposure of humans via the environment, the EUSES section must be used (Section III.5.2).

Concentrations on crops growing on application soil on which the pesticide is applied as well as cows grazing on soil on which pesticide is applied are <u>not</u> taken into account. The table converting the input environmental concentrations to temporary symbols must be amended as follows:

Temporary symbol	**Local concentration**	**Regional concentration**	**Processing in UC=38/39 (pesticide appl.)**
C_{water}	$PEClocal_{water,ann}$	$PECreg_{water}$	C_{river} *or* $Cwater_{pest-365}$ *or* $Clocal_{water,ann}$
C_{air}	$PEClocal_{air,ann}$	$PECreg_{air}$	$PEClocal_{air,ann}$
$C_{grassland}$	$PEClocal_{grassland}$	$PECreg_{agric}$	$PEClocal_{grassland}$
$C_{agric,porew}$	$PEClocal_{agric,porew}$	$PECreg_{agric,porew}$	$PEClocal_{agric,porew}$
$C_{grassland,porew}$	$PEClocal_{grassland,porew}$	$PECreg_{agric,porew}$	$PEClocal_{grassland,porew}$
C_{grw}	$PEClocal_{grw}$	$PECreg_{agric,porew}$	$Cgrw_{pest}$ *or* $PEClocal_{grw}$

In case the substance is applied as particles, only an annual average concentration in water will be known (through drainage). This concentration will then be used in the calculation of $C_{fish-Tx}$ above. If $Cwater_{pest-Tbird}$ and $Cwater_{pest-Tmammal}$ are not specified:

$$Cwater_{pest-Tbird/mammal} = Cwater_{pest-365} \qquad \text{(P-348)}$$

If $Cwater_{pest-365}$ is also not specified, use results from the local distribution module:

$$Cwater_{pest-Tbird/mammal} = PEClocal_{water,ann} \qquad \text{(P-349)}$$

If $Csoil_{pest-Tbird}$ and $Csoil_{pest-Tmammal}$ are not specified:

$$Csoil_{pest-Tbird/mammal} = PEClocal_{agric} \qquad \text{(P-350)}$$

III.5.5.1. Exposure of birds and mammals due to spraying

Initial concentration in food for birds and mammals (via sprays)

Initial concentrations in crops and insects after spraying can be given in the input. If no concentration in feed is known, this concentration can be estimated with the table given below. Hoerger and Kenega (1972) have described a method which estimates the concentration of a pesticide on various types of feed after exposure. It gives a relation by which the mean and maximal concentration directly after an application with a certain dosage can be determined. It must be noted, however, that measured data on feed concentrations is always preferable.

This route is only of importance when the substance is applied as a spray. Only mean concentrations will be used:

Table D-7 *Initial concentration in food for birds and mammals after spraying.*

Type of feed	**Mean concentration on feed (C_{food}; in $kg_c.kg_{food}^{-1}$)**	**Maximal concentration on feed (C_{food}; in $kg_c.kg_{food}^{-1}$)**
short grass	$62 \cdot DOSE_{pest} \cdot 10^{-2}$	$142 \cdot DOSE_{pest} \cdot 10^{-2}$
tall grass	$21 \cdot DOSE_{pest} \cdot 10^{-2}$	$69 \cdot DOSE_{pest} \cdot 10^{-2}$
leaves, leaf crops, forage crops & small seeds	$26 \cdot DOSE_{pest} \cdot 10^{-2}$	$87 \cdot DOSE_{pest} \cdot 10^{-2}$
fruit, pods and large seeds	$2.3 \cdot DOSE_{pest} \cdot 10^{-2}$	$11 \cdot DOSE_{pest} \cdot 10^{-2}$
small insects (foliar application)	$26 \cdot DOSE_{pest} \cdot 10^{-2}$	$87 \cdot DOSE_{pest} \cdot 10^{-2}$
large insects (foliar application)	$2.7 \cdot DOSE_{pest} \cdot 10^{-2}$	$11 \cdot DOSE_{pest} \cdot 10^{-2}$
insects (soil application)	$0.1 \cdot DOSE_{pest} \cdot 10^{-2}$	$1.0 \cdot DOSE_{pest} \cdot 10^{-2}$

If the diet of birds or mammals consists of various kinds of crops or insects, this can be taken into account for the calculation of the C_{food} by manually calculating the feed concentration from the various sources given in the next table.

Input			
$DOSE_{pest}$	single dosage for pesticide	$[kg_c.m^{-2}]$	O
-	type of food for the bird species of choice	[-]	P
-	type of food for the mammalian species of choice	[-]	P
Output			
$Cfood_{bird}$	initial concentration in bird food	$[kg_c.kg_{food}]$	S/O
$Cfood_{mammal}$	initial concentration in mammalian food	$[kg_c.kg_{food}]$	S/O

Concentration in food for birds and mammals (via sprays)

The concentration in feed has to be calculated over 5 days for evaluating acute toxicity and over a longer period of time (depending on the exposure period in the toxicity test for the species) for chronic toxicity. For this calculation it is necessary that the half-life time of the pesticide in crops or insects ($DT50_{food}$) is known. The half-life time should preferably be determined from residue data on crops and insects. If $DT50_{food}$ is unknown, no disappearance of the substance is assumed.

$$k_{food} = \frac{ln\,2}{DT50_{food}} \qquad \text{(P-351)}$$

if $DT50_{food}$ is not given:

$$Cfood_{bird\text{-}5} = \frac{Cfood_{bird}}{k_{food} \cdot 5} \cdot \left(1 - e^{-k_{food} \cdot 5}\right) \qquad \text{(P-352)}$$

$$Cfood_{x\text{-}5} = Cfood_{Tx} = Cfood_{x} \qquad \text{(P-353)}$$

$$Cfood_{Tx} = \frac{Cfood_{x}}{k_{food} \cdot T_{x}} \cdot \left(1 - e^{-k_{food} \cdot T_{x}}\right)$$

$$x \in \{bird, mammal\} \qquad \text{(P-354)}$$

Input			
k_{food}	first order disappearance rate of pesticide in food	$[d^{-1}]$	O
$Cfood_{bird}$	initial concentration in food for birds	$[kg_c.kg_{food}^{-1}]$	S/O
$Cfood_{mammal}$	initial concentration in food for mammals	$[kg_c.kg_{food}^{-1}]$	S/O
$DT50_{food}$	DT50 in food	[d]	S
T_{bird}	duration of chronic toxicity test for birds	[d]	S
T_{mammal}	duration of chronic toxicity test for mammals	[d]	S
Output			
$Cfood_{bird\text{-}5}$	mean concentration in birds food over 5 days	$[kg_c.kg_{food}^{-1}]$	O
$Cfood_{Tbird}$	mean concentration in food over T_{bird} days	$[kg_c.kg_{food}^{-1}]$	O
$Cfood_{Tmammal}$	mean concentration in food over T_{mammal} days	$[kg_c.kg_{food}^{-1}]$	O

Concentration in spray water on leaves and crops

Besides eating granules, treated seeds, crops or insects, birds and mammals can also be exposed to a pesticide by the uptake of water. This can be either surface water or water on leaves and crops. Calculations for this exposure route are based on Luttik (1992).

$$C_{spray} = \frac{DOSE_{pest}}{AMOUNTspray} \qquad \text{(P-355)}$$

Input			
AMOUNTspray	amount of spray liquid used	$[m_{spray}^{3}.m^{-2}]$	S
$DOSE_{pest}$	single dosage for pesticide	$[kg_{c}.m^{-2}]$	O
Output			
C_{spray}	concentration in water on leaves and crops	$[kg_{c}.m_{water}^{-3}]$	O

III.5.5.2. Concentration in earthworms

The uptake of a pesticide by earthworms is calculated by means of the bioconcentration factor (BCF) for soil - earthworm. This BCF should preferably be derived experimentally. If no experimentally obtained data are available, it can be estimated by means of the Quantitative Structure Activity Relationships (QSARs) given in Section III.5.1. BCF worm has to be calculated for the specific properties of application soil:

$$\boldsymbol{BCF_{worm,pest} = K_{worm-porew} \cdot \frac{RHO_{pest}}{K_{pest-water}}} \qquad \text{(P-356)}$$

Input

$K_{worm-porew}$	worm-porewater partition coefficient	$[m^3.kg_{wwt}^{-1}]$	O
RHO_{pest}	wet bulk density of application soil	$[kg.m^{-3}]$	O^c
$K_{pest-water}$	total application soil-water partition coefficient	$[m^3.m^{-3}]$	O

Output

$BCF_{worm,pest}$	bioconcentration factor for earthworms in application soil	$[kg_{wet\ soil}.kg_{wet\ worm}^{-1}]$	O

$$\boldsymbol{C_{worm-Tx} = BCF_{worm,pest} \cdot Csoil_{pest-Tx} \qquad x \in \{bird, mammal\}} \qquad \text{(P-357)}$$

Input

$Csoil_{pest-Tbird}$	mean concentration in soil over T_{bird} days	$[kg_c.kg_{soil}^{-1}]$	O
$Csoil_{pest-Tmammal}$	mean concentration in soil over T_{mammal} days	$[kg_c.kg_{soil}^{-1}]$	O
$BCF_{worm,pest}$	bioconcentration factor for earthworms in application soil	$[kg_{wet\ soil}.kg_{wet\ worm}^{-1}]$	O

Output

$C_{worm-Tbird}$	mean concentration in earthworms for birds	$[kg_c.kg_{wet\ worm}^{-1}]$	O
$C_{worm-Tmammal}$	mean conc. in earthworms for mammals	$[kg_c.kg_{wet\ worm}^{-1}]$	O

III.5.5.3. Concentration in fish

The uptake of pesticides by water organisms is calculated by means of the bioconcentration factor (BCF). If no experimentally derived BCF is available, the QSAR-calculation given in Section III.5.1.1 can be used.

$$\boldsymbol{C_{fish-Tx} = BCF_{fish} \cdot Cwater_{pest-Tx} \qquad x \in \{bird, mammal\}} \qquad \text{(P-358)}$$

Input

$Cwater_{pest-Tbird}$	mean concentration in water over T_{bird} days	$[kg_c.m^{-3}]$	O
$Cwater_{pest-Tmammal}$	mean concentration in water over T_{mammal} days	$[kg_c.m^{-3}]$	O
BCF_{fish}	bioconcentration factor for fish	$[m_{water}^3.kg_{wet\ fish}^{-1}]$	O

Output

$C_{fish-Tbird}$	mean concentration in fish for birds	$[kg_c.kg_{wet\ fish}^{-1}]$	O
$C_{fish-Tmammal}$	mean conc. in fish for mammals	$[kg_c.kg_{wet\ fish}^{-1}]$	O

III.5.6. Total daily intake for humans

Dutch intake figures will be used for the environmental assessment of pesticides instead of the EU-average values as applied in EUSES. Indirect exposure of humans to the pesticide can occur through two routes:

- If the pesticide is applied on application soil, only indirect exposure via the air route (via deposition to crops, cattle and inhalation) and through the concentration in river or ditch water/groundwater (via fish and drinking water) is taken into account.
- If the pesticide is released via the STP, only this route is taken into account for indirect exposure (via volatilisation from STP, sludge and effluent) analogous to non-pesticides.

In Tabe III-23, default values for the intake rate of each medium of interest are shown. These values in column 3 include the highest country-average intake across all EU Member States for each food product (Euromonitor, 1992, as reported by ECETOC, 1994) and are recommended to be used in the TGD for new and existing substances. The default values in Table D-8 are based on the Dutch National Food Consumption Survey 1992 (WVC/LNV, 1992) and are used to calculate the theoretical maximum daily intake of pesticide residues in the Netherlands (van Dooren-Flipsen et al., 1996). These data will also be used here to calculate the indirect exposure of man via the environment outside the target area in the assessment of pesticides. The category ”leaf crops” also includes fruits and cereals. “Root crops” pertain to potatoes in the European diet and also include roots and tubers in the Dutch diet. “Meat” is a general category encompassing beef, veal, pork and poultry and the category “dairy products” includes milk as well as milk products such as butter and cheese. In both cases the intake rates of air and drinking water are 20 $m^3.d^{-1}$ and 2 $l.d^{-1}$, respectively.

Table D-8 *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}	0.010	$[kg_{wwt}.d^{-1}]$	(a)
Daily intake of leaf crops (incl. fruit and cereals)	IH_{leaf}	0.633	$[kg_{wwt}.d^{-1}]$	(a)
Daily intake of root crops	IH_{root}	0.218	$[kg_{wwt}.d^{-1}]$	(a)
Daily intake of meat	IH_{meat}	0.125	$[kg_{wwt}.d^{-1}]$	(a)
Daily intake of dairy products	IH_{milk}	0.402	$[kg_{wwt}.d^{-1}]$	(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: WVC/LNV (1992).
[b] Source: US-EPA (1989).
[c] Source: Vermeire *et al.* (1993b).

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}]	
	specific bacterial population?	[yes/no]	
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}]	
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 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
$PNEC_{micro\text{-}organisms}$	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
$PNECstat_{soil}$	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$_{wwt}^{-1}$]	

III.6.1.1. Aquatic compartment

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:

- algae (primary producers);
- *Daphnia* (primary consumers);
- fish (secondary consumers);
- other species (e.g. decomposers).

This section must also be used to calculate PNECs for pesticides for the aquatic ecosystem.

$$\boldsymbol{LC50\,aqua_{min} = \min\left(LC50\,aqua_i\right)} \tag{137}$$

$$\boldsymbol{NOECaqua_{min} = \min\left(NOECaqua_i\right)} \tag{138}$$

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
	Same taxonomic group as LC50aqua$_{min}$?		
1 NOEC additional (not algae!)	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	yes no	NOECaqua$_{min}$ NOECaqua$_{min}$	50 100
3 NOEC algae, *Daphnia* and fish		NOECaqua$_{min}$	10
3 NOEC *not* algae, *Daphnia* and fish	yes no	NOECaqua$_{min}$ NOECaqua$_{min}$	10 50

$$PNEC_{water} = \frac{TOXaqua}{AFaqua} \tag{139}$$

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
Output			
TOXaqua	toxicological data used for extrapolation of PNEC	$[kg_c.m^{-3}]$	O
AFaqua	assessment factor applied in extrapolation of PNEC	[-]	O
$PNEC_{water}$	PNEC for 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. If no toxicity data are available, equilibrium partitioning will be applied. If for pesticides measured toxicity data for terrestrial organisms are available, the equilibrium partioning method will *not* be used for this group of compounds. As a result, Section III.6.3.1 gives a slightly different assessment scheme for pesticides.

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.

$$LC50terr_{min} = \min\left(LC50terr_i \right) \tag{140}$$

$$NOECterr_{min} = \min\left(NOECterr_i \right) \tag{141}$$

$$PNEC_{soil,ep} = \frac{K_{soil\text{-}water}}{RHO_{soil}} \cdot PNEC_{water} \tag{142}$$

Available ecotox. data		**TOXterr**	**AFterr**
none		$PNEC_{soil,ep}$	1
	Additional criteria		
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
	Same taxonomic group as $LC50terr_{min}$?		
2 NOEC	yes no	$NOECterr_{min}$ $NOECterr_{min}$	50 100
3 NOEC	yes no	$NOECterr_{min}$ $NOECterr_{min}$	10 50

$$PNEC_{soil} = \frac{TOXterr}{AFterr} \tag{143}$$

If $TOXterr = PNEC_{soil,ep}$ then $EPterr$ = 'yes'

Input

$LC50terr_i$	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
$PNEC_{water}$	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

Toxicity data for sediment-dwelling organisms will be scarce. At the moment no standardised test methods or assessment factors have been agreed upon. Therefore, only 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.

In contrast with the other PNECs, the PNEC for sediment is an open parameter to allow for expert estimation from available data outside EUSES.

For pesticides, a PNEC for sediment organisms is derived from experimental data. The assessment scheme in Section III.6.3.2 is analogous with the aquatic system. When no experimental data for sediment are provided, no PNEC will be calculated.

$$PNEC_{sed,ep} = \frac{K_{sed\text{-}water}}{RHO_{sed}} \cdot PNEC_{water} \tag{144}$$

$$PNEC_{sed} = PNEC_{sed,ep} \tag{145}$$

EPsed = 'yes'

Input			
$PNEC_{water}$	PNEC for aquatic organisms	$[kg_c.m^{-3}]$	O^c
$K_{sed\text{-}water}$	sediment-water partition coefficient	$[m^3.m^{-3}]$	O^c
RHO_{sed}	bulk density of sediment	$[kg_{wwt}.m^{-3}]$	O^c
$PNEC_{sed,ep}$	PNEC for sediment-dwelling organisms derived by eq. part.	$[kg_c.kg_{wwt}^{-1}]$	O^c
Output			
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

Depending on the toxicity data available for micro-organisms, assessment factors are selected for extrapolating results from toxicity tests to a PNEC for the sewage treatment plant.

Available ecotox. data	**Specific bacterial population? (e.g. nitrifying bacteria or *P. putida*)**	**TOXmicro**	**AFmicro**
$EC50_{micro}$	yes no	$EC50_{micro}$	10 100
$EC10_{micro}$	yes no	$EC10_{micro}$	1 10
$NOEC_{micro}$	yes no	$NOEC_{micro}$	1 10

If more than one toxicity value is given, the lower of the resulting PNECs is used.

$$PNEC_{micro\text{-}organisms} = \frac{TOXmicro}{AFmicro} \tag{146}$$

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. For pesticides, the derivation of NOEC from NOAEL for UC=38/39 should be skipped. A more specific conversion for the selected species of concern is described in Sections III.63.3-III6.3.5. 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.

Available ecotox. data	**Duration of (sub-)chronic test**	**TOXoral**	**AForal**
$LC50_{bird}$ only		$LC50_{bird}$	1000
$NOEC_{bird}$	28 days 90 days chronic	$NOEC_{bird}$	100 30 10
$NOEC_{mammal,food,chr}$	28 days 90 days chronic	$NOEC_{mammal,food,chr}$	100 30 10

If an NOEC for both birds and mammals is given, the lower of the resulting PNECs is used.

$$PNEC_{oral} = \frac{TOXoral}{AForal} \qquad (147)$$

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:

$$NOEC_{bird} = NOAEL_{bird} \cdot CONV_{bird} \tag{148}$$

$$NOEC_{mammal, food,chr} = NOAEL_{mammal,oral,chr} \cdot CONV_{mammal} \tag{149}$$

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

Table III-31 *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	40
Macaca spp.	20
Microtus spp.	8.3
Mus musculus	8.3
Oryctolagus cuniculus	33.3
Rattus norvegicus (> 6 weeks)	20
Rattus norvegicus (≤ 6 weeks)	10
Gallus domesticus	8

III.6.1.6. Statistical extrapolation method

The Aldenberg and Slob (1993) method is used to support the effects assessment performed with assessment factors. The no-effect level calculated here is the 50% confidence limit of the concentration 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 *E* are dependent on the number of NOECs given. At least four NOECs from different taxonomic groups must be present for this calculation (at most, 10 NOECs can be entered in EUSES). In EUSES, it is not checked whether the toxicity data deviate from the assumed log-logistic distribution. The number of NOECs given is usually too small for the test to be able to reject the log-logistic distribution.

$$AVG_{aqua} = mean\left(\log NOECaqua_i\right) \tag{150}$$

$$STD_{aqua} = standard\ deviation\left(\log NOECaqua_i\right) \tag{151}$$

$$PNECstat_{water} = 10^{AVG_{aqua} - E_{aqua} \cdot STD_{aqua}} \tag{152}$$

$$AVG_{terr} = mean\left(\log NOECterr_i\right) \tag{153}$$

$$STD_{terr} = standard\ deviation\left(\log NOECterr_i\right) \tag{154}$$

$$PNECstat_{soil} = 10^{AVG_{terr} - E_{terr} \cdot STD_{terr}} \tag{155}$$

Input			
$NOECaqua_i$	aquatic NOEC values	$[kg_c m^{-3}]$	S
$NOECterr_i$	terrestrial NOEC values	$[kg_c m^{-3}]$	S
AVG_{aqua}	average of all log-transformed aquatic NOECs	[-]	O^c
STD_{aqua}	standard deviation of all log-transformed aquatic NOECs	[-]	O^c
AVG_{terr}	average of all log-transformed terrestrial NOECs	[-]	O^c
STD_{terr}	standard deviation of all log-transformed terrestrial NOECs	[-]	O^c
E_{aqua}	extrapolation constant, dependent on sample size	[-]	D^c
E_{terr}	extrapolation constant, dependent on sample size	[-]	D^c
Output			
$PNECstat_{water}$	PNEC for aquatic organisms with statistical method	$[kg_c.m^{-3}]$	O^c
$PNECstat_{soil}$	PNEC for terrestrial organisms with statistical method	$[kg_c.m^{-3}]$	O^c

The extrapolation constants for the calculation of one-sided left confidence limits for the logarithmic Hazardous Concentration for 5% of the species on the basis of the logistic distribution are given in Table IV-1. The tabulated values of *E* are such that a one-sided confidence limit for the log *PNEC* is given by log *PNEC* = *AVG* - *E* · *STD*. Here *AVG* and *STD* are the mean and standard deviation, respectively, of a sample of log (*NOEC*) test data of size *m*. Constants are tabulated for a 50% confidence limit. This table is taken from Aldenberg and Slob (1993).

Table IV-1 *Extrapolation constants, one-sided left 50% confidence limit for HC5.*

m	**E**
4	1.92
5	1.85
6	1.81
7	1.78
8	1.76
9	1.75
10	1.73
11	1.72
12	1.72
13	1.71
14	1.70
15	1.70
20	1.68
30	1.66
50	1.65
100	1.64
200	1.63
500	1.63
∞	1.62

III.6.2. Effects assessment for humans

III.6.2.1. Route-to-route extrapolation

For human effects assessment, no extrapolation to no-effect level is performed. In this sub-module the toxicological data can be entered and route-to-route extrapolations are performed when necessary.

Table IV-2 *Defaults: bioavailability for different intake routes.*

Parameter	**Symbol**	**Unit**	**Value**
Bioavailability for oral uptake	BIO_{oral}	[-]	1
Bioavailability for dermal uptake	BIO_{der}	[-]	1
Bioavailability for inhalation	BIO_{inh}	[-]	0.75
Body weight of the human considered	BW	[kg]	70
Daily inhalation rate	IH_{air}	$[m^3.d^{-1}]$	20

These are parameters are already defined in the sub-modules on human indirect exposure and consumer exposure.

Oral-to-dermal route

The extrapolation assumes that the dermal value is the same as the oral value on a mg per kg body-weight basis. If oral and dermal absorption rates are known these can be used to adjust the estimation.

$$LD50_{mammal,der} = LD50_{mammal,oral} \cdot \frac{BIO_{oral}}{BIO_{der}} \tag{156}$$

$$NOAEL_{man,der,acute} = NOAEL_{man,oral,acute} \cdot \frac{BIO_{oral}}{BIO_{der}} \tag{157}$$

$$LOAEL_{man,der,acute} = LOAEL_{man,oral,acute} \cdot \frac{BIO_{oral}}{BIO_{der}} \tag{158}$$

$$NOAEL_{mammal,der,chr} = NOAEL_{mammal,oral,chr} \cdot \frac{BIO_{oral}}{BIO_{der}} \tag{159}$$

$$LOAEL_{mammal,der,chr} = LOAEL_{mammal,oral,chr} \cdot \frac{BIO_{oral}}{BIO_{der}} \tag{160}$$

$$NOAEL_{man,der,chr} = NOAEL_{man,oral,chr} \cdot \frac{BIO_{oral}}{BIO_{der}} \tag{160a}$$

$$LOAEL_{man,der,chr} = LOAEL_{man,oral,chr} \cdot \frac{BIO_{oral}}{BIO_{der}} \tag{160b}$$

Input

$LD50_{mammal,oral}$	oral LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$NOAEL_{man,oral,acute}$	oral NOAEL for man after acute exposure	$[kg_c.kg_{bw}^{-1}]$	S
$LOAEL_{man,oral,acute}$	oral LOAEL for man after acute exposure	$[kg_c.kg_{bw}^{-1}]$	S
$NOAEL_{mammal,oral,chr}$	oral NOAEL for mammals exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$LOAEL_{mammal,oral,chr}$	oral LOAEL for mammals exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$NOAEL_{man,oral,chr}$	oral NOAEL for man exposed (sub-)chronically	$[kg_c.kg_{bw}.d^{-1}]$	S
$LOAEL_{man,oral,chr}$	oral LOAEL for man exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
BIO_{oral}	bioavailability for oral uptake	[-]	D
BIO_{der}	bioavailability for dermal uptake	[-]	D

Output

$LD50_{mammal,der}$	dermal LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S/O
$NOAEL_{man,der,acute}$	dermal NOAEL for man after acute exposure	$[kg_c.kg_{bw}^{-1}]$	S/O
$LOAEL_{man,der,acute}$	dermal LOAEL for man after acute exposure	$[kg_c.kg_{bw}^{-1}]$	S/O
$NOAEL_{mammal,der,chr}$	dermal NOAEL for mammals exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$LOAEL_{mammal,der,chr}$	dermal LOAEL for mammals exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$NOAEL_{man,der,chr}$	dermal NOAEL for man exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$LOAEL_{man,der,chr}$	dermal LOAEL for man exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O

Oral-to-inhalatory route

Two methods are available and the user will have to choose between these. When both mammalian and human data are available, the latter are preferred.

1) This method is applicable to the (sub-)chronic N(L)OAEL: the ratio of the inhalatory LC50 to the oral LD50 is used to estimate the inhalatory N(L)OAEL.

$$\boldsymbol{NOAEL}_{\boldsymbol{mammal,inh,chr}} = \frac{\boldsymbol{LC50}_{\boldsymbol{mammal,inh}}}{\boldsymbol{LD50}_{\boldsymbol{mammal,oral}}} \cdot \boldsymbol{NOAEL}_{\boldsymbol{mammal,oral,chr}} \qquad (161)$$

$$\boldsymbol{LOAEL}_{\boldsymbol{mammal,inh.chr}} = \frac{\boldsymbol{LC50}_{\boldsymbol{mammal,inh}}}{\boldsymbol{LD50}_{\boldsymbol{mammal,oral}}} \cdot \boldsymbol{LOAEL}_{\boldsymbol{mammal,oral,chr}} \qquad (162)$$

$$\boldsymbol{NOAEL}_{\boldsymbol{man,inh,chr}} = \frac{\boldsymbol{LC50}_{\boldsymbol{mammal,inh}}}{\boldsymbol{LD50}_{\boldsymbol{mammal,oral}}} \cdot \boldsymbol{NOAEL}_{\boldsymbol{man,oral,chr}} \qquad (163)$$

$$\boldsymbol{LOAEL}_{\boldsymbol{man,inh,chr}} = \frac{\boldsymbol{LC50}_{\boldsymbol{mammal,inh}}}{\boldsymbol{LD50}_{\boldsymbol{mammal,oral}}} \cdot \boldsymbol{LOAEL}_{\boldsymbol{man,oral,chr}} \qquad (164)$$

Input			
$LD50_{mammal,oral}$	oral LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$LC50_{mammal,inh}$	inhalatory LC50 for mammals	$[kg_c.m^{-3}]$	S/O
$NOAEL_{mammal,oral,chr}$	oral NOAEL for mammals exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$LOAEL_{mammal,oral,chr}$	oral LOAEL for mammals exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$NOAEL_{man,oral,chr}$	oral NOAEL for man exposed (sub-)chronically	$[kg_c.kg_{bw}.d^{-1}]$	S
$LOAEL_{man,oral,chr}$	oral LOAEL for man exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
Output			
$NOAEL_{mammal,inh,chr}$	inh. NOAEL for mammals exposed (sub-)chronically	$[kg_c.m^{-3}]$	S/O
$LOAEL_{mammal,inh,chr}$	inh. LOAEL for mammals exposed (sub-)chronically	$[kg_c.m^{-3}]$	S/O
$NOAEL_{man,inh,chr}$	inh. NOAEL for man exposed (sub-)chronically	$[kg_c.m^{-3}]$	S/O
$LOAEL_{man,inh,chr}$	inh. LOAEL for man exposed (sub-)chronically	$[kg_c.m^{-3}]$	S/O

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.

$$LC50_{mammal,inh} = LD50_{mammal,oral} \cdot \frac{BW}{IH_{air}} \cdot \frac{BIO_{oral}}{BIO_{inh}} \tag{165}$$

$$NOAEL_{man,inh,acute} = NOAEL_{man,oral,acute} \cdot \frac{BW}{IH_{air}} \cdot \frac{BIO_{oral}}{BIO_{inh}} \tag{166}$$

$$LOAEL_{man,inh,acute} = LOAEL_{man,oral,acute} \cdot \frac{BW}{IH_{air}} \cdot \frac{BIO_{oral}}{BIO_{inh}} \tag{167}$$

$$NOAEL_{mammal,inh,chr} = NOAEL_{mammal,oral,chr} \cdot \frac{BW}{IH_{air}} \cdot \frac{BIO_{oral}}{BIO_{inh}} \tag{168}$$

$$LOAEL_{mammal,inh,chr} = LOAEL_{mammal,oral,chr} \cdot \frac{BW}{IH_{inh}} \cdot \frac{BIO_{oral}}{BIO_{inh}} \tag{169}$$

$$NOAEL_{man,inh,chr} = NOAEL_{man,oral,chr} \cdot \frac{BW}{IH_{air}} \cdot \frac{BIO_{oral}}{BIO_{inh}} \tag{170}$$

$$LOAEL_{man,inh,chr} = LOAEL_{man,oral,chr} \cdot \frac{BW}{IH_{air}} \cdot \frac{BIO_{oral}}{BIO_{inh}} \tag{171}$$

Input			
$LD50_{mammal,oral}$	oral LD50 for mammals	$[kg_{c}.kg_{bw}^{-1}]$	S
$NOAEL_{man,oral,acute}$	oral NOAEL for man after acute exposure	$[kg_{c}.kg_{bw}^{-1}]$	S
$LOAEL_{man,oral,acute}$	oral LOAEL for man after acute exposure	$[kg_{c}.kg_{bw}^{-1}]$	S
$NOAEL_{mammal,oral,chr}$	oral NOAEL for mammals exposed (sub-)chronically	$[kg_{c}.kg_{bw}^{-1}.d^{-1}]$	S/O
$LOAEL_{mammal,oral,chr}$	oral LOAEL for mammals exposed (sub-)chronically	$[kg_{c}.kg_{bw}^{-1}.d^{-1}]$	S/O
$NOAEL_{man,oral,chr}$	oral NOAEL for man exposed (sub-)chronically	$[kg_{c}.kg_{bw}.d^{-1}]$	S
$LOAEL_{man,oral,chr}$	oral LOAEL for man exposed (sub-)chronically	$[kg_{c}.kg_{bw}^{-1}.d^{-1}]$	S
BIO_{oral}	bioavailability for oral uptake	[-]	D
BIO_{inh}	bioavailability for inhalation	[-]	D
BW	body weight of the human considered	$[kg_{bw}]$	D
IH_{air}	daily inhalation rate	$[m^{3}.d^{-1}]$	D
Output			
$LC50_{mammal,inh}$	inhalatory LC50 for mammals	$[kg_{c}.m^{-3}]$	S/O
$NOAEL_{man,inh,acute}$	inhalatory NOAEL for man after acute exposure	$[kg_{c}.m^{-3}]$	S/O
$LOAEL_{man,inh,acute}$	inhalatory LOAEL for man after acute exposure	$[kg_{c}.m^{-3}]$	S/O
$NOAEL_{mammal,inh,chr}$	inh. NOAEL for mammals exposed (sub-)chronically	$[kg_{c}.m^{-3}]$	S/O
$LOAEL_{mammal,inh,chr}$	inh. LOAEL for mammals exposed (sub-)chronically	$[kg_{c}.m^{-3}]$	S/O
$NOAEL_{man,inh,chr}$	inh. NOAEL for man exposed (sub-)chronically	$[kg_{c}.m^{-3}]$	S/O
$LOAEL_{man,inh,chr}$	inh. LOAEL for man exposed (sub-)chronically	$[kg_{c}.m^{-3}]$	S/O

III.6.2.2. Conversion of N(L)OEC to N(L)OAEL

If NOAEL is absent and NOEC is available:

$$NOAEL_{mammal,oral,chr} = \frac{NOEC_{mammal,\,food,chr}}{CONV_{mammal}} \qquad (173)$$

If LOAEL is absent and LOEC is available:

$$LOAEL_{mammal,oral,chr} = \frac{LOEC_{mammal,\,food,chr}}{CONV_{mammal}} \qquad (174)$$

Input			
$NOEC_{mammal,food,chr}$	NOEC via food for mammals exposed (sub-)chronically	$[kg_c.kg_{food}^{-1}]$	S/O
$LOEC_{mammal,food,chr}$	LOEC via food for mammals exposed (sub-)chronically	$[kg_c.kg_{food}^{-1}]$	S/O
$CONV_{mammal}$	conversion factor NOAEL to NOEC	$[kg_{bw}.d.kg_{food}^{-1}]$	P/S [a]
Output			
$NOAEL_{mammal,oral,chr}$	oral NOAEL for mammals exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$LOAEL_{mammal,oral,chr}$	oral LOAEL for mammals exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O

[a] see table in Section III.6.1.5.

III.6.3. Effects assessment for pesticides and biocides

Section III.6.1.1 must also be used to calculate PNECs for pesticides for the aquatic ecosystem. For pesticides, when measured toxicity data for terrestrial organisms will be available, the equilibrium partioning method will *not* be used for this group of compounds. As a result, Section III.6.3.1 gives a slightly different assessment scheme for pesticides.

For sediment organisms, a PNEC is derived from experimental data. The assessment scheme in Section III.6.3.2 is analogous with the aquatic system. When no experimental data for sediment are provided, no PNEC will be calculated.

In Section III.6.1.5 of EUSES, skip the derivation NOEC from NOAEL for UC=38/39. A more specific conversion for the selected species of concern is described in Sections III.6.3.3-III.6.3.5.

Input terrestrial and sediment-dwelling organisms

$LC50terr_i$	LC50 for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$
$NOECterr_i$	NOEC for terrestrial organisms, trophic level *i*	$[kg_c.kg_{wwt}^{-1}]$
$LC50_{sed}$	LC50 for sediment-dwelling organism	$[kg_c.kg_{wwt}^{-1}]$
$NOEC_{sed}$	NOEC for sediment-dwelling organism	$[kg_c.kg_{wwt}^{-1}]$

Input birds and mammals

-	bird species of concern	[-]
-	mammalian species of concern	[-]
$NOAEL_{bird}$	NOAEL for birds	$[kg_c.kg_{BW}^{-1}.d^{-1}]$
$NOAEL_{mammal, oral}$	NOAEL for mammals	$[kg_c.kg_{BW}^{-1}.d^{-1}]$

Intermediate results terrestrial and sediment-dwelling organisms

TOXterr	toxicological data used for extrapolation of PNEC	$[kg_c.kg_{wwt}^{-1}]$
AFterr	assessment factor applied in extrapolation of PNEC	[-]
TOXsed	toxicological data used for extrapolation of PNEC	$[kg_c.kg_{wwt}^{-1}]$
AFsed	assessment factor applied in extrapolation of PNEC	[-]

Intermediate results birds and mammals

BW_{bird}	Mean bodyweight of bird species of concern	[kg]
BW_{mammal}	Mean bodyweight of mammalian species of concern	[kg]
DFI_{bird}	daily food intake for bird species of concern	$[kg_{food\ dwt}.d^{-1}]$
DFI_{mammal}	daily food intake for mammalian species of concern	$[kg_{food\ dwt}.d^{-1}]$

Output terrestrial and sediment-dwelling organisms

$PNEC_{soil}$	PNEC for terrestrial organisms	$[kg_c.kg_{wwt}^{-1}]$	c
$PNEC_{sed}$	PNEC for sediment-dwelling organisms	$[kg_c.kg_{wwt}^{-1}]$	c

Output birds and mammals

$NOEC_{bird}$	NOEC for birds in food	$[kg_c.kg_{food}^{-1}]$
$NOEC_{mammal,food,chr}$	NOEC for mammals in food	$[kg_c.kg_{food}^{-1}]$

III.6.3.1. Terrestrial compartment

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.

$$LC50\,terr_{min} = min\left(LC50\,terr_i\right) \tag{P-359}$$

$$NOECterr_{min} = min\left(NOECterr_i\right) \tag{P-360}$$

Available ecotox. data		**TOXterr**	**AFterr**
LC50s		$LC50terr_{min}$	1000
1 NOEC		$NOECterr_{min}$	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
	Same taxonomic group as $LC50terr_{min}$?		
2 NOEC*	yes no	$NOECterr_{min}$ $NOECterr_{min}$	50 100
3 NOEC*	yes no	$NOECterr_{min}$ $NOECterr_{min}$	10 50

*NOECs for species of different trophic levels

$$PNEC_{soil} = \frac{TOXterr}{AFterr} \tag{P-361}$$

Input

$LC50terr_i$	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

Output

TOXterr	toxicological data used for extrapolation of PNEC	$[kg_c.kg_{wwt}^{-1}]$	O
AFterr	assessment factor applied in extrapolation of PNEC	[-]	O
$PNEC_{soil}$	PNEC for terrestrial organisms	$[kg_c.kg_{wwt}^{-1}]$	O^c

III.6.3.2. Sediment compartment

For the sediment-dwelling organisms, a PNEC is derived analogous to the aquatic organisms. When no toxicity data are available for sediment organisms, no PNEC can be calculated. Only one LC50 and NOEC can be entered, when more data are available, the lowest may be used and the assessment factor modified on a case-by-case basis.

Available data	**Additional criteria**	**TOXsed**	**AFsed**
LC50		$LC50_{sed}$	1000
NOEC		$NOEC_{sed}$	100
NOEC and LC50	$LC50_{sed}/1000 < NOEC_{sed}/100$ $LC50_{sed}/1000 \geq NOECaqua_{sed}/100$	$LC50_{sed}$ $NOEC_{sed}$	1000 100

$$PNEC_{sed} = \frac{TOXsed}{AFsed} \tag{P-362}$$

Input

$LC50_{sed}$	LC50 for sediment-dwelling organism	$[kg_c.kg_{wwt}^{-1}]$	S
$NOEC_{sed}$	NOEC for sediment-dwelling organism	$[kg_c.kg_{wwt}^{-1}]$	S

Output

TOXsed	toxicological data used for extrapolation of PNEC	$[kg_c.kg_{wwt}^{-1}]$	O
AFsed	assessment factor applied in extrapolation of PNEC	[-]	O
$PNEC_{sed}$	PNEC for sediment-dwelling organisms	$[kg_c.kg_{wwt}^{-1}]$	O^c

III.6.3.3. Bodyweight of birds and mammals

If the bodyweight is not given in the data set, the user can choose between some species in the table.

Input

Table D-7 *Bodyweight of birds and mammals*

Species	**Range in body weight (g)**	**Mean body weight (g)**
Birds:		
Default	-	10
Quail	-	102
Common Partridge	-	375
Common Pheasant	-	1200
Turtle Dove	-	152
Collared Dove	-	195
Woodpigeon	-	440
Chaffinch	-	22
Goldfinch	-	15
Common Redpoll	-	14
House Sparrow	-	25
Mammals:		
Default	-	6
Hedgehog	400-1000	700
Mole	65-135	100
Woodshrew	6-13	9.5
Hare	2500-6500	4500
Rabbit	1300-2500	1900
Fieldmouse	14-40	27
Woodmouse	14-35	24.5
Brown rat	240-500	370
Badger	7500-15000	11250

-	bird species of concern	[-]	P
-	mammalian species of concern	[-]	P

Output

BW_{bird}	Mean bodyweight of bird species of concern	[kg]	S/O
BW_{mammal}	Mean bodyweight of mammalian species of concern	[kg]	S/O

III.6.3.4. Daily food intake for birds and mammals

If the daily food intake (DFI) is not given in the data set, it can be estimated. The DFI of birds and mammals is strongly correlated to the body weight (BW). Nagy (1987) has derived the relationships presented here based on dry weight.

All birds (default)

$$\log(DFI_{bird} \cdot 1000) = -0.188 + 0.651 \cdot \log(BW_{bird} \cdot 1000) \tag{P-363}$$

Passerines

$$\log(DFI_{bird} \cdot 1000) = -0.4 + 0.85 \cdot \log(BW_{bird} \cdot 1000) \tag{P-364}$$

Non passerines

$$\log(DFI_{bird} \cdot 1000) = -0.521 + 0.751 \cdot \log(BW_{bird} \cdot 1000) \tag{P-365}$$

All mammals (default)

$$\log(DFI_{mammal} \cdot 1000) = -0.629 + 0.822 \cdot \log(BW_{mammal} \cdot 1000) \tag{P-366}$$

Input			
BW_{bird}	mean bodyweight of bird species of concern	[kg]	S/O
BW_{mammal}	mean bodyweight of mammalian species of concern	[kg]	S/O
Output			
DFI_{bird}	daily food intake for bird species of concern	$[kg_{food\ dwt} \cdot d^{-1}]$	S/O
DFI_{mammal}	daily food intake for mammalian species of concern	$[kg_{food\ dwt} \cdot d^{-1}]$	S/O

III.6.3.5. Derivation of the NOEC from NOAEL

If only a NOAEL is given in the input, a NOEC can be converted using the daily food intake and the bodyweight.

$$NOEC_{bird} = \frac{NOAEL_{bird} \cdot BW_{bird}}{DFI_{bird}} \tag{P-367}$$

$$NOEC_{mammal,\,food,chr} = \frac{NOAEL_{mammal,oral,chr} \cdot BW_{mammal}}{DFI_{mammal}} \tag{P-368}$$

Input			
$NOAEL_{bird}$	NOAEL for birds	$[kg_c.kg_{BW}^{-1}.d^{-1}]$	S
$NOAEL_{mammal,\ oral}$	NOAEL for mammals	$[kg_c.kg_{BW}^{-1}.d^{-1}]$	S
BW_{bird}	mean bodyweight of bird species of concern	[kg]	S/O
BW_{mammal}	mean bodyweight of mammalian species of concern	[kg]	S/O
DFI_{bird}	daily food intake for bird species of concern	$[kg_{food\ dwt}.d^{-1}]$	S/O
DFI_{mammal}	daily food intake for mammalian species of concern	$[kg_{food\ dwt}.d^{-1}]$	S/O
Output			
$NOEC_{bird}$	NOEC for birds in food	$[kg_c.kg_{food}^{-1}]$	O
$NOEC_{mammal,food,chr}$	NOEC for mammals in food	$[kg_c.kg_{food}^{-1}]$	O

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, while for the human end-points this is the so-called Margin Of Safety (MOS). 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.

For pesticides also specific RCRs will be calculated. These ratios will be based on the non-extrapolated toxicity data as given in the input data set.

III.7.1. Risk characterisation for the environment

Input			
$PEClocal_{water}$	local PEC in surface water during emission episode	$[kg_c.m^{-3}]$	
$PECreg_{water}$	regional steady-state PEC in surface water	$[kg_c.m^{-3}]$	
$PNEC_{water}$	PNEC for the 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	$[kg_c.kg_{wwt}^{-1}]$	
$PECreg_{sed}$	regional steady-state PEC in sediment	$[kg_c.kg_{wwt}^{-1}]$	
$PNEC_{sed}$	PNEC for the sediment compartment	$[kg_c.kg_{wwt}^{-1}]$	
EPsed	equilibrium partitioning used for PNEC for sediment?	[yes/no]	c
PEC_{stp}	local PEC in STP during emission episode	$[kg_c.m^{-3}]$	
$PNEC_{micro-organisms}$	PNEC for STP micro-organisms	$[kg_c.m^{-3}]$	c
$PEC_{oral,fish}$	PEC in fish (local and regional combined)	$[kg_c.kg_{wwt}^{-1}]$	
$PEC_{oral,worm}$	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
Output			
$RCRlocal_{water}$	RCR for the local water compartment	[-]	c
$RCRreg_{water}$	RCR for the regional 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
$RCRreg_{sed}$	RCR for the regional sediment compartment	[-]	c
RCR_{stp}	RCR for the sewage treatment plant	[-]	c
$RCR_{oral,fish}$	RCR for fish-eating birds and mammals	[-]	c
$RCR_{oral,worm}$	RCR for worm-eating birds and mammals	[-]	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 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.

$$RCRlocal_{water} = \frac{PEClocal_{water}}{PNEC_{water}} \tag{175}$$

$$RCRreg_{water} = \frac{PECreg_{water}}{PNEC_{water}} \tag{176}$$

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
$PNEC_{water}$	PNEC for 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

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 in soil is increased by a factor of 10 to account for uptake via ingestion of soil.

If *EPterr* = yes and log *Kow* > 5 then

$$PEClocal_{soil} = PEClocal_{soil} \cdot 10 \tag{177}$$

If *EPterr* = yes and log *Kow* > 5 then

$$PECreg_{agric} = PECreg_{agric} \cdot 10 \tag{178}$$

$$RCRlocal_{soil} = \frac{PEClocal_{soil}}{PNEC_{soil}} \tag{179}$$

$$RCRreg_{soil} = \frac{PECreg_{agric}}{PNEC_{soil}} \tag{180}$$

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 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 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).

If *EPsed* = yes and log *Kow* > 5 then

$$PEClocal_{sed} = PEClocal_{sed} \cdot 10 \tag{181}$$

If *EPsed* = yes and log *Kow* > 5 then

$$PECreg_{sed} = PECreg_{sed} \cdot 10 \tag{182}$$

$$RCRlocal_{sed} = \frac{PEClocal_{sed}}{PNEC_{sed}} \tag{183}$$

$$RCRreg_{sed} = \frac{PECreg_{sed}}{PNEC_{sed}} \tag{184}$$

Input			
$PEClocal_{sed}$	local PEC in sediment	$[kg_c.kg_{wwt}^{-1}]$	O
$PECreg_{sed}$	regional steady-state PEC in sediment	$[kg_c.kg_{wwt}^{-1}]$	O
$PNEC_{sed}$	PNEC for the sediment compartment	$[kg_c.kg_{wwt}^{-1}]$	O
EPsed	equilibrium partitioning used for PNEC for 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
$RCRreg_{sed}$	RCR for regional 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.

$$\boldsymbol{RCR_{stp} = \frac{PEC_{stp}}{PNEC_{micro\text{-}organisms}}} \qquad (185)$$

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. Fish-eating predators

The concentration of the chemical in fish is compared to the no-effect concentration for birds and mammals. There is only one concentration in fish 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.

$$\boldsymbol{RCR_{oral,fish} = \frac{PEC_{oral,fish}}{PNEC_{oral}}} \qquad (186)$$

Input			
$PEC_{oral,fish}$	PEC in fish (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 and mammals	[-]	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.

$$\boldsymbol{RCR_{oral,fish} = \frac{PEC_{oral,fish}}{PNEC_{oral}}} \qquad (187)$$

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

III.7.2.1. Risk characterisation for humans exposed via the environment

The total daily intake of a substance in food, drinking water and air is compared to the No- or Lowest-Observed-Adverse-Effect Level N(L)OAEL, resulting in 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 (sub-)chronic N(L)OAEL for the inhalation route.

Depending on the available data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$RCRlocal_{man\text{-}env,tot}$	$DOSElocal_{tot}$	$NOAEL_{mammal,oral,chr}$ $LOAEL_{mammal,oral,chr}$ $NOAEL_{man,oral,chr}$ $LOAEL_{man,oral,chr}$
$RCRreg_{man\text{-}env,tot}$	$DOSEreg_{tot}$	$NOAEL_{mammal,oral,chr}$ $LOAEL_{mammal,oral,chr}$ $NOAEL_{man,oral,chr}$ $LOAEL_{man,oral,chr}$
$RCRlocal_{man\text{-}env,inh}$	$PEClocal_{air,ann}$	$NOAEL_{mammal,inh,chr}$ $LOAEL_{mammal,inh,chr}$ $NOAEL_{man,inh,chr}$ $LOAEL_{man,inh,chr}$
$RCRreg_{man\text{-}env,inh}$	$PECreg_{air}$	$NOAEL_{mammal,inh,chr}$ $LOAEL_{mammal,inh,chr}$ $NOAEL_{man,inh,chr}$ $LOAEL_{man,inh,chr}$

Input			
$N(L)OAEL_{mammal,oral,chr}$	oral N(L)OAEL for mammals exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$N(L)OAEL_{man,oral,chr}$	oral N(L)OAEL for man exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$N(L)OAEL_{mammal,inh,chr}$	inh. N(L)OAEL for mammals exposed (sub-)chronically	$[kg_c.m^{-3}]$	S/O
$N(L)OAEL_{man,inh,chr}$	inh. N(L)OAEL for man exposed (sub-)chronically	$[kg_c.m^{-3}]$	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
Output			
$RCRlocal_{man\text{-}env,tot}$	MOS local, total exposure via all media	[-]	O^c
$RCRlocal_{man\text{-}env,inh}$	MOS local, exposure via air	[-]	O^c
$RCRreg_{man\text{-}env,tot}$	MOS regional, total exposure via all media	[-]	O^c
$RCRreg_{man\text{-}env.inh}$	MOS regional, exposure via air	[-]	O^c

III.7.2.2. Risk characterisation for consumers

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 II.6.2.2 for decision rules on the choice of the effect parameter in the risk characterisation for human health.

Inhalation exposure

Depending on the time scale and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$RCRacute_{cons,inh}$	C_{inh}	$LC50_{mammal,inh}$ $NOAEL_{man,inh,acute}$ $LOAEL_{man,inh,acute}$
$RCRchronic_{cons,inh}$	$C_{inh,ann}$	$NOAEL_{mammal,inh,chr}$ $LOAEL_{mammal,inh,chr}$ $NOAEL_{man,inh,chr}$ $LOAEL_{man,inh,chr}$

Input			
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]	S
$LC50_{mammal,inh}$	inhalatory LC50 for mammals	$[kg_c.m^{-3}]$	S/O
$NOAEL_{man,inh,acute}$	inhalatory NOAEL for man after acute exposure	$[kg_c.m^{-3}]$	S/O
$LOAEL_{man,inh,acute}$	inhalatory LOAEL for man after acute exposure	$[kg_c.m^{-3}]$	S/O
$NOAEL_{mammal,inh,chr}$	inh. NOAEL for mammal exposed (sub-)chronically	$[kg_c.m^{-3}]$	S/O
$LOAEL_{mammal,inh,chr}$	inh. LOAEL for mammal exposed (sub-)chronically	$[kg_c.m^{-3}]$	S/O
$NOAEL_{man,inh,chr}$	inh. NOAEL for man exposed (sub-)chronically	$[kg_c.m^{-3}]$	S/O
$LOAEL_{man,inh,chr}$	inh. LOAEL for man exposed (sub-)chronically	$[kg_c.m^{-3}]$	S/O
C_{inh}	concentration in air of room	$[kg_c.m^{-3}]$	O
$C_{inh,ann}$	annual average inhalation exposure concentration	$[kg_c.m^{-3}]$	O
Output			
$RCRacute_{cons,inh}$	MOS acute, exposed by inhalation	[-]	O^c
$RCRchronic_{cons,inh}$	MOS chronic, exposed by inhalation	[-]	O^c

Dermal exposure

Depending on the time scale and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$RCRacute_{cons,der}$	$U_{der,pot}$	$LD50_{mammal,der}$ $NOAEL_{man,der,acute}$ $LOAEL_{man,der,acute}$
	C_{der}	$NOEC_{man,medium,acute}$ $LOEC_{man,medium,acute}$
$RCRchronic_{cons,der}$	$U_{der,pot}$	$NOAEL_{mammal,der,chr}$ $LOAEL_{mammal,der,chr}$ $NOAEL_{man,der,chr}$ $LOAEL_{man,der,chr}$
	$C_{der,ann}$	$NOEC_{man,medium,chr}$ $LOEC_{man,medium,chr}$

Input

TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]	S
$LD50_{mammal,der}$	dermal LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S/O
$NOAEL_{man,der,acute}$	dermal NOAEL for man after acute exposure	$[kg_c.kg_{bw}^{-1}]$	S/O
$LOAEL_{man,der,acute}$	dermal LOAEL for man after acute exposure	$[kg_c.kg_{bw}^{-1}]$	S/O
$NOEC_{man,medium,acute}$	dermal NOEC in a medium for man after acute exposure	$[kg_c.m^{-3}]$	S
$LOEC_{man,medium,acute}$	dermal LOEC in a medium for man after acute exposure	$[kg_c.m^{-3}]$	S
$NOAEL_{mammal,der,chr}$	dermal NOAEL for mammal exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$LOAEL_{mammal,der,chr}$	dermal LOAEL for mammal exposed (sub-)chronically	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$NOAEL_{man,der,chr}$	dermal NOAEL for man exposed (sub-)chronic.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$LOAEL_{man,der,chr}$	dermal LOAEL for man exposed (sub-)chronic.	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$NOEC_{man,medium,chr}$	dermal NOEC in a medium for man exposed (sub-)chronic.	$[kg_c.m^{-3}]$	S
$LOEC_{man,medium,chr}$	dermal LOEC in a medium for man exposed (sub-)chronic.	$[kg_c.m^{-3}]$	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

Output

$RCRacute_{cons,der}$	MOS acute, exposed dermally	[-]	O^c
$RCRchronic_{cons,der}$	MOS chronic, exposed dermally	[-]	O^c

Oral exposure

Depending on the time scale and available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$RCRacute_{cons,oral}$	I_{oral}	$LD50_{mammal,oral}$ $DD_{mammal,oral}$ $NOAEL_{man,oral,acute}$ $LOAEL_{man,oral,acute}$
$RCRchronic_{cons,oral}$	I_{oral}	$NOAEL_{mammal,oral,chr}$ $LOAEL_{mammal,oral,chr}$ $NOAEL_{man,oral,chr}$ $LOAEL_{man,oral,chr}$
	$C_{oral,ann}$ / RHO_{prod}	$NOEC_{mammal,food,chr}$ $LOEC_{mammal,food,chr}$

Input			
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]	S
$LD50_{mammal,oral}$	oral LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$DD_{mammal,oral}$	oral Discriminating Dose for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$NOAEL_{man,oral,acute}$	oral NOAEL for man after acute exposure	$[kg_c.kg_{bw}^{-1}]$	S
$LOAEL_{man,oral,acute}$	oral LOAEL for man after acute exposure	$[kg_c.kg_{bw}^{-1}]$	S
$NOAEL_{mammal,oral,chr}$	oral NOAEL for mammals after chronic exposure	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$LOAEL_{mammal,oral,chr}$	oral LOAEL for mammals after chronic exposure	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$NOAEL_{man,oral,chr}$	oral NOAEL for man after chronic exposure	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$LOAEL_{man,oral,chr}$	oral LOAEL for man after chronic exposure	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$NOEC_{mammal,food,chr}$	NOEC via food for mammals exposed (sub-)chronically	$[kg_c.kg_{food}^{-1}]$	S/O
$LOEC_{mammal,food,chr}$	LOEC via food for mammals exposed (sub-)chronically	$[kg_c.kg_{food}^{-1}]$	S/O
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	$[kg_c.m^{-3}]$	O
Output			
$RCRacute_{cons,oral}$	MOS acute, exposed orally	[-]	O^c
$RCRchronic_{cons,inh}$	MOS chronic, exposed by inhalation	[-]	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**
$RCRacute_{cons,tot}$	U_{tot} / BIO_{oral}	$LD50_{mammal,oral}$ $DD_{mammal,oral}$ $NOAEL_{man,oral,acute}$ $LOAEL_{man,oral,acute}$
$RCRchronic_{cons,tot}$	U_{tot} / BIO_{oral}	$NOAEL_{mammal,oral,chr}$ $LOAEL_{mammal,oral,chr}$ $NOAEL_{man,oral,chr}$ $LOAEL_{man,oral,chr}$

Input			
TIMESCALE	time scale of exposure: acute or (sub-)chronic	[acute/chronic]	S
$LD50_{mammal,oral}$	oral LD50 for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$DD_{mammal,oral}$	oral Discriminating Dose for mammals	$[kg_c.kg_{bw}^{-1}]$	S
$NOAEL_{man,oral,acute}$	oral NOAEL for man after acute exposure	$[kg_c.kg_{bw}^{-1}]$	S
$LOAEL_{man,oral,acute}$	oral LOAEL for man after acute exposure	$[kg_c.kg_{bw}^{-1}]$	S
$NOAEL_{mammal,oral,chr}$	oral NOAEL for mammals after chronic exposure	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$LOAEL_{mammal,oral,chr}$	oral LOAEL for mammals after chronic exposure	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S/O
$NOAEL_{man,oral,chr}$	oral NOAEL for man after chronic exposure	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
$LOAEL_{man,oral,chr}$	oral LOAEL for man after chronic exposure	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	S
BIO_{oral}	bioavailability for oral uptake	[-]	D
U_{tot}	total uptake for one product via different routes	$[kg_c.kg_{bw}^{-1}.d^{-1}]$	O
Output			
$RCRacute_{cons,tot}$	MOS acute, total exposure	[-]	O^c
$RCRchronic_{cons,tot}$	MOS chronic, total exposure	[-]	O^c

III.7.2.3. Risk characterisation for workers

Inhalation exposure

Depending on the available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$RCR_{worker,inh,vapour}$	$C_{inh,worker,vapour}$	$NOAEL_{mammal,inh,chr}$ $LOAEL_{mammal,inh,chr}$ $NOAEL_{man,inh,chr}$ $LOAEL_{man,inh,chr}$
$RCR_{worker,inh,fibre}$	$C_{inh,worker,fibre}$	$NOAEL_{mammal,inh,fibre,chr}$ $LOAEL_{mammal,inh,fibre,chr}$ $NOAEL_{man,inh,fibre,chr}$ $LOAEL_{man,inh,fibre,chr}$
$RCR_{worker,inh,dust}$	$C_{inh,worker,dust}$	$NOAEL_{mammal,inh,chr}$ $LOAEL_{mammal,inh,chr}$ $NOAEL_{man,inh,chr}$ $LOAEL_{man,inh,chr}$

Input			
$NOAEL_{mammal,inh,chr}$	inh. NOAEL for mammals exposed (sub-)chronically	[kg.m^{-3}]	S/O
$LOAEL_{mammal,inh,chr}$	inh. LOAEL for mammals exposed (sub-)chronically	[kg.m^{-3}]	S/O
$NOAEL_{man,inh,chr}$	inh. NOAEL for man exposed (sub-)chronically	[kg.m^{-3}]	S/O
$LOAEL_{man,inh,chr}$	inh. LOAEL for man exposed (sub-)chronically	[kg.m^{-3}]	S/O
$NOAEL_{mammal,inh,fibre,chr}$	inh. NOAEL for mammals exposed to fibers (sub-)chr.	[fibers.m^{-3}]	S
$LOAEL_{mammal,inh,fibre,chr}$	inh. LOAEL for mammals exposed to fibers (sub-)chr.	[fibers.m^{-3}]	S
$NOAEL_{man,inh,fibre,chr}$	inh. NOAEL for man exposed to fibers (sub-)chr.	[fibers.m^{-3}]	S
$LOAEL_{man,inh,fibre,chr}$	inh. LOAEL for man exposed to fibers (sub-)chr.	[fibers.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
Output			
$RCR_{worker,inh,vapour}$	MOS for worker exposed by inhalation of vapour	[-]	O^{c}
$RCR_{worker,inh,fibre}$	MOS for worker exposed inhalation of fibers	[-]	O^{c}
$RCR_{worker,inh,dust}$	MOS for worker exposed inhalation of dust	[-]	O^{c}

Dermal exposure

Depending on the available effects data the following RCRs are possible:

Effects / Exposure	**Exposure**	**Available effects data**
$RCR_{worker,der}$	$U_{der,pot,worker}$	$NOAEL_{mammal,der,chr}$ $LOAEL_{mammal,der,chr}$ $NOAEL_{man,der,chr}$ $LOAEL_{man,der,chr}$
	$W_{der,worker} / (TH_{der,worker} \cdot n_{worker})$	$NOEC_{man,medium,chr}$ $LOEC_{man,medium,chr}$

Input

$NOAEL_{mammal,der,chr}$	dermal NOAEL for mammals exposed (sub-)chronically	$[kg.kg_{bw}^{-1}.d^{-1}]$	S/O
$LOAEL_{mammal,der,chr}$	dermal LOAEL for mammals exposed (sub-)chronically	$[kg.kg_{bw}^{-1}.d^{-1}]$	S/O
$NOAEL_{man,der,chr}$	dermal NOAEL for man exposed (sub-)chronically	$[kg.kg_{bw}^{-1}.d^{-1}]$	S/O
$LOAEL_{man,der,chr}$	dermal LOAEL for man exposed (sub-)chronically	$[kg.kg_{bw}^{-1}.d^{-1}]$	S/O
$NOEC_{man,medium,chr}$	dermal NOEC in a medium for man exposed (sub-)chr.	$[kg.m^{-3}]$	S
$LOEC_{man,medium,chr}$	dermal LOEC in a medium for man exposed (sub-)chr.	$[kg.m^{-3}]$	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

Output

$RCR_{worker,der}$	MOS for worker exposed dermally	[-]	O^{c}

III.7.3. Risk characterisation for specific species due to pesticide application (UC=38/39)

Apart from the risk characterisation ratios mentioned in the previous sections, for pesticides also specific RCRs will be calculated. These ratios will be based on the non-extrapolated toxicity data as given in the input data set.

Input		
BW_{bird}	mean bodyweight of bird species of concern	[kg]
BW_{mammal}	mean bodyweight of mammalian species of concern	[kg]
Input concentrations		
$Cwater_{pest\text{-}T}$	mean concentration in water over T days, $T \in \{0,4,7,21,28\}$	[$kg_c.m_{water}^{-3}$]
$Csoil_{pest\text{-}T}$	mean concentration in soil over T days, $T \in \{0,28\}$	[$kg_c.kg_{soil}^{-1}$]
$Csoil_{pest\text{-}lt}$	concentration in soil after (N_{lt} + 2) years	[$kg_c.kg_{wwt}^{-1}$]
$Csed_{pest\text{-}T}$	mean concentration in sediment over T days, $T \in \{7,28\}$	[$kg_c.kg_{wwt}^{-1}$]
$Csed_{pest\text{-}lt}$	concentration after (N_{lt} + 2) years of applications	[$kg_c.kg_{wwt}^{-1}$]
$C_{worm\text{-}Tbird}$	mean concentration in earthworms over T_{bird} days	[$kg_c.kg_{wet\ worm}^{-1}$]
$C_{worm\text{-}Tmammal}$	mean concentration in earthworms over T_{mammal} days	[$kg_c.kg_{wet\ worm}^{-1}$]
$C_{fish\text{-}Tbird}$	mean concentration in fish over T_{bird} days	[$kg_c.kg_{wet\ fish}^{-1}$]
$C_{fish\text{-}Tmammal}$	mean concentration in fish over T_{mammal} days	[$kg_c.kg_{wet\ fish}^{-1}$]
$Clocal_{air}$	local concentration in air during episode	[$kg_c.m^{-3}$]

Toxicity data birds/mammals

$LD50_{bird}$	LD50 for birds	$[\mathrm{kg_c.kg_{BW}^{-1}}]$	
$LC50_{bird}$	LC50 in food for birds	$[\mathrm{kg_c.kg_{food}^{-1}}]$	
$NOEC_{bird}$	NOEC in food for birds	$[\mathrm{kg_c.kg_{food}^{-1}}]$	
$LD50_{mammal,\ oral}$	LD50 for mammals	$[\mathrm{kg_c.kg_{BW}^{-1}}]$	
$NOEC_{mammal,food,chr}$	NOEC in food for mammals	$[\mathrm{kg_c.kg_{food}^{-1}}]$	
$LC50_{mammal,inh}$	inhalatory LC50 for mammals	$[\mathrm{kg_c.m^{-3}}]$	

Toxicity data terrestrial

$LC50_{worm}$	LC50 for earthworms	$[\mathrm{kg_c.kg_{soil}^{-1}}]$	
$NOEC_{worm}$	NOEC for earthworms	$[\mathrm{kg_c.kg_{soil}^{-1}}]$	
$EC50_{nitr}$	EC50 for nitrificating bacteria in soil	$[\mathrm{kg_c.kg_{soil}^{-1}}]$	
$PNEC_{soil}$	PNEC for terrestrial organisms	$[\mathrm{kg_c.kg_{wwt}^{-1}}]$	c

Toxicity data aquatic

$LC50_{fish}$	LC50 for fish	$[\mathrm{kg_c.m^{-3}}]$	
$NOEC_{fish}$	NOEC for fish	$[\mathrm{kg_c.m^{-3}}]$	
$LC50_{crus}$	LC50 for crustaceans	$[\mathrm{kg_c.m^{-3}}]$	
$NOEC_{crus}$	NOEC for crustaceans	$[\mathrm{kg_c.m^{-3}}]$	
$LC50_{algae}$	EC50 for algae	$[\mathrm{kg_c.m^{-3}}]$	
$NOEC_{algae}$	NOEC for algae	$[\mathrm{kg_c.m^{-3}}]$	
$PNEC_{water}$	PNEC for aquatic organisms	$[\mathrm{kg_c.m^{-3}}]$	c

Toxicity data sediment

$LC50_{sed}$	LC50 for sediment-dwelling organisms	$[\mathrm{kg_c.kg^{-1}}]$	
$NOEC_{sed}$	NOEC for sediment-dwelling organisms	$[\mathrm{kg_c.kg^{-1}}]$	
$PNEC_{sed}$	PNEC for sediment-dwelling organisms	$[\mathrm{kg_c.kg_{wwt}^{-1}}]$	c

Specific inputs sprays and particles

DFI_{bird}	daily food intake for bird species of concern	$[\mathrm{kg_{food\ dwt}.d^{-1}}]$
DFI_{mammal}	daily food intake for mammalian species of concern	$[\mathrm{kg_{food\ dwt}.d^{-1}}]$
$DOSE_{pest}$	dosage	$[\mathrm{kg_c.m^{-2}}]$

Specific inputs sprays only

C_{spray}	concentration in spray water on leaves and crops	$[\mathrm{kg_c.m^{-3}}]$
$Cfood_{x}$	initial concentration in food for *x*	$[\mathrm{kg_c.kg_{food}^{-1}}]$
$Cfood_{x\text{-}5}$	mean concentration in food for *x* over 5 days	$[\mathrm{kg_c.kg_{food}^{-1}}]$
$Cfood_{Tx}$	mean conc. in food over toxicity test duration of *x*	$[\mathrm{kg_c.kg_{food}^{-1}}]$
	$x \in \{bird,mammal\}$	
RHO_{water}	density of water phase	$[\mathrm{kg.m^{-3}}]$
$LD50_{bee}$	lethal dose for 50% of the bees	$[\mathrm{\mu g.bee^{-1}}]$

Specific inputs particles only

$C_{particle}$	concentration of pesticide in granules or treated seeds	$[\mathrm{kg_c.kg_{particle}^{-1}}]$
MIX	mixing with soil	[yes/no]
$W_{particle}$	weight of one granule or treated seed	$[\mathrm{kg_{particle}.particle^{-1}}]$

Output terrestrial			
RCR_{worm-0}	short term RCR for earthworms (PEC/LC50)	[-]	c
$RCR_{worm-28}$	long term RCR for earthworms (PEC/NOEC)	[-]	c
RCR_{nitr-0}	short term RCR for nitrif. bacteria (PEC/EC50)	[-]	c
$RCRworm_{Tbird}$	RCR for worm-eating birds (PEC/NOEC)	[-]	c
$RCRworm_{Tmammal}$	RCR for worm-eating mammals (PEC/NOEC)	[-]	c
RCR_{soil}	RCR for the terrestrial ecosystem	[-]	c
$RCR_{soil-lt}$	RCR for soil after (N_{lt} + 2) years of applications	[-]	c
Output aquatic			
RCR_{fish-4}	short term RCR for fish (PEC/LC50)	[-]	c
$RCR_{fish-28}$	long term RCR for fish (PEC/NOEC)	[-]	c
RCR_{crus-4}	short term RCR for crustaceans (PEC/LC50)	[-]	c
$RCR_{crus-21}$	long term RCR for crustaceans (PEC/NOEC)	[-]	c
$RCR_{algae-4a}$	short term RCR for algae (PEC/EC50)	[-]	c
$RCR_{algae-4b}$	long term RCR for algae (PEC/NOEC)	[-]	c
RCR_{water}	RCR for the aquatic ecosystem	[-]	c
$RCRfish_{bird}$	RCR for fish eating birds (PEC/NOEC)	[-]	c
$RCRfish_{mammal}$	RCR for fish eating mammal (PEC/NOEC)	[-]	c
Output sediment			
RCR_{sed-7}	short term RCR for sediment organisms (PEC/LC50)	[-]	c
RCR_{sed-28}	long term RCR for sediment organisms (PEC/NOEC)	[-]	c
RCR_{sed}	RCR for the sediment ecosystem	[-]	c
RCR_{sed-lt}	RCR for sediment after (N_{lt} + 2) years of applications	[-]	c
Output air			
$RCR_{mammal,inh}$	inhalatory RCR for mammal	[-]	c
Output sprays only			
RCR_{bee}	risk characterisation quotient for bees	$[(g_c.ha^{-1})/(\mu g.bee^{-1})]$	c
$RCRfood_{bird-1}$	RCR for single dose toxicity to birds (PED/LD50)	[-]	c
$RCRfood_{bird-5}$	RCR for acute toxicity to birds (PEC/LC50)	[-]	c
$RCRfood_{Tbird}$	RCR for chronic toxicity to birds (PEC/NOEC)	[-]	c
$RCRfood_{mammal-1}$	RCR for single dose toxicity to mammals (PED/LD50)	[-]	c
$RCRfood_{Tmammal}$	RCR for chronic toxicity to mammals (PEC/NOEC)	[-]	c
$RCRspray_{bird}$	acute RCR for birds, spray water (PEC/LD50)	[-]	c
$RCRsurf_{bird}$	acute RCR for birds, surface water (PEC/LD50)	[-]	c
$RCRsurf_{bird,semi}$	semi-chronic RCR for birds, surface water (PEC/LC50)	[-]	c
$RCRspray_{mammal}$	acute RCR for mammals, spray water (PEC/LD50)	[-]	c
$RCRsurf_{mammal}$	acute RCR for mammals, surface water (PEC/LD50)	[-]	c
Output particles only			
$RCRparticle_{bird}$	RCR for acute toxicity to mammals if granules or seeds are the sole food source (PEC/LC50)	[-]	c
$RCRparticle_{mammal}$	RCR for acute toxicity to birds if granules or seeds are the sole food source (PEC/LC50)	[-]	c
$RCRitem_{bird}$	RCR for items resembling natural food	$[m^{-2}]$	c
$RCRitem_{mammal}$	RCR for items resembling natural food	$[m^{-2}]$	c
Input (bats, scenario timber treatment)			
$DOSE_{wood}$	dosage of a.i. per m^2 wood	$[kg_c.m^{-2}]$	
$LD50_{mammal, oral}$	LD50 for mammals	$[kg_c.kg_{BW}^{-1}]$	
Output			
RCR_{bat}	Relative Toxicity Index (RTI)	$[kg_{BW}.m^{-2}]$	c

III.7.3.1. Filling of the required exposure parameters

The risk characterisation for pesticides departs from the concentrations in the application soil or the ditch surrounding it, averaged over the duration of the toxicity tests ($Csoil_{pest\text{-}T}$ and $Cwater_{pest\text{-}T}$). If these parameters are not specified, they will be filled from the available data.

In case the substance is applied as particles, only an annual average concentration in water will be known (through drainage). This concentration will then be used in the calculation of $C_{fish\text{-}Tx}$ above. If the $Cwater_{pest\text{-}T}$ are not specified:

$$Cwater_{pest\text{-}T} = Cwater_{pest\text{-}365} \quad for\ T \in \{0,4,14,21,28\} \tag{P-369}$$

If $Cwater_{pest\text{-}365}$ is also not specified, use results from the local distribution module:

$$Cwater_{pest\text{-}T} = Clocal_{water} \quad for\ T \in \{0,4\} \tag{P-370}$$

$$Cwater_{pest\text{-}T} = Clocal_{water,ann} \quad for\ T \in \{14,21,28\} \tag{P-371}$$

Input			
$Cwater_{pest\text{-}365}$	mean concentration in water over 365 days	$[kg_c.m_{water}^{-3}]$	O
$Clocal_{water}$	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
Output			
$Cwater_{pest\text{-}0}$	peak concentration in water (dissolved)	$[kg_c.m^{-3}]$	O
$Cwater_{pest\text{-}T}$	mean concentration in water over T days, $T \in \{4,14,21,28\}$	$[kg_c.m_{water}^{-3}]$	O

If the $Csoil_{pest\text{-}T}$ are not specified:

$$\boldsymbol{Csoil_{pest\text{-}0} = Clocal10_{soil}} \tag{P-372}$$

$$\boldsymbol{Csoil_{pest\text{-}28} = Clocal_{soil}} \tag{P-373}$$

Input

$Clocal10_{soil}$	initial concentration in soil in 10th year	$[kg_c.kg_{soil}^{-1}]$	O
$Clocal_{soil}$	concentration in soil averaged over 30 days	$[kg_c.kg_{soil}^{-1}]$	O

Output

$Csoil_{pest\text{-}0}$	peak concentration in soil after N applications	$[kg_c.kg_{soil}^{-1}]$	O
$Csoil_{pest\text{-}28}$	mean concentration in soil over 28 days	[kgc.kgsoil-1]	O

If the sediment concentrations $Csed_{pest\text{-}T}$ are not specified, they are derived form the water concentrations in analogy with Equation P-336:

$$\boldsymbol{Csed_{pest\text{-}T} = \frac{Kp_{susp} \cdot Cwater_{pest\text{-}T}}{CONV_{sed}} \quad for\ T \in \{7,14,28\}} \tag{P-374}$$

Input

$Cwater_{pest\text{-}T}$	mean concentration in water over T days, $T \in \{7,14,28\}$	$[kg_c.m_{water}^{-3}]$	O
Kp_{susp}	solids-water partition coefficient in suspended matter	$[m^3.kg^{-1}]$	S/O
$CONV_{sed}$	conversion factor for sediment concentrations: wwt to dwt	$[kg_{wwt}.kg_{dwt}^{-1}]$	O^c

Output

$Csed_{pest\text{-}T}$	mean concentration in sediment over T days, $T \in \{7,14,28\}$	$[kg_c.kg_{wwt}^{-1}]$	O

III.7.3.2. Risk to bats by remedial timber treatment products used in buildings (only for scenario timber treatment)

The Nature Conservancy Council of Great Britain has developed a Relative Toxicity Index (RTI) which can be used to predict the risk to bats from active ingredients in remedial timber treatments (Mitchell-Jones *et al.*, 1989; Chadwick and Reston, 1993). The RTI is the number of LD50s per square meter for treated wood. In contrast with the original proposed Relative Toxicity Index it is proposed to use the lowest available acute oral toxicity test for mammals instead of the rat oral LD50. Relative Toxicity Index (RTI) for bats is given by:

$$RCR_{bats} = \frac{DOSE_{wood}}{LD50_{mammal,oral}} \qquad \text{(P-375)}$$

Input

$DOSE_{wood}$	dosage of a.i. per m^2 wood	$[kg_c.m^{-2}]$	O
$LD50_{mammal,oral}$	acute oral toxicity for mammals	$[kg_c.kg_{BW}^{-1}]$	S
Output			
RCR_{bats}	Relative Toxicity Index for bats (RTI)	$[kg_{BW}.m^{-2}]$	O^c

III.7.3.3. RCR for bees (via sprays)

Only direct exposure of bees will be taken into account in this version of USES. This will only occur if the pesticide is applied as a spray.

$$RCR_{bee} = \frac{DOSE_{pest} \cdot 10^7}{LD50_{bee}} \qquad \text{(P-376)}$$

The factor 10^7 is used for the conversion of $kg_c.m^{-2}$ to $g.ha^{-1}$. This will turn the RCR for bees into (g/ha)/(µg/bee).

Input

$LD50_{bee}$	lethal dose for 50% of the bees	$[\mu g.bee^{-1}]$	S
$DOSE_{pest}$	dosage of the substance for one application	$[kg_c.m^{-2}]$	S
Output			
RCR_{bee}	risk characterisation quotient for bees	$[(g_c.ha^{-1})/(\mu g.bee^{-1})]$	O^c

III.7.3.4. RCR for birds and mammals exposed through crops and insects (via sprays)

Hazard for birds and mammals eating insects and crops on land after spraying of pesticides will be assessed for chronic and acute exposure separately. The short-term concentration in food is directly compared to the LC50, long-term concentrations in food are directly compared to NOEC values. With the daily food intake (DFI) of the species and its bodyweight, LD50s if present, can be translated to LC50s in food.

$$RCRfood_{bird\text{-}1} = \frac{Cfood_{bird} \cdot DFI_{bird} \cdot 1}{LD50_{bird} \cdot BW_{bird}} \qquad \text{(P-377)}$$

$$RCRfood_{bird\text{-}5} = \frac{Cfood_{bird\text{-}5}}{LC50_{bird}} \qquad \text{(P-378)}$$

$$RCRfood_{Tbird} = \frac{Cfood_{Tbird}}{NOEC_{bird}} \qquad \text{(P-379)}$$

The *1* in the formula above is the number of feeding days assumed to be representative with respect to the single dose toxicity value (LD50) used.

$$RCRfood_{mammal\text{-}1} = \frac{Cfood_{mammal} \cdot DFI_{mammal} \cdot 1}{LD50_{mammal,oral} \cdot BW_{mammal}} \qquad \text{(P-380)}$$

$$RCRfood_{Tmammal} = \frac{Cfood_{Tmammal}}{NOEC_{mammal,food,chr}} \qquad \text{(P-381)}$$

Input

$LD50_{bird}$	LD50 for birds	$[kg_c.kg_{BW}^{-1}]$	S
$LC50_{bird}$	LC50 in food for birds	$[kg_c.kg_{food}^{-1}]$	S
$NOEC_{bird}$	NOEC in food for birds S/O	$[kg_c.kg_{food}^{-1}]$	
$LD50_{mammal, oral}$	LD50 for mammals	$[kg_c.kg_{BW}^{-1}]$	S
$NOEC_{mammal,food,chr}$	NOEC in food for mammals S/O	$[kg_c.kg_{food}^{-1}]$	
DFI_{bird}	daily food intake for bird species of concern S/O	$[kg_{food\ dwt}.d^{-1}]$	
DFI_{mammal}	daily food intake for mammalian species of concern S/O	$[kg_{food\ dwt}.d^{-1}]$	
$Cfood_x$	initial concentration in food for x S/O	$[kg_c.kg_{food}^{-1}]$	
$Cfood_{x-5}$	mean concentration in food for x over 5 days	$[kg_c.kg_{food}^{-1}]$	O
$Cfood_{Tx}$	mean conc. in food over toxicity test duration of x $x \in \{bird,mammal\}$	$[kg_c.kg_{food}^{-1}]$	O
BW_{bird}	mean bodyweight of bird species of concern S/O	[kg]	
BW_{mammal}	mean bodyweight of mammalian species of concern S/O	[kg]	

Output

$RCRfood_{bird-1}$	RCR for single dose toxicity to birds (PED/LD50)	[-]	O^c
$RCRfood_{bird-5}$	RCR for acute toxicity to birds (PEC/LC50)	[-]	O^c
$RCRfood_{Tbird}$	RCR for chronic toxicity to birds (PEC/NOEC)	[-]	Oc
RCRfoodmammal-1	RCR for single dose toxicity to mammals (PED/LD50)	[-]	Oc
RCRfoodTmammal	RCR for chronic toxicity to mammals (PEC/NOEC)	[-]	O^c

III.7.3.5. RCR for birds and mammals exposed through granules or treated seeds

By eating granules or treated seeds, birds and mammals can be exposed to pesticides. The calculations for these exposure routes are developed by Luttik (1992).

The term *particle* in the formula symbols is used for granules and treated seeds.

One particle criteria

$$RCRone\_particle_{bird} = \frac{C_{particle} \cdot W_{particle}}{LD50_{bird} \cdot BW_{bird}} \qquad \text{(P-382)}$$

$$RCRone\_particle_{mammal} = \frac{C_{particle} \cdot W_{particle}}{LD50_{mammal,oral} \cdot BW_{mammal}} \qquad \text{(P-383)}$$

RCR for birds and mammals if treated seeds or granules are sole food source

$$RCRparticle_{bird} = \frac{C_{particle} \cdot DFI_{bird} \cdot 1}{LD50_{bird} \cdot BW_{bird}} \qquad \text{(P-384)}$$

$$RCRparticle_{mammal} = \frac{C_{particle} \cdot DFI_{mammal} \cdot 1}{LD50_{mammal,oral} \cdot BW_{mammal}} \qquad \text{(P-385)}$$

The *1* in the formula above is the number of feeding days assumed to be representative with respect to the single dose toxicity value (LD50) used.

LD50 in number of particles

$$LD50particle_{bird} = \frac{LD50_{bird} \cdot BW_{bird}}{C_{particle} \cdot W_{particle}} \qquad \text{(P-386)}$$

$$LD50particle_{mammal} = \frac{LD50_{mammal,oral} \cdot BW_{mammal}}{C_{particle} \cdot W_{particle}} \qquad \text{(P-387)}$$

RCR for items resembling natural food

$$DOSE_{particle} = \frac{DOSE_{pest}}{C_{particle}} \quad \text{(P-388)}$$

if MIX = "yes" $F_{mix} = 0.01$
if MIX = "no" $F_{mix} = 1$

$$N_{particles} = \frac{DOSE_{particle}}{W_{particle}} \cdot F_{mix} \quad \text{(P-389)}$$

$$RCRitem_{bird} = \frac{N_{particles}}{LD50particle_{bird}} \quad \text{(P-390)}$$

$$RCRitem_{mammal} = \frac{N_{particles}}{LD50particle_{mammal}} \quad \text{(P-391)}$$

Input			
$LD50_{bird}$	LD50 for birds	$[kg_c.kg_{BW}^{-1}]$	S
$LD50_{mammal,oral}$	LD50 for mammals (oral)	$[kg_c.kg_{BW}^{-1}]$	S
DFI_{bird}	daily food intake for bird species of concern	$[kg_{food\ dwt}.d^{-1}]$	S
DFI_{mammal}	daily food intake for mammalian species of concern	$[kg_{food\ dwt}.d^{-1}]$	S
BW_{bird}	mean bodyweight of bird species of concern	[kg]	O
BW_{mammal}	mean bodyweight of mammalian species of concern	[kg]	O
$C_{particle}$	concentration of pesticide in granules or treated seeds	$[kg_c.kg_{particle}^{-1}]$	S
MIX	mixing with soil	[yes/no]	P
F_{mix}	fraction of particles available at surface	[-]	O
$DOSE_{pest}$	dosage	$[kg_c.m^{-2}]$	S
$DOSE_{particle}$	dosage of particles	$[kg_{particle}.m^{-2}]$	O
$W_{particle}$	weight of one granule or treated seed	$[kg_{particle}.particle^{-1}]$	S
$N_{particles}$	number of particles per m^2	$[particles.m^{-2}]$	O
Output			
RCRone $particle_{bird}$	One particle criteria for acute toxicity to mammals (PED/LD50)	[-]	O^c
RCRone $particle_{mammal}$	One particle criteria for acute toxicity to birds (PED/LD50)	[-]	O^c
$RCRparticle_{bird}$	RCR for acute toxicity to mammals if granules or seeds are the sole food source (PED/LD50)	[-]	O^c
$RCRparticle_{mammal}$	RCR for acute toxicity to birds if granules or seeds are the sole food source (PED/LD50)	[-]	O^c
$LD50particle_{bird}$	LD50 recalculated per granule or treated seed	[particles]	O^c
$LD50particle_{mammal}$	LD50 recalculated per granule or treated seed	[particles]	O^c
$RCRitem_{bird}$	RCR for items resembling natural food	$[m^{-2}]$	O^c
$RCRitem_{mammal}$	RCR for items resembling natural food	$[m^{-2}]$	O^c

III.7.3.6. Daily water intake of birds and mammals

The daily requirement for water intake varies greatly between species of different habits, and according to a wide range of stresses. Robbins (1983) has reviewed information on water turnover rates (which gives a rough estimate of water intake) for wild birds and mammals, providing the following predictive equations for unstressed animals with free access to water:

$$DWI_{bird} = 1.19 \cdot 10^{-4} \cdot BW_{bird}^{\ 0.75} \tag{P-392}$$

$$DWI_{mammal} = 1.20 \cdot 10^{-4} \cdot BW_{mammal}^{\ 0.84} \tag{P-393}$$

Input			
BW_{bird}	mean bodyweight of bird species of concern	$[kg_{bw}]$	S/O
BW_{mammal}	mean bodyweight of mammalian species of concern	$[kg_{bw}]$	S/O
Output			
DWI_{bird}	daily water intake of bird species of choice	$[m_{water}^3.d^{-1}]$	O^c
DWI_{mammal}	daily water intake of mammalian species of choice	$[m_{water}^3.d^{-1}]$	O^c

III.7.3.7. RCR for birds and mammals exposed through uptake of water (via sprays)

Besides eating granules, treated seeds, crops or insects, birds and mammals can also be exposed to a pesticide by the uptake of water. This can be either surface water or water on leaves and crops. Calculations for this exposure route are based on Luttik (1992). This route will only be used if the pesticide is applied as spray.

$$RCRspray_{bird} = \frac{C_{spray} \cdot DWI_{bird} \cdot 1}{LD50_{bird} \cdot BW_{bird}} \qquad \text{(P-394)}$$

$$RCRsurf_{bird} = \frac{Cwater_{pest\text{-}0} \cdot DWI_{bird} \cdot 1}{LD50_{bird} \cdot BW_{bird}} \qquad \text{(P-395)}$$

$$RCRsurf_{bird,semi} = \frac{Cwater_{pest\text{-}4}}{LC50_{bird} \cdot RHO_{water}} \qquad \text{(P-396)}$$

$$RCRspray_{mammal} = \frac{C_{spray} \cdot DWI_{mammal} \cdot 1}{LD50_{mammal,oral} \cdot BW_{mammal}} \qquad \text{(P-397)}$$

$$RCRsurf_{mammal} = \frac{Cwater_{pest\text{-}0} \cdot DWI_{mammal} \cdot 1}{LD50_{mammal,oral} \cdot BW_{mammal}} \qquad \text{(P-398)}$$

Input			
$LD50_{bird}$	LD50 for birds	$[kg_c.kg_{BW}^{-1}]$	S
$LD50_{mammal,oral}$	LD50 for mammals (oral)	$[kg_c.kg_{BW}^{-1}]$	S
$LC50_{bird}$	LC50 in food for birds	$[kg_c.kg_{food}^{-1}]$	S
DWI_{bird}	daily water intake of bird species of choice	$[m_{water}^3.d^{-1}]$	O/S
DWI_{mammal}	daily water intake of mammalian species of choice	$[m_{water}^3.d^{-1}]$	O/S
BW_{bird}	mean bodyweight of bird species of concern	$[kg_{bw}]$	O
BW_{mammal}	mean bodyweight of mammalian species of concern	$[kg_{bw}]$	O
C_{spray}	concentration in spray water on leaves and crops	$[kg_c.m^{-3}]$	O
$Cwater_{pest\text{-}0}$	initial concentration in surface water	$[kg_c.m^{-3}]$	O
$Cwater_{pest\text{-}4}$	mean concentration in water over 4 days	$[kg_c.m^{-3}]$	O
RHO_{water}	density of water phase	$[kg.m^{-3}]$	D
Output			
$RCRspray_{bird}$	acute RCR for birds, surface water (PED/LD50)	[-]	O^c
$RCRsurf_{bird}$	acute RCR for birds, surface water (PED/LD50)	[-]	O^c
$RCRsurf_{bird,semi}$	semi-chronic RCR for birds, surface water (PEC/LC50)	[-]	O^c
$RCRspray_{mammal}$	acute RCR for mammals, spray water (PED/LD50)	[-]	O^c
$RCRsurf_{mammal}$	acute RCR for mammals, spray water (PED/LD50)	[-]	O^c

III.7.3.8. RCR for terrestrial organisms (earthworms and nitrificating bacteria)

Earthworms and bacteria are exposed to concentrations in target soil. For earthworms both acute and chronic exposure are assessed, for bacteria only acute toxicity is considered. If there is no application of the pesticide on target soil, the concentration on agricultural soil (non-target area) is taken.

$$RCR_{worm\text{-}0} = \frac{Csoil_{pest\text{-}0}}{LC50_{worm}} \tag{P-399}$$

$$RCR_{worm\text{-}28} = \frac{Csoil_{pest\text{-}28}}{NOEC_{worm}} \tag{P-400}$$

$$RCR_{nitr\text{-}0} = \frac{Csoil_{pest\text{-}0}}{EC50_{nitr}} \tag{P-401}$$

For pesticides also an RCR for the ecosystem will be calculated analogous to non-pesticides (see Section III.7.1.2). A $PNEC_{soil}$ is derived according to the procedure described in Section III.6.3.1. The PEC used for the risk characterisation ratio will be the exposure concentration for the earthworms.

$$RCR_{soil} = \frac{Csoil_{pest\text{-}28}}{PNEC_{soil}} \tag{P-402}$$

This PNEC is also used in comparison with the long-term soil concentration:

$$RCR_{soil\text{-}lt} = \frac{Csoil_{pest\text{-}lt}}{PNEC_{soil}} \tag{P-403}$$

Input			
$Csoil_{pest\text{-}0}$	initial concentration in soil	$[kg_c.kg_{wwt}^{-1}]$	O
$Csoil_{pest\text{-}28}$	mean concentration in soil over 28 days	$[kg_c.kg_{wwt}^{-1}]$	O
$Csoil_{pest\text{-}lt}$	concentration in soil after (N_{lt} + 2) years	$[kg_c.kg_{wwt}^{-1}]$	O
$LC50_{worm}$	LC50 for earthworms	$[kg_c.kg_{wwt}^{-1}]$	S
$NOEC_{worm}$	NOEC for earthworms	$[kg_c.kg_{wwt}^{-1}]$	S
$EC50_{nitr}$	EC50 for nitrificating bacteria in soil	$[kg_c.kg_{wwt}^{-1}]$	S
$PNEC_{soil}$	PNEC for terrestrial organisms	$[kg_c.kg_{wwt}^{-1}]$	O^c
Output			
$RCR_{worm\text{-}0}$	short term RCR for earthworms (PEC/LC50)	[-]	O^c
$RCR_{worm\text{-}28}$	long term RCR for earthworms (PEC/NOEC)	[-]	O^c
$RCR_{nitr\text{-}0}$	short term RCR for nitrif. bacteria (PEC/EC50)	[-]	O^c
RCR_{soil}	RCR for the soil ecosystem	[-]	O^c
$RCR_{soil\text{-}lt}$	RCR for soil after (N_{lt} + 2) years of applications	[-]	O^c

III.7.3.9. RCR for birds and mammals exposed through earthworms

The uptake of terrestrial organisms by birds and mammals, in other words, the secondary poisoning of birds and mammals, has been described by Romijn *et al.* (1991b). Worms will be caught exclusively on application soil unless there is no application of the pesticide on soil. In the latter case agricultural soil (non-target area) will be used.

It has to be noticed that in this calculation, unlike the research of Romijn *et al.* (1991b), extrapolation methods are not applied to derive a NOEC for birds or mammals.

$$\boldsymbol{RCRworm_{Tbird}} = \frac{\boldsymbol{C_{worm\text{-}Tbird}}}{\boldsymbol{NOEC_{bird}}} \qquad \text{(P-404)}$$

$$\boldsymbol{RCRworm_{Tmammal}} = \frac{\boldsymbol{C_{worm\text{-}Tmammal}}}{\boldsymbol{NOEC_{mammal,\,food,chr}}} \qquad \text{(P-405)}$$

Input			
$NOEC_{bird}$	NOEC for birds	$[kg_c.kg_{wet\ food}^{-1}]$	S
$NOEC_{mammal,food,chr}$	NOEC for mammal	$[kg_c.kg_{wet\ food}^{-1}]$	S/O
$C_{worm\text{-}Tbird}$	mean concentration in earthworms over T_{bird} days	$[kg_c.kg_{wet\ worm}^{-1}]$	O
$C_{worm\text{-}Tmammal}$	mean concentration in earthworms over T_{mammal} days	$[kg_c.kg_{wet\ worm}^{-1}]$	O
Output			
$RCRworm_{Tbird}$	RCR for worm-eating birds (PEC/NOEC)	[-]	O^c
$RCRworm_{Tmammal}$	RCR for worm-eating mammals (PEC/NOEC)	[-]	O^c

III.7.3.10. RCR for aquatic organisms

The water organisms fish, crustaceans and algae are supposed to be exposed to water concentrations in the ditch that are the mean of the concentration over a period of time. For acute exposure a value of 4 days is taken, for chronic exposure a different value is used, depending on the exposure period in the toxicity test. If there is only release through an STP, the concentration in the effluent after dilution and sorption to suspended matter will be used as exposure concentration.

$$RCR_{fish\text{-}0} = \frac{Cwater_{pest\text{-}0}}{LC50_{fish}} \tag{P-406}$$

$$RCR_{fish\text{-}28} = \frac{Cwater_{pest\text{-}28}}{NOEC_{fish}} \tag{P-407}$$

$$RCR_{crus\text{-}0} = \frac{Cwater_{pest\text{-}0}}{LC50_{crus}} \tag{P-408}$$

$$RCR_{crus\text{-}21} = \frac{Cwater_{pest\text{-}21}}{NOEC_{crus}} \tag{P-409}$$

$$RCR_{algae\text{-}0a} = \frac{Cwater_{pest\text{-}0}}{EC50_{a\lg ae}} \tag{P-410}$$

$$RCR_{algae\text{-}0b} = \frac{Cwater_{pest\text{-}0}}{NOEC_{algae}} \tag{P-411}$$

For pesticides also an RCR for the ecosystem will be calculated analogous to non-pesticides in III.7.1.1. A $PNEC_{water}$ is derived according to the procedure described in section III.6.1.1. The PEC used will be the exposure concentration calculated for the duration of the test for the most sensitive organisms (i.e. the species with the lowest NOEC).

Exposure/Effects	**Exposure**		**Effects**
RCR_{water}	if $NOEC_{algae}$ = lowest:	$Cwater_{pest\text{-}0}$	$PNEC_{water}$
	if $NOEC_{crus}$ = lowest:	$Cwater_{pest\text{-}21}$	
	if $NOEC_{fish}$ = lowest:	$Cwater_{pest\text{-}28}$	

Input

$Cwater_{pest-T}$	mean concentration in water over *T* days, T ∈ {4,21,28}	$[kg_c.m_{water}^{-3}]$	O
$LC50_{fish}$	LC50 for fish	$[kg_c.m^{-3}]$	S
$NOEC_{fish}$	NOEC for fish	$[kg_c.m^{-3}]$	S
$LC50_{crus}$	LC50 for crustaceans	$[kg_c.m^{-3}]$	S
$NOEC_{crus}$	NOEC for crustaceans	$[kg_c.m^{-3}]$	S
$LC50_{algae}$	EC50 for algae	$[kg_c.m^{-3}]$	S
$NOEC_{algae}$	NOEC for algae	$[kg_c.m^{-3}]$	S
$PNEC_{water}$	PNEC for aquatic organisms	$[kg_c.m^{-3}]$	O^c

Output

RCR_{fish-0}	short term RCR for fish (PEC/LC50)	[-]	O^c
$RCR_{fish-28}$	long term RCR for fish (PEC/NOEC)	[-]	O^c
RCR_{crus-0}	short term RCR for crustaceans (PEC/LC50)	[-]	O^c
$RCR_{crus-21}$	long term RCR for crustaceans (PEC/NOEC)	[-]	O^c
$RCR_{algae-0a}$	short term RCR for algae (PEC/EC50)	[-]	O^c
$RCR_{algae-0b}$	long term RCR for algae (PEC/NOEC)	[-]	O^c
RCR_{water}	RCR for the aquatic ecosystem	[-]	O^c

III.7.3.11. RCR for sediment-dwelling organisms

$$RCR_{sed\text{-}7} = \frac{Csed_{pest\text{-}7}}{LC50_{sed}} \qquad \text{(P-412)}$$

$$RCR_{sed\text{-}14} = \frac{Csed_{pest\text{-}14}}{NOEC_{sed}} \qquad \text{(P-413)}$$

$$RCR_{sed\text{-}28} = \frac{Csed_{pest\text{-}28}}{NOEC_{sed}} \qquad \text{(P-414)}$$

$$RCR_{sed} = \frac{Csed_{pest\text{-}28}}{PNEC_{sed}} \qquad \text{(P-415)}$$

$$RCR_{sed\text{-}lt} = \frac{Csed_{pest\text{-}lt}}{PNEC_{sed}} \qquad \text{(P-416)}$$

Input			
$Csed_{pest\text{-}T}$	mean concentration in sediment over T days, $T \in \{7,14,28\}$	$[kg_c.kg_{wwt}^{-1}]$	O
$Csed_{pest\text{-}lt}$	concentration after (N_{lt} + 2) years of applications	$[kg_c.kg_{wwt}^{-1}]$	O
$LC50_{sed}$	LC50 for sediment-dwelling organisms	$[kg_c.kg_{wwt}^{-1}]$	S
$NOEC_{sed}$	LC50 for sediment-dwelling organisms	$[kg_c.kg_{wwt}^{-1}]$	S
$PNEC_{sed}$	PNEC for sediment-dwelling organisms	$[kg_c.kg_{wwt}^{-1}]$	O
Output			
$RCR_{sed\text{-}7}$	short term RCR for sediment organisms(PEC/LC50)	[-]	O^c
$RCR_{sed\text{-}14}$	long term RCR for sediment organisms (PEC/NOEC)	[-]	O^c
$RCR_{sed\text{-}28}$	long term RCR for sediment organisms (PEC/NOEC)	[-]	O^c
$RCR_{sed\text{-}lt}$	RCR for sediment after (N_{lt} + 2) years of applications	[-]	O^c

III.7.3.12. RCR for birds and mammals exposed through fish

The uptake of pesticides by water organisms is calculated by means of the bioconcentration factor (BCF). If no experimentally derived BCF is available, the QSAR-calculation given in Section III.5.1.1 is used. Uptake of water organisms by birds and mammals (secondary poisoning) has been described by Romijn *et al.* (1991a).

$$RCRfish_{bird} = \frac{C_{fish\text{-}Tbird}}{NOEC_{bird}} \qquad \text{(P-417)}$$

$$RCRfish_{mammal} = \frac{C_{fish\text{-}Tmammal}}{NOEC_{mammal,food,chr}} \qquad \text{(P-418)}$$

Input			
$NOEC_{bird}$	NOEC for fish eating bird	$[kg_c.kg_{wet\ food}^{-1}]$	S/O
$NOEC_{mammal,food,chr}$	NOEC for fish eating mammal	$[kg_c.kg_{wet\ food}^{-1}]$	S/O
$C_{fish\text{-}Tbird}$	mean concentration in fish over T_{bird} days	$[kg_c.kg_{wet\ fish}^{-1}]$	O
$C_{fish\text{-}Tmammal}$	mean concentration in fish over T_{mammal} days	$[kg_c.kg_{wet\ fish}^{-1}]$	O
Output			
$RCRfish_{bird}$	RCR for fish eating birds (PEC/NOEC)	[-]	O^c
$RCRfish_{mammal}$	RCR for fish eating mammal (PEC/NOEC)	[-]	O^c

III.7.3.13. RCR for mammals after inhalation of air

The risk characterisation ratio for mammals after inhalation of contaminated air is calculated by comparing the established LC50-value from toxicological experiments with the calculated PEC in air according the appropriate scenario.

$$RCR_{mammal,inh} = \frac{Clocal_{air}}{LC50_{mammal,inh}} \qquad \text{(P-419)}$$

Input			
$Clocal_{air}$	local concentration in air during episode	$[kg_c.m^{-3}]$	O
$LC50_{mammal,inh}$	inhalatory LC50 for mammals	$[kg_c.m^{-3}]$	S/O
Output			
$RCR_{mammal,inh}$	inhalatory RCR for mammal	[-]	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.

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I. Glossary of abbreviations

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
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 organized and how it can produce valid data; GLP principles are described by OECD
HEDSET	Harmonized 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 greates 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	Organization for Economic Cooperation 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
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)

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II. List of symbols applied in (E)USES 4.0

This appendix contains a list of all parameter symbols applied in EUSES. The symbols are grouped according to subject and given with a description, units (internal and on-screen), flags, value (for defaults, on-screen unit), type (for which assessment types is the parmeter used) and range (minimum-maximum). The flags are used as follows:

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). Sets of changed default values can be saved.
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.
*	An asterisk is added when a parameter can be set to a different value on the regional and continental spatial scale.
^{c}	Default or output parameter is closed and cannot be changed by the user.
^{d}	A superscript 'd' is added to closed outputs which are shown with the defaults. These parameters are displayed to help the user set certain defaults. For example, the effluent discharge rate of the local STP is sometimes known but cannot be changed without changing the defaults of inhabitant number and wastewater per inhabitant.

For parameters with an S or D status, ranges are specified. The ranges are advised ranges, they are not used as strict limits. When a value is applied outside this range, a warning will be given by the computer program. Ranges are specified as [min,max] or <min,max> etc. Square brackets are used when the minimum or maximum is included in the range, pointed brackets when they are excluded.

The on-screen units are the standard units used for input and output to screen. However, EUSES allows the user to choose between different logical units for several parameters, if appropriate. Internally, all parameters are converted to SI units. Several alternative input units are shown in the table below.

Soil and sediment concentr.	Water and air concentr.	Temperature	Fractions	Rate constants/ half-lifes	Emissions, tonnage etc.
[mg.kg$_{wwt}^{-1}$]	[mg.l^{-1}]	[^{o}C]	[-]	[d^{-1}]	[kg.d^{-1}]
[μg.kg$_{wwt}^{-1}$]	[μg.l^{-1}]	[K]	[%]	[d]	[kg.yr^{-1}]
[mg.kg$_{dwt}^{-1}$]	[mg.m^{-3}]			[s^{-1}]	[tonnes.yr^{-1}]
[μg.kg$_{dwt}^{-1}$]	[μg.m^{-3}]			[s]	[tonnes.d^{-1}]

The column 'Type' is used to indicate the basic scope of the assessment and is defined as follows:

Assessment

A. Assessment of new and existing chemicals

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.

B. Assessment of plant protection products and biocides

Block method

- Block method for mixtures, local and regional scale

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Input substance identification							
---	general name			S		I-V	
---	CAS no.			S		I-V	
---	EC notification no.			S		I-V	
---	EINECS no.			S		I-V	
Input physico-chemical properties							
MOLW	molecular weight	[kg.mol^{-1}]	[g.mol^{-1}]	S		I-III	[40,2000]
Kow	octanol-water partition coefficient	[-]	[-]	S		I-III	log: [-1,7]
SOL	water solubility	[kg.m^{-3}]	[mg.l^{-1}]	S		I-III	[1e-3,1e5]
H$_{0\ solution}$	enthalpy of solution	[J. .mol^{-1}]	[J. .mol^{-1}]	S		I-III	[10]
VP	vapour pressure	[Pa]	[Pa]	S		I-III	[1e-6,1e6]
H$_{0\ vapourisation}$	enthalpy of solution	[J. .mol^{-1}]	[J. .mol^{-1}]	S		I-III	[50]
TEMPboil	boiling point	[K]	[C]	S		I-III	[-100,500]
TEMPmelt	melting point	[K]	[C]	S		I-III	[-100,500]
Release estimation	i ∈ {prod,form,proc,priv,rec} j ∈ {air,water,ind,surf,agric}						
PRODVOL	production volume of chemical in EU	[kg.d^{-1}]	[tonnes.yr^{-1}]	S		I-III	[0,1e6]
HPVC	high-production volume chemical	[yes/no]	[yes/no]	P	"no"	I-III	
IMPORT	volume of chemical imported to EU	[kg.d^{-1}]	[tonnes.yr^{-1}]	S		I-III	[0,1e6]
EXPORT	volume of chemical exported from EU	[kg.d^{-1}]	[tonnes.yr^{-1}]	S		I-III	[0,1e6]
INDCAT	industrial category	[-]	[-]	P		I-III	
USECAT	use category	[-]	[-]	P		I-III	
MAINCAT	main category (for existing substances)	[-]	[-]	P		I-III	
Ftonnage$_k$	fraction of total tonnage for application *k*	[-]	[-]	S		I-III	<0,1]
Fchem$_{form}$	fraction of chemical in formulation	[-]	[-]	S	1	I-III	
---	specific information on substance use pattern			P		I-III	
---	relevant steps in life cycle			P		I-III	
PRODVOLreg	regional production volume of substance	[kg.d^{-1}]	[tonnes.yr^{-1}]	O		I-III	[0,1e6]
PRODVOLcont	continental production volume of substance	[kg.d^{-1}]	[tonnes.yr^{-1}]	O^c		I-III	[0,1e6]
TONNAGE	tonnage in EU	[kg.d^{-1}]	[tonnes.yr^{-1}]	O		I-III	[0,1e6]
TONNAGEreg	tonnage in region	[kg.d^{-1}]	[tonnes.yr^{-1}]	O		I-III	[0,1e6]
TONNAGEreg$_{form}$	regional tonnage of formulation used	[kg.d^{-1}]	[tonnes.yr^{-1}]	O^c		I-III	
TONNAGEcont	tonnage in continent	[kg.d^{-1}]	[tonnes.yr^{-1}]	O^c		I-III	[0,1e6]
TONNAGE$_k$	relevant tonnage for application *k*	[kg.d^{-1}]	[tonnes.yr^{-1}]	O		I-III	[0,1e6]
Fprodvol$_{reg}$	fraction of EU production volume for region	[-]	[-]	D	0.10	I-III	[0,1]
Fconnect$_{stp}$	fraction connected to sewer systems region/continent	[-]	[-]	D	0.70	I-IIIb	[0,1]
F$_{i,j}$	fraction of tonnage released during stage *i* to compartment *j*	[-]	[-]	O	App. IA	I-III	[0,1]
Fmainsource$_i$	fraction of the main local source during life-cycle stage *i*	[-]	[-]	O	App. IB	I-IIIa	[0,1]
Temission$_i$	number of days per year for the emission in stage *i*	[d.yr^{-1}]	[-]	O	App. IB	I-IIIa	[1,365]
RELEASEcont$_{i,j}$	continental release during life-cycle stage *i* to compartment *j*	[kg.d^{-1}]	[kg.yr^{-1}]	O		I-IIIb	
RELEASEreg$_{i,j}$	regional release during life-cycle stage *i* to compartment *j*	[kg.d^{-1}]	[kg.yr^{-1}]	O		I-III	
Elocal$_{i,j}$	local emission during episode to comp. *j* during stage *i*	[kg.d^{-1}]	[kg.d^{-1}]	O		I-IIIa	
Ereg$_j$	total regional emission to compartment *j* (annual average flux) j ∈ {water,surface water,agric,ind,air}	[kg.d^{-1}]	[kg.d^{-1}]	O		I-IIIb	
Ereg$_{direct\text{-}water}$	direct regional emission to surface water (annual average)	[kg.d^{-1}]	[kg.d^{-1}]	O		I-IIIb	

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Econt$_{j}$	total continental emission to compartment *j* (annual average flux) j ∈{water,surface water,agric,ind,air}	[kg.d^{-1}]	[kg.d^{-1}]	O		I-IIIb	
Econt$_{direct\text{-}water}$	direct continental emission to surface water (annual average)	[kg.d^{-1}]	[kg.d^{-1}]	O		I-IIIb	
Characteristics of compartments							
Fwater$_{soil}$	volume fraction of water in soil	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	D	0.2	I-III	[0,0.7]
Fsolid$_{soil}$	volume fraction of solids in soil	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	D	0.6	I-III	[0.3,0.7]
Fair$_{soil}$	volume fraction of air in soil	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	D	0.2	I-III	[0,0.7]
Fwater$_{sed}$	volume fraction of water in sediment	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	D	0.8	I-III	[0.5,0.9]
Fsolid$_{sed}$	volume fraction of solids in sediment	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	D	0.2	I-III	[0.1,0.4]
Fwater$_{susp}$	volume fraction of water in suspended matter	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	D	0.9	I-III	[0.8,0.95]
Fsolid$_{susp}$	volume fraction of solids in suspeneded matter	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	D	0.1	I-III	[0.05,0.2]
RHOsolid	density of solid phase	[kg.m^{-3}]	[kg.l^{-1}]	D	2.5	I-III	[2,3]
RHOwater	density of water phase	[kg.m^{-3}]	[kg.l^{-1}]	D	1.0	I-III	[0.90,1.1]
RHOair	density of air phase [0.001,0.002]	[kg.m^{-3}]	[kg.l^{-1}]	D	0.0013	I-III	
RHO$_{soil}$	wet bulk density of soil	[kg.m^{-3}]	[kg.l^{-1}]	O^{cd}		I-III	
RHO$_{sed}$	wet bulk density of sediment	[kg.m^{-3}]	[kg.l^{-1}]	O^{cd}		I-III	
RHO$_{susp}$	wet bulk density of suspended matter	[kg.m^{-3}]	[kg.l^{-1}]	O^{cd}		I-III	
CONV$_{soil}$	conversion factor for soil concentrations: wwt to dwt	[kg.kg^{-1}]	[kg.kg^{-1}]	O^{cd}		I-III	
CONV$_{sed}$	conversion factor for sediment concentrations: wwt to dwt	[kg.kg^{-1}]	[kg.kg^{-1}]	O^{cd}		I-III	
Foc$_{soil}$	weight fraction of organic carbon in soil	[kg.kg^{-1}]	[kg.kg^{-1}]	D	0.02	I-III	[0.01,0.20]
Foc$_{sed}$	weight fraction of organic carbon in sediment	[kg.kg^{-1}]	[kg.kg^{-1}]	D	0.05	I-III	[0.01,0.20]
Foc$_{susp}$	weight fraction of organic carbon in suspended matter	[kg.kg^{-1}]	[kg.kg^{-1}]	D	0.1	I-III	[0.01,0.20]
Foc$_{PS}$	fraction of organic carbon solids primary settler of STP	[kg.kg^{-1}]	[kg.kg^{-1}]	D	0.3	I-III	[0.10,0.40]
Foc$_{RS}$	fraction of organic carbon solids raw sewage of STP	[kg.kg^{-1}]	[kg.kg^{-1}]	D	0.3	I-III	[0.10,0.40]
Foc$_{A}$	fraction of organic carbon solids aeration tank of STP	[kg.kg^{-1}]	[kg.kg^{-1}]	D	0.37	I-III	[0.10,0.40]
Foc$_{SLS}$	fraction of organic carbon solids solids-liquid sep. of STP	[kg.kg^{-1}]	[kg.kg^{-1}]	D	0.37	I-III	[0.10,0.40]
CONjunge	constant of Junge equation	[Pa.m]	[Pa.m]	D \			
				>	product: 10^{-4} Pa	I-III	[1e-6,1e-2]
SURF$_{aer}$	surface area of aerosol particles	[m^{2}.m^{-3}]	[m^{2}.m^{-3}]	D /			
TEMP	environmental temperature	[K]	[C]	D	12	I-III	[0,25]
R	gas constant	[Pa.m^{3}.mol^{-1}.K^{-1}]	[Pa.m^{3}.mol^{-1}.K^{-1}]	D^{c}	8.314	I-III	---
Partition coefficients							
VP$_{L}$	sub-cooled liquid vapour pressure	[Pa]	[Pa]	O		I-III	[1e-6,1e6]
Koc	organic carbon-water partition coefficient	[m^{3}.kg^{-1}]	[l.kg^{-1}]	O		I-III	[1,1e6]
Fass$_{aer}$	fraction of chemical associated with aerosol particles	[-]	[-]	O		I-III	[0,1]
HENRY	Henry's law constant	[Pa.m^{3}.mol^{-1}]	[Pa.m^{3}.mol^{-1}]	O		I-III	[4e-10,1e12]
Kp$_{susp}$	solids-water partition coefficient in suspended matter	[m^{3}.kg^{-1}]	[l.kg^{-1}]	O		I-III	[0.01,1e5]
Kp$_{sed}$	solids-water partition coefficient in sediment	[m^{3}.kg^{-1}]	[l.kg^{-1}]	O		I-III	[0.01,1e5]
Kp$_{soil}$	solids-water partition coefficient in soil	[m^{3}.kg^{-1}]	[l.kg^{-1}]	O		I-III	[0.01,1e5]
K$_{air\text{-}water}$	air-water partition coefficient	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	O^{cd}		I-III	
K$_{soil\text{-}water}$	soil-water partition coefficient	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	O^{c}		I-III	

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$K_{susp\text{-}water}$	suspended matter-water partition coefficient	$[m^3.m^{-3}]$	$[m^3.m^{-3}]$	O^c		I-III	
$K_{sed\text{-}water}$	sediment-water partition coefficient	$[m^3.m^{-3}]$	$[m^3.m^{-3}]$	O^c		I-III	
Kp_{RS}	solids-water partition coeff. in raw sewage sludge	$[m^3.kg^{-1}]$	$[l.kg^{-1}]$	O		I-III	[1e-5,1e5]
Kp_{PS}	solids-water partition coeff. in settled sewage sludge	$[m^3.kg^{-1}]$	$[l.kg^{-1}]$	O		I-III	[1e-5,1e5]
Kp_{A}	solids-water partition coeff. in activated sewage sludge	$[m^3.kg^{-1}]$	$[l.kg^{-1}]$	O		I-III	[1e-5,1e5]
Kp_{SLS}	solids-water partition coeff. in effluent sewage sludge	$[m^3.kg^{-1}]$	$[l.kg^{-1}]$	O		I-III	[1e-5,1e5]
Degradation and transformation rates							
k_{OH}	specific degradation rate constant with OH-radicals	$[m^3.molec^{-1}.d^{-1}]$	$[cm^3.molec^{-1}.s^{-1}]$	S	0	I-III	[0,1e-10]
$OHCONC_{air}$	concentration of OH-radicals in atmosphere	$[molec.m^{-3}]$	$[molec.cm^{-3}]$	D	5.10^5	I-III	[1e5,1e6]
$kdeg_{air}$	rate constant for degradation in air	$[d^{-1}]$	$[d^{-1}]$	O		I-III	[0,0.7]
$DT50hydr_{water}$	half-life for hydrolysis in water	[d]	[d]	S	1e6	I-III	[1,1e6]
$khydr_{water}$	rate constant for hydrolysis in surface water	$[d^{-1}]$	$[d^{-1}]$	O		I-III	[0,0.7]
$DT50photo_{water}$	half-life for photolysis in water	[d]	[d]	S	1e6	I-III	[1,1e6]
$kphoto_{water}$	rate constant for photolysis in surface water	$[d^{-1}]$	$[d^{-1}]$	O		I-III	[0,0.7]
---	characterisation of biodegradability (ready/inherent/non-biodegradable/specific criteria)		[-]	P	non-biodegr.	I-III	
$DT50bio_{stp}$	half-life for biodegradation in STP	[d]	[d]	O		I-III	□0,10]
$kbio_{stp}$	rate constant for biodegradation in STP	$[d^{-1}]$	$[d^{-1}]$	O		I-III	[0,30]
$kabio_{stp}$	rate constant for abiotic degradation in STP	$[d^{-1}]$	$[d^{-1}]$	D	0	I-III	[0,30]
$kdeg_{stp}$	total rate constant for degradation in STP	$[d^{-1}]$	$[d^{-1}]$	O		I-III	[0,30]
$DT50bio_{water}$	half-life for biodegradation in bulk surface water	[d]	[d]	O		I-III	[1,1e6]
$kbio_{water}$	rate constant for biodegradation in bulk surface water	$[d^{-1}]$	$[d^{-1}]$	O		I-III	[0,0.7]
$kdeg_{water}$	total rate constant for degradation in bulk surface water	$[d^{-1}]$	$[d^{-1}]$	O		I-III	[0,0.7]
$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]	[d]	O		I-III	[1,1e6]
$kbio_{soil}$	rate constant for biodegradation in bulk soil	$[d^{-1}]$	$[d^{-1}]$	O		I-III	[0,0.7]
$kabio_{soil}$	rate constant for abiotic degradation in bulk soil	$[d^{-1}]$	$[d^{-1}]$	D	0	I-III	[0,0.7]
$kdeg_{soil}$	total rate constant for degradation in bulk soil	$[d^{-1}]$	$[d^{-1}]$	O		I-III	[0,0.7]
$DT50bio\text{-}aer_{sed}$	half-life for biodegradation in aerated sediment	[d]	[d]	O		I-III	[1,1e6]
$kbio\text{-}aer_{sed}$	rate constant for biodegradation in aerated sediment	$[d^{-1}]$	$[d^{-1}]$	O		I-III	[0,0.7]
$kabio_{sed}$	rate constant for abiotic degradation in bulk sediment	$[d^{-1}]$	$[d^{-1}]$	D	0	I-III	[0,0.7]
$kbio\text{-}anaer_{sed}$	rate constant for anaerobic biodegradation in sediment	$[d^{-1}]$	$[d^{-1}]$	D	0	I-III	[0,0.7]
$kdeg_{sed}$	total rate constant for degradation in bulk sediment	$[d^{-1}]$	$[d^{-1}]$	O		I-III	[0,0.7]
$Faer_{sed}$	fraction of sediment compartment that is aerated	$[m^3.m^{-3}]$	$[m^3.m^{-3}]$	D	0.10	I-III	[0,1]
Sewage treatment							
$Estp_{air}$	local indirect emission to air from STP during episode	$[kg.d^{-1}]$	$[kg.d^{-1}]$	O		I-III	
$Clocal_{eff}$	concentration of chemical (total) in the STP-effluent	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O		I-III	
$Clocal_{inf}$	concentration in untreated wastewater	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O		I-III	
C_{sludge}	concentration in dry sewage sludge	$[kg.kg^{-1}]$	$[mg.kg^{-1}]$	O		I-III	
PEC_{stp}	PEC for micro-organisms in the STP	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O		I-III	
$Estp\text{-}reg_{air}$	regional indirect emission to air from STP	$[kg.d^{-1}]$	$[kg.d^{-1}]$	O		I-III	
$Estp\text{-}reg_{water}$	regional indirect emission to surface water from STP	$[kg.d^{-1}]$	$[kg.d^{-1}]$	O		I-III	
$Estp\text{-}reg_{agric}$	regional indirect emission to agricultural soil from STP	$[kg.d^{-1}]$	$[kg.d^{-1}]$	O		I-III	

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Estp-cont$_{air}$	continental indirect emission to air from STP	$[kg.d^{-1}]$	$[kg.d^{-1}]$	O		I-III	
Estp-cont$_{water}$	continental indirect emission to surface water from STP	$[kg.d^{-1}]$	$[kg.d^{-1}]$	O		I-III	
Estp-cont$_{agric}$	continental indirect emission to agricultural soil from STP	$[kg.d^{-1}]$	$[kg.d^{-1}]$	O		I-III	
EFFLUENTlocal$_{stp}$	effluent discharge rate of local STP	$[m^3.d^{-1}]$	$[l.d^{-1}]$	O^{cd}		I-IIIa	
EFFLUENT$_{stp}$	effluent discharge rate of STP	$[m^3.d^{-1}]$	$[l.d^{-1}]$	O^{*c}		I-III	
Fstp$_{water}$	fraction of emission directed to water by STP	[-]	[-]	O		I-IIIa	[0,1]
Fstp$_{air}$	fraction of emission directed to air by STP	[-]	[-]	O		I-IIIa	[0,1]
Fstp$_{sludge}$	fraction of emission directed to sludge by STP	[-]	[-]	O		I-IIIa	[0,1]
Fstp$_{degr}$	fraction of the emission degraded in STP	[-]	[-]	O		I-IIIa	[0,1]
Fstp-reg$_{water}$	fraction of emission directed to water by regional STP	[-]	[-]	O		I-IIIb	[0,1]
Fstp-reg$_{air}$	fraction of emission directed to air by regional STP	[-]	[-]	O		I-IIIb	[0,1]
Fstp-reg$_{sludge}$	fraction of emission directed to sludge by regional STP	[-]	[-]	O		I-IIIb	[0,1]
Fstp-reg$_{degr}$	fraction of the emission degraded in regional STP	[-]	[-]	O		I-IIIb	[0,1]
Fstp-cont$_{water}$	fraction of emission directed to water by continental STP	[-]	[-]	O		I-IIIb	[0,1]
Fstp-cont$_{air}$	fraction of emission directed to air by continental STP	[-]	[-]	O		I-IIIb	[0,1]
Fstp-cont$_{sludge}$	fraction of emission directed to sludge by continental STP	[-]	[-]	O		I-IIIb	[0,1]
Fstp-cont$_{degr}$	fraction of the emission degraded in continental STP	[-]	[-]	O		I-IIIb	[0,1]
Nlocal	number of inhabitants feeding one STP	[eq]	[eq]	D	10000	I-IIIa	[1e3,1e5]
N *	number of inhabitants feeding regional system	[eq]	[eq]	D	2.0.10^{7}	I-IIIb	[1e3,5e9]
	number of inhabitants feeding continental system	[eq]	[eq]	O^{cd}		I-IIIb	
	number of inhabitants in the EU	[eq]	[eq]	D	3.7.10^{8}	I-IIIb	[1e3,5e9]
Q$_{stp}$	sewage flow	$[m^3.eq^{-1}.d^{-1}]$	$[l.eq^{-1}.d^{-1}]$	D	200	I-III	[100,300]
k$_{SLR}$	sludge loading rate	$[kg.kg^{-1}.d^{-1}]$	$[kg.kg^{-1}.d^{-1}]$	D	0.15	I-III	[0.01,1]
TEMPstp$_{air}$	temperature of air above aeration tank	[K]	[C]	D	15	I-III	
TEMPstp$_{water}$	temperature of water in aeration tank	[K]	[C]	D	15	I-III	
M	mode of aeration: surface (s) or bubble aeration (b)	[-]	[-]	D	s	I-III	{s,b}
BOD	mass of O_2 binding material per person per day	$[kg.eq^{-1}.d^{-1}]$	$[g.eq^{-1}.d^{-1}]$	D	54	I-III	[10,100]
SOLIDS	dry weight solids produced per person per day	$[kg.eq^{-1}.d^{-1}]$	$[kg.eq^{-1}.d^{-1}]$	D	0.09	I-III	[0.05,0.5]
RHO$_{RS}$	density solids in raw sewage	$[kg.m^{-3}]$	$[kg.l^{-1}]$	D	1.5	I-III	[±10%]
DEPTH$_{PS}$	depth of primary settler	[m]	[m]	D	4	I-III	[±10%]
HRT$_{PS}$	hydraulic retention time of primary settler	[d]	[hr]	D	2	I-III	[±10%]
RHO$_{PS}$	density suspended and settled solids in primary settler	$[kg.m^{-3}]$	$[kg.l^{-1}]$	D	1.5	I-III	[±10%]
DEPTH$_{A}$	depth of aeration tank	[m]	[m]	D	3	I-III	[±10%]
RHO$_{A}$	density solids of activated sludge	$[kg.m^{-3}]$	$[kg.l^{-1}]$	D	1.300	I-III	[±10%]
CAS	concentration solids of activated sludge	$[kg.m^{-3}]$	$[kg.m^{-3}]$	D	4	I-III	[±10%]
COX	steady state O_2 concentration in activated sludge	$[kg.m^{-3}]$	$[kg\ m^{-3}]$	D	0.002	I-III	[±10%]
G	aeration rate of bubble aeration	$[m^3.d^{-1}.eq^{-1}]$	$[m^3.s^{-1}.eq^{-1}]$	D	1.31.10^{-5}	I-III	[±10%]
DEPTH$_{SLS}$	depth of solids-liquid separator	[m]	[m]	D	3	I-III	[±10%]
RHO$_{SLS}$	density suspended and settled solids in solids-liquid separator	$[kg.m^{-3}]$	$[kg.l^{-1}]$	D	1.300	I-III	[±10%]
SUSP$_{eff}$	concentration solids in effluent	$[kg.m^{-3}]$	$[mg.l^{-1}]$	D	30	I-III	[±10%]
HRT$_{SLS}$	hydraulic retention time of solids-liquid separator	[d]	[hr]	D	6	I-III	[±10%]

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Parameters for regional and continental distribution							
AREA *	area of regional system	[m^2]	[km^2]	D	4.0.10^4	I-IIIb	[400,512e6]
	area of continental system	[m^2]	[km^2]	O^{cd}		I-IIIb	
	area of EU	[m^2]	[km^2]	D	3.56.10^6	I-IIIb	[400,512e6]
HEIGHT$_{air}$	atmospheric mixing height	[m]	[m]	D	1000	I-IIIb	[100,2000]
WINDSPEED	windspeed in the system	[m.d^{-1}]	[m.s^{-1}]	D	3	I-IIIb	[1,10]
TAU$_{air}$	residence time of air in system	[d]	[d]	O*^{cd}		I-IIIb	
DEPRATE$_{aer}$	aerosol deposition velocity	[m.d^{-1}]	[m.s^{-1}]	D	10^{-3}	I-IIIb	[1e-4,1e-2]
COLLEFF$_{aer}$	aerosol collection efficiency	[-]	[-]	D	2.10^5	I-IIIb	[2e4,2e6]
Fflow$_{out}$ *	fraction of water flow from global scale to continent	[-]	[-]	D*^{c}	0	I-IIIb	
	fraction of water flow from continental scale to region	[-]	[-]	D*	0.034	I-IIIb	[0,1]
FLOW$_{water}$	total water flow through system	[m^3.d^{-1}]	[m^3.d^{-1}]	O*^{c}		I-IIIb	
WASTEW	wastewater produced by inhabitants system	[m^3.d^{-1}]	-	O*^{c}		I-IIIb	
RAINDIRECT	rainfall directly into surface water	[m^3.d^{-1}]	-	O*^{c}		I-IIIb	
RUNOFF	rainwater run-off from soil	[m^3.d^{-1}]	-	O*^{c}		I-IIIb	
RAINRATE	average daily precipitation	[m.d^{-1}]	[mm.yr^{-1}]	D	700	I-IIIb	[200,2000]
F$_{water}$	area fraction of water of the system system	[-]	[-]	D*	0.03	I-IIIb	[0,1]
DEPTH$_{water}$	water depth of system	[m]	[m]	D*	3	I-IIIb	[1,15]
TAU$_{water}$	residence time of water in system	[d]	[d]	O*^{cd}		I-IIIb	
SUSP$_{water}$ *	suspended solids concentration of continental system	[kg.m^{-3}]	[mg.l^{-1}]	D*	25	I-IIIb	[1,100]
	suspended solids concentration of regional system	[kg.m^{-3}]	[mg.l^{-1}]	D*	15	I-IIIb	[1,100]
BIOTA$_{water}$	concentration biota	[kg.m^{-3}]	[mg.l^{-1}]	D	1	I-IIIb	[10,1000]
BCF$_{biota}$	BCF for aquatic biota in regional/continental model	[m^3.kg^{-1}]	[l.kg^{-1}]	O^{c}		I-IIIb	
DEPTH$_{sed}$	sediment mixing depth	[m]	[m]	D	0.03	I-IIIb	[0,1e10]
SETTLRATE$_{susp}$	settling velocity of suspended solids	[m.d^{-1}]	[m.d^{-1}]	D	2.5	I-IIIb	[1,5]
SUSPPROD$_{water}$	(biogenic) production of suspended solids in water	[kg.d^{-1}]	[kg.d^{-1}]	D	0	I-IIIb	[0,0.01]
NETsedrate	net sedimentation rate	[m.d^{-1}]	[mm.yr^{-1}]	O*^{cd}		I-IIIb	
F$_{natural}$	area fraction of natural soil	[-]	[-]	D*	0.60	I-IIIb	[0,1]
DEPTH$_{natural}$	mixing depth natural soil	[m]	[m]	D	0.05	I-IIIb	[0.01,0.50]
F$_{agric}$	area fraction of agricultural soil	[-]	[-]	D*	0.27	I-IIIb	[0,1]
DEPTH$_{agric}$	mixing depth agricultural soil	[m]	[-]	D	0.2	I-IIIb	[0.01,0.50]
F$_{ind}$	area fraction of industrial/urban soil	[-]	[-]	D*	0.10	I-IIIb	[0,1]
DEPTH$_{ind}$	mixing depth industrial/urban soil	[m]	[m]	D	0.05	I-IIIb	[0.01,0.50]
Finf$_{soil}$	fraction of rain water infiltrating soil	[-]	[-]	D	0.25	I-IIIb	[0,1]
Frunoff$_{soil}$	fraction of rain water running off soil	[-]	[-]	D	0.25	I-IIIb	[0,1]
EROSION	soil erosion rate of regional system	[m.d^{-1}]	[mm.yr^{-1}]	D	0.03	I-IIIb	[0,10]
kasl$_{air}$	air-film partial mass-transfer coefficient (air-soil interface)	[m.d^{-1}]	[m.s^{-1}]	D	1.39.10^{-3}	I-III	[± factor 3]
kaw$_{air}$	air-film partial-mass transfer coefficient (air-water interface)	[m.d^{-1}]	[m.s^{-1}]	D	1.39.10^{-3}	I-III	[± factor 3]
kaw$_{water}$	water-film partial mass-transfer coefficient (air-water interface)	[m.d^{-1}]	[m.s^{-1}]	D	1.39.10^{-5}	I-III	[± factor 3]
kasl$_{soilair}$	soil-air partial mass-transfer coefficient (air-soil interface)	[m.d^{-1}]	[m.s^{-1}]	D	5.56.10^{-6}	I-III	[± factor 3]
kasl$_{soilwater}$	soilwater-water film partial mass-transfer coefficient (air-soil interface)	[m.d^{-1}]	[m.s^{-1}]	D	5.56.10^{-10}	I-III	[± factor 3]
kws$_{water}$	water-film partial mass-transfer coefficient (sediment-water interface)	[m.d^{-1}]	[m.s^{-1}]	D	2.78.10^{-6}	I-III	[± factor 3]
kws$_{sed}$	pore water partial mass-transfer coefficient (sediment-water interface)	[m.d^{-1}]	[m.s^{-1}]	D	2.78.10^{-8}	I-III	[± factor 3]

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Continental concentrations							
PECcont$_{water}$	continental PEC in surface water (dissolved)	[kg.m^{-3}]	[mg.l^{-1}]	O^c		I-IIIb	
PECcont$_{water,tot}$	continental PEC in surface water (total)	[kg.m^{-3}]	[mg.l^{-1}]	O^c		I-IIIb	
PECcont$_{air}$	continental PEC in air (total)	[kg.m^{-3}]	[mg.m^{-3}]	O^c		I-IIIb	
PECcont$_{agric}$	continental PEC in agricultural soil (total)	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c		I-IIIb	
PECcont$_{agric,porew}$	continental PEC in pore water of agricultural soils	[kg.m^{-3}]	[mg.l^{-1}]	O^c		I-IIIb	
PECcont$_{natural}$	continental PEC in natural soil (total)	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c		I-IIIb	
PECcont$_{ind}$	continental PEC in industrial soil (total)	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c		I-IIIb	
PECcont$_{sed}$	continental PEC in sediment (total)	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c		I-IIIb	
Regional concentrations							
PECreg$_{water}$	regional PEC in surface water (dissolved)	[kg.m^{-3}]	[mg.l^{-1}]	O		I-IIIb	
PECreg$_{air}$	regional PEC in air (total)	[kg.m^{-3}]	[mg.m^{-3}]	O		I-IIIb	
PECreg$_{agric}$	regional PEC in agricultural soil (total)	[kg.kg^{-1}]	[mg.kg^{-1}]	O		I-IIIb	
PECreg$_{agric,porew}$	regional PEC in pore water of agricultural soils	[kg.m^{-3}]	[mg.l^{-1}]	O		I-IIIb	
PECreg$_{natural}$	regional PEC in natural soil (total)	[kg.kg^{-1}]	[mg.kg^{-1}]	O		I-IIIb	
PECreg$_{ind}$	regional PEC in industrial soil (total)	[kg.kg^{-1}]	[mg.kg^{-1}]	O		I-IIIb	
PECreg$_{sed}$	regional PEC in sediment (total)	[kg.kg^{-1}]	[mg.kg^{-1}]	O		I-IIIb	
Local environmental concentrations							
Clocal$_{air}$	local concentration in air during emission episode	[kg.m^{-3}]	[mg.m^{-3}]	O		I-IIIa	
Clocal$_{air,ann}$	annual average concentration in air, 100 m from point source	[kg.m^{-3}]	[mg.m^{-3}]	O		IIIa	
Clocal$_{water}$	local concentration in surface water during emission episode	[kg.m^{-3}]	[mg.l^{-1}]	O		I-IIIa	
Clocal$_{water,ann}$	annual average local concentration in surface water during	[kg.m^{-3}]	[mg.l^{-1}]	O		IIIa	
Clocal$_{soil}$	local concentration in agric. soil averaged over 30 days	[kg.kg^{-1}]	[mg.kg^{-1}]	O		Ia	
Clocal$_{agric}$	local concentration in agric. soil averaged over 180 days	[kg.kg^{-1}]	[mg.kg^{-1}]	O		II-IIIa	
Clocal$_{grassland}$	local concentration in grassland averaged over 180 days	[kg.kg^{-1}]	[mg.kg^{-1}]	O		II-IIIa	
Fst-st$_{i}$	fraction of steady-state situation achieved in soil *i* {soil,agric,grassland}	[-]	[-]	O^c		I-IIIa	
PEClocal$_{air,ann}$	annual average local PEC in air (total)	[kg.m^{-3}]	[mg.m^{-3}]	O		IIIa	
PEClocal$_{water}$	local PEC during emission episode	[kg.m^{-3}]	[mg.l^{-1}]	O		I-IIIa	
PEClocal$_{water,ann}$	annual average local PEC in surface water (dissolved)	[kg.m^{-3}]	[mg.l^{-1}]	O		II-IIIa	
PEClocal$_{sed}$	local PEC in sediment during emission episode	[kg.kg^{-1}]	[mg.kg^{-1}]	O		Ia	
PEClocal$_{soil}$	local PEC in agric. soil (total) averaged over 30 days	[kg.kg^{-1}]	[mg.kg^{-1}]	O		Ia	
PEClocal$_{agric}$	local PEC in agric. soil (total) averaged over 180 days	[kg.kg^{-1}]	[mg.kg^{-1}]	O		II-IIIa	
PEClocal$_{grassland}$	local PEC in grassland (total) averaged over 180 days	[kg.kg^{-1}]	[mg.kg^{-1}]	O		II-IIIa	
PEClocal$_{agric,porew}$	local PEC in pore water of agricultural soil	[kg.m^{-3}]	[mg.l^{-1}]	O		IIIa	
PEClocal$_{grassland,porew}$	local PEC in pore water of grassland	[kg.m^{-3}]	[mg.l^{-1}]	O		IIIa	
PEClocal$_{grw}$	local PEC in groundwater under agricultural soil	[kg.m^{-3}]	[mg.l^{-1}]	O		IIIa	

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Parameters for local distribution							
Cstd$_{air}$	concentration in air at source strength 1 kg.d^{-1}	[kg.m^{-3}]	[mg.m^{-3}]	D	2.78.10^{-4}	I-IIIa	[1e-5,1e-3]
DEPstd$_{aer}$	standard deposition flux of aerosol-bound compounds at source strength of 1 kg.d^{-1}	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	D	1.10^{-2}	I-IIIa	[1e-3,0.1]
DEPstd$_{gas}$	deposition flux of gaseous compounds as function of Henry's Law coefficient, at source strength of 1 kg.d^{-1}	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	D	Table	I-IIIa	
DEPtotal	total deposition flux during emission episode	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O		I-IIIa	
DEPtotal$_{ann}$	annual average total deposition flux	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O		I-IIIa	
DILUTION	dilution factor	[-]	[-]	D/O^{cd}	10	I-IIIa	[1,1e5]
FLOW	flow rate of the river	[m^{3}.d^{-1}]	[m^{3}.d^{-1}]	D	18000	I-IIIa	[0,1e8]
DEPTH$_{soil}$	mixing depth of soil (for terrestrial ecosystem)	[m]	[m]	D	0.20	I-IIIa	[0.01,0.50]
DEPTH$_{agric}$	mixing depth of agricultural soil	[m]	[m]	D	0.20	I-III	[0.01,0.50]
DEPTH$_{grassland}$	mixing depth of grassland soil	[m]	[m]	D	0.10	I-IIIa	[0.01,0.50]
k$_{volat\ i}$	rate constant for volatilisation from soil *i*	[d^{-1}]	[d^{-1}]	O		I-IIIa	[0,0.7]
k$_{leach\ i}$	rate constant for leaching from soil *i*	[d^{-1}]	[d^{-1}]	O		I-IIIa	[0,0.7]
k$_{i}$	total rate constant for removal from top soil *i*	[d^{-1}]	[d^{-1}]	O		I-IIIa	[0,0.7]
D$_{air\ i}$	aerial deposition flux per kg of soil *i*	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	O^{c}		I-IIIa	
Cdep10$_{i}$	concentration in soil *i* due to sludge in 10th year at t=0	[kg.kg^{-1}]	[mg.kg^{-1}]	O^{c}		I-IIIa	
APPLsludge$_{soil}$	dry sludge application rate on soil	[kg.m^{-2}.yr^{-1}]	[kg.ha^{-1}.yr^{-1}]	D	5000	I-IIIa	[0,8000]
APPLsludge$_{agric}$	dry sludge application rate on agricultural soil	[kg.m^{-2}.yr^{-1}]	[kg.ha^{-1}.yr^{-1}]	D	5000	I-IIIa	[0,8000]
APPLsludge$_{grassland}$	dry sludge application rate on grassland	[kg.m^{-2}.yr^{-1}]	[kg.ha^{-1}.yr^{-1}]	D	1000	I-IIIa	[0,8000]
Facc$_{i}$	fraction accumulated in one year in soil *i*	[-]	[-]	O^{c}		I-IIIa	
Csludge1$_{i}$	concentration in soil *i* due to sludge in first year at t=0	[kg.kg^{-1}]	[mg.kg^{-1}]	O^{c}		I-IIIa	
Csludge10$_{i}$	concentration in soil *i* due to sludge in 10th year at t=0	[kg.kg^{-1}]	[mg.kg^{-1}]	O^{c}		I-IIIa	
Clocal10$_{i}$	initial concentration soil *i* (after 10 years)	[kg.kg^{-1}]	[mg.kg^{-1}]	O^{c}		I-IIIa	
T$_{soil}$	averaging time soil (for terrestrial ecosystem)	[d]	[d]	D	30	Ia	[1,100]
T$_{agric}$	averaging time agricultural soil	[d]	[d]	D	180	II-IIIa	[10,300]
T$_{grassland}$	averaging time grassland	[d]	[d]	D	180	II-IIIa	[10,300]
Clocal$_{i}$	average concentration in soil *i* over T days	[kg.kg^{-1}]	[mg.kg^{-1}]	O		I-IIaI	
Cinf$_{i}$	initial concentration in soil *i* in steady-state situation	[kg.kg^{-1}]	[mg.kg^{-1}]	O^{c}		I-IIIa	
Fst-st$_{i}$	fraction of steady-state situation achieved in soil *i*	[-]	[-]	O^{c}		I-IIIa	
Parameters for human and predator exposure via the environment							
BCF$_{fish}$	bioconcentration factor for fish	[m^{3}.kg^{-1}]	[l.kg^{-1}]	O		II-III	[1,1e5]
K$_{worm\text{-}porew}$	partition coefficient worm-porewater	[m^{3}.kg^{-1}]	[l.kg^{-1}]	O		II	[1,1e6]
BCF$_{worm}$	bioconcentration factor for earthworms	[kg.kg^{-1}]	[kg.kg^{-1}]	O		II	[0,100]
PEC$_{oral,fish}$	concentration in fish from surface water for predators	[kg.kg^{-1}]	[mg.kg^{-1}]	O		II	
PEC$_{oral,worm}$	local concentration in earthworms from agricultural soil	[kg.kg^{-1}]	[mg.kg^{-1}]	O		II	
Fwater$_{plant}$	volume fraction of water in plant tissue	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	D	0.65	III	[0.4,0.8]
Flipid$_{plant}$	volume fraction of lipids in plant tissue	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	D	0.01	III	[0.001,0.03]
Fair$_{plant}$	volume fraction of air in plant tissue	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	D	0.30	III	[0.20,0.40]
b	correction for differences between plant lipids and octanol	[-]	[-]	D	0.95	III	[0.9,1]
RHOplant	bulk density of plant tissue (wet weight)	[kg.m^{-3}]	[kg.l^{-1}]	D	0.7	III	[0.5,1]
kmetab$_{plant}$	rate constant for metabolism in plants	[d^{-1}]	[d^{-1}]	D	0	III	[0,0.7]

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$kphoto_{plant}$	rate constant for photolysis in plants	[d^{-1}]	[d^{-1}]	D	0	III	[0,0.7]
$kelim_{plant}$	rate constant for total elimination in plants	[d^{-1}]	[d^{-1}]	O^c		III	[0,0.7]
$K_{leaf-air}$	partition coefficient between leaves and air	[m^3.m^{-3}]	[m^3.m^{-3}]	O		III	[1,1e8]
$K_{plant-water}$	partition coefficient between plant tissue and water	[m^3.m^{-3}]	[m^3.m^{-3}]	O		III	[1,1e5]
TSCF	transpiration-stream concentration factor	[-]	[-]	O		III	[0,1]
$AREA_{plant}$	leaf surface area	[m^2]	[m^2]	D	5	III	[2,10]
g_{plant}	conductance (0.001 m.s^{-1})	[m.d^{-1}]	[m.s^{-1}]	D	0.001	III	[1e-4,0.01]
V_{leaf}	shoot volume	[m^3]	[l]	D	2	III	[1,4]
$kgrowth_{plant}$	rate constant for dilution by growth	[d^{-1}]	[d^{-1}]	D	0.035	III	[0.01,0.05]
Qtransp	transpiration stream	[m^3.d^{-1}]	[l.d^{-1}]	D	1	III	[0.5,2]
ALPHA	sink term of differential equation	[d^{-1}]	---	O^c		III	
$BETA_{agric}$	source term of differential equation, agricultural soil	[kg.m^{-3}.d^{-1}]	---	O^c		III	
$BETA_{grass}$	source term of differential equation, grassland	[kg.m^{-3}.d^{-1}]	---	O^c		III	
BAF_{meat}	bioaccumulation factor for meat	[d.kg^{-1}]	[d.kg^{-1}]	O		III	[1e-6,0.1]
BAF_{milk}	bioaccumulation factor for milk	[d.kg^{-1}]	[d.kg^{-1}]	O		III	[1e-6,0.1]
$ICdwt_{grass}$	daily intake for cattle of grass (dryweight)	[kg.d^{-1}]	[kg.d^{-1}]	D	16.9	III	[10,20]
$CONV_{grass}$	conversion factor grass from dryweight to wetweight	[kg.kg^{-1}]	[kg.kg^{-1}]	D	4	III	[2,6]
$ICdwt_{soil}$	daily intake of soil (dryweight)	[kg.d^{-1}]	[kg.d^{-1}]	D	0.41	III	[0.1,0.6]
IC_{grass}	daily intake for cattle of grass (wet weight)	[kg.d^{-1}]	[kg.d^{-1}]	O^{cd}		III	
IC_{soil}	daily intake for cattle of soil (wet weight)	[kg.d^{-1}]	[kg.d^{-1}]	O^{cd}		III	
IC_{air}	daily inhalation rate for cattle	[m^3.d^{-1}]	[m^3.d^{-1}]	D	122	III	[100,150]
IC_{drw}	daily intake of drinking water for cattle	[m^3.d^{-1}]	[l.d^{-1}]	D	55	III	[30,70]
F_{pur}	purification factor for surface water	[-]	[-]	D	Table	III	[0,1]
Parameters for humans							
IH_{drw}	daily intake of drinking water	[m^3.d^{-1}]	[l.d^{-1}]	D	2	III	[1,4]
IH_{fish}	daily intake of fish	[kg.d^{-1}]	[kg.d^{-1}]	D	0.115	III	[0,0.4]
IH_{leaf}	daily intake of leaf crops (incl. fruit and cereals)	[kg.d^{-1}]	[kg.d^{-1}]	D	1.20	III	[0,2]
IH_{root}	daily intake of root crops	[kg.d^{-1}]	[kg.d^{-1}]	D	0.384	III	[0,1]
IH_{meat}	daily intake of meat	[kg.d^{-1}]	[kg.d^{-1}]	D	0.301	III	[0,1]
IH_{milk}	daily intake of dairy products	[kg.d^{-1}]	[kg.d^{-1}]	D	0.561	III	[0,1]
IH_{air}	inhalation rate for humans	[m^3.d^{-1}]	[m^3.d^{-1}]	D	20	III-V	[5,30]
BIO_{oral}	bioavailability for oral uptake	[-]	[-]	D	1	III-V	[0,1]
BIO_{inh}	bioavailability for inhalation	[-]	[-]	D	0.75	III-V	[0,1]
BIO_{der}	bioavailability for dermal uptake	[-]	[-]	D	1	IV-V	[0,1]
BW	bodyweight of the human considered	[kg]	[kg]	D	70	III-V	[40,150]
Locally defined symbols in indirect exposure sub-module							
C_{agric}	total concentration in soil (wet weight)	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c		III	
C_{air}	total concentration in air	[kg.m^{-3}]	[mg.m^{-3}]	O^c		III	
C_{water}	concentration in surface water (dissolved)	[kg.m^{-3}]	[mg.l^{-1}]	O^c		III	
$C_{grassland}$	concentration in grassland soil	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c		III	
$C_{agric,porew}$	concentration in pore water of agricultural soil	[kg.m^{-3}]	[mg.l^{-1}]	O^c		III	

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$C_{grassland,porew}$	concentration in pore water of grassland soil	[kg.m^{-3}]	[mg.l^{-1}]	O^{c}		III	
C_{grw}	concentration in groundwater	[kg.m^{-3}]	[mg.l^{-1}]	O^{c}		III	
C_{fish}	concentration in wet fish	[kg.kg^{-1}]	[mg.kg^{-1}]	O^{c}		III	
$Croot_{plant}$	concentration in root tissue of plant	[kg.kg^{-1}]	[mg.kg^{-1}]	O^{c}		III	
C_{leaf}	concentration in leaves of plant	[kg.kg^{-1}]	[mg.kg^{-1}]	O^{c}		III	
C_{grass}	concentration in grass (wet weight)	[kg.kg^{-1}]	[mg.kg^{-1}]	O^{c}		III	
$Fleaf_{porew}$	fraction of total uptake by crops from porewater	[-]	[-]	O^{c}		III	
$Fleaf_{air}$	fraction of total uptake by crops from air	[-]	[-]	O^{c}		III	
$Fgrass_{porew}$	fraction of total uptake by grass from porewater	[-]	[-]	O^{c}		III	
$Fgrass_{air}$	fraction of total uptake by grass from air	[-]	[-]	O^{c}		III	
C_{drw}	concentration in drinking water	[kg.m^{-3}]	[mg.l^{-1}]	O^{c}		III	
C_{meat}	concentration in meat (wet weight)	[kg.kg^{-1}]	[mg.kg^{-1}]	O^{c}		III	
C_{milk}	concentration in milk (wet weight)	[kg.kg^{-1}]	[mg.kg^{-1}]	O^{c}		III	
$Fcattle_{i}$	fraction of total intake by cattle through medium *i* $i \in$ {grass,drw,air,grassland}	[-]	[-]	O^{c}		III	
$DOSE_{i}$	daily dose through intake of *i*	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	O^{c}		III	
$Fdose_{i}$	fraction of total dose through intake of medium *i* $i \in$ {drw,fish,leaf,root,meat,milk,air}	[-]	[-]	O^{c}		III	
$DOSE_{tot}$	total daily intake for humans	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	O^{c}		III	
Global variables indirect human exposure							
$Clocal_{fish}$	local concentration in wet fish	[kg.kg^{-1}]	[mg.kg^{-1}]	O		III	
$Creg_{fish}$	regional concentration in wet fish	[kg.kg^{-1}]	[mg.kg^{-1}]	O		III	
$Clocal_{leaf}$	local concentration in leaves of plant	[kg.kg^{-1}]	[mg.kg^{-1}]	O		III	
$Creg_{leaf}$	regional concentration in leaves of plant	[kg.kg^{-1}]	[mg.kg^{-1}]	O		III	
$Clocal_{root}$	local concentration in root tissue of plant	[kg.kg^{-1}]	[mg.kg^{-1}]	O		III	
$Creg_{root}$	regional concentration in root tissue of plant	[kg.kg^{-1}]	[mg.kg^{-1}]	O		III	
$Clocal_{grass}$	local concentration in grass (wet weight)	[kg.kg^{-1}]	[mg.kg^{-1}]	O		III	
$Creg_{grass}$	regional concentration in grass (wet weight)	[kg.kg^{-1}]	[mg.kg^{-1}]	O		III	
$Flocal\text{-}leaf_{porew}$	local fraction of total uptake by crops from pore water	[-]	[-]	O^{c}		III	
$Flocal\text{-}leaf_{air}$	local fraction of total uptake by crops from air	[-]	[-]	O^{c}		III	
$Flocal\text{-}grass_{porew}$	local fraction of total uptake by grass from pore water	[-]	[-]	O^{c}		III	
$Flocal\text{-}grass_{air}$	local fraction of total uptake by grass from air	[-]	[-]	O^{c}		III	
$Freg\text{-}leaf_{porew}$	regional fraction of total uptake by crops from pore water	[-]	[-]	O^{c}		III	
$Freg\text{-}leaf_{air}$	regional fraction of total uptake by crops from air	[-]	[-]	O^{c}		III	
$Freg\text{-}grass_{porew}$	regional fraction of total uptake by grass from pore water	[-]	[-]	O^{c}		III	
$Freg\text{-}grass_{air}$	regional fraction of total uptake by grass from air	[-]	[-]	O^{c}		III	
$Clocal_{meat}$	local concentration in meat (wet weight)	[kg.kg^{-1}]	[mg.kg^{-1}]	O		III	
$Creg_{meat}$	regional concentration in meat (wet weight)	[kg.kg^{-1}]	[mg.kg^{-1}]	O		III	
$Clocal_{milk}$	local concentration in milk (wet weight)	[kg.kg^{-1}]	[mg.kg^{-1}]	O		III	
$Creg_{milk}$	regional concentration in milk (wet weight)	[kg.kg^{-1}]	[mg.kg^{-1}]	O		III	
$Clocal_{drw}$	local concentration in drinking water	[kg.m^{-3}]	[mg.l^{-1}]	O		III	
$Creg_{drw}$	regional concentration in drinking water	[kg.m^{-3}]	[mg.l^{-1}]	O		III	

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
DOSElocal$_{tot}$	local total daily intake for humans	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	O		III	
DOSEreg$_{tot}$	regional total daily intake for humans	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	O		III	
Fleaf-local$_{porew}$	fraction of total uptake by crops from pore water	[-]	[-]	O^c		III	
Fleaf-reg$_{porew}$	fraction of total uptake by crops from pore water	[-]	[-]	O^c		III	
Fleaf-local$_{air}$	fraction of total uptake by crops from air	[-]	[-]	O^c		III	
Fleaf-reg$_{air}$	fraction of total uptake by crops from air	[-]	[-]	O^c		III	
Fgrass-local$_{porew}$	fraction of total uptake by grass from pore water	[-]	[-]	O^c		III	
Fgrass-reg$_{porew}$	fraction of total uptake by grass from pore water	[-]	[-]	O^c		III	
Fgrass-local$_{air}$	fraction of total uptake by grass from air	[-]	[-]	O^c		III	
Fgrass-reg$_{air}$	fraction of total uptake by grass from air	[-]	[-]	O^c		III	
Fcattle-local$_i$	fraction of total intake by cattle through medium *i*	[-]	[-]	O^c		III	
Fcattle-reg$_i$	fraction of total intake by cattle through medium *i*	[-]	[-]	O^c		III	
	$i \in$ {grass,drw,air,soil}						
Fdose-local$_i$	fraction of total dose through intake of medium *i*	[-]	[-]	O^c		III	
Fdose-reg$_i$	fraction of total dose through intake of medium *i*	[-]	[-]	O^c		III	
	$i \in$ {drw,fish,leaf,root,meat,milk,air}						
Exposure variables workers							
TEMPwork	average temperature on the workplace	[K]	[C]	D	20	V	[10,30]
-	specific questions on exposure (see decision trees Appendix V)			S		V	
W$_{der,worker}$	dermal weight of substance on the skin of workers	[kg.m^{-2}.d^{-1}]	[kg.cm^{-2}.d^{-1}]	O		V	
C1$_{inh,worker,vapour}$	vapour concentration in air for workers	[ppm]	[ppm]	O		V	
C$_{inh,worker,vapour}$	vapour concentration in air for workers	[kg.m^{-3}]	[mg.m^{-3}]	O		V	
C$_{inh,worker,fibre}$	fibre concentration in air for workers	[fibres.m^{-3}]	[fibres.m^{-3}]	O		V	
C$_{inh,worker,dust}$	dust concentration in air for workers	[kg.m^{-3}]	[mg.m^{-3}]	O		V	
U$_{der,pot,worker}$	potential dermal uptake for workers	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	O		V	
-	logfile of EASE			O		V	
AREA$_{der,worker}$	area of contact between substance and skin	[m^2]	[cm^{-2}]	S		V	
TH$_{der,worker}$	thickness of product	[m]	[cm]	D	0.01	V	
n$_{worker}$	mean number of events per day	[d^{-1}]	[d^{-1}]	S		V	
Exposure variables consumers							
Q$_{prod}$	amount of undiluted product used	[kg]	[mg]	S		IV	[0,1e7]
RHO$_{prod}$	density of product before dilution	[kg.m^{-3}]	[g.cm^{-3}]	S		IV	<0,5]
V$_{prod}$	volume of undiluted product used	[m^3]	[cm^3]	S		IV	<0,1e4]
V$_{appl}$	applicated/ingested volume of product	[m^3]	[cm^3]	S		IV	[0,1e4]
V$_{room}$	room volume	[m^3]	[m^3]	S		IV	[1,500]
F$_{oral}$	fraction of product swallowed	[-]	[-]	S		IV	[0,1]
F$_{resp}$	respirable fraction of inhaled substance	[-]	[-]	D	1	IV	[0,1]
T$_{contact}$	duration of exposure or contact	[d]	[d]	S		IV	[0,365]
Fc$_{prod}$	weight fraction of substance in product	[-]	[-]	S		IV	[0,1]
Fc$_{migr}$	fraction of substance migrating from article	[d^{-1}]	[h^{-1}]	S		IV	[0,1]
D	dilution factor	[-]	[-]	S		IV	[1,100]

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
C_{prod}	average concentration of substance in undiluted product	[kg.m^{-3}]	[mg.cm^{-3}]	S		IV	[0,∞>
$AREA_{art}$	surface area of article in contact with food	[m^{2}]	[cm^{2}]	S		IV	<0,1e5]
n	number of events	[d^{-1}]	[d^{-1}]	S		IV	[0,10]
TH_{art}	thickness of article in contact with food	[m]	[cm]	S		IV	<0,10]
C_{art}	concentration of substance in article	[kg.m^{-3}]	[mg.cm^{-3}]	S		IV	
TH_{der}	thickness of layer of product on skin	[m]	[cm]	D	0.01	IV	<0,1]
W_{der}	weight of substance on skin per event	[kg.m^{-2}]	[mg.cm^{-2}]	S		IV	
$AREA_{der}$	surface area of exposed skin	[m^{2}]	[cm^{2}]	P/S	Table	IV	<0,2e4]
C_{inh}	concentration in air of room	[kg.m^{-3}]	[mg.m^{-3}]	O		IV	
I_{inh}	inhalatory intake	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	O		IV	
C_{der}	average concentration of substance in product	[kg.m^{-3}]	[mg.cm^{-3}]	O		IV	
A_{der}	amount of substance on skin	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	O		IV	
$A_{migr,der}$	amount of substance on skin due to migration	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	O		IV	
$U_{der,pot}$	potential dermal uptake	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	O		IV	
C_{oral}	concentration in product swallowed	[kg.m^{-3}]	[mg.cm^{-3}]	O		IV	
I_{oral}	ingestion rate of substance	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	O		IV	
$C_{inh,ann}$	annual average inhalation exposure concentration	[kg.m^{-3}]	[mg.m^{-3}]	O		IV	
$C_{der,ann}$	annual average dermal exposure concentration	[kg.m^{-3}]	[mg.m^{-3}]	O		IV	
$C_{oral,ann}$	annual average oral exposure concentration	[kg.m^{-3}]	[mg.m^{-3}]	O		IV	
U_{tot}	total uptake via different routes for one product	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	O		IV	
Micro-organism effects assessment							
$EC50_{micro}$	EC50 for micro-organisms in a STP	[kg.m^{-3}]	[mg.l^{-1}]	S		I	[1e-5,1e5]
$EC10_{micro}$	EC10 for micro-organisms in a STP	[kg.m^{-3}]	[mg.l^{-1}]	S		I	[1e-5,1e5]
$NOEC_{micro}$	NOEC for micro-organisms in a STP	[kg.m^{-3}]	[mg.l^{-1}]	S		I	[1e-5,1e5]
---	specific bacterial population?	[yes/no]	[yes/no]	S		I	{yes,no}
TOXmicro	toxicological data used for extrapolation of PNEC	[kg.m^{-3}]	[mg.l^{-1}]	O		I	[1e-5,1e5]
AFmicro	assessment factor applied in extrapolation of PNEC	[-]	[-]	O		I	[1,1000]
Aquatic effects assessment							
$LC50aqua_{i}$	LC50 for aquatic organisms, trophic level *i*	[kg.m^{-3}]	[mg.l^{-1}]	S		I	[1e-5,1e5]
$NOECaqua_{i}$	NOEC for aquatic organisms, trophic level *i* $i \in \{1,2,3,4\}$	[kg.m^{-3}]	[mg.l^{-1}]	S		I	[1e-5,1e5]
TOXaqua	toxicological data used for extrapolation of PNEC	[kg.m^{-3}]	[mg.l^{-1}]	O		I	[1e-5,1e5]
AFaqua	assessment factor applied in extrapolation of PNEC	[-]	[-]	O		I	[1,1000]
AVG_{aqua}	average of all log-transformed aquatic NOECs	[-]	[-]	O^{c}		I	
STD_{aqua}	standard deviation of all log-transformed aquatic NOECs	[-]	[-]	O^{c}		I	
E_{aqua}	extrapolation constant dependent on sample size	[-]	[-]	D^{c}	Table	I	

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Terrestrial effects assessment							
LC50terr$_i$	LC50 for terrestrial organisms, trophic level *i*	[kg.kg^{-1}]	[mg.kg^{-1}]	S		I	
NOECterr$_i$	NOEC for terrestrial organisms, trophic level *i*	[kg.kg^{-1}]	[mg.kg^{-1}]	S		I	
	$i \in \{1,2,3,4\}$						
TOXterr	toxicological data used for extrapolation of PNEC	[kg.kg^{-1}]	[mg.kg^{-1}]	O		I	
AFterr	assessment factor applied in extrapolation of PNEC	[-]	[-]	O		I	
EPterr	equilibrium partitioning used for PNEC in soil?	[yes/no]	[yes/no]	O^c		I	
AVG$_{terr}$	average of all log-transformed terrestrial NOECs	[-]	[-]	O^c		I	
STD$_{terr}$	standard deviation of all log-transformed terrestrial NOECs	[-]	[-]	O^c		I	
E$_{terr}$	extrapolation constant dependent on sample size	[-]	[-]	D^c	Table	I	
Sediment effects assessment							
EPsed	equilibrium partitioning used for PNEC in sediment?	[yes/no]	[yes/no]	O^c		I	
Input bird / mammalian effects data							
LC50$_{bird}$	LC50 in avian dietary study (5 days)	[kg.kg^{-1}]	[mg.kg^{-1}]	S		II	
LD50$_{mammal,oral}$	oral LD50 for mammals	[kg.kg^{-1}]	[mg.kg^{-1}]	S		II-V	
DD$_{mammal,oral}$	oral Discriminating Dose for mammals	[kg.kg^{-1}]	[mg.kg^{-1}]	S		IV,V	
LD50$_{mammal,der}$	dermal LD50 for mammals	[kg.kg^{-1}]	[mg.kg^{-1}]	S/O		IV,V	
LC50$_{mammal,inh}$	inhalatory LC50 for mammals	[kg.m^{-3}]	[mg.m^{-3}]	S/O		IV,V	
NOAEL$_{man,oral,acute}$	oral NOAEL for man after acute exposure	[kg.kg^{-1}]	[mg.kg^{-1}]	S		IV,V	
LOAEL$_{man,oral,acute}$	oral LOAEL for man after acute exposure	[kg.kg^{-1}]	[mg.kg^{-1}]	S		IV,V	
NOAEL$_{man,inh,acute}$	inhalatory NOAEL for man after acute exposure	[kg.m^{-3}]	[mg.m^{-3}]	S/O		IV,V	
LOAEL$_{man,inh,acute}$	inhalatory LOAEL for man after acute exposure	[kg.m^{-3}]	[mg.m^{-3}]	S/O		IV,V	
NOAEL$_{man,der,acute}$	dermal NOAEL for man after acute exposure	[kg.kg^{-1}]	[mg.kg^{-1}]	S/O		IV,V	
LOAEL$_{man,der,acute}$	dermal LOAEL for man after acute exposure	[kg.kg^{-1}]	[mg.kg^{-1}]	S/O		IV,V	
NOEC$_{man,medium,acute}$	dermal NOEC in a medium for man after acute exposure	[kg.m^{-3}]	[mg.cm^{-3}]	S		IV,V	
LOEC$_{man,medium,acute}$	dermal LOEC in a medium for man after acute exposure	[kg.m^{-3}]	[mg.cm^{-3}]	S		IV,V	
NOEC$_{bird}$	NOEC for birds	[kg.kg^{-1}]	[mg.kg^{-1}]	S/O		II	
NOEC$_{mammal,food,chr}$	NOEC via food for mammals exposed (sub)chronically	[kg.kg^{-1}]	[mg.kg^{-1}]	S/O		II-IV	
LOEC$_{mammal,food,chr}$	LOEC via food for mammals exposed (sub)chronically	[kg.kg^{-1}]	[mg.kg^{-1}]	S/O		II-IV	
NOAEL$_{bird}$	NOAEL for birds	[kg.kg.d^{-1}]	[mg.kg^{-1}.d^{-1}]	S		II	
NOAEL$_{mammal,oral,chr}$	oral NOAEL for mammals exposed (sub)chronically	[kg.kg.d^{-1}]	[mg.kg^{-1}.d^{-1}]	S/O		II-V	
NOAEL$_{man,oral,chr}$	oral NOAEL for man exposed (sub)chronically	[kg.kg.d^{-1}]	[mg.kg^{-1}.d^{-1}]	S		III-V	
LOAEL$_{mammal,oral,chr}$	oral LOAEL for mammals exposed (sub)chronically	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	S/O		II-V	
LOAEL$_{man,oral,chr}$	oral LOAEL for man exposed (sub)chronically	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	S		III-V	
NOAEL$_{mammal,inh,chr}$	inhalatory NOAEL for mammals exposed (sub)chronically	[kg.m^{-3}]	[mg.m^{-3}]	S/O		IV-V	
LOAEL$_{mammal,inh,chr}$	inhalatory LOAEL for mammals exposed (sub)chronically	[kg.m^{-3}]	[mg.m^{-3}]	S/O		IV-V	
NOAEL$_{man,inh,chr}$	inhalatory NOAEL for man exposed (sub-)chronically	[kg.m^{-3}]	[mg.m^{-3}]	S/O		IV-V	
LOAEL$_{man,inh,chr}$	inhalatory LOAEL for man exposed (sub-)chronically	[kg.m^{-3}]	[mg.m^{-3}]	S/O		IV-V	
NOAEL$_{mammal,der,chr}$	dermal NOAEL for mammals exposed (sub)chronically	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	S/O		IV-V	
LOAEL$_{mammal,der,chr}$	dermal LOAEL for mammals exposed (sub)chronically	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	S/O		IV-V	
NOAEL$_{man,der,chr}$	dermal NOAEL for man exposed (sub)chronically	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	S/O		IV-V	

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$LOAEL_{man,der,chr}$	dermal LOAEL for man exposed (sub)chronically	[kg.kg^{-1}.d^{-1}]	[mg.kg^{-1}.d^{-1}]	S/O		IV-V	
$NOEC_{man,medium,chr}$	dermal NOEC in a medium for man exposed (sub)chronically	[kg.m^{-3}]	[mg.cm^{-3}]	S		IV-V	
$LOEC_{man,medium,chr}$	dermal LOEC in a medium for man exposed (sub)chronically	[kg.m^{-3}]	[mg.cm^{-3}]	S		IV-V	
$NOAEL_{mammal,inh,fibre,chr}$	inhalatory NOAEL for mammals exposed to fibers (sub-)chronically	[fibers.m^{-3}]	[fibers.m^{-3}]	S		V	
$LOAEL_{mammal,inh,fibre,chr}$	inhalatory LOAEL for mammals exposed to fibers (sub-)chronically	[fibers.m^{-3}]	[fibers.m^{-3}]	S		V	
$NOAEL_{man,inh,fibre,chr}$	inhalatory NOAEL for man exposed to fibers (sub-)chr.	[fibers.m^{-3}]	[fibers.m^{-3}]	S		V	
$LOAEL_{man,inh,fibre,chr}$	inhalatory LOAEL for man exposed to fibers (sub-)chr.	[fibers.m^{-3}]	[fibers.m^{-3}]	S		V	
T_{bird}	duration of (sub-)chronic test with birds	[d]	[d]	P		II	
T_{mammal}	duration of (sub-)chronic test with mammals	[d]	[d]	P		II	
$CONV_{bird}$	conversion factor NOAEL to NOEC for birds	[kg.d.kg^{-1}]	[kg.d.kg^{-1}]	S		II	
$CONV_{mammal}$	conversion factor NOAEL to NOEC for mammals	[kg.d.kg^{-1}]	[kg.d.kg^{-1}]	P/S	Table	II-V	
TOXoral	toxicological data used for extrapolation of PNEC	[kg.kg^{-1}]	[mg.kg^{-1}]	O		II	
AForal	assessment factor applied in extrapolation of PNEC	[-]	[-]	O		II	
PNECs							
$PNEC_{water}$	PNEC for aquatic organisms	[kg.m^{-3}]	[mg.l^{-1}]	O^c		I	
$PNEC_{micro-organisms}$	PNEC for micro-organisms in a STP	[kg.m^{-3}]	[mg.l^{-1}]	O^c		I	
$PNEC_{oral}$	PNEC for secondary poisoning of birds and mammals	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c		II	
$PNEC_{soil}$	PNEC for terrestrial organisms	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c		I	
$PNEC_{soil,ep}$	PNEC for terrestrial organisms derived by eq. part.	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c		I	
$PNEC_{sed}$	PNEC for sediment-dwelling organisms	[kg.kg^{-1}]	[mg.kg^{-1}]	O		I	
$PNEC_{sed,ep}$	PNEC for sediment-dwelling organisms derived by eq. part.	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c		I	
$PNECstat_{water}$	PNEC for aquatic organisms with statistical method	[kg.m^{-3}]	[mg.l^{-1}]	O^c		I	
$PNECstat_{soil}$	PNEC for terrestrial organisms with statistical method	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c		I	
Risk characterisation ratios environment							
$RCRlocal_{water}$	RCR for the local water compartment	[-]	[-]	O^c		Ia	
$RCRreg_{water}$	RCR for the regional water compartment	[-]	[-]	O^c		Ib	
$RCRlocal_{soil}$	RCR for the local soil compartment	[-]	[-]	O^c		Ia	
$RCRreg_{soil}$	RCR for the regional soil compartment	[-]	[-]	O^c		Ib	
$RCRlocal_{sed}$	RCR for the local sediment compartment	[-]	[-]	O^c		Ia	
$RCRreg_{sed}$	RCR for the regional sediment compartment	[-]	[-]	O^c		Ib	
RCR_{stp}	RCR for the sewage treatment plant	[-]	[-]	O^c		Ia	
$RCR_{oral,fish}$	RCR for fish-eating birds and mammals	[-]	[-]	O^c		II	
$RCR_{oral,worm}$	RCR for worm-eating birds and mammals	[-]	[-]	O^c		II	
Risk characterisation ratios workers							
$RCR_{worker,inh,vapour}$	MOS for worker exposed by inhalation of vapour	[-]	[-]	O^c		V	
$RCR_{worker,inh,fibre}$	MOS for worker exposed inhalation of fibers	[-]	[-]	O^c		V	
$RCR_{worker,inh,dust}$	MOS for worker exposed inhalation of dust	[-]	[-]	O^c		V	
$RCR_{worker,der}$	MOS for worker exposed dermally	[-]	[-]	O^c		V	

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Risk characterisation ratios consumers							
$RCRacute_{cons,inh}$	MOS acute, exposed by inhalation	[-]	[-]	O^c		IV	
$RCRacute_{cons,der}$	MOS acute, exposed dermally	[-]	[-]	O^c		IV	
$RCRacute_{cons,oral}$	MOS acute, exposed orally	[-]	[-]	O^c		IV	
$RCRacute_{cons,tot}$	MOS acute, total exposure	[-]	[-]	O^c		IV	
$RCRchronic_{cons,inh}$	MOS chronic, exposed by inhalation	[-]	[-]	O^c		IV	
$RCRchronic_{cons,der}$	MOS chronic, exposed dermally	[-]	[-]	O^c		IV	
$RCRchronic_{cons,oral}$	MOS chronic, exposed orally	[-]	[-]	O^c		IV	
$RCRchronic_{cons,tot}$	MOS chronic, total exposure	[-]	[-]	O^c		IV	
Risk chracterisation ratios man exposed via the environment							
$RCRlocal_{man-env,tot}$	MOS local, total exposure via all media	[-]	[-]	O^c		III	
$RCRlocal_{man-env,inh}$	MOS local, exposure via air	[-]	[-]	O^c		III	
$RCRreg_{man-env,tot}$	MOS regional, total exposure via all media	[-]	[-]	O^c		III	
$RCRreg_{man-env.inh}$	MOS regional, exposure via air	[-]	[-]	O^c		III	

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Application input							
-	scenario choice for agricultural pesticides	[-]	[-]	P		B	
-	scenario choice for biocides	[-]	[-]	P		B	
DOSE$_{pest}$	single dosage for pesticide	[kg.m^{-2}]	[kg.ha^{-1}]	S	1	B	[0,2000]
DOSE$_{pest,gh}$	single dosage in case of pesticide in greenhouse	[kg]	[kg]	S	1	B	[0,2000]
DOSE$_{max}$	apparent maximum dosage	[kg.m^{-2}]	[kg.ha^{-1}]	O		B	
DOSE$_{wood}$	dosage of a.i. per m^2 of wood	[kg.m^{-2}]	[kg.m^{-2}]	O		B	
N$_{appl}$	number of applications in one year	[-]	[-]	S	1	B	[1,52]
T$_{interval}$	application interval	[d]	[d]	S	1	B	[1,52]
N$_{lt}$	number of application periods per registration period	[-]	[-]	S	9	B	[1,520]
T$_{interval\text{-}lt}$	long term interval for application periods	[d]	[d]	S	365	B	[365,3650]
AMOUNTspray	amount of spray liquid used	[m^3.m^{-2}]	[l.ha^{-1}]	S	400	B	[200,1500]
DRAINS	is drainage present?	[yes/no]	[yes/no]	P	no	B	
MIX	mixing with soil	[yes/no]	[yes/no]	P	no	B	
---	choice of crop and growing stage	[-]	[-]	P		B	
F$_{int}$	fraction of dosage intercepted by crops	[-]	[-]	O		B	[0,1]
F$_{air}$	fraction of dosage emitted to air	[-]	[-]	O		B	[0,1]
F$_{soil}$	fraction of dosage that reaches the soil	[-]	[-]	O		B	[0,1]
---	choice of application	[-]	[-]	P		B	
F$_{drift}$	fraction drift related to location and way of application	[-]	[-]	O		B	[0,1]
---	choice of reduction measure	[-]	[-]	P		B	
REDUCTION	reduction measure applicable?	[yes/no]	[yes/no]	P		B	
Fred$_{drift}$	fraction emission reduction for drift	[-]	[-]	O		B	[0,1]
T$_{bird}$	test duration for bird toxicity test	[d]	[d]	S	28	B	[1,730]
T$_{mammal}$	test duration for mammalian toxicity test	[d]	[d]	S	28	B	[1,730]
Season	choice of season (spring/autumn)	[spring/autumn]	[spring/autumn]	P		B	
Characteristics of application soil							
Fwater$_{satsoil}$	volume fraction of water in saturated soil	[m^3.m^{-3}]	[m^3.m^{-3}]	D	0.4	I-III	[0,0.7]
Fwater$_{pest}$	volume fraction of water in application soil	[m^3.m^{-3}]	[m^3.m^{-3}]	D	0.2	B	[0,0.7]
Fsolid$_{pest}$	volume fraction of solids in application soil	[m^3.m^{-3}]	[m^3.m^{-3}]	D	0.6	B	[0.3,0.7]
Fair$_{pest}$	volume fraction of air in application soil	[m^3.m^{-3}]	[m^3.m^{-3}]	D	0.2	B	[0,0.7]
Foc$_{pest}$	weight fraction of organic carbon in application soil	[kg.kg^{-1}]	[kg.kg^{-1}]	D	0.029	B	[0.01,0.20]
Fom$_{pest}$	weight fraction of organic matter in application soil	[kg.kg^{-1}]	[kg.kg^{-1}]	D	0.05	B	[0.01,0.30]
RHO$_{satsoil}$	wet bulk density of saturated soil	[kg.m^{-3}]	[kg.l^{-1}]	O^{cd}		I-III	
RHO$_{pest}$	wet bulk density of application soil	[kg$_{wwt}$.m^{-3}]	[kg.l^{-1}]	O^{c}		B	
DEPTH$_{pest}$	mixing depth of application soil	[m]	[m]	O		B	[0.01,0.50]
Characateristics of ditch							
Fom$_{ditch}$	weight fraction organic matter in suspended matter of ditch	[kg.kg^{-1}]	[kg.kg^{-1}]	D	0.085	B	[0.01,0.30]
DEPTH$_{ditch}$	depth of ditch	[m]	[m]	D	0.30	B	[0.1,5]
DILUTION$_{ditch}$	dilution factor ditch to surface water (river)	[-]	[-]	D	10	B	[1,1000]
DILUTION$_{drai}$	dilution factor for drainage water reaching the surface water	[-]	[-]	D	10	B	[1,1000]

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
DT50$_{advec}$	half-lifetime for advection	[d]	[d]	D	50	B	[1,1e4]
SETTLRATE$_{ditch}$	settling velocity of suspended particles	[m.d^{-1}]	[m.d^{-1}]	D	3	B	[0.1,30]
WIDTH$_{ditch}$	width of ditch	[m]	[m]	D	1	B	[0.5,5]
AREA$_{ditch}$	cross section of water layer in ditch	[m^{2}]	[m^{2}]	D	0.21	B	[0.1,1]
DEPTH$_{ditch,pest}$	depth of ditch	[m]	[m]	O		B	
SUSP$_{water}$	concentration suspended solids in the ditch	[kg.m^{-3}]	[mg.l^{-1}]	D	15	B	[1,100]
TEMPwater	default temperature of water compartment	[10/12°C]	[10/12°C]	P		B	
TEMPwater$_{test}$	temperature of water compartment under test conditions	[°C]	[°C]	D	20	B	
TEMP$_{TOXSWA}$	temperature of water compartment in TOXSWA	[283K]	[10°C]	D		B	
Partitioning and degradation							
Kom	organic matter-water partition coefficient	[m^{3}.kg^{-1}]	[l.kg^{-1}]	O			[1,1e6]
Kp$_{pest}$	solids-water partition coefficient in application soil	[m^{3}.kg^{-1}]	[l.kg^{-1}]	O		B	[0.01,1e5]
K$_{pest-water}$	total soil-water partition coefficient in application soil	[m^{3}.m^{-3}]	[m^{3}.m^{-3}]	O^{c}		B	
Fdiss$_{ditch}$	fraction of the chemical in the water phase of the ditch	[-]	[-]	O^{c}		B	
Foc$_{susp,pest}$	weight fraction of organic carbon in suspended matter for pesticides	[kg.kg^{-1}]	[kg.kg^{-1}]	D	0.0294	B	[0.01,0.2]
Fom$_{susp,pest}$	weight fraction of organic matter in suspended matter for pesticides	[kg.kg^{-1}]	[kg.kg^{-1}]	D	0.050	B	[0.01,0.30]
Koc	organic carbon-water partition coefficient	[m^{3}.kg^{-1}]	[l.kg^{-1}]	O		B	
Kp$_{susp,pest}$	solids-water partition coefficient in suspended matter for pesticides	[m^{3}.kg^{-1}]	[l.kg^{-1}]	O		B	
K$_{air-water}$	air-water partition coefficient	[-]	[-]	O^{c}			
Distribution water							
VOLAT$_{ditch}$	overall mass transfer coefficient for volatilization referenced to water	[m.d^{-1}]	[m.d^{-1}]	O		B	
kaw-pest$_{water}$	partial mass transfer coeff. at the water-side of the air-water interface	[m.d^{-1}]	[m.d^{-1}]	O		B	
kaw-pest$_{air}$	partial mass transfer coeff. at the air-side of the air-water interface	[m.d^{-1}]	[m.d^{-1}]	O		B	
k$_{volat}$	first order rate constant for volatilisation	[d^{-1}]	[d^{-1}]	O		B	
k$_{advec}$	first order rate constant for advection in the ditch	[d^{-1}]	[d^{-1}]	O		B	
k$_{sedim}$	first order rate constant for sedimentation	[d^{-1}]	[d^{-1}]	O		B	
k$_{resusp}$	first order rate constant for resuspention	[d^{-1}]	[d^{-1}]	O		B	
k$_{ditch}$	total rate constant for removal in the ditch	[d^{-1}]	[d^{-1}]	O		B	
E$_{avg}$	average emission during the year as result of drift	[kg.d^{-1}.m^{-3}]	[kg.d^{-1}.m^{-3}]	O^{c}		B	
k$_{ditch-365}$	removal rate constant in ditch during one year	[d^{-1}]	[d^{-1}]	O		B	
Cwater$_{pest-1\ appl}$	concentration in surface water after one application	[kg.m^{-3}]	[mg.l^{-1}]	O		B	
Cwater$_{drift-365}$	annual average concentration in ditch year as result of drift	[kg.m^{-3}]	[mg.l^{-1}]	O		B	
C$_{drai}$	concentration in drainage water	[kg.m^{-3}]	[mg.l^{-1}]	O		B	
C$_{shallow\ grw}$	concentration in shallow ground water (PESTLA)	[kg.m^{-3}]	[mg.l^{-1}]	O		B	
Cwater$_{drai-365}$	total concentration in surface water as result of drainage	[kg.m^{-3}]	[mg.l^{-1}]	O		B	
F$_{rw}$	fraction of the chemical remaining in water after one interval	[-]	[-]	O^{c}			
DT50$_{water}$	half-life time for degradation in water (under test conditions)	[d]	[d]	S		B	
DT50$_{water,temp}$	half-life time for degradation in water corrected for the temperature	[d]	[d]	O		B	
kdeg$_{water}$	first order rate constant for degradation in surface water	[d^{-1}]	[d^{-1}]	O		B	
kdeg$_{water,temp}$	temperature dependent rate constant for degradation in water	[d^{-1}]	[d^{-1}]	O		B	
k$_{volat,temp}$	temperature dependent first order rate constant for volatilisation in ditch	[d^{-1}]	[d^{-1}]	O		B	
k$_{ditch,temp}$	temperature dependent total rate constant for removal in the ditch	[d^{-1}]	[d^{-1}]	O		B	

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Distribution soil							
$Csoil_{pest\text{-}1\ appl}$	concentration in application soil after one application	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Csoil_{pest\text{-}0,lt}$	peak concentration in soil after long-term applications	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c			
$Csoil_{pest\text{-}1}$	concentration in plough layer after 1 year	[kg.kg^{-1}]	[kg.kg^{-1}]	O^c			
F_{rs}	fraction of the concentration remaining in soil after one interval	[-]	[-]	O^c			
F_{lt}	fraction of the concentration remaining after time $T_{interval,lt}$	[-]	[-]	O^c			
$Csoil_{std,pest\text{-}1}$	standard concentration in plough layer after one year	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c			
F_{bound}	fraction of bound residues at end of metabolism study	[-]	[-]	S			
$Cres\_bound_{pest\text{-}1}$	concentration of bound residues after 1 year	[kg.m^{-3}]	[kg.m^{-3}]	O^c			
Distribution sediment							
$Csed_{pest\text{-}0,lt}$	peak concentration in sediment after long-term applications	[kg.kg^{-1}]	[mg.kg^{-1}]	O^c			
F_{lts}	fraction of the concentration remaining in sediment after long-term interval	[-]	[-]	O^c			
Distribution air							
$Estd_{field,\ air,\ 1h}$	standard 1 hour emission strength of the field	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$Estd_{field,\ air,\ 24h}$	standard 24 hour emission strength of the field	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$Estd_{greenhouse,air,1h}$	standard 1 hour emission strength of the greenhouse	[kg.d^{-1}]	[mg.d^{-1}]	O			
$Estd_{greenhouse,air,24h}$	standard 24 hour emission strength of the greenhouse	[kg.d^{-1}]	[mg.d^{-1}]	O			
$E_{field,air,1h}$	1 hour emission strength of the field	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$E_{field,air,24h}$	24 hour emission strength of the field	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$E_{greenhouse,air,1h}$	1 hour emission strength of the greenhouse	[kg.d^{-1}]	[mg.d^{-1}]	O			
$E_{greenhouse,air,24h}$	24 hour emission strength of the greenhouse	[kg.d^{-1}]	[mg.d^{-1}]	O			
$Cstd_{field,air,1h}$	1 hour avg. concentration at downwind of field with standard source	[kg.m^{-3}]	[kg.m^{-3}]	D	1.28e-4		
$Cstd_{greenhouse,air,1h}$	1 hour avg. concentration from greenhouse with standard source strength	[kg.m^{-3}]	[mg.m^{-3}]	O			
$C_{field,air,1h}$	1 hour averaged conc. at 10 meters downwind of field	[kg.m^{-3}]	[mg.m^{-3}]	O			
$C_{greenhouse,air,1h}$	1 hour averaged conc. in the lee side eddy of the greenhouse	[kg.m^{-3}]	[mg.m^{-3}]	O			
K	coefficient dependent on wind direction to front of greenh.	[-]	[-]	D	0.2		
A	area of standard greenhouse perpendicular to wind direction	[m^{2}]	[m^{2}]	D	350		
u	windspeed at the roof top	[m.d^{-1}]	[m.s^{-1}]	D	3		
P_{1h}	1 hour averaged precipitation intensity	[m.d^{-1}]	[m.d^{-1}]	D	0.060		
P_{24h}	24 hours averaged precipitation intensity	[m.d^{-1}]	[m.d^{-1}]	D	0.015		
$DEPRATE_{dry}$	dry deposition velocity	[m.d^{-1}]	[m.s^{-1}]	D	0.001		
$DEPstd_{gas\text{-}dry,field,1h}$	standard 1 hour avg. dry deposition flux for field application	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$DEPstd_{gas\text{-}dry,greenhouse,1h}$	standard 1 hour avg. dry deposition flux for greenhouse	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$DEP_{gas\text{-}dry,\ field,1h}$	1 hour averaged dry deposition flux for field application	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$DEP_{gas\text{-}dry,\ greenhouse,1h}$	1 hour averaged dry deposition flux for greenhouse	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$DEP_{gas\text{-}dry,\ field,24h}$	24 hour averaged dry deposition flux for field application	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$DEP_{gas\text{-}dry,\ greenhouse,24h}$	24 hour averaged dry deposition flux for greenhouse	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$DEP_{gas\text{-}wet,field,1h}$	1 hour averaged wet deposition flux downwind of field	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$DEP_{gas\text{-}wet,field,24h}$	24 hours averaged wet deposition flux downwind of field	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$DEP_{gas\text{-}wet,greenhouse,1h}$	1 hour averaged wet dep. flux downwind for greenhouse	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$DEP_{gas\text{-}wet,greenhouse,24h}$	24 hours averaged wet dep. flux downwind for greenhouse	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$DEP_{total,field,1h}$	1 hour averaged total deposition flux downwind of field	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$DEP_{total,field,24h}$	24 hours averaged total deposition flux downwind of field	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$DEP_{total,greenhouse,1h}$	1 hour averaged total dep. flux downwind of greenhouse	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
$DEP_{total,greenhouse,24h}$	24 hours averaged total dep. flux downwind of greenhouse	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	O			
Pesticide-specific exposure concentrations							
$Cwater_{pest-0}$	peak concentration in water (dissolved)	[kg.m^{-3}]	[mg.l^{-1}]	O			
$Cwater_{pest-4}$	average concentration in ditch over 4 days (dissolved)	[kg.m^{-3}]	[mg.l^{-1}]	O			
$Cwater_{pest-7}$	average concentration in ditch over 7 days (dissolved)	[kg.m^{-3}]	[mg.l^{-1}]	O			
$Cwater_{pest-21}$	average concentration in ditch over 21 days (dissolved)	[kg.m^{-3}]	[mg.l^{-1}]	O			
$Cwater_{pest-28}$	average concentration in ditch over 28 days (dissolved)	[kg.m^{-3}]	[mg.l^{-1}]	O			
$Cwater_{pest-Tbird}$	average concentration in the ditch over T_{bird} days (dissolved)	[kg.m^{-3}]	[mg.l^{-1}]	O			
$Cwater_{pest-Tmammal}$	average concentration in the ditch over T_{mammal} days (dissolved)	[kg.m^{-3}]	[mg.l^{-1}]	O			
$Cwater_{pest-365}$	annual average concentration in ditch	[kg.m^{-3}]	[mg.l^{-1}]	O			
C_{river}	average concentration in a river for human exposure	[kg$_c$.m^{-3}]	[mg.l^{-1}]	O			
$Csoil_{pest-0}$	peak concentration in soil after applications	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Csoil_{pest-28}$	average concentration in application soil over 28 days	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Csoil_{pest-Tbird}$	average concentration in soil over T_{bird} days	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Csoil_{pest-Tmammal}$	average concentration in soil over T_{mammal} days	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Csoil_{pest-lt}$	soil concentration after long-term application	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Csoil_{pest-10}$	peak concentration in plough layer after 10 years	[kg.m^{-3}]	[kg.m^{-3}]	O			
$Csoil_{pest-11}$	peak concentration in plough layer after 11 years	[kg.m^{-3}]	[kg.m^{-3}]	O			
$Csoil_{pest-12}$	peak concentration in plough layer after 12 years	[kg.m^{-3}]	[kg.m^{-3}]	O			
$Csed_{pest-7}$	average concentration in sediment over 7 days	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Csed_{pest-14}$	average concentration in sediment over 14 days	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Csed_{pest-28}$	average concentration in sediment over 28 days	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Csed_{pest-lt}$	sediment concentration after long-term application	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Cstd_{shallow\ grw}$	standard concentration in upper groundwater	[(kg.m^{-3})/(kg.m^{-2})]		O			
$Cgrw_{pest}$	concentration in ground water	[kg.m^{-3}]	[mg.l^{-1}]	O			
$Cwater_{pest-T}$	average concentration in water over *T* days	[kg$_c$.m^{-3}]	[mg$_c$.l^{-1}]	O			
$Cwater_{pest-standard}$	total conc. resulting from input of 1 mg m^{-2} at water surface	[kg$_c$.m^{-3}]	[mg$_c$.l^{-1}]	D	4.76		[0.5,50]
$Cwater_{pest-1appl}$	total concentration in ditch after one application	[kg$_c$.m^{-3}]	[mg$_c$.l^{-1}]	O			
$Cwater_{pest-T,spring}$	concentration in ditch over T days in spring	[kg$_c$.m^{-3}]	[mg$_c$.l^{-1}]	O			
$Cwater_{pest-T,autumn}$	concentration in ditch over T days in autumn	[kg$_c$.m^{-3}]	[mg$_c$.l^{-1}]	O			
Discharge via settling tank on a sewage treatment plant							
$DOSE_{cell}$	dosage per cell	[kg.cell^{-1}]	[kg.cell^{-1}]	O^c			
SUMDOSE	total dosage	[kg]	[kg]	O^c			
$AREA_{cell}$	area of one cell	[m^2.cell^{-1}]	[m^2.cell^{-1}]	D	200		
N_{cells}	number of cells	[cell]	[cell]	D	5		
$Temission_{stp}$	emission period for discharge to STP	[d]	[d]	D	25		
Agricultural pesticides used in amenity use							
$Cwater_{au}$	water concentration for amenity use scenario (total)	[kg.m^{-3}]	[mg.l^{-1}]	O			

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Paved areas							
w_{pavem}	discharge coefficient pavement	[-]	[-]	D	0.8		
$WIDTH_d$	width of paved dike or slope	[m]	[m]	D	4		
$WIDTH_{water\ d}$	width of city water course	[m]	[m]	D	10		
$DEPTH_{water\ d}$	depth of city water course	[m]	[m]	D	1.5		
V_{rain}	volume of rain flowing into separated sewage system	$[m^3]$	$[m^3]$	O^c			
i_{rain}	rain intensity, worst case situation	[m]	[m]	D	0.007		
$AREAroofs_L$	surface of roofs in model town (Lelystad)	$[m^2]$	$[m^2]$	D	$1.2.10^6$		
$AREApavem_L$	surface of pavements (excl. roofs) in model town (Lelystad)	$[m^2]$	$[m^2]$	D	$3.0.10^6$		
w_{roof}	discharge coefficient roof	[-]	[-]	D	0.9		
$AREAtreat_L$	treated area of pavements in model town (Lelystad)	$[m^2]$	$[m^2]$	O^c			
$C_{rainflow}$	concentration in discharged rain water	$[kg_c.m^{-3}]$	$[mg.l^{-1}]$	O^c			
$DILUTION_{ss}$	dilution factor for stagnant surface water	[-]	[-]	D	3		
$AREAroofs_R$	surface of roofs in model town (Raamsdonk-Dorp)	$[m^2]$	$[m^2]$	D	$3.83.10^3$		
$AREApavem_R$	surface of pavements (excl. roofs) in model town (Raamsdonk-Dorp)	$[m^2]$	$[m^2]$	D	$7.77.10^3$		
F_{treat}	fraction treated area	[-]	[-]	D	0.9		
$AREAtreat_R$	treated area of pavements in model town (Raamsdonk-Dorp)	$[m^2]$	$[m^2]$	O^c			
$AREAroofs_D$	surface of roofs in model area (Dongemond)	$[m^2]$	$[m^2]$	D	$1.82.10^6$		
$AREApavem_D$	surface of pavements (excl. roofs) in model area (Dongemond)	$[m^2]$	$[m^2]$	D	$3.69.10^6$		
F_{dry}	fraction dry weather in spring campaign	[-]	[-]	D	0.1		
$AREAtreat_D$	treated area of pavements in model area (Dongemond)	$[m^2]$	$[m^2]$	O^c			
DWA_{day}	daily dry weather flow of STP	$[m^3.d^{-1}]$	$[m^3.d^{-1}]$	D	16000		
F_{DWA}	fraction dry weather discharge during storm event	[-]	[-]	D	0.1		
$Ftime_{DWA}$	fraction of time for dry weather discharge	[d]	[d]	D	0.33		
DWA	dry weather flow in model area	$[m^3.d^{-1}]$	$[l.d^{-1}]$	O^c			
C_{infl}	influent concentration STP	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O^c			
$Fpur_{pest}$	purification factor STP	[-]	[-]	S	0		[0,1]
$DILUTION_{ls}$	dilution factor for large surface water with low flow	[-]	[-]	D	10		
Plantations							
$Ftreat_p$	fraction treated area	[-]	[-]	D	0.5		
$Fdrift_p$	fraction drift	[-]	[-]	D	0.01		
$DEPTH_{water\ p}$	depth of city water course	[m]	[m]	D	0.25		
Water courses							
-	direct application to water course?	[yes/no]	[yes/no]	P	no		
$Fdrift_w$	fraction drift	[-]	[-]	D	0.1		
$DEPTH_{water\ w}$	depth of city water course	[m]	[m]	D	0.25		
Paved dike bodies and slopes							
SPOT	spotwise application	[yes/no]	[yes/no]	P			
$Ftreat_s$	fraction surface application	[-]	[-]	O			
$Fdrift_s$	fraction drift	[-]	[-]	D	0.1		
$DEPTH_{water\ s1}$	depth of city water course	[m]	[m]	D	2		

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$DEPTH_{water\ s2}$	depth of small water course	[m]	[m]	D	0.25		
$WIDTH_{s}$	width of paved dike or slope	[m]	[m]	D	4		
$WIDTH_{water\ s3}$	width of receiving surface water (large river)	[m]	[m]	D	10		
$DEPTH_{water\ s3}$	depth of water (large river)	[m]	[m]	D	2		
$WIDTH_{water\ s4}$	width of receiving surface water (small river)	[m]	[m]	D	2		
$DEPTH_{water\ s4}$	depth of water (small river)	[m]	[m]	D	0.25		
Application of pesticides for seed treatment							
$DOSE_{pest\_particle}$	dosage pesticide for seed treatment	[$kg_{c}.m^{-2}$]	[$kg_{c}.ha^{-1}$]	S/O			[0,2000]
MIX_{soil}	mixing of seed with soil	[yes/no]	[yes/no]	D/S			
DRAINS	drainage present	[yes/no]	[yes/no]	D/S			
$RAD_{particle}$	radius seed	[m]	[m]	D/S			[0.0001-0.01]
$RAD_{influence,particle}$	radius range of influence seed	[m]	[m]	D	0.05		[0.005-0.1]
$RADtotal_{influence,particle}$	total radius range of influence seed	[m]	[m]	O			
CONSTANT	constant belonging to a sphere or half a sphere	[-]	[-]	O			
$V_{soil,influence,particle}$	volume soil of range of influence seed	[m^{3}]	[m^{3}]	O			
$Nparticle_{area}$	number of seed per m^{2}	[m^{-2}]	[ha^{-1}]	S			[5e4,7e7]
$V_{soil,influence,particle}$	volume soil of range of influence seed	[m^{3}]	[m^{3}]	O			
$Vsoil_{max\_particle}$	maximum volume soil of range of influence seed	[$m^{3}.m^{-2}$]	[$m^{3}.ha^{-1}$]	D	500		
$Vsoil_{total\_particle}$	total volume soil of range of influence seed	[$m^{3}.m^{-2}$]	[$m^{3}.ha^{-1}$]	O			
Cparticle	concentration of pesticide in granules or treated seed	[$kg_{c}.kg_{par}^{-1}$]	[$mg.kg^{-1}$]	S/O			
WEIGHTparticle	weight of one granule or treated seed	[$kg_{part}.part^{-1}$]	[$mg_{c}.kg_{part}^{-1}$]	S/O			
$Nparticle_{weight}$	Number of granules or seed per kg	[kg_{part}^{-1}]	[kg_{part}^{-1}]	S/O			
$Nparticle_{area}$	number of granules or seed per m^{2}	[m^{-2}]	[m^{-2}]	S/O			
Application of non-agricultural pesticides (processing in UC 39)							
Private use of human hygiene biocidal products							
Nlocal	number of inhabitants feeding one STP	[eq]	[eq]	D	10,000		
$F_{4,water}$	fraction released to wastewater	[-]	[-]	D	1		
$Cform_{volume}$	active substance in product	[$kg_{c}.m^{-3}$]	[$g_{c}.l^{-1}$]	S			
$Cform_{weight}$	active substance in product	[$kg.kg^{-1}$]	[$g.kg^{-1}$]	S			
-	type of product	[-]		P			
$Vform_{inh}$	consumption per inhabitant	[$m^{3}.d^{-1}$]	[$ml.d^{-1}$]	O			
$Qform_{inh}$	consumption per inhabitant	[$kg.d^{-1}$]	[$g.d^{-1}$]	O			
$Vform_{appl}$	consumption per application	[m^{3}]	[ml]	O			
$Qform_{appl}$	consumption per application	[kg]	[g]	O			
Nappl	number of applications	[-]	[-]	O			
Finh	fradtion of inhabitants using the product	[-]	[-]	O			
Fpenetr	Penetration factor of disinfectant	[-]	[-]	D	0.5		
RHOform	Specific density of product	[$kg.m^{-3}$]	[$kg.m^{-3}$]	D	1000		

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Industrial use of human hygiene biocidal products							
Nbeds$_{pres}$	number of beds in model hospital	[-]	[-]	D	400		
Foccup	occupancy rate	[-]	[-]	D	0.75		
Nbeds$_{occup}$	number of occupied beds in model hospital	[-]	[-]	D	300		
F$_{3,water}$	fraction released to wastewater	[-]	[-]	D	1		
-	specification of type of active ingredient used	[-]	[-]	P			
Qsubst$_{pres\_bed}$	consumption of active ingredient per bed	[kg.d^{-1}]	[g.d^{-1}]	O			
-	specification of type of active ingredient used	[-]	[-]	P			
Qsubst$_{occup\_bed}$	consumption of active ingredient per occupied bed	[kg.d^{-1}]	[g.d^{-1}]	O			
Disinfectants in swimming water, discharged to STP							
AREA$_{swimw}$	water surface	[m^2]	[m^2]	D	440		
DEPTH$_{swimw}$	average depth of water	[m]	[m]	D	1.8		
N$_{visit}$	number of visitors per day	[-]	[-]	D	400		
C$_{swimw}$	concentration in swimming water	[kg.m^{-3}]	[mg.l^{-1}]	S			
Q$_{repl}$	water replaced per visitor	[m^3]	[m^3]	D	0.05		
Temission$_{swimw,ac}$	number of emission days 'acute'	[d]	[d]	D	2		
Temission$_{swimw,chr}$	number of emission days 'acute'	[d]	[d]	D	300		
Disinfectants in swimming water, discharged to surface water							
POOLTYPE	type of swimming pool	[public/private]	[public/private]	P	public		
DILUTION$_{public}$	dilution factor of receiving surface water public pools	[-]	[-]	D	4		
DILUTION$_{private}$	dilution factor of receiving surface water private pools	[-]	[-]	D	2		
Private use of disinfectant used for sanitary purposes							
Nlocal	Number of inhabitants feeding one STP	[-]	[-]	D	10,000		
F$_{4,water}$	Fraction released to waste water	[-]	[-]	D	1		
Cform	concentration active substance in biocidal product	[kg.m^{-3}]	[g.l^{-1}]	S			
Fpenetr	Penetration factor of disinfectant	[-]	[-]	D	0.5		
-	type of application	[-]	[-]	P			
Vform	Consumption per capita	[m^3.cap^{-1}.d^{-1}]	[m^3.cap^{-1}.d^{-1}]	O			
Disinfectants in horticulture							
Qsubst	amount of active ingredient used	[kg]	[kg]	S			
Fret	fraction of retention in goods	[-]	[-]	D	0.02		
Fdisin	fraction of disintegration	[-]	[-]	D	0.001		
Temission$_{fogging}$	number of emission days for fogging	[d]	[d]	D	1		
Biocides used in medical sector, sanitary purposes							
Fsan	fraction released to waste water for sanitary purposes	[-]	[-]	D	0.55		
Fobj	fraction released to waste water for brushes	[-]	[-]	D	0.95		
Cproc$_{san}$	concentration at which active substance is used, sanitary purposes	[kg.m^{-3}]	[kg.l^{-1}]	S			
Cproc$_{obj}$	concentration at which active substance is used, brushes	[kg.m^{-3}]	[kg.l^{-1}]	S			
Vcons$_{san}$	amount of water with active substance, sanitary purpose	[m^3.d^{-1}]	[l.d^{-1}]	D	25		

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$Vcons_{obj}$	amount of water with active substance, brushes	$[m^3.d^{-1}]$	$[l.d^{-1}]$	D	25		
Biocides used in medical sector, disinfection of instruments in washers							
Cproc	working concentration of active ingredient	$[kg.m^{-3}]$	$[g.l^{-1}]$	S			
$Nmax_{mach}$	number of washers or disinfectors	[-]	[-]	D	3		
-	type of washer	[-]	[-]	P			
Vproc	volume of solution in machine	$[m^3]$	[l]	O			
$Tint_{repl}$	Replacement interval	[d]	[d]	D	14		
Fcarry-over	Fraction carry-over	[-]	[-]	D	0.015		
$kdeg_{disinf}$	Rate constant for chemical conversion	$[d^{-1}]$	$[d^{-1}]$	S/D	0		
Biocides used in medical sector, disinfection of instruments in baths							
$Tint_{repl}$	average time disinfection solution is in use (replacement interval)	[d]	[d]	O			
Qsubst	amount of active substance used	$[kg.d^{-1}]$	$[kg.yr^{-1}]$	D	250		
$Temission_3$	emission day, i.e., replacements	$[d^{-1}]$	$[d^{-1}]$	D	100		
$kdeg_{disinf}$	rate constant for chemical conversion	$[d^{-1}]$	$[d^{-1}]$	S/D	0		
Biocides used in medical sector, disinfection of laundry in washing streets							
Nmach	number of washing tubes (with disinfectant)	[-]	[-]	D	3		
Qmat	capacity of washing tube	$[kg.d^{-1}]$	$[kg.d^{-1}]$	D	8000		
$Vform_{kg}$	amount of disinfectant for laundry	$[m^3.kg^{-1}]$	$[l.kg^{-1}]$	S			
Cform	concentration of active substance in disinfectant solution	$[kg.m^{-3}]$	$[kg.l^{-1}]$	S			
Fred	concentration reduction in washing process	[-]	[-]	D	0		
Biocides used in medical sector, disinfection of laundry in tumbler washing machines							
Nbatch	number of batches	$[d^{-1}]$	$[d^{-1}]$	D	3		
Qmat	capacity of machines	[kg]	[kg]	D	25		
$Vform_{kg}$	amount of disinfectant for laundry	$[m^3.kg^{-1}]$	$[l.kg^{-1}]$	S			
Cform	concentration of active substance in disinfectant solution	$[kg.m^{-3}]$	$[kg.l^{-1}]$	S			
Fred	concentration reduction in washing process	[-]	[-]	D	0		
Disinfectants for sewage and waste water							
$Clocal_{eff}$	working concentration of the active substance in effluent	$[kg.m^{-3}]$	$[mg.l^{-1}]$	S			
DILUTION	dilution factor for receiving surface water	[-]	[-]	D	10		
$Clocal_{water}$	concentration in receiving surface water	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
In-can preservatives, washing and cleaning fluids, human hygiene products and cosmetics							
Nlocal	number of inhabitants feeding one STP	[eq]	[eq]	D	10,000		
$F_{4,water}$	fraction released to wastewater	[-]	[-]	D	1		
$Cform_{volume}$	active substance in product	$[kg_c.m^{-3}]$	$[g_c.l^{-1}]$	S			
$Cform_{weight}$	active substance in product	$[kg.kg^{-1}]$	$[g.kg^{-1}]$	S			
-	type of product	[-]	[-]	P			
$Vform_{inh}$	consumption per inhabitant	$[l.d^{-1}]$	$[ml.d^{-1}]$	O			
$Qform_{inh}$	consumption per inhabitant	$[kg.d^{-1}]$	$[g.d^{-1}]$	O			

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$Vform_{appl}$	consumption per application	[l]	[ml]	O			
$Qform_{appl}$	consumption per application	[kg]	[g]	O			
Nappl	number of applications	[d^{-1}]	[-]	O			
Finh	fraction of inhabitants using the product	[-]	[-]	O			
Fpenetr	fraction of inhabitants using the product	[-]	[-]	D	0.5		
RHOform	specific density of product	[kg.m^{-3}]	[kg.m^{-3}]	D	1000		
In-can preservatives, paints and coatings, waste treatment							
$Fsubst\_prod_i$	fraction of biocide (by weight) in the product	[-]	[-]	D	0.02		
$Qreg\_prod_i$	quantity of product i in the region	[kg.d^{-1}]	[ktonnes.yr^{-1}]	D	210		
$Fpres\_prod_i$	fraction of product with a biocid added	[-]	[-]	D	0.8		
$Fpenetr_i$	penetration factor	[-]	[-]	D	0.25		
$Fdiff_i$	fraction lost due to diffuse releases	[-]	[-]	D	0.25		
$Fdeg_i$	fraction lost due to degradation	[-]	[-]	D	0		
$Flandf_i$	fraction of product waste landfilled	[-]	[-]	D	0.75		
$Flandf_{total}$	fraction of (total) waste landfilled	[-]	[-]	D	0.6		
Qwaste_reg	total quantity of waste in the region	[kg.d^{-1}]	[ktonnes.yr^{-1}]	D	11880		
$Qsubst\_reg_i$	quantity of biocide for application in product *i* in total waste in the region	[kg.d^{-1}]	[kg.yr^{-1}]	O			
$Csubst\_landf_i$	ìnitial concentration of biocide in landfilled waste	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
In-can preservatives, fluids used in paper production, drying sections							
Vform	quantity of product with preservative applied per quantity of paper	[m^{3}.kg^{-1}]	[l.tonne^{-1}]	S			
Cform	concentration fo active substance in the biocidal product	[kg.m^{-3}]	[g.l^{-1}]	S			
Qsubst	quantity of active substance applied per quantity of paper	[kg.kg^{-1}]	[kg.tonne^{-1}]	S/O			
-	type of paper produced	[-]	[-]	P			
Qpaper	quantity of coated paper produced per day	[kg.d^{-1}]	[tonnes.d^{-1}]	O			
VP	vapour pressure	[Pa]	[Pa]	S			
Fevap	fraction evaporated	[-]	[-]	O			
In-can preservatives, fluids used in paper production, broke							
Vform	quantity of product with preservative applied per quantity of paper	[m^{3}.kg^{-1}]	[l.tonne^{-1}]	S			
Cform	concentration fo active substance in the biocidal product	[kg.m^{-3}]	[g.l^{-1}]	S			
Qsubst	quantity of active substance applied per quantity of paper	[kg.kg^{-1}]	[kg.tonne^{-1}]	S/O			
-	type of paper produced	[-]	[-]	P			
Qpaper	quantity of coated paper produced per day	[kg.d^{-1}]	[tonnes.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			
In-can preservatives, fluids used in paper production, paper recycling							
TONNAGE	relevant tonnage in EU for this application	[kg.d^{-1}]	[tonnes.yr^{-1}]	S			
TONNAGEreg	relevant tonnage in the region for this application	[kg.d^{-1}]	[tonnes.yr^{-1}]	S/O			
$Fprodvol_{reg}$	fraction for the region	[-]	[-]	D	0.1		
$Fmainsource_5$	fraction of the main source (local STP)	[-]	[-]	D	0.1		

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
-	type of paper recycled	[-]	[-]	P			
Frec	fraction of paper recycled	[-]	[-]	O	0.5		
Fdeink	fraction of preservatives released at deinking	[-]	[-]	D	1		
Fdecomp	fraction decomposed during deinking	[-]	[-]	D	0		
-	degree of solubility	[-]	[-]	P			
Fprelim	fraction removed from waste water during preliminary on-site treatment	[-]	[-]	O			
Nwdays	number of working days	[d]	[d.yr^{-1}]	D	320		
In-can preservatives, fluids used in textile production							
Vform$_i$	quantity of fluid applied per quantity of fibres / fabric for treatment step i	[m^3.kg^{-1}]	[l.tonne^{-1}]	S			
Cform$_i$	concentration fo active substance in the biocidal product for treatment step i	[kg.m^{-3}]	[mg.l^{-1}]	S			
Qsubst$_i$	quantity of active substance applied per quantity of fibres for treatment step i	[kg.kg^{-1}]	[kg.tonne^{-1}]	S/O			
-	type of fibre produced	[-]	[-]	P			
Qfibres	quantity of fibres / fabrics treated per day	[kg.d^{-1}]	[tonnes.d^{-1}]	O			
Ffix	fixation fraction	[-]	[-]	D	0		
Elocal_water$_i$	local emission of active substance to waste water for treatment step i	[kg$_c$.d^{-1}]	[kg$_c$.d^{-1}]	O			
In-can preservatives, fluids used in leather production							
Vform$_i$	quantity of fluid applied per quantity of fibres / fabric for treatment step i	[m^3.kg^{-1}]	[l.tonne^{-1}]	S			
Cform$_i$	concentration fo active substance in the biocidal product for treatment step i	[kg.m^{-3}]	[mg.l^{-1}]	S			
Qsubst$_i$	quantity of active substance applied per quantity of fibres for treatment step i	[kg.kg^{-1}]	[kg.tonne^{-1}]	S/O			
-	type of fibre produced	[-]	[-]	P			
Qleather	quantity of raw hides treated per day	[kg.d^{-1}]	[tonnes.d^{-1}]	O	15		
Ffix	fixation fraction	[-]	[-]	D	0		
Elocal_water$_i$	local emission of active substance to waste water for treatment step i	[kg$_c$.d^{-1}]	[kg$_c$.d^{-1}]	O			
Film preservatives, glues and adhesives, waste treatment							
Fsubst_prod$_i$	fraction of biocide (by weight) in the product	[-]	[-]	D	0.003		
Qreg_prod$_i$	quantity of product i in the region	[kg.d^{-1}]	[ktonnes.yr^{-1}]	D			
Fpres_prod$_i$	fraction of product with a biocid added	[-]	[-]	D	0.8		
Fpenetr$_i$	penetration factor	[-]	[-]	D	0.25		
Fdiff$_i$	fraction lost due to diffuse releases	[-]	[-]	D			
Fdeg$_i$	fraction lost due to degradation	[-]	[-]	D	0		
Flandf$_i$	fraction of product waste landfilled	[-]	[-]	D	0.75		
Flandf$_{total}$	fraction of (total) waste landfilled	[-]	[-]	D	0.6		
Qwaste_reg	total quantity of waste in the region	[kg.d^{-1}]	[ktonnes.yr^{-1}]	D	11880		

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Qsubst_reg$_i$	quantity of biocide for application in product *i* in total waste in the region	[kg.d^{-1}]	[kg.yr^{-1}]	O			
Csubst_landf$_i$	initial concentration of biocide in landfilled waste	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
Film preservatives, paper and cardboard production, drying sections							
Qform	quantity of product with preservative applied per quantity of paper	[kg.kg^{-1}]	[kg.tonne^{-1}]	S			
Vform	volume of product with preservative applied per quantity of paper	[m^3.kg^{-1}]	[l.tonne^{-1}]	S			
Cform$_{solid}$	concentration fo active substance in the biocidal product	[kg.kg^{-1}]	[g.kg^{-1}]	S			
Cform$_{liquid}$	concentration fo active substance in the biocidal product	[kg.m^{-3}]	[g.l^{-1}]	S			
Qsubst	quantity of active substance applied per quantity of paper	[kg.kg^{-1}]	[kg.tonne^{-1}]	S/O			
-	type of paper produced	[-]	[-]	P			
Qpaper	quantity of coated paper produced per day	[kg.d^{-1}]	[tonnes.d^{-1}]	O			
VP	vapour pressure	[Pa]	[Pa]	S			
Fevap	fraction evaporated	[-]	[-]	O			
Fdecomp	fraction decomposing during drying	[-]	[-]	D	0		
Film preservatives, paper and cardboard production, broke							
Qform	quantity of product with preservative applied per quantity of paper for each application step	[kg.kg^{-1}]	[kg.tonne^{-1}]	S			
Vform	volume of product with preservative applied per quantity of paper for each application step	[m^3.kg^{-1}]	[l.tonne^{-1}]	S			
Cform$_{solid}$	concentration fo active substance in the biocidal product	[kg.kg^{-1}]	[g.kg^{-1}]	S			
Cform$_{liquid}$	concentration fo active substance in the biocidal product	[kg.m^{-3}]	[g.l^{-1}]	S			
Qsubst	quantity of active substance applied per quantity of paper	[kg.kg^{-1}]	[kg.tonne^{-1}]	S/O			
Fbroke	fraction of coated broke produced compared to overall production	[-]	[-]	D	0.2		
Ffix	fixation fraction	[-]	[-]	D	0		
-	type of paper produced	[-]	[-]	P			
Qpaper	quantity of coated paper produced per day	[kg.d^{-1}]	[tonnes.d^{-1}]	O			
Fclosure	degree of closure of the water system	[-]	[-]	O			
Film preservatives, paper and cardboard production, recycling							
TONNAGE	relevant tonnage in EU for this application	[kg.d^{-1}]	[tonnes.yr^{-1}]	S			
TONNAGEreg	relevant tonnage in the region for this application	[kg.d^{-1}]	[tonnes.yr^{-1}]	S/O			
Fprodvol$_{reg}$	fraction for the region	[-]	[-]	D	0.1		
Fmainsource$_5$	fraction of the main source (local STP)	[-]	[-]	D	0.1		
-	type of paper recycled	[-]	[-]	P			
Frec	fraction of paper recycled	[-]	[-]	O			
Fdeink	fraction of preservatives released at deinking	[-]	[-]	D	1		
Fdecomp	fraction decomposed during deinking	[-]	[-]	D	0		
-	degree of solubilty	[-]	[-]	P			
Fprelim	fraction removed from waste water during preliminary on-site treatment	[-]	[-]	O			
Nwdays	number of working days	[d]	[d.yr^{-1}]	D	320		

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Creosote impregnation							
$Q_{mater,creos}$	quantity of wood impregnated	$[m^3.d^{-1}]$	$[m^3.d^{-1}]$	S	50		
Q_{creos}	quantity of creosote per m^3 wood	$[kg.m^{-3}]$	$[kg.m^{-3}]$	S	80		
F_{creos}	fraction of substance in creosote	[-]	[-]	S	0.05		
$F_{ws,creos}$	fraction released to water/soil	[-]	[-]	O			
$F_{w,creos}$	fraction to waste water	[-]	[-]	S	0.99		
$F_{a,creos}$	fraction released to air	[-]	[-]	O			
$F_{s,creos}$	fraction released to soil	[-]	[-]	O^c			
D_{wood}	storage density of treated wood per m^2	$[m^3.m^{-2}]$		S	0.76		
$Temission_{creos}$	number of emission days for creosote impregnation	[d]	[d]	D	250		
$T_{interval,creos}$	application interval for creosote impregnation	[d]	[d]	D	70		
$N_{appl,creos}$	number of applications in one year for creosote impregnation	[-]	[-]	D	5		
Salt impregnation							
$Q_{mater,salt}$	quantity of wood impregnated	$[m^3.d^{-1}]$	$[m^3.d^{-1}]$	S	50		
Q_{salt}	quantity of salt per m^3 wood	$[kg.m^{-3}]$	$[kg.m^{-3}]$	S	2		
$F_{ws,salt}$	fraction released to water/soil	[-]	[-]	S	0.0001		
$F_{w,salt}$	fraction released to waste water	[-]	[-]	S	0.99		
$F_{s,salt}$	fraction released to soil	[-]	[-]	O^c			
$D_{wood,salt}$	storage density of treated wood per m^2	$[m^3.m^{-2}]$	$[m^3.m^{-2}]$	S	0.76		
$Temission_{salt}$	number of emission days for salt impregnation	[d]	[d]	D	250		
$T_{interval,salt}$	application interval for salt impregnation	[d]	[d]	D	36		
$N_{appl,salt}$	number of applications in one year for salt impregnation	[-]	[-]	D	10		
Drenching and dipping							
$Q_{mater,drench}$	quantity of wood impregnated	$[m^3.d^{-1}]$	$[m^3.d^{-1}]$	S	2		
$Q_{ai,drench}$	quantity of a.i. per m^3 wood	$[kg.m^{-3}]$	$[kg.m^{-3}]$	S	1		
$F_{ws,drench}$	fraction released to water/soil	[-]	[-]	S	0.0005		
$F_{w,drench}$	fraction released to waste water	[-]	[-]	S	0.9		
$F_{s,drench}$	fraction released to soil	[-]	[-]	O^c			
$D_{wood,drench}$	storage density of treated wood per m^2	$[m^3.m^{-2}]$	$[m^3.m^{-2}]$	S	0.76		
$F_{a,drench}$	fraction released to air	[-]	[-]	O			
$Temission_{drench}$	number of emission days for drenching	[d]	[d]	D	50		
$T_{interval,drench}$	application interval for drenching	[d]	[d]	D	35		
$N_{appl,drench}$	number of applications in one year for drenching	[-]	[-]	D	10		
Remedial timber treatment in buildings							
$F_{ai,remed}$	fraction of a.i. in formulation	[-]	[-]	S			
$APPL_{solid}$	solid application rate of formulation	$[kg.m^{-2}]$	$[kg.m^{-2}]$	S			
$APPL_{fluid}$	fluid application rate of formulation	$[m^3.m^{-2}]$	$[l.m^{-2}]$	S			
RHO_{form}	density	$[kg.m^{-3}]$	$[kg.l^{-1}]$	S			
Leaching from impregnated wood to surface water							
$DEPTH_{wway}$	waterway depth	[m]	[m]	D	1.5		

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$WIDTH_{wway}$	waterway width	[m]	[m]	D	5		
TAU_{wway}	residence time of waterway water	[d]	[d]	D	20		
$DIAM_{pole}$	diameter of poles	[m]	[m]	D	0.1		
N_{pole}	number of poles per meter (both sides)	[m^{-1}]	[m^{-1}]	D	5		
$AREA_{leach}$	leaching surface of impregnated wood per meter model waterway	[m^{2}.m^{-1}]	[m^{2}.m^{-1}]	O^{c}			
$Cwater_{pest,eq}$	equilibrium concentration in waterway	[kg.m^{-3}]	[mg.l^{-1}]	O^{c}			
a	regression constant a (from curve fitting)	[-]	[-]	S			
e^{b}	regression constant e^{b} (from curve fitting)	[-]	[-]	S			
$FLUX_{avg}$	mean flux of compound over a certain period	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	S			
Leaching from impregnated wood to groundwater							
$FLUX_{comp}$	mean flux of compound	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	S			
$AREA_{leach}$	leaching area	[m^{2}]	[m^{2}]	O^{c}			
$DEPTH_{pole}$	part of pole in saturated zone	[m]	[m]	D	0.1		
RAD_{pole}	radius of pole	[m]	[m]	D	0.05		
Q_{pole}	amount of substance leached over 1 year	[kg]	[kg]	O^{c}			
V_{soil}	volume of soil around pole	[m^{3}]	[m^{3}]	O^{c}			
RAD_{soil}	radius of soil area	[m]	[m]	D	0.1		
$F_{influence}$	fraction influenced area per ha	[-]	[-]	O^{c}			
M_{soil}	soil mass around pole	[kg]	[kg]	O^{c}			
V_{pore}	pore water volume around pole	[m^{3}]	[m^{3}]	O^{c}			
C_{porew}	concentration of leached substance in porewater	[kg.m^{-3}]	[kg.m^{-3}]	O			
Leaching from impregnated wood to soil							
$DEPTH_{fence}$	depth of soil layer	[m]	[m]	D	0.05		
$WIDTH_{fence}$	width of soil layer	[m]	[m]	D	0.025		
$HEIGHT_{fence}$	height of the fence	[m]	[m]	D	2		
$LENGTH_{fence}$	length of fence	[m]	[m]	D	1		
T_{rain}	number of days with leaching	[d]	[d]	D	35		
$FLUX_{fence}$	mean flux of compound over 1 year	[kg.m^{-2}.d^{-1}]	[mg.m^{-2}.d^{-1}]	S			
$AREA_{fence}$	leaching surface of impregnated fence per m length	[m^{2}]	[m^{2}]	O^{c}			
Q_{fence}	quantity leached per m length of fence	[kg$_{c}$]	[kg]	O^{c}			
V_{soil}	volume of soil around fence	[m^{3}]	[m^{3}	O^{c}			
M_{soil}	soil mass around fence	[kg]	[kg]	O^{c}			
V_{pore}	pore water volume around fence	[m^{3}]	[m^{2}]	O^{c}			
C_{porew}	concentration in porewater of soil	[kg.m^{-3}]	[kg.m^{-3}]	O			
Wood preservatives at landfilling							
-	type of biocide/preservative	[-]	[-]	P			
$Qsubst\_prep_{i}$	quantity of biocide for application in preparation i in total waste	[kg.d^{-1}]	[ktonnes.yr^{-1}]	O			
Fsubst	fraction of component in wood preservative	[-]	[-]	O			
$Fsubst\_prod_{i}$	fraction of biocide in the product (by weight) before application	[-]	[-]	D	0.1		
$Qreg\_prod_{i}$	quantity of product i in the region	[kg.d^{-1}]	[ktonnes.yr^{-1}]	D	4.5		
$Fpenetr_{i}$	penetration factor	[-]	[-]	D			
$Fdiff_{i}$	fraction lost due to diffuse releases	[-]	[-]	D	0		

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$Flandf_i$	fraction of product waste landfilled	[-]	[-]	D	0.6		
$Flandf_{total}$	fraction of (total) waste landfilled	[-]	[-]	D	0.6		
Qwaste_reg	total quantity of waste in the region	[kg.d^{-1}]	[ktonnes.yr^{-1}]	D	11880		
$Qsubst\_reg_i$	quantity of biocide in total waste in the region	[kg.d^{-1}]	[kg.yr^{-1}]	O^c			
$Csubst\_landf_0$	initial concentration of biocide in landfilled waste	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
Fibre, leather, rubber and polymerised materials preservatives							
Textile and fabrics preservatives, imported material							
-	type of imported fibre treated	[-]	[-]	P			
Qfibres	quantity of fibres / fabrics treated per day	[kg.d^{-1}]	[tonnes.d^{-1}]	O			
-	type of material imported	[-]	[-]	P			
Cmat	estimated content of active substance present in imported material	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Eimport_{water}$	local emission of active substance to waste water due to imported material	[kg.d^{-1}]	[kg.d^{-1}]	O			
Textile and fabrics preservatives, production							
-	type of fibre treated	[-]	[-]	P			
Qfibres	quantity of fibres / fabrics treated per day	[kg.d^{-1}]	[tonnes.d^{-1}]	O			
$Qsubst_i$	quantity of active substance applied per quantity of fibres / fabrics for treatment stepi	[kg.kg^{-1}]	[kg.tonne^{-1}]	S			
Ffix	fixation fraction	[-]	[-]	S/D			
$Eimport_{water}$	local emission of active substance to waste water due to imported material	[kg.d^{-1}]	[kg.d^{-1}]	O			
$Elocal\_water_i$	local emission of active substance to waste water for one treatment step	[kg.d^{-1}]	[kg.d^{-1}]	O			
Textile and fabrics preservatives, service life							
$Qsubst\_tot_k$	annual input of the substance in article k	[kg.d^{-1}]	[tonnes.yr^{-1}]	S			
$Fprodvol_{reg}$	fraction of the region	[-]	[-]	D			
-	type of article	[-]	[-]	P			
$Tservice_k$	service life of article k	[d]	[yr]	O			
$F_{service,j}$	average (over one year) fraction of mass released in one day during service life to compartment j	[-]	[-]	D			
$Temission_{service}$	emission duration per year	[d]	[d.yr^{-1}]	D			
$Fmainsource_{service}$	fraction of the main source	[-]	[-]	D			
$RELEASEreg_{k,service,j}$	regional release for the stage of service life to compartment j for biocide for product k	[kg.d^{-1}]	[kg.d^{-1}]	O			
$RELEASEreg_{service,j}$	total regional release for the stage of service life to compartment j for biocide for all m products with the biocide	[kg.d^{-1}]	[kg.d^{-1}]	O			
$Elocal_{service,j}$	total local emission for the stage of service life to compartment j from all products	[kg.d^{-1}]	[kg.d^{-1}]	O			

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Leather and hides preservatives							
Vform$_i$	quantity of fluid applied per quantity of leather for treatment step i	[kg.kg^{-1}]	[l.tonne^{-1}]	S			
Cform$_i$	concentration fo active substance in the biocidal product for treatment step i	[kg.m^{-3}]	[mg.l^{-1}]	S			
-	process step	[-]	[-]	P			
Qsubst$_i$	quantity of active substance applied per quantity of leather for	[kg.kg^{-1}]	[kg.tonne^{-1}]	O			
Qleather	quantity of leather treated per day, treatment step i	[kg.d^{-1}]	[tonnes.d^{-1}]	D	15		
Ffix	fixation fraction	[-]	[-]	D	0.95		
Elocal_water$_i$	local emission of active substance to waste water for treatment step i	[kg$_c$.d^{-1}]	[kg$_c$.d^{-1}]	O			
Paper and cardboard preservatives, drying sections							
Vform	quantity of product with preservative applied per quantity of paper	[m^3.kg^{-1}]	[l.tonne^{-1}]	S			
Cform	concentration fo active substance in the biocidal product	[kg.m^{-3}]	[g.l^{-1}]	S			
Qsubst	quantity of active substance applied per quantity of paper	[kg.kg^{-1}]	[kg.tonne^{-1}]	S			
-	type of paper produced	[-]	[-]	P			
Qpaper	quantity of coated paper produced per day	[kg.d^{-1}]	[tonnes.d^{-1}]	O			
VP	vapour pressure	[Pa]	[Pa]	P			
Fdecomp	decomposition rate during drying	[-]	[-]	D	0		
Fevap	fraction evaporated	[-]	[-]	O			
Paper and cardboard preservatives, broke							
Vform	quantity of product with preservative applied per quantity of paper	[m^3.kg^{-1}]	[m^3.kg^{-1}]	S			
Cform	concentration fo active substance in the biocidal product	[kg.m^{-3}]	[kg.m^{-3}]	S			
Qsubst	quantity of active substance applied per quantity of paper	[kg.kg^{-1}]	[kg.kg^{-1}]	S			
-	type of paper produced	[-]	[-]	P			
Qpaper	quantity of coated paper produced per day	[kg.d^{-1}]	[kg.d^{-1}]	O			
Fbroke	fraction of coated broke produced compared to overall production	[-]	[-]	D	0.2		
Ffix	fixation fraction	[-]	[-]	D	0		
-	type of paper produced	[-]	[-]	P			
Fclosure	degree of closure of the water system	[-]	[-]	O			
Paper and cardboard preservatives, recycling							
TONNAGE	relevant tonnage in EU for this application	[kg.d^{-1}]	[tonnes.yr^{-1}]	S			
TONNAGEreg	relevant tonnage in the region for this application	[kg.d^{-1}]	[tonnes.yr^{-1}]	S/O			
Fprodvol$_{reg}$	fraction for the region	[-]	[-]	D	0.1		
Fmainsource$_5$	fraction of the main source (local STP)	[-]	[-]	D	0.1		
-	type of paper recycled	[-]	[-]	P			
Frec	fraction of paper recycled	[-]	[-]	O	0.5		
Fdeink	fraction of preservatives released at deinking	[-]	[-]	D	1		
Fdecomp	fraction decomposed during deinking	[-]	[-]	D	0		
-	degree of solubility	[-]	[-]	P			
Fprelim	fraction removed from waste water during preliminary on site treatment	[-]	[-]	O			
Nwdays	number of working days	[d]	[d.yr^{-1}]	D	320		

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Biocides in process and cooling-water installations							
COOLTYPE	type of cooling water system (open circulation/contin. flow)	[open/cont]	[open/cont]	P	open		
$\text{DILUTION}_{cooling}$	dilution factor in receiving surface water	[-]	[-]	D	3		
$C_{ai,cooling}$	concentration of a.i. in cooling water	[kg.m^{-3}]	[mg.l^{-1}]	S	0.5		
Q_{circ}	quantity of water in circulation	[m^3.d^{-1}]	[m^3.d^{-1}]	S	10,000		
F_{depos}	fraction of water lost due to spray and wind drift	[-]	[-]	S	0.00025		
$\text{AREA}_{soil,cooling}$	soil surface where deposition occurs	[m^2]	[m^2]	S	100		
$T_{interval,cooling}$	time period between two emission events	[d]	[d]	D	1		
$N_{appl,cooling}$	number of applications in one year	[-]	[-]	D	300		
Slimicides							
Qform_uins	amount of biocide prescribed in user's instructions per unit of mass of dry paper or per unit of volume process water	[kg.kg^{-1}]	[kg.kg^{-1}]	S			
Cform	content of active ingredient in biocidal product	[kg$_c$.m^{-3}]	[kg$_c$.m^{-3}]	S			
RHOform	specific density of biocide formulation	[kg.m^{-3}]	[kg.m^{-3}]	S	1000		
Vww	amount of waste water per quantity of dry paper	[m^3.kg^{-1}]	[m^3.kg^{-1}]	D	20		
APPL	treatment of both long and short circulation with slimicide	[yes/no]	[yes/no]	P	yes		
Fww1	fraction of the total waste water flow coming from the short circulation of the wire part	[-]	[-]	O			
CONN	connection to pulp mill	[yes/no]	[yes/no]	P	no		
Fww2	fraction dilution of waste water wit waste water from pulping	[-]	[-]	O			
Cproc	concentration of process water prescribed in the user's intructions	[kg.m^{-3}]	[mg.l^{-1}]	S			
Qsubst	amount of active ingredient per quantity of dry paper	[kg$_c$.kg^{-1}]	[kg$_c$.kg^{-1}]	O			
Cinf	theoretical concentration of active ingredient in effluent from paper mill (influent waste water treatment plant)	[kg.m^{-3}]	[kg.m^{-3}]	O			
$\text{EFFLUENTlocal}_{stp}$	effluent discharge of STP for paper plant	[m^3.d^{-1}]	[m^3.d^{-1}]	D	5000		
Temission_3	number of emission days	[d]	[d]	D	300		
Nlocal_3	capacity of local STP of paper plant	[eq]	[eq]	D	25,000		
DILUTION_3	dilution factor for receiving surface water	[-]	[-]	D	10		
DT50hydr_{acid}	half-life time for hydrolysis in acid circumstances	[d]	[d]	S			
DT50hydr_{water}	half-life time for hydrolysis in neutral circumstances	[d]	[d]	S			
DT50hydr_{alkal}	half-life time for hydrolysis in alkaline circumstances	[d]	[d]	S			
DT50bio_{water}	half-life time for biodegradation in water	[d]	[d]	S			
DT50bio_{stp}	half-life time for for biodegradation in activated sludge	[d]	[d]	S			
$\text{DT50photo}_{wate}\text{r}$	half-lifte time for photolysis in water	[d]	[d]	S			
TESTTYPE	type of biodegradation test	[dark/light-dark]	[dark/light-dark]	P	light-dark		
DT50bioI_{water}	half-life for biodegradation in water from biodegradation test 12 hours light/12 hours dark	[d]	[d]	S			
DT50bioII_{water}	half-life for biodegradation niwater from biodegradation test in the dark	[d]	[d]	S			
kbiotot_{water}	rate constant for biodegradation in water including hydrolysis and photolysis	[d^{-1}]	[d^{-1}]	O			
kbioh_{water}	rate constant for biodegradation in water including hydrolysis	[d^{-1}]	[d^{-1}]	O			

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$khydr_{water}$	rate constant for degradation due to hydrolysis at neutral (pH≈7) conditions	$[d^{-1}]$	$[d^{-1}]$	O			
$kphoto_{water}$	rate constant for photolysis	$[d^{-1}]$	$[d^{-1}]$	O			
$khydr_{acid}$	rate constant for degradation due to hydrolysis at acid (pH≈5) conditions	$[d^{-1}]$	$[d^{-1}]$	O			
$khydr_{alkal}$	rate constant for degradation due to hydrolysis at alkaline (pH≈8) conditions	$[d^{-1}]$	$[d^{-1}]$	O			
$kbio_{water}$	rate constant for biodegradation in water	$[d^{-1}]$	$[d^{-1}]$	O			
$kbiotot_{stp}$	rate constant for biodegradation in STPs including hydrolysis	$[d^{-1}]$	$[d^{-1}]$	O			
$kphototot_{water}$	rate constant for photolysis including hydrolysis	$[d^{-1}]$	$[d^{-1}]$	O			
Tpr	retention time for paper making process	[d]	[d]	D			
Tps	retention time for primary settling	[d]	[d]	D			
Tas	retention time for the activated sludge unit	[d]	[d]	D			
Tss	retention time for secondary settling	[d]	[d]	D			
Tmc	retention time for chemical/mechanical treatment	[d]	[d]	D			
Tbt	retention time for long-term biological treatment	[d]	[d]	D			
Cacid	concentration after primary settling for acid process conditions	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
Cneutr	concentration after primary settling for neutral process conditions	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
Calkal	concentration after primary settling for alkaline process conditions	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
$Cacid_{AS}$	concentration after secondary settling for acid process conditions	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
$Cneutr_{AS}$	concentration after secondary settling for neutral process conditions	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
$Calkal_{AS}$	concentration after secondary settling for alkaline process conditions	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
$Cacid_{CM}$	concentration after chemical/mechanical treatment for acid process conditions	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
$Cneutr_{CM}$	concentration after chemical/mechanical treatment for neutral process conditions	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
$Calkal_{CM}$	concentration after chemical/mechanical treatment for alkaline process conditions	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
$Cacid_{BT}$	concentration after long-term biological treatment for acid process conditions	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
$Cneutr_{BT}$	concentration after long-term biological treatment for neutral process conditions	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
$Calkal_{BT}$	concentration after long-term biological treatment for alkaline process conditions	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
$PEC_{AS\_stp\_acid}$	predicted environmental concentration for assessment of micro-organisms in STP with activated sludge for acid conditions at the paper making process	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			
$PEC_{AS\_stp\_neutr}$	predicted environmental concentration for assessment of micro-organisms in STP with activated sludge for neutral conditions at the paper making process	$[kg.m^{-3}]$	$[mg.l^{-1}]$	O			

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$PEC_{AS\_stp\_alkal}$	predicted environmental concentration for assessment of micro-organisms in STP with activated sludge for alkaline conditions at the paper making process	[kg.m^{-3}]	[mg.l^{-1}]	O			
$PEC_{BT\_stp\_acid}$	predicted environmental concentration for assessment of micro-organisms in STP with a long-term biological treatment for acid conditions at the paper making process	[kg.m^{-3}]	[mg.l^{-1}]	O			
$PEC_{BT\_stp\_neutr}$	predicted environmental concentration for assessment of micro-organisms in STP with a long-term biological treatment for neutral conditions at the paper making process	[kg.m^{-3}]	[mg.l^{-1}]	O			
$PEC_{BT\_stp\_alkal}$	predicted environmental concentration for assessment of micro-organisms in STP with a long-term biological treatment for alkaline conditions at the paper making process	[kg.m^{-3}]	[mg.l^{-1}]	O			
$PEClocal_{AS\_water\_acid}$	predicted Environmental Concentration in receiving surface water after activated sludge treatment for acid process conditions at paper making	[kg.m^{-3}]	[mg.l^{-1}]	O			
$PEClocal_{AS\_water\_alkal}$	predicted Environmental Concentration in receiving surface water after activated sludge treatment for alkaline process conditions at paper making	[kg.m^{-3}]	[mg.l^{-1}]	O			
$PEClocal_{AS\_water\_neutr}$	predicted Environmental Concentration in receiving surface water after activated sludge treatment for neutral process conditions at paper making	[kg.m^{-3}]	[mg.l^{-1}]	O			
$PEClocal_{CM\_water\_acid}$	predicted Environmental Concentration in receiving surface water after chemical/mechanical treatment for acid process conditions at paper making	[kg.m^{-3}]	[mg.l^{-1}]	O			
$PEClocal_{CM\_water\_alkal}$	predicted Environmental Concentration in receiving surface water after chemical/mechanical treatment for alkaline process conditions at paper making	[kg.m^{-3}]	[mg.l^{-1}]	O			
$PEClocal_{CM\_water\_neutr}$	predicted Environmental Concentration in receiving surface water after chemical/mecanical treatment for neutral process conditions at paper making	[kg.m^{-3}]	[mg.l^{-1}]	O			
$PEClocal_{BT\_water\_acid}$	predicted Environmental Concentration in receiving surface water after long-term biological treatment for acid process conditions at paper making	[kg.m^{-3}]	[mg.l^{-1}]	O			
$PEClocal_{BT\_water\_alkal}$	predicted Environmental Concentration in receiving surface water afte long-term biological treatment for alkaline process conditions at paper making	[kg.m^{-3}]	[mg.l^{-1}]	O			
$PEClocal_{BT\_water\_neutr}$	predicted Environmental Concentration in receiving surface water after long-term biological treatment for neutral process conditions at paper making	[kg.m^{-3}]	[mg.l^{-1}]	O			
Preservative in metal industry							
Q_{pres}	system capacity	[kg]	[kg]	S	100		
F_{suppl}	fraction of fluid supplemented per day	[d^{-1}]	[d^{-1}]	S	0.035		
-	type of preservative	[-]	[-]	P	unknown		

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$F_{ai,pres}$	fraction of active ingredient in (diluted) fluid	[-]	[-]	O			
$Temission_{pres}$	number of emission days for preservative	[d]	[d]	D	300		
Rodenticides							
Q_{subst}	amount used	[kg]	[kg]	S			
F_{ret}	fraction of retention in goods	[-]	[-]	D	0.02		
F_{disin}	fraction of disintegration	[-]	[-]	D	0.001		
$Temission_{fogging}$	number of emission days for fogging	[d]	[d]	D	1		
Antifoulings							
N_{ship}	number of yachts in yacht-basin	[-]	[-]	D	250		
$AREA_{deck}$	mean ship deck area	[m^2]	[m^2]	D	10		
$F_{water\text{-}ship}$	ratio water/ship in yacht-basin	[-]	[-]	D	3		
-	specification of season for fraction of ships in water	[-]	[-]	P	Whole year		
F_{ship}	fraction ships in water	[-]	[-]	O			[0,1]
V_{anti}	volume of paint per yacht	[m^3]	[l]	S	2		
$AREAlitre_{anti}$	cover of antifouling paint	[$m^2.m^{-3}$]	[$m^2.l^{-1}$]	S	2.5		
$DEPTH_{basin}$	depth of yacht-basin	[m]	[m]	D	2.5		
$F_{s\text{-}ns}$	fraction ships in yacht-basin	[-]	[-]	D	0.71		
$FLUX_{anti}$	mean flux of compound	[$kg.m^{-2}.d^{-1}$]	[$mg.m^{-2}.d^{-1}$]	S	25		
$DT50_{advec,basin}$	advection half-life time in basin	[d]	[d]	D	50		
$AREA_{ship}$	necessary harbour area per yacht	[m^2]	[m^2]	O^c			
V_{basin}	amount of water in yacht-basin	[m^3]	[m^3]	O^c			
$AREA_{anti}$	antifouling surface per yacht-basin	[m^2]	[m^2]	O^c			
$k_{advec,basin}$	rate constant for advection	[d^{-1}]	[d^{-1}]	O^c			
k_{basin}	overall rate constant for removal from basin	[d^{-1}]	[d^{-1}]	O^c			
Embalming and taxidermist fluids, taxidermy							
Qskin	quantity of treated drained skin per day	[$kg.d^{-1}$]	[$kg.d^{-1}$]	D	4		
-	type of agent per treatment step	[-]	[-]	P			
Qsubst	quantity of active substance applied per kg of drained skin	[$kg.kg^{-1}$]	[$kg.kg^{-1}$]	D/O	0.02		
Ffix	fixation fraction	[-]	[-]	S/D	0.95		
$Elocal\_water_i$	local emission of active substance to waste water for treatment step i	[$kg.d^{-1}$]	[$kg.d^{-1}$]	O			
Embalming and taxidermist fluids, embalming process							
-	type of preservation	[short/long]	[short/long]	P			
-	type of biocide applied	[-]	[-]	P			
$Vform_{arterial}$	volume of solution applied per embalmed corpse for arterial injection	[m^3]	[l]	O			
$Vform_{cavity}$	volume of solution applied per embalmed corpse for cavity treatment	[m^3]	[l]	O			
RHOform	specific mass of solution	[$kg.m^{-3}$]	[$kg.m^{-3}$]	D	1,000		
$Cform_{arterial}$	content of active substance in solution for arterial injection	[$kg.kg^{-1}$]	[$kg.kg^{-1}$]	S			
$Cform_{cavity}$	content of active substance in solution for cavity treatment	[$kg.kg^{-1}$]	[$kg.kg^{-1}$]	S			
$Fret_{arterial}$	retention rate of arterial fluid	[-]	[-]	S/O			
$Fret_{cavity}$	retention rate of cavity fluid	[-]	[-]	S/O			

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Embalming and taxidermist fluids, releases in cemeteries							
-	type of preservation	[-]	[-]	P			
-	type of biocide applied	[-]	[-]	P			
$Vform_{arterial}$	volume of solution applied per embalmed corpse for arterial injection	[m^3]	[l]	O			
$Vform_{cavity}$	volume of solution applied per embalmed corpse for cavity treatment	[m^3]	[l]	O			
RHOform	specific mass of solution	[kg.m^{-3}]	[kg.m^{-3}]	D	1,000		
$Cform_{arterial}$	content of active substance in solution for arterial injection	[kg.kg^{-1}]	[kg.kg^{-1}]	S			
$Cform_{cavity}$	content of active substance in solution for cavity treatment	[kg.kg^{-1}]	[kg.kg^{-1}]	S			
$Fret_{arterial}$	retention rate of arterial fluid	[-]	[-]	S/O			
$Fret_{cavity}$	retention rate of cavity fluid	[-]	[-]	S/O			
Freact	factor for reaction with body	[-]	[-]	S/D	0		
Ncorpse	number of embalmed corpses burried per day	[-]	[-]	D	24		
LENGTHcem	length of cemetery	[m]	[m]	D	100		
WIDTHcem	widht of cemetery	[m]	[m]	D	100		
$DEPTHmix_{cem-soil}$	mixing depth of soil	[m]	[m]	D	0.5		
RHOsoil	bulk density of soil	[kg$_{wwt}$.m^{-3}]	[kg$_{wwt}$.m^{-3}]	D	1,700		
$K_{soil-water}$	soil-water partition coefficient	[m^3.m^{-3}]	[m^3.m^{-3}]	O^c			
$krem_{soil}$	first order rate constant for removal in soil	[d^{-1}]	[d^{-1}]	O			
$Elocal_{soil}$	daily average input of active substance to the cemetery	[kg.d^{-1}]	[kg.yr^{-1}]	O			
$Csoil\_av_{cem}$	average concentration in soil	[kg.kgwwt^{-1}]	[mg.kg$_{wwt}^{-1}$]	O			
$Cporew\_av_{cem}$	average concentration in soil porewater	[kg.m^{-3}]	[mg.l^{-1}]	O			
Waste treatment, landfill model							
AREAlandf	bottom surface of the landfill	[m^2]	[m^2]	D	300,000		
DEPTHwaste	total height of waste dumped	[m]	[m]	D	20		
RHOwaste	density of waste	[kg. m^{-3}]	[kg. m^{-3}]	D	1,000		
Tutil	utilisation period	[d]	[d]	D	15		
Vlandf	total volume of landfill	[m^3]	[m^3]	O^c			
$Qwaste_{landf}$	mass of waste dumped daily	[kg.d^{-1}]	[kg.d^{-1}]	O^c			
RAINRATE	wet precipitation	[m.d^{-1}]	[m.yr^{-1}]	D	0.8		
WS_{bare}	precipitation surplus in sector with a surface without vegetation	[m.d^{-1}]	[m.yr^{-1}]	D	0.45		
WS_{veg}	precipitation surplus in sector with a surface with vegetation	[m.d^{-1}]	[m.yr^{-1}]	D	0.3		
WS_{final}	precipitation surplus in sector with a surface with top seal	[m.d^{-1}]	[m.yr^{-1}]	D	0.05		
$Vwater_{produced}$	water produced in waste sector	[m^3.d^{-1}]	[m^3.d^{-1}]	D	0		
$Vwater_{dump}$	amount of percolating water in section where dumping takes	[m^3.d^{-1}]	[m^3.d^{-1}]	O^c			
$Vwater_{veg}$	amount of percolating water in a section where dumping has taken place in one of the previous years during the utilitsation period	[m^3.d^{-1}]	[m^3.d^{-1}]	O^c			
$Vwater_{final}$	amount of percolating water in section where dumping has taken place after closure of the landfill and application of final seal	[m^3.d^{-1}]	[m^3.d^{-1}]	O^c			
$Vwater_{open}$	amount of water in section where dumping stil has to take palce in future year	[m^3.d^{-1}]	[m^3.d^{-1}]	O^c			
$Vwater\_percol_i$	amount of percolating water for year i = 1…Tutil +5 in the entire landfill entire landfill	[m^3.d^{-1}]	[m^3.d^{-1}]	O^c			
$Fgas_{formation}$	factor of (gas) formation	[-]	[-]	D	0.58		

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$Vgas_{orgC}$	volume of landfill gas produced from organic carbon	[m^3.kg]	[m^3.kg]	D	1.87		
-	type of waste, inorganic or domestic	[inorg/domestic]	[inorg/domestic]	P			
$Corg_{landf}$	content of biodegradable organic carbon in waste	[kg.kg^{-1}]	[kg.tonne^{-1}]	O			
$kdeg_{waste\_orgC}$	rate constant for biodegradation of organic carbon inwaste	[d^{-1}]	[yr^{-1}]	D	0.094		
$kdeg_{soil}$	rate constant for degradation in bulk soil	[d^{-1}]	[d^{-1}]	O			
$Vgas\_landf_i$	total amount of gas produced in year i in the entire landfill for i = 1…Tutil+5	[m^3.d^{-1}]	[m^3.d^{-1}]	O^c			
$kdeg_{waste\text{-}subst}$	rate constant for degradation of substance in waste	[d^{-1}]	[d^{-1}]	O^c			
$K_{soil\text{-}water}$	soil-water partition coefficient	[m^3.m^{-3}]	[m^3.m^{-3}]	O^c			
$K_{air\text{-}water}$	air-water partition coefficient	[m^3.m^{-3}]	[m^3.m^{-3}]	O^c			
$kasl_{air}$	partial mass transfer coefficient at air side of air–soil interface	[m.d^{-1}]	[m.d^{-1}]	D	$1.39.10^{-3}$		
$kasl_{soil\text{-}air}$	partial mass transfer coefficient at soil-air side of air-soil interface	[m.d^{-1}]	[m.d^{-1}]	D	$5.56.10^{-6}$		
$kasl_{soil\text{-}water}$	partial mass transfer coefficient at soil-water side of soil-water interface	[m.d^{-1}]	[m.d^{-1}]	D	$5.56.10^{-6}$		
$kleach_{bare}$	rate constant for leaching of substance in sector with a surface without vegetation	[d^{-1}]	[d^{-1}]	O^c			
$kleach_{veg}$	rate constant for leaching of substance in sector with a surface with vegetation	[d^{-1}]	[d^{-1}]	O^c			
$kleach_{final}$	rate constant for leaching of substance in sector with a surface with top seal	[d^{-1}]	[d^{-1}]	O^c			
$kvolat_{waste}$	rate constant for volatilisation of substance without vegetation	[d^{-1}]	[d^{-1}]	O^c			
$krem_{bare}$	overall removal rate constant in sector with a surface without vegetation	[d^{-1}]	[d^{-1}]	O^c			
$krem_{veg}$	overall removal rate constant in sector with a surface with vegetation	[d^{-1}]	[d^{-1}]	O^c			
$krem_{final}$	overall removal rate constant in sector with a surface with top seal	[d^{-1}]	[d^{-1}]	O^c			
$Csubst\_landf_i$	concentration in waste at beginning of year i in a sector for i = 1..Tutil+5	[kg.kg^{-1}]	[kg.kg^{-1}]	O^c			
$Qrem\_sec_i$	amount removed from waste in a sector in year i for i = 1…Tutil+5	[kg.d^{-1}]	[kg.d^{-1}]	O^c			
$Qleach\_sec_i$	amount of substance leached from a sector in year i for i = 1…Tutil+5	[kg.d^{-1}]	[kg.d^{-1}]	O^c			
$Qleach\_landf_i$	total amount of substance leached from landfill in year i for i = 1…Tutil+5	[kg.d^{-1}]	[kg.d^{-1}]	O^c			
$Qvolat\_sec_i$	amount of substance volatilised from a sector in year i for i = 1…Tutil+5	[kg.d^{-1}]	[kg.d^{-1}]	O^c			
$Qvolat\_landf_i$	total amount of substance volatilised from landfill in year i for i = 1…Tutil+5	[kg.d^{-1}]	[kg.d^{-1}]	O^c			
$Fleach_{subsoi}l$	fraction of substance leached and penetrating into the subsoil	[-]	[-]	D	0.05		
Fvolat	fraction of substance volatilised and escaping into the air	[-]	[-]	D	0.15		
$Csubst\_landf_0$	initial concentration of substance in landfilled waste	[kg.kg^{-1}]	[kg.kg^{-1}]	O			
$Qsubst\_STP_i$	amount of substance leached per day in year i and transported to the STP for i = 1…Tuitl+5	[kg]	[kg]	O			
$Qsubst\_soil_i$	amount of substance leached per day in year i and penetrated into the subsoil for i = 1…Tuitl+5	[kg]	[kg]	O			
$Qsubst\_air_i$	amount of substance volatilised per day in year i and escaped to the air for i = 1…Tuitl+5	[kg]	[kg]	O			
$Csubst\_perc_i$	concentration of substance in percolating water in year i for i = 1…Tutil+5	[kg.m^{-3}]	[kg.m^{-3}]	O			
$Qsubst\_gas_i$	concentration of substance in landfill gas in year i and transported to the STP for i = 1…Tuitl+5	[kg.m^{-3}]	[kg.m^{-3}]	O			

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
Exposure of birds/mammals							
$BCF_{worm,pest}$	bioconcentration factor for earthworms in application soil	[kg.kg^{-1}]	[kg.kg^{-1}]	O			
$DT50_{food}$	DT50 in food	[d]	[d]	S	1e6		
k_{food}	first order disappearance rate of pesticide in food	[d^{-1}]	[d^{-1}]	O			
---	type of food for the bird species of choice	[-]	[-]	P			
---	type of food for the mammalian species of choice	[-]	[-]	P			
$Cfood_{bird}$	initial concentration in bird food	[kg.kg]	[mg.kg^{-1}]	S/O			
$Cfood_{mammal}$	initial concentration in mammalian food	[kg.kg]	[mg.kg^{-1}]	S/O			
$Cfood_{bird-5}$	mean concentration in birds food over 5 days	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Cfood_{mammal-5}$	mean concentration in mammal food over 5 days	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Cfood_{Tbird}$	mean concentration in food over T_{bird} days	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$Cfood_{Tmammal}$	mean concentration in food over T_{mammal} days	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
AMOUNTspray	amount of spray liquid used	[m^{3}.m^{-2}]	[l.ha^{-1}]	S			[1,1500]
$C_{particle}$	concentration of pesticide in granules or treated seeds	[kg.kg^{-1}]	[mg.kg^{-1}]	S			
$DOSE_{particle}$	dosage of particles	[kg.m^{-2}]	[kg.m^{-2}]	O			
$W_{particle}$	weight of one granule or treated seed	[kg.particle^{-1}]		S			
F_{mix}	fraction of particles available at surface	[-]	[-]	O			
$N_{particles}$	number of particles per m^{2}	[particles.m^{-2}]		O			
$C_{fish-Tbird}$	mean concentration in fish for birds	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$C_{fish-Tmammal}$	mean concentration in fish for mammals	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$C_{worm-Tbird}$	mean concentration in earthworms for birds	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
$C_{worm-Tmammal}$	mean conc. in earthworms for mammals	[kg.kg^{-1}]	[mg.kg^{-1}]	O			
C_{spray}	concentration in water on leaves and crops	[kg.m^{-3}]	[mg.l^{-1}]	O			
Parameters for birds/mammals							
---	bird species of concern	[-]	[-]	P			
---	mammalian species of concern	[-]	[-]	P			
BW_{bird}	Mean bodyweight of bird species of concern	[kg]	[kg]	S/O	0.010		[0.005,10]
BW_{mammal}	Mean bodyweight of mammalian species of concern	[kg]	[kg]	S/O	0.006		[0.005,15]
DFI_{bird}	daily food intake for bird species of concern	[kg.d^{-1}]	[kg.d^{-1}]	S/O	0.0029		
DFI_{mammal}	daily food intake for mammalian species of concern	[kg.d^{-1}]	[kg.d^{-1}]	S/O	0.001		
DWI_{bird}	daily water intake of bird species of choice	[m^{3}.d^{-1}]	[l.d^{-1}]	O			
DWI_{mammal}	daily water intake of mammalian species of choice	[m^{3}.d^{-1}]	[l.d^{-1}]	O			
Toxicity data							
$LD50_{bee}$	lethal dose for 50% of the bees	[µg.bee^{-1}]	[µg.bee^{-1}]	S			
$LD50_{bird}$	LD50 for birds	[kg.kg^{-1}]	[mg.kg^{-1}]	S			
$LC50_{bird}$	LC50 in food for birds	[kg.kg^{-1}]	[mg.kg^{-1}]	S			
$LD50particle_{bird}$	LD50 recalculated per granule or treated seed	[particles]		O^{c}			
$LD50particle_{mammal}$	LD50 recalculated per granule or treated seed	[particles]		O^{c}			
$LC50_{worm}$	LC50 for earthworms	[kg.kg^{-1}]	[mg.kg^{-1}]	S			
$NOEC_{worm}$	NOEC for earthworms	[kg.kg^{-1}]	[mg.kg^{-1}]	S			

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$\mathrm{EC50_{nitr}}$	EC50 for nitrificating bacteria in soil	$[\mathrm{kg.kg^{-1}}]$	$[\mathrm{mg.kg^{-1}}]$	S			
TOXterr	toxicological data used for extrapolation of PNEC	$[\mathrm{kg.kg^{-1}}]$	$[\mathrm{mg.kg^{-1}}]$	O			
AFterr	assessment factor applied in extrapolation of PNEC	[-]	[-]	O			
$\mathrm{PNEC_{soil}}$	PNEC for terrestrial organisms	$[\mathrm{kg.kg^{-1}}]$	$[\mathrm{mg.kg^{-1}}]$	$\mathrm{O^c}$			
$\mathrm{LC50_{fish}}$	LC50 for fish	$[\mathrm{kg.m^{-3}}]$	$[\mathrm{mg.l^{-1}}]$	S			
$\mathrm{NOEC_{fish}}$	NOEC for fish	$[\mathrm{kg.m^{-3}}]$	$[\mathrm{mg.l^{-1}}]$	S			
$\mathrm{LC50_{crus}}$	LC50 for crustaceans	$[\mathrm{kg.m^{-3}}]$	$[\mathrm{mg.l^{-1}}]$	S			
$\mathrm{NOEC_{crus}}$	NOEC for crustaceans	$[\mathrm{kg.m^{-3}}]$	$[\mathrm{mg.l^{-1}}]$	S			
$\mathrm{LC50_{algae}}$	EC50 for algae	$[\mathrm{kg.m^{-3}}]$	$[\mathrm{mg.l^{-1}}]$	S			
$\mathrm{NOEC_{algae}}$	NOEC for algae	$[\mathrm{kg.m^{-3}}]$	$[\mathrm{mg.l^{-1}}]$	S			
$\mathrm{PNEC_{water}}$	PNEC for aquatic organisms	$[\mathrm{kg.m^{-3}}]$	$[\mathrm{mg.l^{-1}}]$	$\mathrm{O^c}$			
$\mathrm{LC50_{sed}}$	LC50 for sediment-dwelling organism	$[\mathrm{kg.kg^{-1}}]$	$[\mathrm{mg.kg^{-1}}]$	S			
$\mathrm{NOEC_{sed}}$	LC50 for sediment-dwelling organism	$[\mathrm{kg.kg^{-1}}]$	$[\mathrm{mg.kg^{-1}}]$	S			
TOXsed	toxicological data used for extrapolation of PNEC	$[\mathrm{kg.kg^{-1}}]$	$[\mathrm{mg.kg^{-1}}]$	O			
AFsed	assessment factor applied in extrapolation of PNEC	[-]	[-]	O			
$\mathrm{PNEC_{sed}}$	PNEC for sediment-dwelling organisms	$[\mathrm{kg.kg^{-1}}]$	$[\mathrm{mg.kg^{-1}}]$	$\mathrm{O^c}$			
Risk characterisation quotients for pesticides							
$\mathrm{RCR_{bats}}$	Relative Toxicity Index for bats (RTI)	$[\mathrm{kg.m^{-2}}]$		O			
$\mathrm{RRC_{bee}}$	risk characterisation quotient for bees	$[(\mathrm{g.ha^{-1}})/(\mathrm{\mu g.bee^{-1}})]$		$\mathrm{O^c}$			
$\mathrm{RCRfood_{bird\text{-}1}}$	RCR for single-dose toxicity to birds (PED/LD50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRfood_{bird\text{-}5}}$	RCR for acute toxicity to birds (PEC/LC50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRfood_{Tbird}}$	RCR for chronic toxicity to birds (PEC/NOEC)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRfood_{mammal\text{-}1}}$	RCR for single-dose toxicity to mammals (PED/LD50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRfood_{Tmammal}}$	RCR for chronic toxicity to mammals (PEC/NOEC)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRitem_{bird}}$	RCR birds for items resembling natural food	$[\mathrm{m^{-2}}]$	$[\mathrm{m^{-2}}]$	$\mathrm{O^c}$			
$\mathrm{RCRitem_{mammal}}$	RCR mammals for items resembling natural food	$[\mathrm{m^{-2}}]$	$[\mathrm{m^{-2}}]$	$\mathrm{O^c}$			
$\mathrm{RCRone\ particle_{bird}}$	One particle RCR for birds (PED/LD50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRone\ particle_{mammal}}$	One particle RCR for mammals (PED/LD50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRparticle_{bird}}$	RCR birds if particles are sole food source (PED/LD50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRparticle_{mammal}}$	RCR mammals if particles are the sole food source (PED/LD50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRspray_{bird}}$	acute RCR for birds, spray water (PED/LD50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRsurf_{bird}}$	acute RCR for birds, surface water (PED/LD50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRsurf_{bird,semi}}$	semi-chronic RCR for birds, surface water (PEC/LC50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRspray_{mammal}}$	acute RCR for mammals, spray water (PED/LD50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRsurf_{mammal}}$	acute RCR for mammals, surface water (PED/LD50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCR_{worm\text{-}0}}$	short-term RCR for earthworms (PEC/LC50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCR_{worm\text{-}28}}$	long-term RCR for earthworms (PEC/NOEC)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCR_{nitr\text{-}0}}$	short-term RCR for nitrif. bacteria (PEC/EC50)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCR_{soil}}$	RCR for the soil ecosystem	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCR_{soil\text{-}lt}}$	RCR for soil after (N_{lt} + 2) years of applications	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRworm_{Tbird}}$	RCR for worm-eating birds (PEC/NOEC)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCRworm_{Tmammal}}$	RCR for worm-eating mammals (PEC/NOEC)	[-]	[-]	$\mathrm{O^c}$			
$\mathrm{RCR_{fish\text{-}4}}$	short-term RCR for fish (PEC/LC50)	[-]	[-]	$\mathrm{O^c}$			

Symbol	Explanation	Unit int.	Unit scr	Flags	Value (D,scr.)	Type	Range
$RCR_{fish\text{-}28}$	long-term RCR for fish (PEC/NOEC)	[-]	[-]	O^c			
$RCR_{crus\text{-}4}$	short-term RCR for crustaceans (PEC/LC50)	[-]	[-]	O^c			
$RCR_{crus\text{-}21}$	long-term RCR for crustaceans (PEC/NOEC)	[-]	[-]	O^c			
$RCR_{algae\text{-}4a}$	short-term RCR for algae (PEC/EC50)	[-]	[-]	O^c			
$RCR_{algae\text{-}4b}$	long-term RCR for algae (PEC/NOEC)	[-]	[-]	O^c			
RCR_{water}	RCR for the aquatic ecosystem	[-]	[-]	O^c			
$RCR_{sed\text{-}7}$	short-term RCR for sediment organisms (PEC/LC50)	[-]	[-]	O^c			
$RCR_{sed\text{-}14}$	long-term RCR for sediment organisms(PEC/NOEC)	[-]	[-]	O^c			
$RCR_{sed\text{-}28}$	long-term RCR for sediment organisms(PEC/NOEC)	[-]	[-]	O^c			
RCR_{sed}	RCR for the sediment ecosystem	[-]	[-]	O^c			
$RCR_{sed\text{-}lt}$	RCR for sediment after (N_{lt} + 2) years of applications	[-]	[-]	O^c			
$RCRfish_{bird}$	RCR for fish eating birds (PEC/NOEC)	[-]	[-]	O^c			
$RCRfish_{mammal}$	RCR for fish eating mammal (PEC/NOEC)	[-]	[-]	O^c			
$RCR_{mammal,inh}$	inhalatory RCR for mammal	[-]	[-]	O^c			

III. 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

IV. 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) processing, (4) private use and (5) recovery; these estimates have been collected in the 'A-tables'.

2. The fraction of the main source and the number of emission days (point sources); these estimates have been collected in the 'B-tables'.

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). 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 processing
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 processing. 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 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 recovery
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 recovery is relevant.

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

PROCESSING 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	areosol propellants		1	0	0
9, 10, 36	cleaning/washing agents and additives + colourants + odour agents		0	0.1	0.4
19	fertilizers		0	0.05	0*
26	food/feedstuff additives		0	0	0.05
50	surfactants		0.05	0.1	0*
41	pharmaceuticals (external application)		0	0	0.1
41	pharmaceuticals (internal application)0		0	0	
48	solvents		1	0	0
38, 39	pesticides + biocides		0	0	0*

* It should be noted that direct emission to agricultural soil, as well as processing of pesticides (UC=38) and biocides (UC=39), is outside the scope of EUSES.

PRIVATE USE Not applicable

RECOVERY Not applicable

IC=2: CHEMICAL INDUSTRY: BASIC CHEMICALS

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING Table A3.2

Conditions		Emission factors		
Sol. (mg/l)	Vap. (Pa)	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

RECOVERY Not applicable
(Emissions at recovery of chemicals such as catalysts are included in the emissions at processing)

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		Emission factors			
	Sol. (mg/l)	Vap. (Pa)	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
	T (tonnes/year)					
Waste water	<1,000		0.02			
	≥1,000		0.003			

PRODUCTION Table A1.2 for UC = 33 (intermediates) **Continued**

Compartment	Conditions		Emission factors All MC's	MC=1a	MC=1b	MC=1c
Soil				0	0.00001	0.0001

FORMULATION Table A2.1

PROCESSING 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
	T (tonnes/year)					
Waste water	<1,000		0.02			
	≥1,000		0.007	0.0005		
Soil			0.0001			

(1) Default

Remark: The releases at processing 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

RECOVERY Not applicable

IC = 4: ELECTRICAL/ELECTRONIC INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING 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

PROCESSING 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

RECOVERY Not applicable

IC = 5: PERSONAL /DOMESTIC

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING 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, 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

PRIVATE USE Table A4.1 **Continued**

Compartment	Conditions			Emission factors
	Use category	Sol. (mg/l)	Vap. (Pa)	
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	
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, 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

PRIVATE USE Table A4.1 **Continued**

Compartment	Conditions			Emission factors
	Use category	Sol. (mg/l)	Vap. (Pa)	
Waste water	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
Soil	2			0.0001
	3, 36, 41			0
	5			0.0005
	7			0.001
	8 (household products)			0.01
	(cosmetics)			0.001
	9, 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

RECOVERY Not applicable

IC = 6: PUBLIC DOMAIN

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING Table A3.5

Conditions Use categories		Emission factors Air	Waste water	Soil
9	(cleaning/washing agents)	0.0025	0.9	0.05
39	(pesticides, non-agricultural)	0.1	0.05	0.8
All	other	0.05	0.45	0.45

PRIVATE USE Not applicable

RECOVERY Not applicable

IC = 7: LEATHER PROCESSING INDUSTRY

PRODUCTION Table A1.1 for UC ≠ 10 (colourants)
Table A1.3 for UC = 10 (colourants)

UC = 10 (Colourants)

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

PROCESSING 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

RECOVERY 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

PROCESSING 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
RECOVERY	Not applicable

IC = 9: MINERAL OIL AND FUEL INDUSTRY

PRODUCTION	Table A1.1
FORMULATION	Table A2.1
PROCESSING	Table A3.8

Compartment	Conditions		Emission factors
	Sol. (mg/l)	Vap. (Pa)	
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		Emission factors
		Vap. (Pa)	
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

RECOVERY	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		Emission factors
		Vap. (Pa)	
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	0.99
	Other functions	0.002
Soil		0.00025

(1) Default

PROCESSING Table A3.9

Compartment	Conditions		Emission factors	
		Vap. (Pa)	MC=2	MC=3 (1)
Air	Solid materials (e.g. films)		0	
	Else	<1		0.000035
		1-10		0.00025
		10-100		0.0075
		100-1,000		0.025
		≥1,000		0.075
Waste water	Solid materials (e.g. fims)		0	
	Aqueous solutions:			
	- coupler of dye			0.15
	- else			0.8
Soil	Solid materials (e.g. fims)		0	
	Else			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

RECOVERY Table A5.1

Compartment	Conditions UC=42 (photochemicals), for aqueous solutions only!	Vap. (Pa)	Emission factors
Air		<1	0.000005
		1-10	0.000025
		10-100	0.00075
		100-1,000	0.0025
		≥1,000	0.01
Waste water			0.2
Soil			0

IC = 11: POLYMERS INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING Table A3.10 for polymerization processes

In the polymers industry polymers are produced by:
A) Polymerization 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), Vulcanizing agents (UC 53 Vulcanizing 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

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

PROCESSING Table A3.10 for polymerization 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

PROCESSING 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 (Colourants)
		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)

Compartment	Conditions Vap. (Pa)	Boiling point (°C)	Emission factors A	Emission factors B	Type of 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	

PROCESSING Table A3.11 for polymer processing **Continued**

Compartment	Conditions		Emission factors		Type of
	Vap. (Pa)	Boiling point (°C)	A	B	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

RECOVERY Not considered yet

IC = 12: PULP, PAPER AND BOARD INDUSTRY

PRODUCTION Table A1.1 for UC ≠ 10 (colourants)
Table A1.3 for UC = 10 (colourants)

FORMULATION Table A2.1 for UC ≠ 45 (reprographic agents)
Table A2.1 for UC = 45 (reprographic agents)

PROCESSING Table A3.12 for printing and allied processes

Compartment	Conditions		Emission factors	
	Use categories	Vap. (Pa)	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

PROCESSING Table A3.12 for pulp, paper and board production

Compartment	Conditions		Emission factors			
	Use category	Sol. (mg/l)	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

PROCESSING Table A3.12 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

RECOVERY 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
PROCESSING	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 (colourants):
Emission factor (EF) = Emission factor dyeing proces (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

PROCESSING 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 (Colourants) only, i.e. types used normally by industry for batch dyeing

5. RECOVERY Not applicable

IC = 14: PAINTS, LACQUERS AND VARNISHES INDUSTRY

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING 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

RECOVERY Not applicable

IC = 16: ENGINEERING INDUSTRY: CIVIL AND MECHANICAL

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING 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

PROCESSING 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

RECOVERY Not applicable

IC = 0: OTHERS

PRODUCTION Table A1.1

FORMULATION Table A2.1

PROCESSING Table A3.16

B-tables: Estimates for the fraction of the main source and the number of days for emissions

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

PROCESSING 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

RECOVERY 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

PROCESSING 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

RECOVERY 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!	
PROCESSING	Table B3.2
PRIVATE USE	Not applicable
RECOVERY	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
PROCESSING	Table B3.2
PRIVATE USE	Not applicable
RECOVERY	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
PROCESSING	Not applicable
PRIVATE USE	Table B4.1

Only for waste water!

T (tonnes/year)	f main source	No. of days:
	0.002	365

RECOVERY 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
PROCESSING	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
RECOVERY	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

PROCESSING 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

RECOVERY 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

PROCESSING 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

PROCESSING 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

RECOVERY 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

PROCESSING 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!

RECOVERY 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

PROCESSING 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 processing 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

RECOVERY 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

PROCESSING 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

RECOVERY 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

PROCESSING 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

RECOVERY 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

PROCESSING 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

PROCESSING 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

RECOVERY 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

PROCESSING 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

RECOVERY 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

PROCESSING 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

RECOVERY 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
PROCESSING	Table B3.14
PRIVATE USE	Table B4.5
RECOVERY	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

IVa. 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	Coloring 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

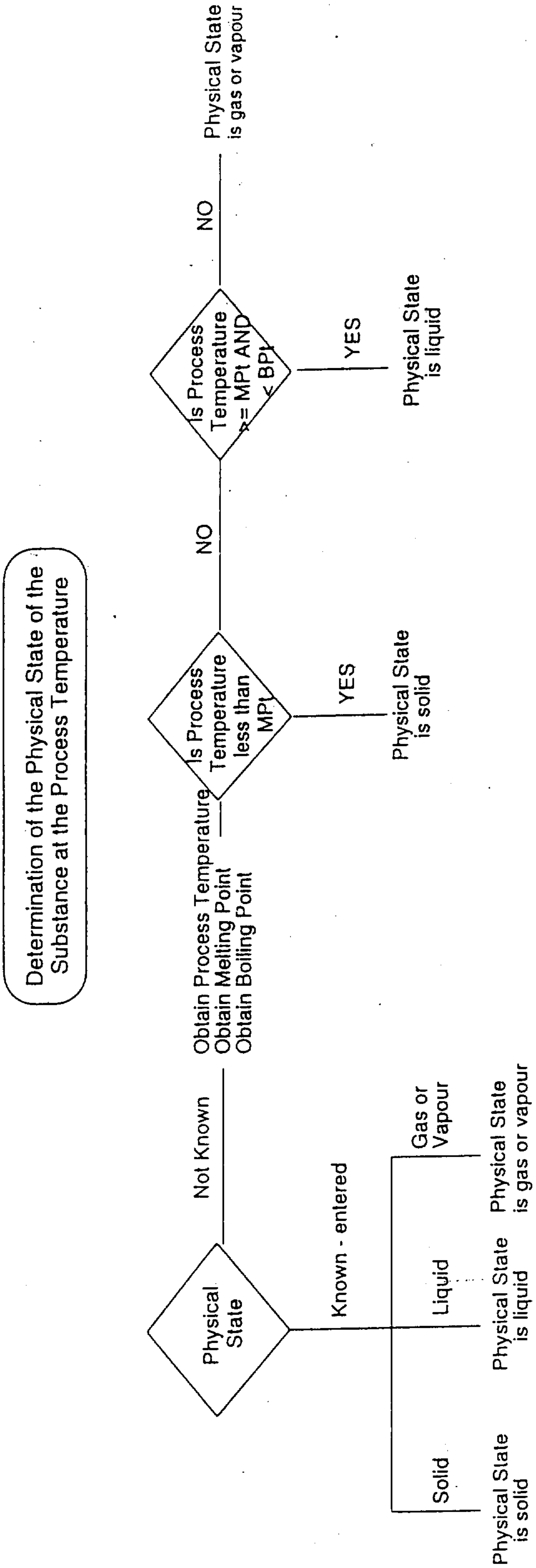
IVb. Synonyms for functions according to ChemUSES (US-EPA, 1980)

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

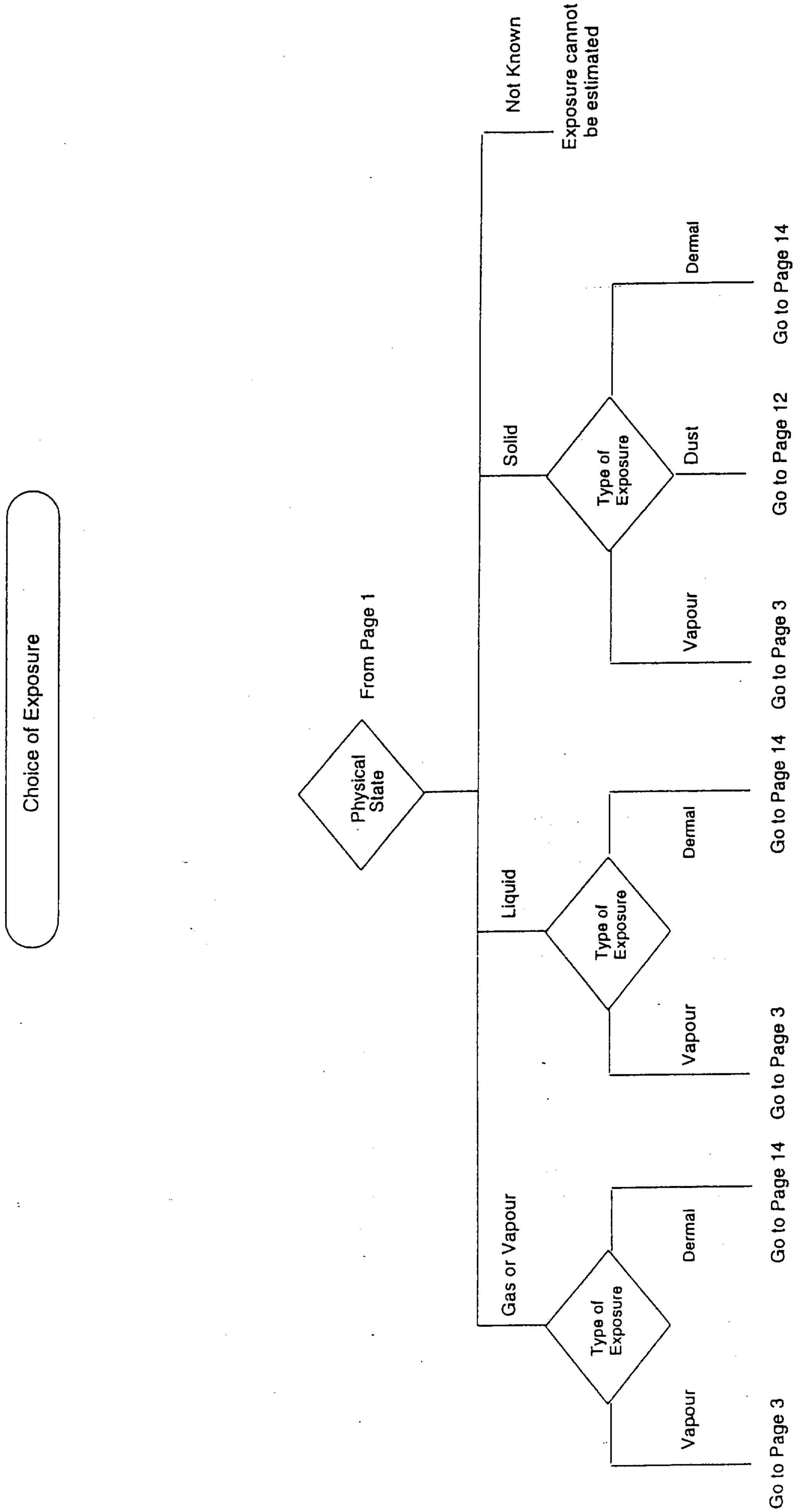
No.	ChemUSES Function	Use category EU (No.)
49	Descaling agents	0
198	Desensitizers (explosives)	42
299	Desensitizers (photography)	42
292	Desizing agents	43
300	Detackifiers	6
173	Detergents	9
179	Detonators	18
182	Developers	42
231	Devulcanizing agents	47
205	Dewatering aids	0
82	Dewaxing solvents	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

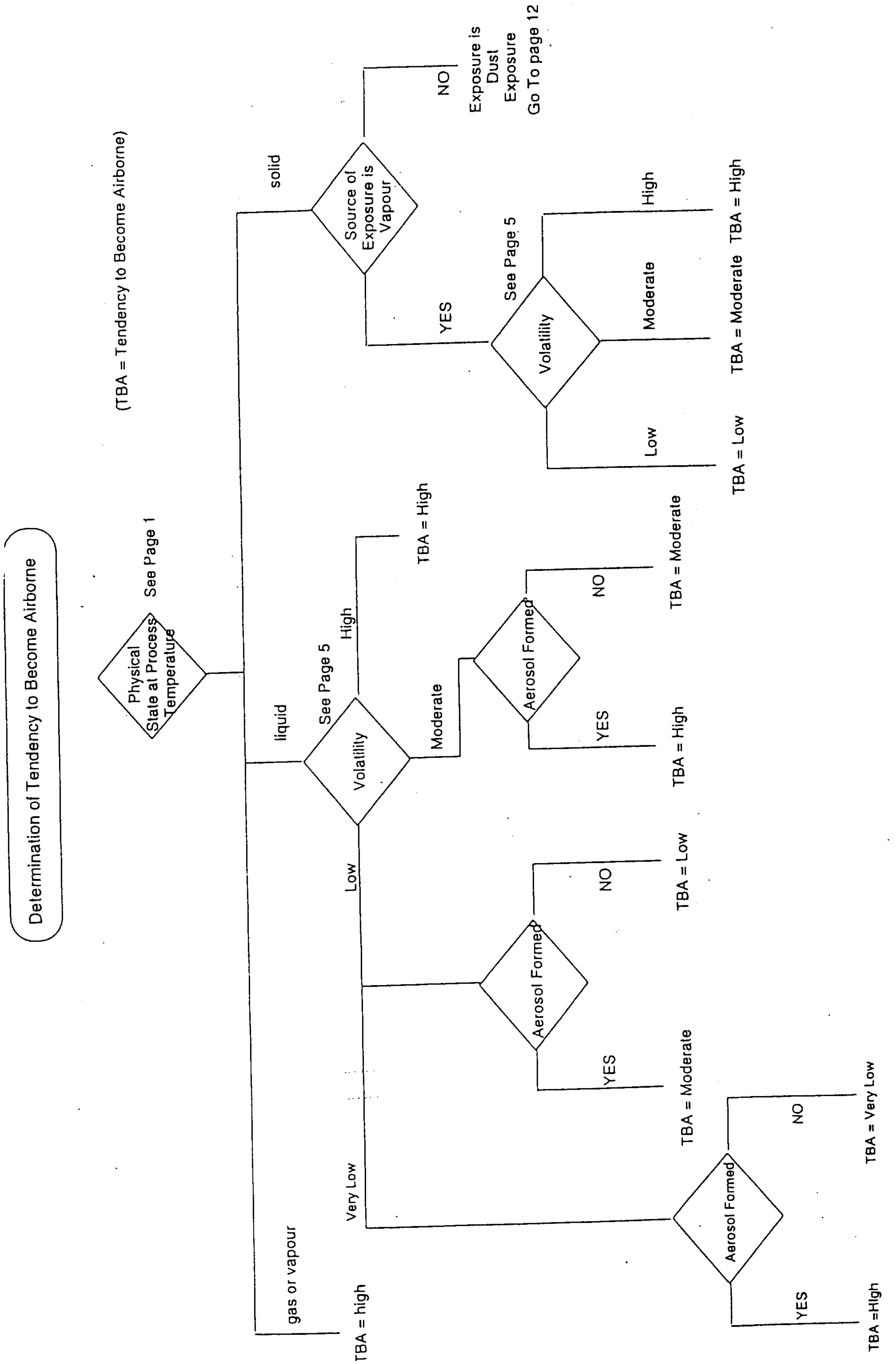
No.	ChemUSES Function	Use category EU (No.)
290	Organic intermediates	33
382	Osmotic membranes	0
325	Oxidation-reduction indicators	34
149	Oxidizers	37
320	Paint and varnish removers	48
17	Papermaking agents	0
144	Parting agents	6
139	Pearlizing agents	10
249	Penetrants	35
96	Peptizing agents	43
253	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

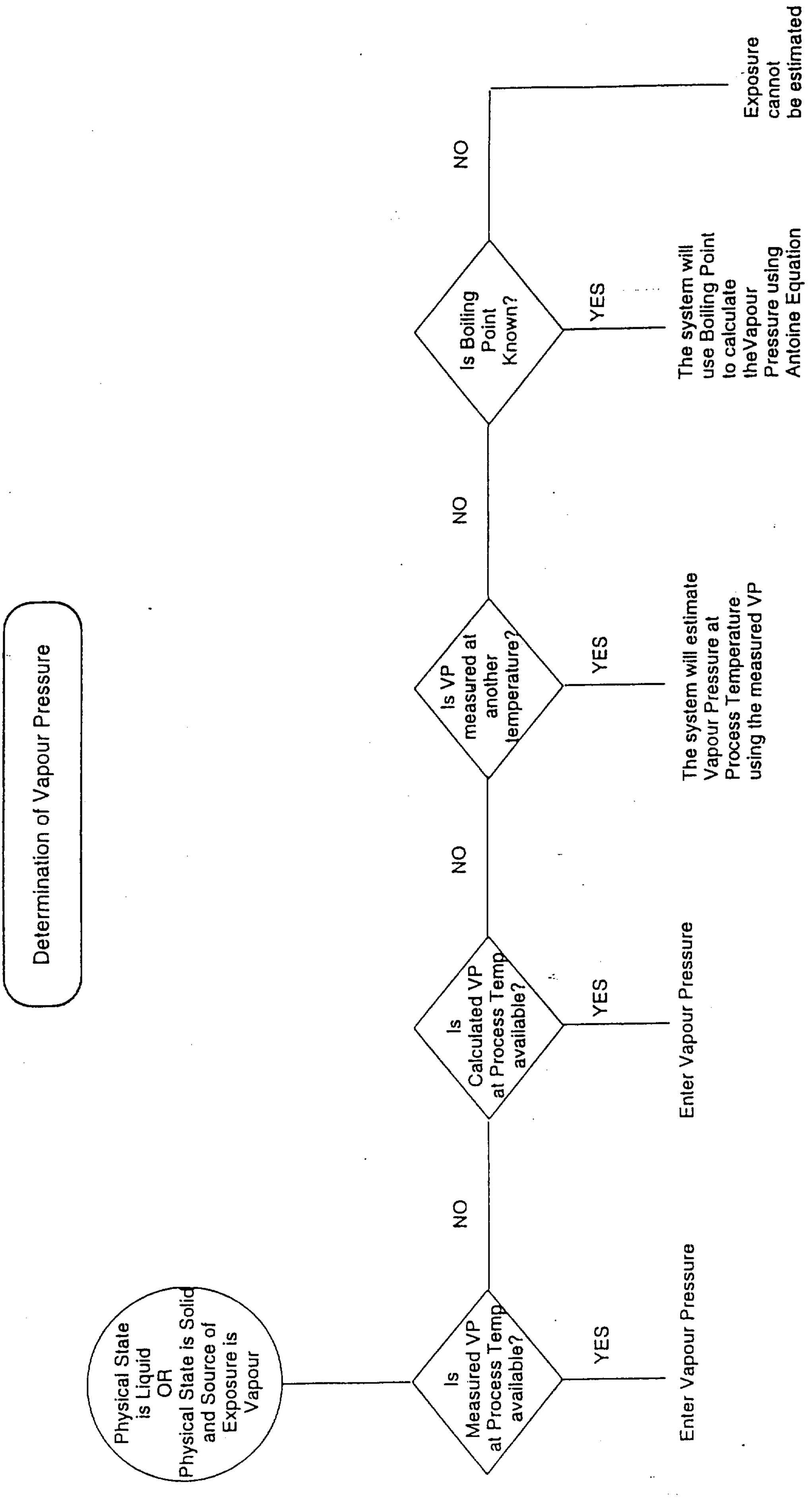
V. Flow diagrams of EASE

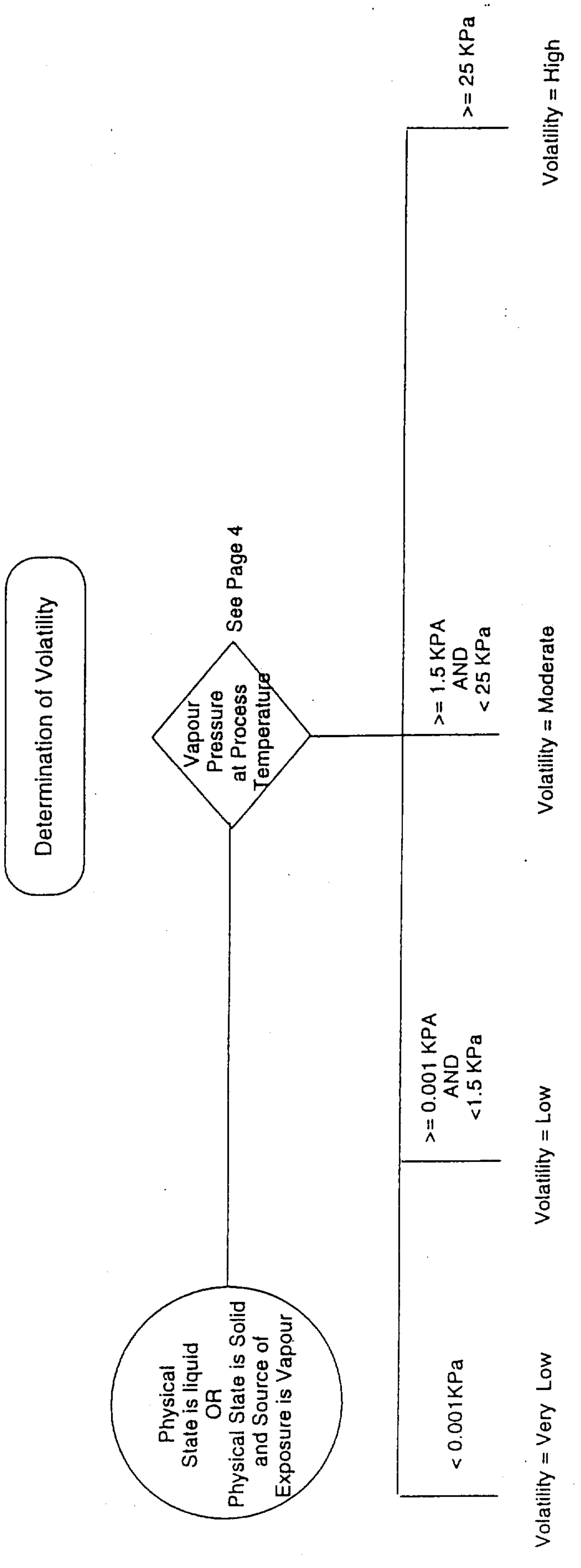


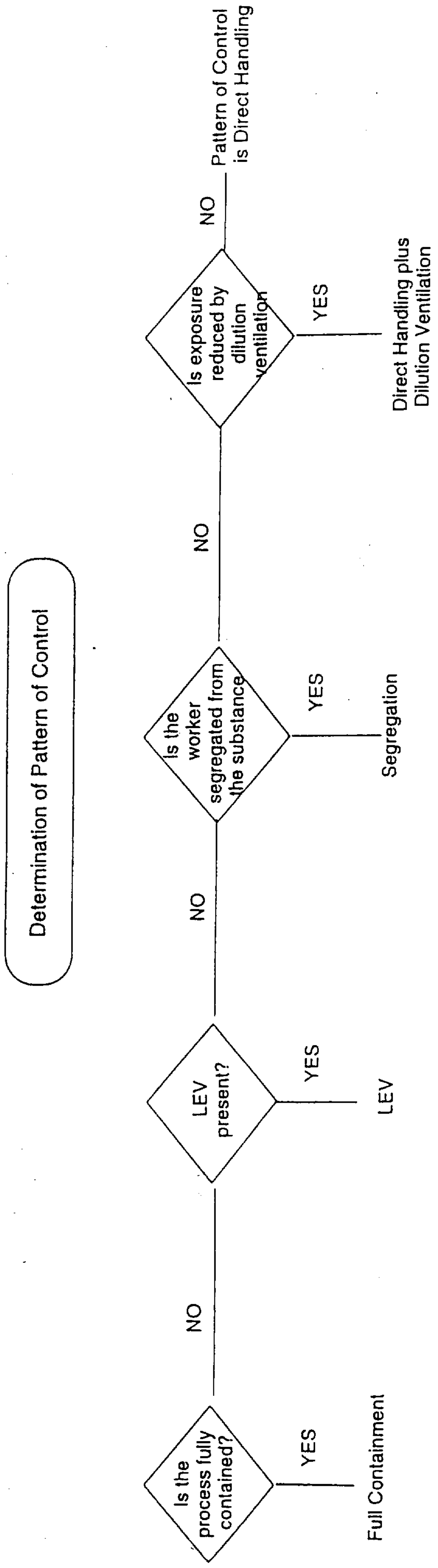
Determination of the Physical State of the Substance at the Process Temperature

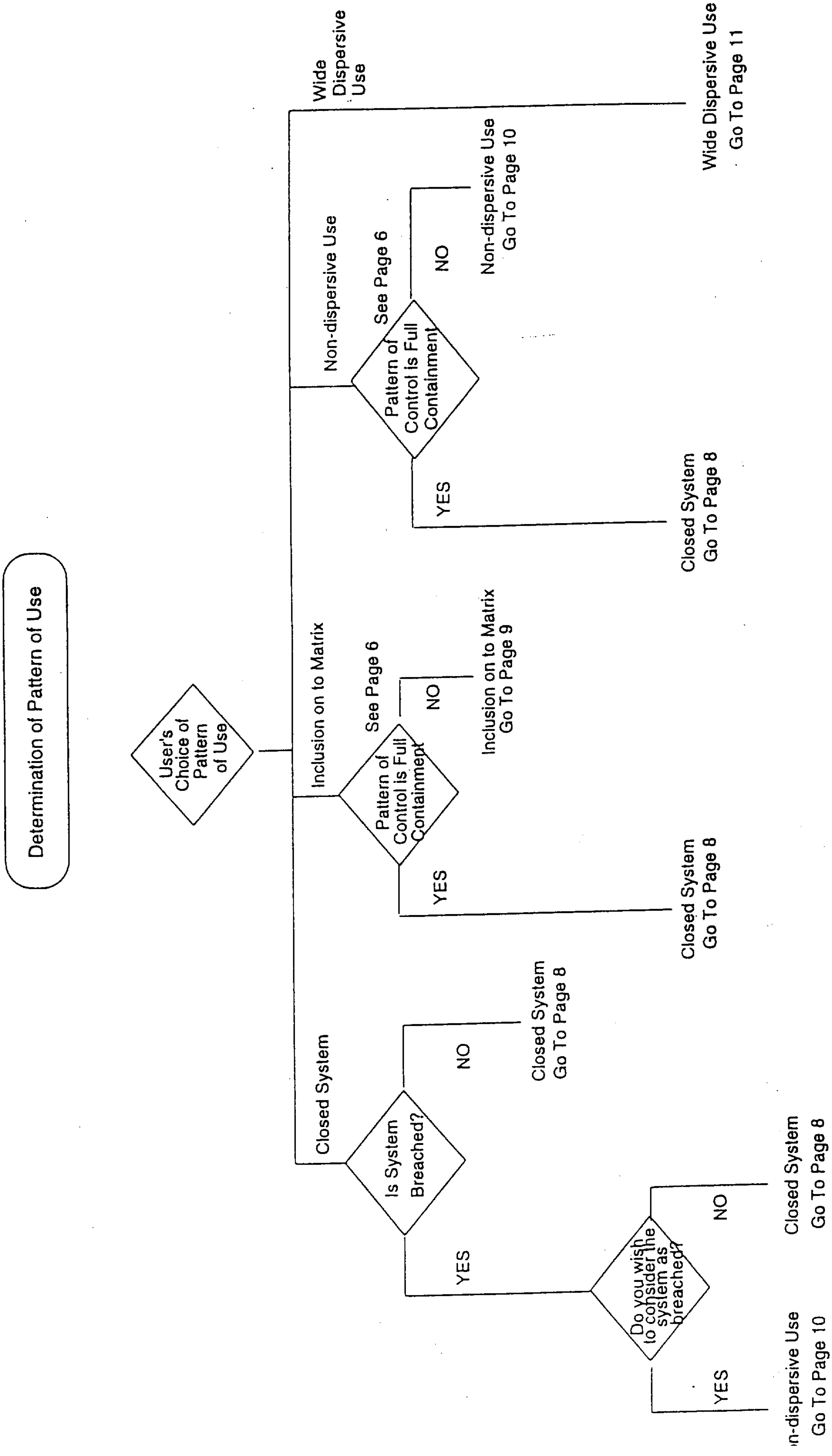

Choice of Exposure
From Page 1
Physical State
Gas or Vapour
Liquid
Solid
Not Known
Exposure cannot be estimated
Type of Exposure
Vapour
Dermal
Go to Page 3
Go to Page 14
Type of Exposure
Vapour
Dermal
Go to Page 3
Go to Page 14
Type of Exposure
Vapour
Dust
Dermal
Go to Page 3
Go to Page 12
Go to Page 14


Determination of Tendency to Become Airborne
(TBA = Tendency to Become Airborne)
Physical State at Process Temperature
See Page 1
solid
Source of Exposure is Vapour
NO
Exposure is Dust Exposure Go To page 12
YES
Volatility
See Page 5
High
TBA = High
Moderate
TBA = Moderate
Low
TBA = Low
liquid
Volatility
See Page 5
High
TBA = High
Moderate
Aerosol Formed
NO
TBA = Moderate
YES
TBA = High
Low
Aerosol Formed
NO
TBA = Low
YES
TBA = Moderate
Very Low
Aerosol Formed
NO
TBA = Very Low
YES
TBA =High
gas or vapour
TBA = high


Determination of Vapour Pressure
Physical State is Liquid OR Physical State is Solid and Source of Exposure is Vapour
Is Measured VP at Process Temp available?
YES
Enter Vapour Pressure
NO
Is Calculated VP at Process Temp available?
YES
Enter Vapour Pressure
NO
Is VP measured at another temperature?
YES
The system will estimate Vapour Pressure at Process Temperature using the measured VP
NO
Is Boiling Point Known?
YES
The system will use Boiling Point to calculate theVapour Pressure using Antoine Equation
NO
Exposure cannot be estimated


Determination of Volatility
Physical State is liquid OR Physical State is Solid and Source of Exposure is Vapour
Vapour Pressure at Process Temperature
See Page 4
< 0.001KPa
>= 0.001 KPA AND <1.5 KPa
>= 1.5 KPA AND < 25 KPa
>= 25 KPa
Volatility = Very Low
Volatility = Low
Volatility = Moderate
Volatility = High

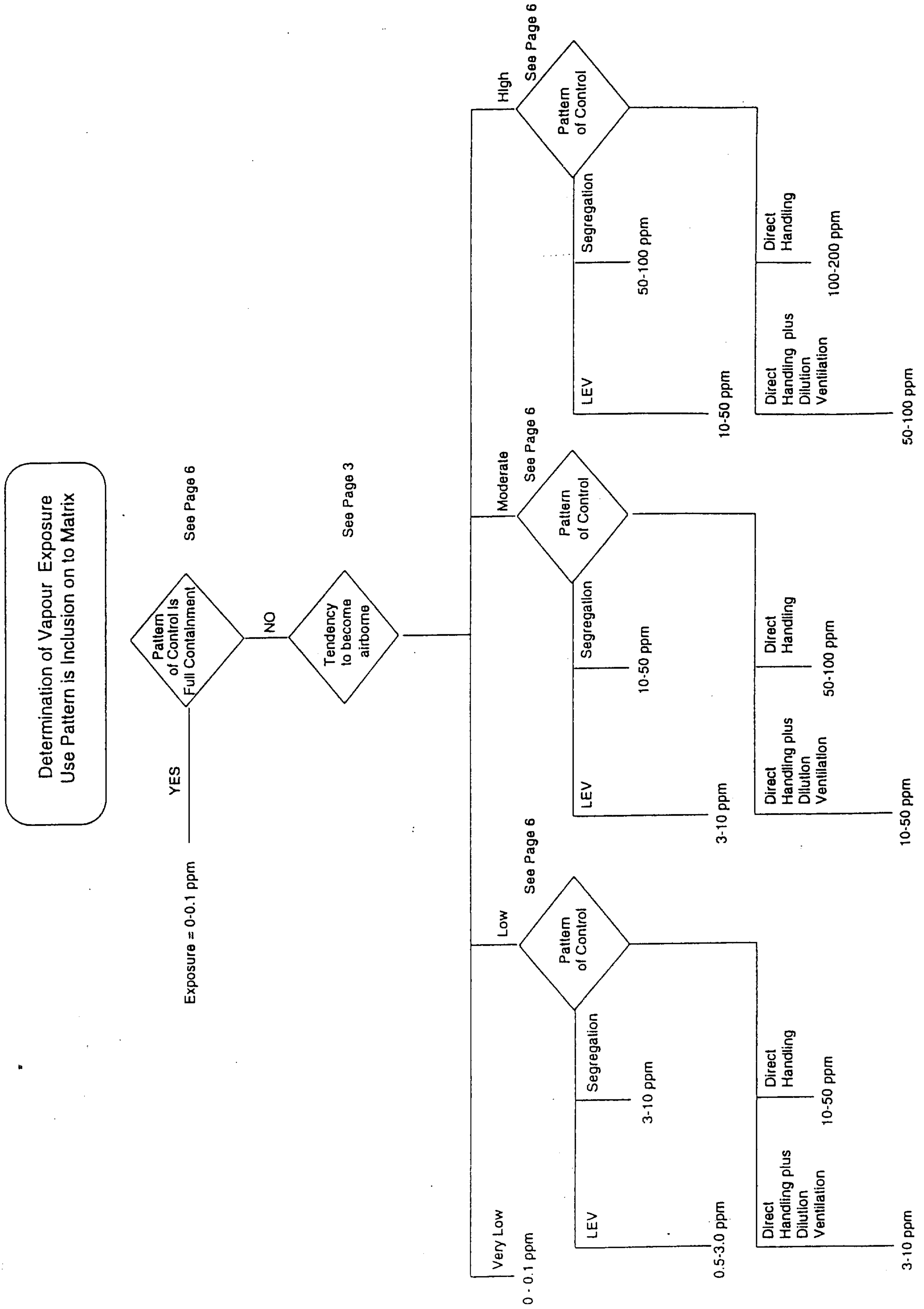

Determination of Pattern of Control
Is the process fully contained?
YES
Full Containment
NO
LEV present?
YES
LEV
NO
Is the worker segregated from the substance
YES
Segregation
NO
Is exposure reduced by dilution ventilation
YES
Direct Handling plus Dilution Ventilation
NO
Pattern of Control is Direct Handling

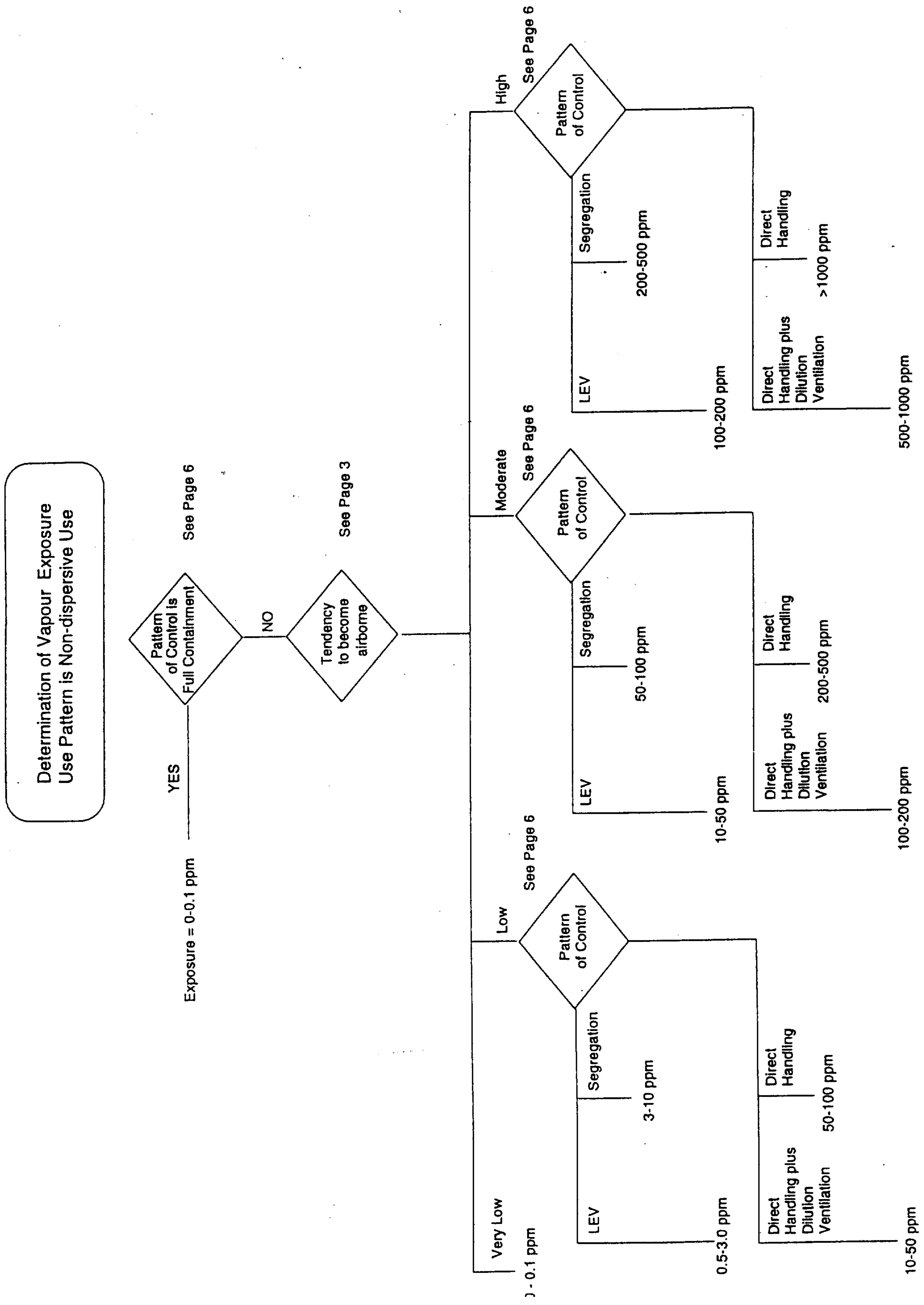

Determination of Pattern of Use
User's Choice of Pattern of Use
Closed System
Is System Breached?
NO
Closed System Go To Page 8
YES
Do you wish to consider the system as breached?
NO
Closed System Go To Page 8
YES
n-dispersive Use Go To Page 10
Inclusion on to Matrix
See Page 6
Pattern of Control is Full Containment
NO
Inclusion on to Matrix Go To Page 9
YES
Closed System Go To Page 8
Non-dispersive Use
See Page 6
Pattern of Control is Full Containment
NO
Non-dispersive Use Go To Page 10
YES
Closed System Go To Page 8
Wide Dispersive Use
Wide Dispersive Use Go To Page 11

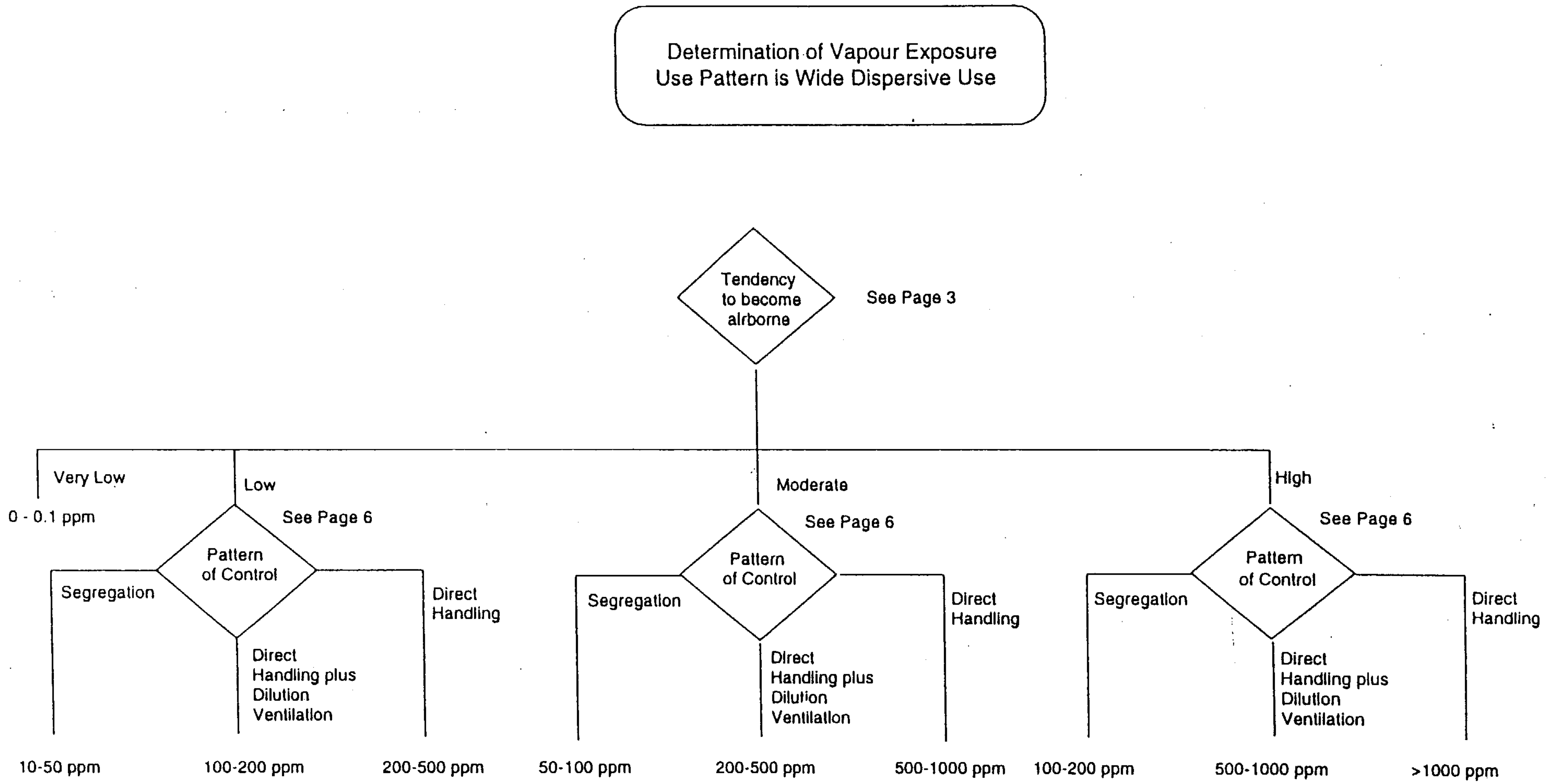
Determination of Vapour Exposure

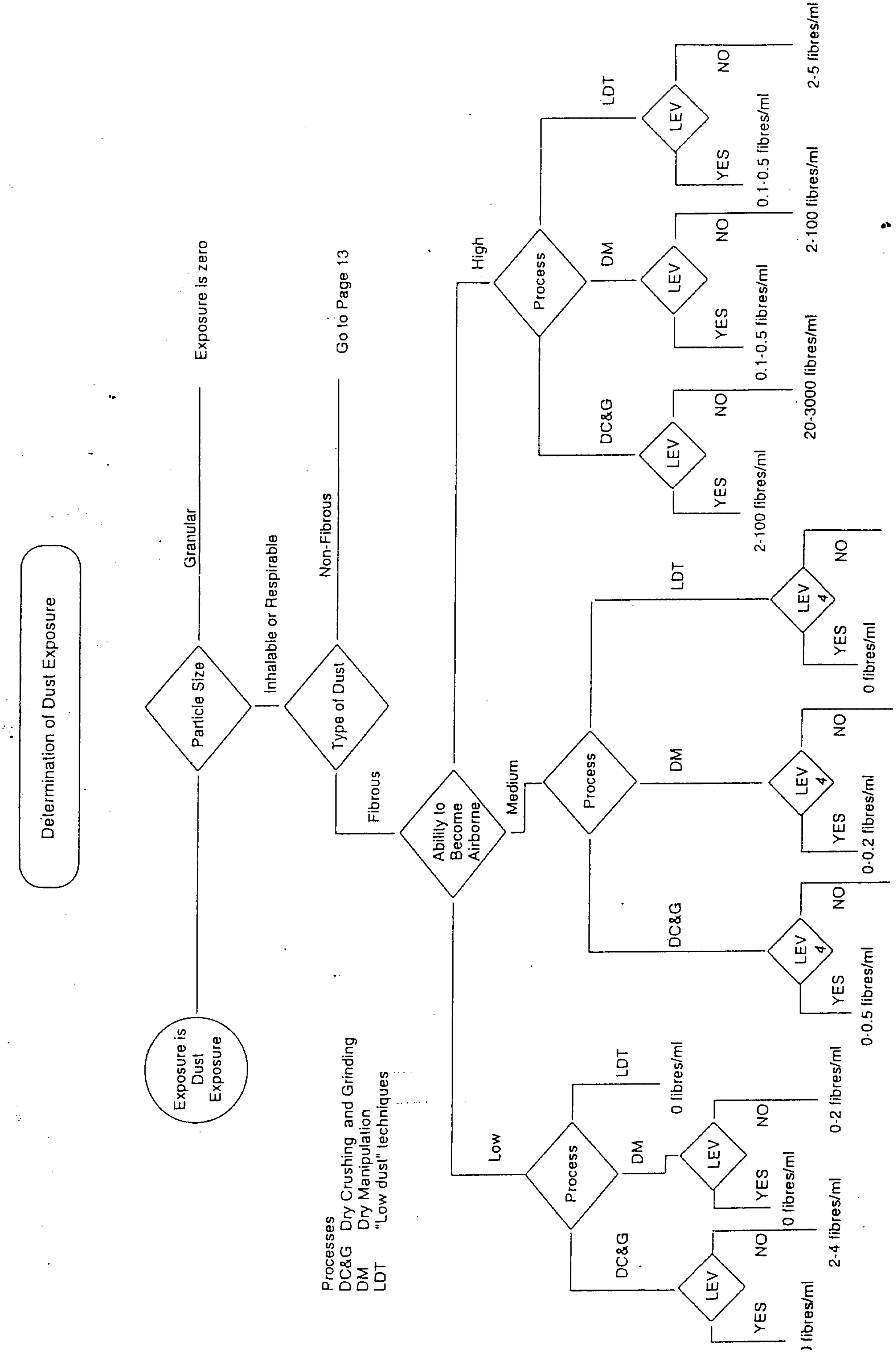
Use Pattern is Closed System

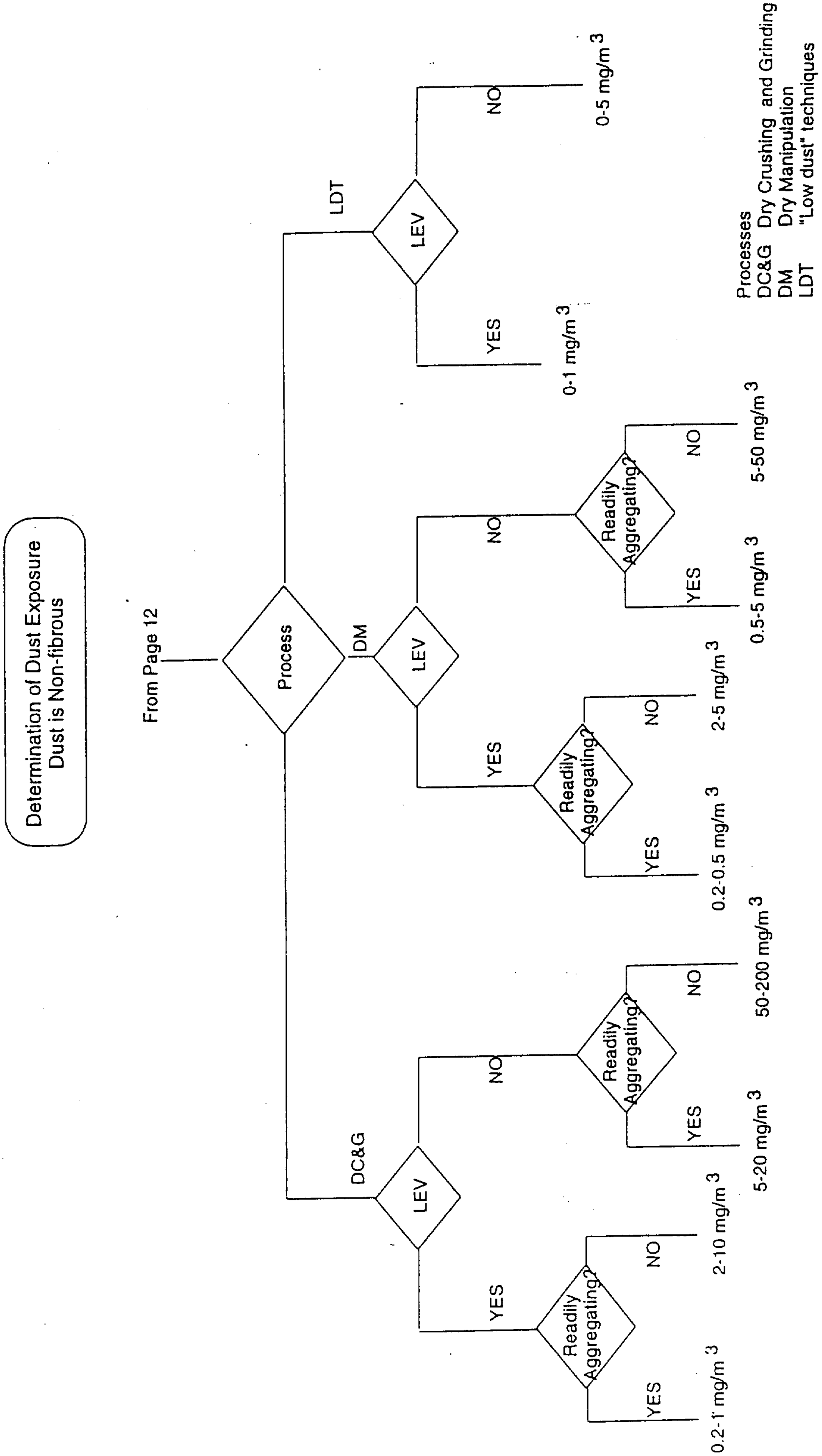
Exposure = 0-0.1 ppm

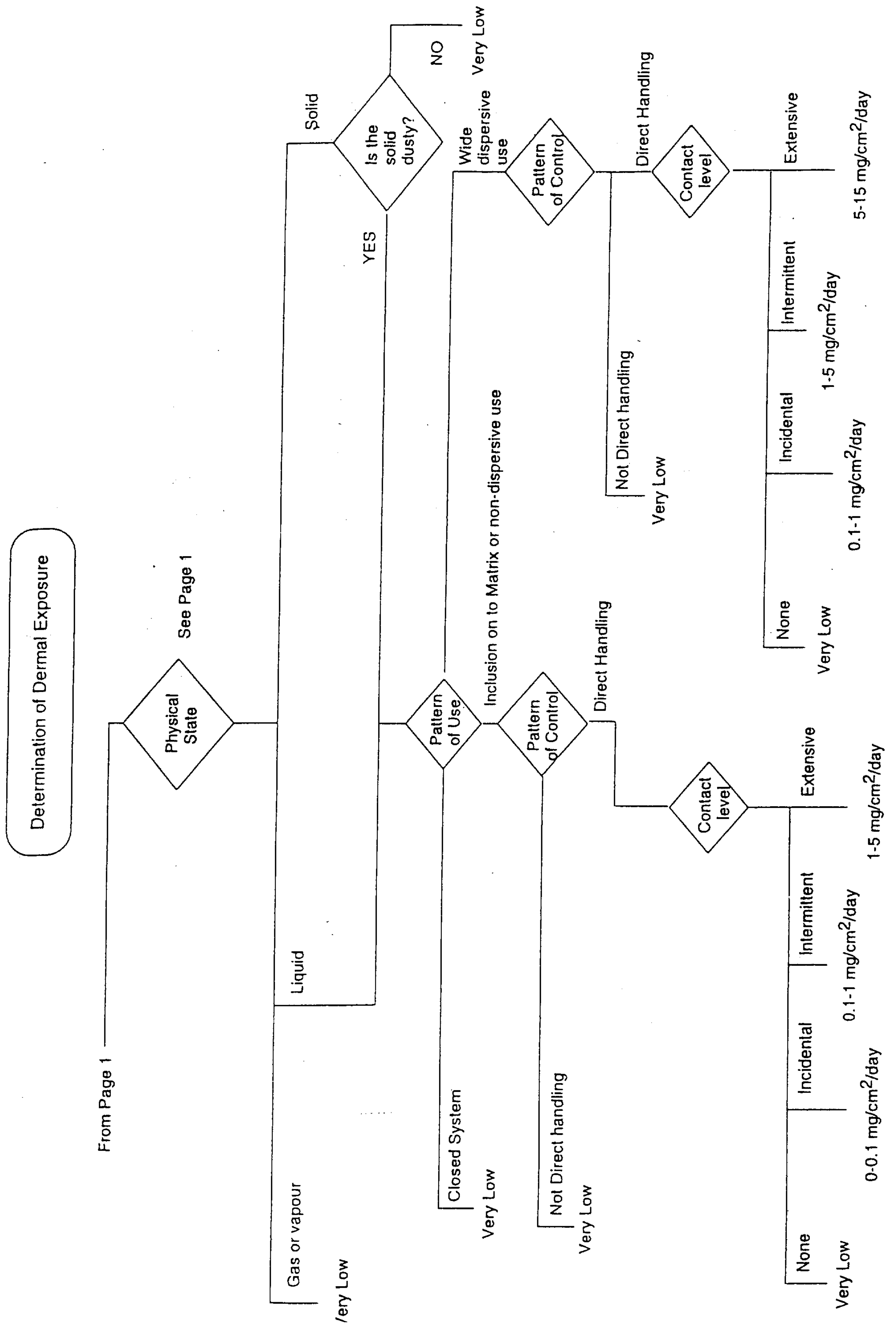

Determination of Vapour Exposure
Use Pattern is Inclusion on to Matrix
Pattern of Control is Full Containment
See Page 6
YES
Exposure = 0-0.1 ppm
NO
Tendency to become airborne
See Page 3
Very Low
0 - 0.1 ppm
Low
See Page 6
Pattern of Control
LEV
0.5-3.0 ppm
Segregation
3-10 ppm
Direct Handling plus Dilution Ventilation
3-10 ppm
Direct Handling
10-50 ppm
Moderate
See Page 6
Pattern of Control
LEV
3-10 ppm
Segregation
10-50 ppm
Direct Handling plus Dilution Ventilation
10-50 ppm
Direct Handling
50-100 ppm
High
See Page 6
Pattern of Control
LEV
10-50 ppm
Segregation
50-100 ppm
Direct Handling plus Dilution Ventilation
50-100 ppm
Direct Handling
100-200 ppm


Determination of Vapour Exposure
Use Pattern is Non-dispersive Use
Pattern of Control is Full Containment
See Page 6
YES
Exposure = 0-0.1 ppm
NO
Tendency to become airborne
See Page 3
Very Low
- 0.1 ppm
Low
See Page 6
Pattern of Control
Segregation
3-10 ppm
LEV
0.5-3.0 ppm
Direct Handling
50-100 ppm
Direct Handling plus Dilution Ventilation
10-50 ppm
Moderate
See Page 6
Pattern of Control
Segregation
50-100 ppm
LEV
10-50 ppm
Direct Handling
200-500 ppm
Direct Handling plus Dilution Ventilation
100-200 ppm
High
See Page 6
Pattern of Control
Segregation
200-500 ppm
LEV
100-200 ppm
Direct Handling
>1000 ppm
Direct Handling plus Dilution Ventilation
500-1000 ppm


Determination of Vapour Exposure
Use Pattern is Wide Dispersive Use
Tendency to become airborne
See Page 3
Very Low
0 - 0.1 ppm
Low
See Page 6
Pattern of Control
Segregation
Direct Handling plus Dilution Ventilation
Direct Handling
10-50 ppm
100-200 ppm
200-500 ppm
Moderate
See Page 6
Pattern of Control
Segregation
Direct Handling plus Dilution Ventilation
Direct Handling
50-100 ppm
200-500 ppm
500-1000 ppm
High
See Page 6
Pattern of Control
Segregation
Direct Handling plus Dilution Ventilation
Direct Handling
100-200 ppm
500-1000 ppm
>1000 ppm


Determination of Dust Exposure
Exposure is Dust Exposure
Particle Size
Granular
Exposure is zero
Inhalable or Respirable
Type of Dust
Non-Fibrous
Go to Page 13
Fibrous
Ability to Become Airborne
High
Medium
Low
Process
DC&G
DM
LDT
LEV
4
YES
NO
2-100 fibres/ml
20-3000 fibres/ml
0.1-0.5 fibres/ml
2-100 fibres/ml
0.1-0.5 fibres/ml
2-5 fibres/ml
0-0.5 fibres/ml
20-100 fibres/ml
0-0.2 fibres/ml
2-20 fibres/ml
0 fibres/ml
0-2 fibres/ml
fibres/ml
2-4 fibres/ml
0 fibres/ml
0-2 fibres/ml
0 fibres/ml
Processes
DC&G Dry Crushing and Grinding
DM Dry Manipulation
LDT "Low dust" techniques


Determination of Dust Exposure
Dust is Non-fibrous
From Page 12
Process
DC&G
LEV
YES
Readily Aggregating?
YES
0.2-1 mg/m 3
NO
2-10 mg/m 3
NO
Readily Aggregating?
YES
5-20 mg/m 3
NO
50-200 mg/m 3
DM
LEV
YES
Readily Aggregating?
YES
0.2-0.5 mg/m 3
NO
2-5 mg/m 3
NO
Readily Aggregating?
YES
0.5-5 mg/m 3
NO
5-50 mg/m 3
LDT
LEV
YES
0-1 mg/m 3
NO
0-5 mg/m 3
Processes
DC&G Dry Crushing and Grinding
DM Dry Manipulation
LDT "Low dust" techniques


Determination of Dermal Exposure
From Page 1
Physical State
See Page 1
Solid
Is the solid dusty?
NO
Very Low
YES
Liquid
Gas or vapour
Very Low
Pattern of Use
Closed System
Very Low
Inclusion on to Matrix or non-dispersive use
Wide dispersive use
Pattern of Control
Direct Handling
Not Direct handling
Very Low
Contact level
None
Very Low
Incidental
0-0.1 mg/cm2/day
Intermittent
0.1-1 mg/cm2/day
Extensive
1-5 mg/cm2/day
Pattern of Control
Direct Handling
Not Direct handling
Very Low
Contact level
None
Very Low
Incidental
0.1-1 mg/cm2/day
Intermittent
1-5 mg/cm2/day
Extensive
5-15 mg/cm2/day

VI. Valid IC/UC combinations

Table of valid and non-valid IC-UC combinations (UC vertical, IC horizontal)

Explanation of symbols:

X	Valid combination (distinguished in relevant IC scenario)
@	Combination is valid (not specifically distinguished in relevant IC scenario)
?	The combination does not seem to be likely, but is regarded as UC = 0
-	Invalid combination

UC \ IC	1	2	3	4	5	6	7	8
1	?	@	@	-	?	?	?	-
2	?	?	?	@	X	@	?	-
3	X	?	?	-	X	?	-	-
4	?	@	@	-	?	?	-	-
5	?	@	@	-	X	?	-	?
6	?	@	@	?	@	@	X	?
7	?	@	@	@	X	?	-	-
8	?	@	@	?	X	?	@	-
9	X	?	?	@	X	X	X	@
10	X	?	?	@	X	?	X	?
11	?	?	?	-	X	-	-	-
12	?	@	@	@	-	-	-	?
13	?	-	-	-	?	?	-	?
14	?	?	?	?	X	?	-	@
15	?	-	-	-	@	-	-	-
16	?	-	-	?	-	?	-	-
17	?	-	-	@	-	-	-	@
18	?	-	-	-	-	-	-	-
19	X	?	?	-	X	@	-	-
20	?	?	?	-	-	-	-	-
21	?	?	?	?	-	-	?	-
22	?	-	-	@	?	?	-	-
23	?	-	-	-	-	-	-	@
24	?	-	-	?	-	-	-	@
25	?	-	-	-	-	-	-	-
26	X	-	-	-	X	-	-	-
27	?	-	-	-	@	@	-	?
28	?	-	-	-	@	@	-	?
29	?	?	?	@	?	?	-	X
30	@	-	-	-	?	?	-	?
31	?	-	-	@	?	?	X	-
32	?	?	?	@	@	@	-	-
33	-	-	X	-	-	-	-	-
34	-	@	@	-	?	-	-	-
35	@	-	-	?	X	@	-	X

UC \ IC	1	2	3	4	5	6	7	8
36	X	-	-	-	X	?	-	?
37	?	@	@	-	?	?	-	?
38	X	-	-	-	X	X	-	-
39	X	-	-	-	@	@	@	@
40	?	@	@	-	?	?	?	?
41	X	-	-	-	X	-	-	-
42	?	-	-	@	-	-	-	-
43	?	@	@	?	?	?	-	?
44	?	@	@	?	?	?	-	?
45	?	-	-	-	?	?	-	-
46	?	-	-	@	-	-	-	-
47	?	-	-	?	X	?	-	-
48	X	@	@	@	X	@	?	@
49	?	@	@	?	?	-	-	?
50	X	@	@	@	X	@	?	@
51	?	@	@	-	-	-	@	-
52	?	-	-	-	-	-	-	-
53	?	-	-	-	-	-	-	-
54	?	-	-	@	-	-	-	@
0	X	@	@	@	X	X	@	@

UC \ IC	9	10	11	12	13	14	16	0
1	-	-	-	-	?	-	@	@
2	-	-	-	@	-	-	@	@
3	-	-	-	-	-	X	-	@
4	-	-	-	-	-	@	-	@
5	@	-	-	-	-	?	-	@
6	-	-	X	@	@	-	?	@
7	@	-	X	-	@	-	?	@
8	-	@	-	-	@	-	-	@
9	-	-	@	X	@	-	?	@
10	@	@	X	X	X	X	?	@
11	-	-	-	-	-	-	-	@
12	-	-	@	-	-	-	-	@
13	-	-	-	-	-	-	@	@
14	-	-	-	-	-	X	-	@
15	-	-	-	-	-	-	-	@
16	-	-	-	-	-	-	-	@
17	-	-	?	-	-	-	-	@
18	-	-	-	-	-	-	-	@
19	-	-	-	-	-	-	-	@
20	-	-	X	X	-	X	-	@
21	-	-	-	-	-	-	-	@

UC \ IC	9	10	11	12	13	14	16	0
22	-	-	X	?	@	-	@	@
23	-	-	-	@	-	-	-	@
24	-	-	@	-	-	-	-	@
25	-	-	@	-	-	-	-	@
26	-	-	-	-	-	-	-	@
27	X	-	-	-	-	-	-	@
28	X	-	-	-	-	-	-	@
29	-	-	-	-	-	-	-	@
30	-	-	-	-	-	-	-	@
31	-	-	-	X	@	-	-	@
32	-	-	-	-	-	-	@	@
33	X	-	-	-	-	-	-	@
34	-	-	-	-	-	-	-	@
35	-	-	X	-	-	-	-	@
36	-	-	-	-	-	-	-	@
37	-	?	-	-	-	@	-	@
38	-	-	-	-	-	?	-	@
39	-	?	?	@	-	-	@	@
40	-	-	-	-	-	-	-	@
41	-	-	-	-	-	@	-	@
42	-	X	-	-	-	-	-	@
43	-	?	X	-	-	-	-	@
44	-	-	-	-	-	-	-	@
45	-	-	-	X	-	-	-	@
46	-	-	-	-	-	-	-	@
47	-	-	X	-	-	X	-	@
48	-	-	X	X	@	X	@	@
49	@	-	X	-	-	?	-	@
50	-	?	?	-	@	X	-	@
51	-	-	-	-	-	-	-	@
52	@	-	-	-	-	X	-	@
53	-	-	X	-	-	-	-	@
54	-	-	-	-	-	-	-	@
0	@	?	X	X	@	X	@	@

APPENDIX VII: PEARL tables, Concentration in Groundwater (μg/l)

spring	Kom (l/kg)																				
DT50bio,soil (days) at 20 °C	0	1	2.5	5	7.5	10	12.5	15	20	25	30	40	50	60	70	80	90	100	125	150	175	200
2.5	1.59E-07	2.23E-08	8.26E-09	1.17E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5	5.66E-03	2.72E-03	7.22E-05	4.90E-06	2.53E-07	8.83E-09	1.78E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7.5	5.81E-02	3.44E-02	1.42E-02	3.45E-03	5.76E-04	9.04E-05	1.73E-05	3.28E-06	1.14E-07	1.68E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
10	2.37E-01	1.55E-01	8.16E-02	3.14E-02	1.43E-02	7.38E-03	3.95E-03	1.86E-03	3.84E-04	6.65E-05	8.54E-06	4.18E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
12.5	6.25E-01	4.47E-01	2.77E-01	1.40E-01	8.13E-02	4.99E-02	3.98E-02	1.85E-02	6.12E-03	1.67E-03	3.85E-04	9.84E-06	7.53E-08	1.00E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
15	1.27E+00	9.77E-01	6.74E-01	4.02E-01	2.65E-01	1.79E-01	1.20E-01	7.76E-02	3.07E-02	1.07E-02	3.29E-03	1.33E-04	2.57E-06	1.38E-08	1.38E-11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
20	3.36E+00	2.81E+00	2.20E+00	1.58E+00	1.19E+00	8.87E-01	6.45E-01	4.64E-01	2.22E-01	9.53E-02	3.73E-02	4.42E-03	4.08E-04	2.89E-05	1.29E-06	3.12E-08	3.57E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
25	6.27E+00	5.52E+00	4.61E+00	3.66E+00	2.94E+00	2.31E+00	1.79E+00	1.36E+00	7.21E-01	3.49E-01	1.56E-01	2.58E-02	3.75E-03	5.21E-04	5.58E-05	4.25E-06	2.10E-07	6.03E-09	0.00E+00	0.00E+00	0.00E+00	0.00E+00
30	9.67E+00	8.77E+00	7.70E+00	6.44E+00	5.39E+00	4.37E+00	3.54E+00	2.78E+00	1.58E+00	8.25E-01	4.03E-01	8.35E-02	1.66E-02	3.34E-03	6.64E-04	1.32E-04	2.28E-05	3.02E-06	3.96E-09	0.00E+00	0.00E+00	0.00E+00
40	1.69E+01	1.59E+01	1.47E+01	1.31E+01	1.15E+01	9.88E+00	8.34E+00	6.80E+00	4.23E+00	2.44E+00	1.34E+00	3.78E-01	1.10E-01	3.34E-02	1.00E-02	3.03E-03	8.84E-04	2.43E-04	7.77E-05	8.28E-08	1.85E-10	0.00E+00
50	2.38E+01	2.29E+01	2.19E+01	2.02E+01	1.81E+01	1.62E+01	1.40E+01	1.17E+01	7.68E+00	4.74E+00	2.81E+00	9.80E-01	3.60E-01	1.34E-01	5.02E-02	1.90E-02	7.01E-03	2.51E-03	1.88E-04	1.16E-05	3.76E-07	4.25E-09
60	3.00E+01	2.94E+01	2.85E+01	2.70E+01	2.47E+01	2.25E+01	1.97E+01	1.68E+01	1.15E+01	7.44E+00	4.69E+00	1.90E+00	8.00E-01	3.40E-01	1.47E-01	6.40E-02	2.73E-02	1.16E-02	1.35E-03	1.45E-04	1.35E-05	8.74E-07
70	3.55E+01	3.51E+01	3.45E+01	3.31E+01	3.09E+01	2.85E+01	2.53E+01	2.19E+01	1.54E+01	1.04E+01	6.83E+00	3.07E+00	1.43E+00	6.66E-01	3.16E-01	1.52E-01	7.24E-02	3.44E-02	5.35E-03	8.07E-04	1.11E-04	1.40E-05
80	4.03E+01	4.02E+01	3.98E+01	3.87E+01	3.66E+01	3.41E+01	3.05E+01	2.67E+01	1.92E+01	1.33E+01	9.13E+00	4.42E+00	2.22E+00	1.11E+00	5.69E-01	2.94E-01	1.51E-01	7.79E-02	1.49E-02	2.84E-03	5.13E-04	8.67E-05
90	4.44E+01	4.46E+01	4.46E+01	4.36E+01	4.12E+01	3.91E+01	3.53E+01	3.11E+01	2.29E+01	1.63E+01	1.15E+01	5.91E+00	3.13E+00	1.66E+00	9.02E-01	4.92E-01	2.68E-01	1.47E-01	3.31E-02	7.47E-03	1.65E-03	3.44E-04
100	4.81E+01	4.86E+01	4.88E+01	4.81E+01	4.65E+01	4.37E+01	3.98E+01	3.53E+01	2.64E+01	1.92E+01	1.39E+01	7.52E+00	4.13E+00	2.29E+00	1.31E+00	7.45E-01	4.25E-01	2.46E-01	6.25E-02	1.60E-02	4.03E-03	1.02E-03
125	5.55E+01	5.66E+01	5.73E+01	5.72E+01	5.62E+01	5.35E+01	4.92E+01	4.43E+01	3.43E+01	2.59E+01	1.96E+01	1.16E+01	6.88E+00	4.16E+00	2.56E+00	1.59E+00	9.86E-01	6.25E-01	1.98E-01	6.43E-02	2.11E-02	6.88E-03
150	6.12E+01	6.27E+01	6.39E+01	6.42E+01	6.38E+01	6.12E+01	5.68E+01	5.16E+01	4.09E+01	3.19E+01	2.50E+01	1.56E+01	9.74E+00	6.25E+00	4.07E+00	2.65E+00	1.75E+00	1.17E+00	4.31E-01	1.62E-01	6.24E-02	2.42E-02
175	6.57E+01	6.74E+01	6.91E+01	6.98E+01	6.99E+01	6.74E+01	6.30E+01	5.76E+01	4.65E+01	3.70E+01	2.97E+01	1.93E+01	1.25E+01	8.39E+00	5.68E+00	3.84E+00	2.65E+00	1.84E+00	7.55E-01	3.16E-01	1.35E-01	5.88E-02
200	6.92E+01	7.12E+01	7.32E+01	7.43E+01	7.49E+01	7.25E+01	6.81E+01	6.27E+01	5.13E+01	4.16E+01	3.39E+01	2.26E+01	1.52E+01	1.05E+01	7.31E+00	5.10E+00	3.64E+00	2.60E+00	1.16E+00	5.25E-01	2.43E-01	1.15E-01

autumn	Kom (l/kg)																				
DT50bio,soil (days) at 20 °C	0	1	2.5	5	7.5	10	12.5	15	20	25	30	40	50	60	70	80	90	100	125	150	175	200
1	1.34E-04	3.96E-05	5.78E-06	1.97E-07	3.68E-09	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2.5	2.42E-01	1.50E-01	7.27E-02	2.15E-02	6.23E-03	1.62E-03	3.47E-04	6.84E-05	1.93E-06	2.55E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5	4.75E+00	3.54E+00	2.25E+00	1.04E+00	4.70E-01	2.04E-01	8.54E-02	3.41E-02	4.62E-03	2.31E-04	1.22E-05	4.94E-09	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7.5	1.47E+01	1.17E+01	8.22E+00	4.40E+00	2.28E+00	1.14E+00	5.47E-01	2.56E-01	4.94E-02	7.80E-03	8.21E-04	3.84E-06	2.23E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
10	2.70E+01	2.22E+01	1.63E+01	9.42E+00	5.26E+00	2.86E+00	1.50E+00	7.61E-01	1.74E-01	3.39E-02	5.52E-03	3.21E-05	4.53E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
12.5	3.95E+01	3.32E+01	2.51E+01	1.52E+01	9.06E+00	5.17E+00	2.85E+00	1.52E+00	3.91E-01	8.78E-02	1.71E-02	4.70E-04	8.76E-06	9.36E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
15	5.12E+01	4.36E+01	3.36E+01	2.15E+01	1.32E+01	7.80E+00	4.45E+00	2.47E+00	6.97E-01	1.75E-01	3.97E-02	1.82E-03	7.80E-05	2.52E-06	4.47E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
20	7.14E+01	6.18E+01	5.02E+01	3.37E+01	2.17E+01	1.35E+01	8.16E+00	4.81E+00	1.57E+00	4.69E-01	1.37E-01	1.46E-02	1.95E-03	1.69E-04	1.13E-05	4.29E-07	7.94E-09	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
25	8.76E+01	7.82E+01	6.47E+01	4.49E+01	3.00E+01	1.94E+01	1.22E+01	7.53E+00	2.73E+00	9.57E-01	3.52E-01	6.27E-02	1.27E-02	2.44E-03	4.32E-04	6.38E-05	6.92E-06	5.12E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00
30	1.02E+02	9.19E+01	7.71E+01	5.48E+01	3.77E+01	2.51E+01	1.63E+01	1.04E+01	4.17E+00	1.69E+00	7.47E-01	1.78E-01	4.55E-02	1.10E-02	2.53E-03	5.46E-04	9.53E-05	1.28E-05	1.96E-08	0.00E+00	0.00E+00	0.00E+00
40	1.24E+02	1.13E+02	9.66E+01	7.15E+01	5.12E+01	3.56E+01	2.44E+01	1.66E+01	7.80E+00	3.92E+00	2.11E+00	7.00E-01	2.32E-01	7.44E-02	2.37E-02	7.25E-03	2.15E-03	6.42E-04	2.36E-05	2.74E-07	6.74E-10	0.00E+00
50	1.40E+02	1.29E+02	1.12E+02	8.48E+01	6.25E+01	4.51E+01	3.22E+01	2.30E+01	1.22E+01	6.98E+00	4.20E+00	1.63E+00	6.30E-01	2.41E-01	9.27E-02	3.52E-02	1.33E-02	5.05E-03	4.02E-04	2.85E-05	9.77E-07	1.23E-08
60	1.51E+02	1.40E+02	1.23E+02	9.56E+01	7.21E+01	5.34E+01	3.94E+01	2.92E+01	1.69E+01	1.05E+01	6.77E+00	2.91E+00	1.25E+00	5.46E-01	2.38E-01	1.03E-01	4.51E-02	2.00E-02	2.40E-03	2.77E-04	2.90E-05	1.95E-06
70	1.61E+02	1.50E+02	1.33E+02	1.05E+02	8.03E+01	6.09E+01	4.61E+01	3.53E+01	2.18E+01	1.41E+01	9.59E+00	4.45E+00	2.07E+00	9.92E-01	4.74E-01	2.26E-01	1.10E-01	5.35E-02	8.56E-03	1.33E-03	1.99E-04	2.71E-05
80	1.68E+02	1.57E+02	1.40E+02	1.12E+02	8.74E+01	6.75E+01	5.23E+01	4.09E+01	2.65E+01	1.79E+01	1.25E+01	6.15E+00	3.06E+00	1.56E+00	8.01E-01	4.11E-01	2.15E-01	1.12E-01	2.22E-02	4.30E-03	8.18E-04	1.48E-04
90	1.74E+02	1.63E+02	1.47E+02	1.18E+02	9.36E+01	7.34E+01	5.78E+01	4.62E+01	3.10E+01	2.17E+01	1.55E+01	7.94E+00	4.16E+00	2.25E+00	1.21E+00	6.59E-01	3.66E-01	2.02E-01	4.67E-02	1.06E-02	2.42E-03	5.35E-04
100	1.79E+02	1.69E+02	1.52E+02	1.24E+02	9.91E+01	7.87E+01	6.29E+01	5.10E+01	3.53E+01	2.52E+01	1.83E+01	9.78E+00	5.38E+00	3.02E+00	1.70E+00	9.67E-01	5.62E-01	3.25E-01	8.49E-02	2.20E-02	5.72E-03	1.47E-03
125	1.89E+02	1.79E+02	1.62E+02	1.35E+02	1.10E+02	8.97E+01	7.37E+01	6.13E+01	4.46E+01	3.33E+01	2.51E+01	1.44E+01	8.60E+00	5.20E+00	3.16E+00	1.96E+00	1.23E+00	7.10E-01	2.49E-01	8.18E-02	2.69E-02	8.92E-03
150	1.96E+02	1.86E+02	1.70E+02	1.43E+02	1.19E+02	9.83E+01	8.24E+01	6.97E+01	5.22E+01	4.02E+01	3.10E+01	1.88E+01	1.18E+01	7.54E+00	4.83E+00	3.18E+00	2.10E+00	1.39E+00	5.18E-01	1.98E-01	7.59E-02	2.94E-02
175	2.01E+02	1.91E+02	1.76E+02	1.49E+02	1.25E+02	1.05E+02	8.94E+01	7.69E+01	5.85E+01	4.61E+01	3.62E+01	2.28E+01	1.49E+01	9.87E+00	6.59E+00	4.52E+00	3.10E+00	2.13E+00	8.80E-01	3.73E-01	1.60E-01	6.93E-02
200	2.04E+02	1.95E+02	1.80E+02	1.54E+02	1.31E+02	1.11E+02	9.52E+01	8.27E+01	6.42E+01	5.12E+01	4.06E+01	2.64E+01	1.78E+01	1.21E+01	8.36E+00	5.88E+00	4.16E+00	2.96E+00	1.32E+00	6.03E-01	2.82E-01	1.33E-01

APPENDIX VII: PEARL tables, Concentration in Plough layer after one year (mg/kg)

spring	Kom (l/kg)																				
DT50bio,soil (days) at 20 °C	0	1	2.5	5	7.5	10	12.5	15	20	25	30	40	50	60	70	80	90	100	125	150	175	200
2.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002
20	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0002	0.0003	0.0004	0.0005	0.0006	0.0008	0.0009	0.0010	0.0010	0.0011	0.0011	0.0011	0.0012	0.0012	0.0012
25	0.0000	0.0000	0.0000	0.0001	0.0001	0.0002	0.0003	0.0005	0.0008	0.0011	0.0014	0.0019	0.0024	0.0027	0.0030	0.0032	0.0033	0.0034	0.0036	0.0037	0.0037	0.0037
30	0.0000	0.0000	0.0000	0.0001	0.0002	0.0005	0.0007	0.0010	0.0016	0.0022	0.0029	0.0040	0.0049	0.0057	0.0063	0.0067	0.0070	0.0073	0.0077	0.0079	0.0080	0.0080
40	0.0000	0.0000	0.0001	0.0002	0.0006	0.0011	0.0017	0.0024	0.0039	0.0054	0.0070	0.0099	0.0123	0.0143	0.0159	0.0171	0.0180	0.0187	0.0199	0.0204	0.0207	0.0209
50	0.0000	0.0000	0.0001	0.0004	0.0010	0.0018	0.0028	0.0040	0.0066	0.0093	0.0120	0.0171	0.0214	0.0249	0.0277	0.0300	0.0317	0.0330	0.0351	0.0362	0.0368	0.0371
60	0.0000	0.0000	0.0001	0.0006	0.0014	0.0025	0.0040	0.0056	0.0094	0.0133	0.0172	0.0245	0.0308	0.0361	0.0403	0.0436	0.0462	0.0482	0.0514	0.0531	0.0540	0.0545
70	0.0000	0.0000	0.0002	0.0007	0.0018	0.0032	0.0051	0.0072	0.0120	0.0171	0.0222	0.0318	0.0401	0.0470	0.0526	0.0570	0.0605	0.0632	0.0675	0.0698	0.0710	0.0716
80	0.0000	0.0000	0.0002	0.0009	0.0021	0.0039	0.0061	0.0087	0.0146	0.0207	0.0269	0.0387	0.0488	0.0573	0.0642	0.0697	0.0740	0.0774	0.0828	0.0856	0.0872	0.0880
90	0.0000	0.0000	0.0002	0.0010	0.0024	0.0045	0.0071	0.0101	0.0169	0.0241	0.0313	0.0450	0.0569	0.0669	0.0750	0.0815	0.0866	0.0906	0.0970	0.1000	0.1020	0.1030
100	0.0000	0.0001	0.0003	0.0011	0.0027	0.0050	0.0080	0.0133	0.0190	0.0271	0.0353	0.0508	0.0643	0.0756	0.0849	0.0923	0.0981	0.1030	0.1100	0.1140	0.1160	0.1170
125	0.0000	0.0001	0.0003	0.0013	0.0033	0.0062	0.0098	0.0140	0.0234	0.0336	0.0438	0.0632	0.0801	0.0944	0.1061	0.1155	0.1230	0.1290	0.1380	0.1440	0.1460	0.1480
150	0.0000	0.0001	0.0004	0.0015	0.0038	0.0071	0.0113	0.0161	0.0270	0.0387	0.0505	0.0731	0.0928	0.1100	0.1231	0.1341	0.1430	0.1500	0.1610	0.1670	0.1700	0.1720
175	0.0000	0.0001	0.0004	0.0017	0.0042	0.0078	0.0124	0.0178	0.0298	0.0429	0.0560	0.0810	0.1030	0.1220	0.1369	0.1493	0.1590	0.1670	0.1800	0.1860	0.1900	0.1920
200	0.0000	0.0001	0.0004	0.0018	0.0045	0.0084	0.0134	0.0191	0.0322	0.0462	0.0605	0.0876	0.1110	0.1320	0.1483	0.1617	0.1720	0.1810	0.1950	0.2020	0.2060	0.2080

autumn	Kom (l/kg)																				
DT50bio,soil (days) at 20 °C	0	1	2.5	5	7.5	10	12.5	15	20	25	30	40	50	60	70	80	90	100	125	150	175	200
2.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0002	0.0002	0.0000	0.0002	0.0002	0.0002	0.0002	0.0002
20	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0002	0.0002	0.0003	0.0004	0.0005	0.0007	0.0008	0.0009	0.0010	0.0011	0.0011	0.0011	0.0012	0.0012	0.0012	0.0012
25	0.0000	0.0000	0.0000	0.0001	0.0002	0.0003	0.0005	0.0006	0.0009	0.0013	0.0016	0.0021	0.0025	0.0028	0.0031	0.0033	0.0034	0.0035	0.0037	0.0037	0.0038	0.0038
30	0.0000	0.0000	0.0001	0.0002	0.0004	0.0006	0.0010	0.0013	0.0020	0.0026	0.0033	0.0044	0.0053	0.0060	0.0065	0.0070	0.0073	0.0075	0.0078	0.0080	0.0081	0.0081
40	0.0000	0.0000	0.0001	0.0004	0.0009	0.0016	0.0024	0.0032	0.0048	0.0065	0.0081	0.0110	0.0133	0.0152	0.0167	0.0178	0.0186	0.0193	0.0202	0.0207	0.0210	0.0211
50	0.0000	0.0001	0.0002	0.0007	0.0016	0.0027	0.0040	0.0055	0.0084	0.0113	0.0142	0.0192	0.0233	0.0267	0.0293	0.0313	0.0328	0.0340	0.0358	0.0367	0.0372	0.0374
60	0.0000	0.0001	0.0003	0.0010	0.0023	0.0039	0.0058	0.0079	0.0120	0.0163	0.0204	0.0278	0.0339	0.0388	0.0426	0.0456	0.0479	0.0497	0.0524	0.0538	0.0545	0.0549
70	0.0000	0.0001	0.0004	0.0013	0.0029	0.0050	0.0075	0.0102	0.0158	0.0212	0.0266	0.0362	0.0442	0.0506	0.0558	0.0597	0.0628	0.0651	0.0689	0.0707	0.0717	0.0722
80	0.0001	0.0002	0.0005	0.0016	0.0035	0.0061	0.0091	0.0123	0.0191	0.0258	0.0323	0.0441	0.0539	0.0619	0.0682	0.0731	0.0769	0.0798	0.0804	0.0868	0.0880	0.0886
90	0.0001	0.0002	0.0005	0.0019	0.0041	0.0070	0.0105	0.0143	0.0223	0.0300	0.0377	0.0514	0.0630	0.0723	0.0798	0.0856	0.0901	0.0935	0.0990	0.1020	0.1030	0.1040
100	0.0001	0.0002	0.0006	0.0021	0.0046	0.0079	0.0119	0.0161	0.0251	0.0339	0.0426	0.0582	0.0713	0.0820	0.0904	0.0970	0.1020	0.1060	0.1120	0.1160	0.1170	0.1180
125	0.0001	0.0003	0.0008	0.0026	0.0057	0.0098	0.0147	0.0200	0.0312	0.0422	0.0531	0.0727	0.0810	0.1030	0.1130	0.1220	0.1280	0.1330	0.1410	0.1450	0.1470	0.1490
150	0.0001	0.0003	0.0009	0.0030	0.0065	0.0113	0.0170	0.0231	0.0361	0.0488	0.0615	0.0842	0.1030	0.1190	0.1320	0.1410	0.1490	0.1550	0.1640	0.1690	0.1720	0.1730
175	0.0001	0.0003	0.0010	0.0033	0.0072	0.0125	0.0188	0.0256	0.0401	0.0542	0.0682	0.0936	0.1150	0.1330	0.1470	0.1580	0.1660	0.1730	0.1830	0.1890	0.1920	0.1930
200	0.0001	0.0003	0.0010	0.0036	0.0078	0.0135	0.0203	0.0277	0.0433	0.0586	0.0738	0.1010	0.1250	0.1440	0.1590	0.1710	0.1800	0.1870	0.1990	0.2050	0.2080	0.2100

Water phase (dummy data)

Spring	**One application**				
	Interval not relevant				
DT50water,temp	**PEC0**	**PEC4**	**PEC14**	**PEC21**	**PEC28**
[d]	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**
0.1	4.73	0.17	0.05	0.03	0.02
0.2	4.73	0.33	0.09	0.06	0.05
0.3	4.73	0.50	0.20	0.10	0.07
0.4	4.73	0.67	0.30	0.13	0.10
0.5	4.73	0.83	0.40	0.16	0.12
0.6	4.73	0.98	0.50	0.19	0.14
0.7	4.73	1.13	0.60	0.22	0.17
0.8	4.73	1.27	0.70	0.26	0.19
0.9	4.73	1.40	0.80	0.29	0.22
1.0	4.73	1.53	0.90	0.32	0.24
2.0	4.73	2.39	1.00	0.63	0.47
3.0	4.73	2.85	1.30	0.91	0.70
4.0	4.73	3.14	1.60	1.17	0.90
5.0	4.73	3.33	2.00	1.39	1.09
6.0	4.73	3.46	2.20	1.59	1.27
7.0	4.73	3.56	2.40	1.76	1.42
8.0	4.73	3.64	2.50	1.90	1.56
9.0	4.73	3.71	2.60	2.03	1.68
10.0	4.73	3.76	2.80	2.14	1.79
15.0	4.73	3.92	3.00	2.54	2.20
20.0	4.73	4.01	3.20	2.79	2.47
30.0	4.73	4.09	3.35	3.06	2.78
40.0	4.73	4.14	3.50	3.22	2.96
50.0	4.73	4.16	3.60	3.32	3.08
100.0	4.73	4.22	3.75	3.53	3.33
200.0	4.73	4.25	3.80	3.64	3.46
500.0	4.73	4.26	3.85	3.71	3.55
1000.0	4.73	4.27	3.90	3.73	3.58

Water phase (dummy data)

Spring	**Two Applications**									
	Interval: 7 days					**Interval: 10 days**				
DT50water,temp	**PEC0**	**PEC4**	**PEC14**	**PEC21**	**PEC28**	**PEC0**	**PEC4**	**PEC14**	**PEC21**	**PEC28**
[d]	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**
0.1	4.73	0.17	0.09	0.06	0.05	4.73	0.17	0.09	0.06	0.05
0.2	4.73	0.34	0.20	0.13	0.10	4.73	0.34	0.20	0.13	0.10
0.3	4.73	0.50	0.30	0.19	0.14	4.73	0.50	0.30	0.19	0.14
0.4	4.73	0.67	0.40	0.26	0.19	4.73	0.67	0.40	0.26	0.19
0.5	4.74	0.83	0.50	0.32	0.24	4.73	0.83	0.50	0.32	0.24
0.6	4.74	0.99	0.60	0.38	0.29	4.74	0.98	0.60	0.38	0.29
0.7	4.75	1.14	0.70	0.45	0.34	4.74	1.13	0.70	0.45	0.34
0.8	4.76	1.28	0.80	0.51	0.38	4.74	1.28	0.80	0.51	0.38
0.9	4.77	1.42	0.90	0.57	0.43	4.74	1.41	0.90	0.57	0.43
1.0	4.79	1.55	1.00	0.64	0.48	4.75	1.54	1.00	0.64	0.48
2.0	5.15	2.64	1.60	1.24	0.94	4.91	2.50	1.50	1.23	0.94
3.0	5.59	3.44	2.20	1.78	1.38	5.20	3.18	2.10	1.74	1.37
4.0	5.98	4.06	2.80	2.25	1.78	5.50	3.72	2.60	2.18	1.76
5.0	6.29	4.55	3.30	2.65	2.14	5.78	4.16	3.00	2.54	2.11
6.0	6.54	4.93	3.50	2.98	2.46	6.02	4.52	3.30	2.84	2.41
7.0	6.75	5.24	3.80	3.27	2.75	6.23	4.82	3.60	3.10	2.68
8.0	6.92	5.50	4.00	3.51	3.00	6.41	5.08	3.80	3.32	2.91
9.0	7.06	5.72	4.20	3.72	3.22	6.56	5.30	4.00	3.50	3.12
10.0	7.18	5.90	4.50	3.90	3.41	6.69	5.48	4.30	3.67	3.30
15.0	7.58	6.51	5.00	4.54	4.13	7.15	6.13	4.70	4.24	3.96
20.0	7.80	6.85	5.60	4.93	4.58	7.43	6.52	5.30	4.62	4.38
30.0	8.04	7.22	6.10	5.53	5.11	7.73	6.94	5.80	5.28	4.86
40.0	8.17	7.42	6.50	5.91	5.41	7.89	7.17	6.20	5.66	5.13
50.0	8.25	7.54	6.65	6.15	5.60	8.00	7.31	6.50	5.92	5.33
100.0	8.42	7.80	7.15	6.67	6.12	8.21	7.61	6.90	6.45	5.83
200.0	8.50	7.93	7.30	6.95	6.42	8.33	7.77	7.10	6.75	6.12
500.0	8.56	8.01	7.45	7.13	6.61	8.40	7.87	7.25	6.94	6.31
1000.0	8.57	8.04	7.50	7.19	6.68	8.42	7.91	7.40	7.00	6.37

Water phase (dummy data)

Spring	Three Applications									
	Interval: 7 days					Interval: 10 days				
DT50water,temp	**PEC0**	**PEC4**	**PEC14**	**PEC21**	**PEC28**	**PEC0**	**PEC4**	**PEC14**	**PEC21**	**PEC28**
[d]	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**
0.1	4.73	0.17	0.09	0.10	0.07	4.73	0.17	0.09	0.10	0.07
0.2	4.73	0.34	0.20	0.19	0.15	4.73	0.34	0.20	0.19	0.15
0.3	4.73	0.51	0.30	0.29	0.22	4.73	0.50	0.30	0.28	0.22
0.4	4.74	0.67	0.40	0.39	0.29	4.73	0.67	0.40	0.36	0.29
0.5	4.74	0.83	0.50	0.48	0.36	4.73	0.83	0.50	0.44	0.36
0.6	4.74	0.99	0.60	0.58	0.43	4.74	0.99	0.60	0.51	0.43
0.7	4.75	1.14	0.70	0.67	0.50	4.74	1.14	0.70	0.59	0.50
0.8	4.76	1.29	0.80	0.76	0.58	4.74	1.28	0.80	0.66	0.57
0.9	4.77	1.42	0.90	0.86	0.65	4.75	1.41	0.90	0.73	0.65
1.0	4.79	1.56	1.00	0.95	0.72	4.75	1.54	1.00	0.79	0.71
2.0	5.21	2.68	2.00	1.80	1.40	4.93	2.52	1.70	1.41	1.37
3.0	5.81	3.60	2.80	2.51	2.04	5.28	3.24	2.30	1.94	1.94
4.0	6.41	4.39	3.40	3.09	2.60	5.69	3.87	2.90	2.43	2.43
5.0	6.94	5.06	3.90	3.57	3.09	6.10	4.42	3.40	2.93	2.85
6.0	7.40	5.64	4.20	3.96	3.51	6.49	4.91	3.80	3.38	3.21
7.0	7.79	6.12	4.70	4.29	3.88	6.84	5.35	4.30	3.77	3.52
8.0	8.13	6.54	5.00	4.58	4.21	7.16	5.74	4.60	4.13	3.78
9.0	8.43	6.91	5.60	4.90	4.49	7.45	6.08	5.00	4.44	4.02
10.0	8.68	7.23	6.00	5.21	4.74	7.71	6.39	5.50	4.72	4.23
15.0	9.59	8.34	7.00	6.33	5.64	8.67	7.53	6.20	5.75	5.21
20.0	10.13	9.01	7.70	7.02	6.37	9.28	8.25	6.90	6.41	5.90
30.0	10.74	9.78	8.50	7.83	7.25	10.01	9.10	7.60	7.17	6.72
40.0	11.07	10.19	9.00	8.29	7.76	10.42	9.59	8.20	7.61	7.20
50.0	11.28	10.46	9.30	8.58	8.09	10.68	9.90	8.60	7.90	7.51
100.0	11.72	11.02	10.00	9.27	8.81	11.25	10.58	9.20	8.52	8.18
200.0	11.96	11.32	10.20	9.71	9.20	11.56	10.94	9.80	8.91	8.55
500.0	12.10	11.50	10.50	9.99	9.45	11.75	11.17	10.00	9.16	8.78
1000.0	12.15	11.57	10.60	10.09	9.53	11.82	11.25	10.10	9.25	8.86

Water phase (dummy data)

Spring	Four Applications									
	Interval: 7 days					Interval: 10 days				
DT50water,temp	**PEC0**	**PEC4**	**PEC14**	**PEC21**	**PEC28**	**PEC0**	**PEC4**	**PEC14**	**PEC21**	**PEC28**
[d]	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**
0.1	4.73	0.17	0.13	0.12	0.10	4.73	0.17	0.13	0.10	0.07
0.2	4.73	0.34	0.25	0.22	0.19	4.73	0.34	0.25	0.19	0.15
0.3	4.73	0.51	0.37	0.31	0.29	4.73	0.50	0.37	0.28	0.22
0.4	4.74	0.67	0.48	0.41	0.39	4.73	0.67	0.48	0.36	0.29
0.5	4.74	0.83	0.59	0.50	0.48	4.74	0.83	0.59	0.44	0.36
0.6	4.74	0.99	0.72	0.60	0.58	4.74	0.99	0.72	0.52	0.43
0.7	4.75	1.14	0.78	0.69	0.67	4.74	1.14	0.78	0.59	0.51
0.8	4.76	1.29	0.90	0.78	0.77	4.74	1.28	0.90	0.66	0.58
0.9	4.78	1.43	1.00	0.87	0.86	4.75	1.41	1.00	0.73	0.65
1.0	4.80	1.56	1.10	0.97	0.95	4.75	1.54	1.10	0.80	0.72
2.0	5.23	2.70	2.10	1.87	1.82	4.94	2.52	1.80	1.45	1.40
3.0	5.88	3.66	3.00	2.72	2.58	5.30	3.26	2.50	2.06	2.04
4.0	6.57	4.52	3.80	3.47	3.22	5.74	3.91	3.00	2.62	2.62
5.0	7.23	5.30	4.60	4.12	3.78	6.20	4.50	3.60	3.13	3.15
6.0	7.82	5.99	5.20	4.69	4.25	6.65	5.04	4.00	3.58	3.63
7.0	8.36	6.61	5.60	5.19	4.65	7.07	5.53	4.50	4.04	4.06
8.0	8.83	7.15	6.00	5.62	5.05	7.47	5.97	5.00	4.46	4.44
9.0	9.27	7.64	6.30	6.00	5.45	7.83	6.37	5.30	4.85	4.77
10.0	9.64	8.07	6.80	6.33	5.81	8.16	6.74	5.80	5.20	5.08
15.0	11.05	9.68	8.00	7.53	7.14	9.45	8.14	7.00	6.53	6.22
20.0	11.93	10.69	9.20	8.51	7.98	10.32	9.06	8.00	7.41	6.94
30.0	12.97	11.89	10.40	9.70	8.98	11.38	10.18	9.00	8.47	7.83
40.0	13.55	12.57	11.10	10.38	9.55	12.00	10.84	9.70	9.09	8.40
50.0	13.93	13.00	11.60	10.82	9.95	12.40	11.27	10.10	9.49	8.79
100.0	14.74	13.95	12.60	11.78	10.90	13.30	12.21	10.90	10.37	9.67
200.0	15.18	14.46	13.20	12.30	11.45	13.80	12.73	11.40	10.85	10.16
500.0	15.45	14.78	13.50	12.63	11.79	14.11	13.06	11.80	11.16	10.47
1000.0	15.54	14.89	13.60	12.74	11.91	14.22	13.17	11.90	11.26	10.57

Water phase (dummy data)

Spring	**Five or more applications**				
	Interval: 7 days				
DT50water,temp	**PEC0**	**PEC4**	**PEC14**	**PEC21**	**PEC28**
[d]	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**
0.1	4.73	0.17	0.13	0.12	0.11
0.2	4.73	0.34	0.25	0.22	0.21
0.3	4.73	0.51	0.36	0.31	0.31
0.4	4.74	0.67	0.50	0.41	0.40
0.5	4.74	0.83	0.60	0.50	0.50
0.6	4.74	0.99	0.70	0.60	0.59
0.7	4.75	1.14	0.80	0.69	0.69
0.8	4.77	1.29	0.90	0.79	0.78
0.9	4.78	1.43	1.00	0.88	0.87
1.0	4.80	1.56	1.20	0.97	0.97
2.0	5.24	2.70	2.10	1.89	1.88
3.0	5.91	3.68	3.00	2.78	2.74
4.0	6.64	4.58	3.90	3.61	3.52
5.0	7.36	5.40	4.70	4.37	4.22
6.0	8.03	6.16	5.30	5.05	4.83
7.0	8.65	6.84	6.00	5.65	5.37
8.0	9.22	7.46	6.60	6.19	5.85
9.0	9.74	8.02	7.10	6.68	6.27
10.0	10.21	8.53	7.60	7.12	6.65
15.0	12.01	10.46	9.40	8.73	8.10
20.0	13.19	11.72	10.30	9.76	9.18
30.0	14.62	13.26	11.70	11.00	10.49
40.0	15.45	14.15	12.50	11.78	11.25
50.0	15.99	14.73	13.00	12.31	11.74
100.0	17.18	16.00	14.40	13.52	12.81
200.0	17.83	16.70	15.00	14.19	13.40
500.0	18.24	17.14	15.40	14.61	13.77
1000.0	18.38	17.29	15.60	14.76	13.90

Water phase (dummy data)

Autumn	One application				
	Interval not relevant				
DT50water,temp	PEC0	PEC4	PEC14	PEC21	PEC28
[d]	[µg/l]	[µg/l]	[µg/l]	[µg/l]	[µg/l]
0.1	4.73	0.17	0.05	0.03	0.02
0.2	4.73	0.33	0.09	0.06	0.05
0.3	4.73	0.50	0.20	0.10	0.07
0.4	4.73	0.66	0.30	0.13	0.10
0.5	4.73	0.82	0.40	0.16	0.12
0.6	4.73	0.96	0.50	0.19	0.14
0.7	4.73	1.10	0.55	0.21	0.16
0.8	4.73	1.22	0.65	0.24	0.18
0.9	4.73	1.33	0.75	0.26	0.19
1.0	4.73	1.44	0.85	0.28	0.21
2.0	4.73	2.10	0.90	0.41	0.31
3.0	4.73	2.43	1.00	0.48	0.36
4.0	4.73	2.63	1.20	0.52	0.39
5.0	4.73	2.76	1.30	0.54	0.41
6.0	4.73	2.84	1.40	0.56	0.42
7.0	4.73	2.91	1.50	0.57	0.43
8.0	4.73	2.96	1.55	0.58	0.44
9.0	4.73	3.00	1.60	0.59	0.44
10.0	4.73	3.04	1.65	0.60	0.45
15.0	4.73	3.14	1.70	0.62	0.47
20.0	4.73	3.19	1.75	0.63	0.47
30.0	4.73	3.25	1.80	0.64	0.48
40.0	4.73	3.28	1.85	0.65	0.49
50.0	4.73	3.29	1.90	0.65	0.49
100.0	4.73	3.33	1.95	0.66	0.49
200.0	4.73	3.34	2.00	0.66	0.50
500.0	4.73	3.35	2.05	0.66	0.50
1000.0	4.73	3.36	2.10	0.66	0.50

Water phase (dummy data)

Autumn	Two Applications									
	Interval: 7 days					Interval: 10 days				
DT50water,temp	PEC0	PEC4	PEC14	PEC21	PEC28	PEC0	PEC4	PEC14	PEC21	PEC28
[d]	[μg/l]	[μg/l]	[μg/l]	[μg/l]	[μg/l]	[μg/l]	[μg/l]	[μg/l]	[μg/l]	[μg/l]
0.1	4.73	0.17	0.05	0.06	0.05	4.73	0.17	0.05	0.06	0.05
0.2	4.73	0.34	0.09	0.13	0.10	4.73	0.34	0.09	0.13	0.10
0.3	4.73	0.50	0.20	0.19	0.14	4.73	0.50	0.20	0.19	0.14
0.4	4.73	0.67	0.30	0.26	0.19	4.73	0.66	0.30	0.26	0.19
0.5	4.74	0.82	0.40	0.32	0.24	4.73	0.82	0.40	0.32	0.24
0.6	4.74	0.97	0.50	0.37	0.28	4.73	0.96	0.50	0.37	0.28
0.7	4.74	1.10	0.55	0.42	0.32	4.74	1.10	0.55	0.42	0.32
0.8	4.74	1.23	0.65	0.47	0.36	4.74	1.22	0.65	0.47	0.36
0.9	4.74	1.34	0.75	0.52	0.39	4.74	1.34	0.75	0.52	0.39
1.0	4.74	1.44	0.85	0.56	0.42	4.74	1.44	0.85	0.56	0.42
2.0	4.75	2.12	1.10	0.82	0.62	4.74	2.11	1.10	0.82	0.62
3.0	4.76	2.45	1.30	0.95	0.72	4.75	2.44	1.30	0.95	0.72
4.0	4.76	2.65	1.40	1.03	0.78	4.75	2.64	1.40	1.03	0.78
5.0	4.77	2.78	1.45	1.08	0.81	4.75	2.77	1.45	1.08	0.81
6.0	4.77	2.87	1.49	1.12	0.84	4.75	2.86	1.49	1.12	0.84
7.0	4.77	2.93	1.50	1.15	0.86	4.75	2.92	1.50	1.14	0.86
8.0	4.77	2.99	1.55	1.17	0.88	4.75	2.98	1.55	1.17	0.88
9.0	4.77	3.03	1.60	1.18	0.89	4.75	3.02	1.60	1.18	0.89
10.0	4.77	3.06	1.65	1.20	0.90	4.75	3.05	1.65	1.19	0.90
15.0	4.77	3.17	1.70	1.24	0.93	4.75	3.15	1.70	1.24	0.93
20.0	4.77	3.22	1.75	1.26	0.95	4.75	3.21	1.75	1.26	0.95
30.0	4.77	3.28	1.80	1.28	0.96	4.75	3.26	1.80	1.28	0.96
40.0	4.77	3.30	1.85	1.29	0.97	4.75	3.29	1.85	1.29	0.97
50.0	4.77	3.32	1.90	1.30	0.98	4.75	3.31	1.90	1.30	0.98
100.0	4.77	3.36	1.95	1.31	0.99	4.75	3.34	1.95	1.31	0.99
200.0	4.77	3.37	2.00	1.32	0.99	4.75	3.36	2.00	1.32	0.99
500.0	4.77	3.38	2.05	1.32	1.00	4.75	3.37	2.05	1.32	0.99
1000.0	4.77	3.39	2.10	1.33	1.00	4.75	3.37	2.10	1.32	1.00

Water phase (dummy data)

Autumn	Three Applications									
	Interval: 7 days					Interval: 10 days				
DT50water,temp	**PEC0**	**PEC4**	**PEC14**	**PEC21**	**PEC28**	**PEC0**	**PEC4**	**PEC14**	**PEC21**	**PEC28**
[d]	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**	**[µg/l]**
0.1	4.73	0.17	0.11	0.10	0.07	4.73	0.17	0.11	0.10	0.07
0.2	4.73	0.34	0.24	0.19	0.15	4.73	0.34	0.24	0.19	0.15
0.3	4.73	0.50	0.37	0.29	0.22	4.73	0.50	0.37	0.28	0.22
0.4	4.74	0.67	0.50	0.38	0.29	4.73	0.67	0.50	0.36	0.29
0.5	4.74	0.82	0.60	0.47	0.36	4.73	0.82	0.60	0.43	0.36
0.6	4.74	0.97	0.70	0.56	0.42	4.74	0.96	0.70	0.50	0.42
0.7	4.74	1.10	0.80	0.64	0.48	4.74	1.10	0.80	0.56	0.48
0.8	4.74	1.23	0.90	0.71	0.53	4.74	1.22	0.90	0.62	0.53
0.9	4.75	1.34	1.00	0.77	0.58	4.74	1.34	1.00	0.67	0.58
1.0	4.75	1.45	1.05	0.84	0.63	4.74	1.44	1.05	0.71	0.63
2.0	4.76	2.12	1.45	1.23	0.93	4.75	2.11	1.20	1.01	0.93
3.0	4.77	2.46	1.67	1.43	1.08	4.75	2.45	1.40	1.15	1.07
4.0	4.77	2.66	1.85	1.54	1.16	4.75	2.64	1.50	1.23	1.16
5.0	4.77	2.78	1.93	1.62	1.22	4.75	2.77	1.60	1.28	1.22
6.0	4.77	2.88	1.95	1.67	1.26	4.75	2.86	1.70	1.32	1.26
7.0	4.77	2.94	1.97	1.71	1.29	4.75	2.93	1.80	1.35	1.29
8.0	4.78	2.99	2.00	1.74	1.32	4.76	2.98	1.90	1.37	1.31
9.0	4.78	3.04	2.05	1.77	1.33	4.76	3.02	2.00	1.39	1.33
10.0	4.78	3.07	2.10	1.79	1.35	4.76	3.06	2.10	1.40	1.34
15.0	4.78	3.18	2.12	1.85	1.40	4.76	3.16	2.12	1.45	1.39
20.0	4.78	3.23	2.15	1.88	1.42	4.76	3.21	2.15	1.47	1.41
30.0	4.78	3.29	2.17	1.91	1.44	4.76	3.27	2.17	1.49	1.44
40.0	4.78	3.31	2.22	1.93	1.46	4.76	3.30	2.22	1.50	1.45
50.0	4.78	3.33	2.25	1.94	1.46	4.76	3.31	2.25	1.51	1.46
100.0	4.78	3.36	2.28	1.96	1.48	4.76	3.35	2.28	1.53	1.47
200.0	4.78	3.38	2.30	1.97	1.49	4.76	3.37	2.30	1.53	1.48
500.0	4.78	3.39	2.35	1.98	1.49	4.76	3.38	2.35	1.54	1.49
1000.0	4.78	3.40	2.40	1.98	1.49	4.76	3.38	2.40	1.54	1.49

Water phase (dummy data)

Autumn	Four Applications									
	Interval: 7 days					Interval: 10 days				
DT50water,temp	PEC0	PEC4	PEC14	PEC21	PEC28	PEC0	PEC4	PEC14	PEC21	PEC28
[d]	[μg/l]	[μg/l]	[μg/l]	[μg/l]	[μg/l]	[μg/l]	[μg/l]	[μg/l]	[μg/l]	[μg/l]
0.1	4.73	0.17	0.11	0.12	0.10	4.73	0.17	0.11	0.10	0.07
0.2	4.73	0.34	0.24	0.22	0.19	4.73	0.34	0.24	0.19	0.15
0.3	4.73	0.51	0.37	0.31	0.29	4.73	0.50	0.37	0.28	0.22
0.4	4.74	0.67	0.50	0.41	0.38	4.73	0.67	0.50	0.36	0.29
0.5	4.74	0.82	0.60	0.50	0.47	4.73	0.82	0.60	0.43	0.36
0.6	4.74	0.97	0.70	0.58	0.56	4.74	0.97	0.70	0.50	0.42
0.7	4.74	1.10	0.80	0.66	0.64	4.74	1.10	0.80	0.56	0.48
0.8	4.74	1.23	0.90	0.73	0.71	4.74	1.22	0.90	0.62	0.53
0.9	4.75	1.34	1.00	0.79	0.78	4.74	1.34	1.00	0.67	0.58
1.0	4.75	1.45	1.05	0.85	0.84	4.74	1.44	1.05	0.72	0.63
2.0	4.76	2.12	1.40	1.24	1.23	4.75	2.12	1.20	1.01	0.93
3.0	4.77	2.46	1.65	1.44	1.43	4.75	2.45	1.40	1.15	1.08
4.0	4.77	2.66	1.80	1.56	1.55	4.75	2.65	1.60	1.24	1.17
5.0	4.77	2.79	1.85	1.63	1.62	4.76	2.77	1.70	1.29	1.22
6.0	4.78	2.88	1.90	1.69	1.68	4.76	2.87	1.90	1.33	1.26
7.0	4.78	2.95	1.95	1.73	1.72	4.76	2.93	1.95	1.36	1.29
8.0	4.78	3.00	1.98	1.76	1.75	4.76	2.98	1.98	1.38	1.32
9.0	4.78	3.04	2.00	1.78	1.77	4.76	3.03	2.00	1.40	1.33
10.0	4.78	3.07	2.10	1.80	1.79	4.76	3.06	2.10	1.41	1.35
15.0	4.78	3.18	2.12	1.87	1.85	4.76	3.16	2.12	1.45	1.40
20.0	4.79	3.23	2.15	1.90	1.89	4.76	3.22	2.15	1.48	1.42
30.0	4.79	3.29	2.17	1.93	1.92	4.76	3.27	2.17	1.50	1.45
40.0	4.79	3.32	2.22	1.95	1.93	4.76	3.30	2.22	1.51	1.46
50.0	4.79	3.34	2.25	1.96	1.94	4.76	3.32	2.25	1.52	1.47
100.0	4.79	3.37	2.28	1.98	1.97	4.76	3.35	2.28	1.53	1.48
200.0	4.79	3.39	2.30	1.99	1.98	4.76	3.37	2.30	1.54	1.49
500.0	4.79	3.40	2.35	2.00	1.98	4.76	3.38	2.35	1.55	1.49
1000.0	4.79	3.40	2.40	2.00	1.98	4.76	3.38	2.40	1.55	1.49

Water phase (dummy data)

Autumn	**Five or more applications**				
	Interval: 7 days				
DT50water,temp	**PEC0**	**PEC4**	**PEC14**	**PEC21**	**PEC28**
[d]	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**	**[μg/l]**
0.1	4.73	0.17	0.11	0.12	0.11
0.2	4.73	0.34	0.24	0.22	0.21
0.3	4.73	0.51	0.37	0.31	0.31
0.4	4.74	0.67	0.50	0.41	0.40
0.5	4.74	0.82	0.60	0.50	0.49
0.6	4.74	0.97	0.70	0.58	0.57
0.7	4.74	1.10	0.80	0.66	0.65
0.8	4.75	1.23	0.90	0.73	0.72
0.9	4.75	1.34	1.00	0.79	0.79
1.0	4.75	1.45	1.05	0.85	0.85
2.0	4.76	2.13	1.40	1.25	1.24
3.0	4.77	2.46	1.60	1.45	1.44
4.0	4.77	2.66	1.70	1.56	1.56
5.0	4.78	2.79	1.80	1.64	1.63
6.0	4.78	2.88	1.90	1.70	1.69
7.0	4.78	2.95	1.95	1.74	1.73
8.0	4.78	3.00	1.98	1.77	1.76
9.0	4.78	3.04	2.00	1.79	1.78
10.0	4.78	3.08	2.10	1.81	1.80
15.0	4.79	3.18	2.12	1.87	1.87
20.0	4.79	3.24	2.15	1.91	1.90
30.0	4.79	3.29	2.17	1.94	1.93
40.0	4.79	3.32	2.22	1.96	1.95
50.0	4.79	3.34	2.25	1.97	1.96
100.0	4.79	3.37	2.28	1.99	1.98
200.0	4.79	3.39	2.30	2.00	1.99
500.0	4.79	3.40	2.35	2.00	2.00
1000.0	4.79	3.40	2.40	2.01	2.00

IX. Differences between emission scenarios for the local situation

In general two types of emission scenarios may be distinguished, viz one based on the regional tonnage and the other on the consumption.

1. Emission scenario based on tonnages

In general no regional tonnage will be known for an arbitrary substance. In that case the regional tonnage is derived from the EU tonnage by multiplication by 0.1 (10 % rule). This is about twice the amount that may be expected on account of the fraction of inhabitants in the region of the EU (see 4). Such a situation will not be unlikely in most cases as it may be expected that the more densely populated areas will have more industrial activities than the rural areas.

For diffuse emissions caused by e.g. households the standard STP with 10,000 inhabitants feeding the system and an amount of 0.2 m^3 wastewater per inhabitant per day is considered as a point source. If the use of a substance would be evenly distributed over the population (consumers) and STPs in a region and over the week, the fraction of this substance reaching the standard STP of EUSES would be *number of inhabitants connected to the STP (Nlocal) / number of inhabitants in the region (N)*. This means a fraction of 10,000 / 20.0.106 = 0.0005 with the defaults of EUSES. As the use of (formulation containing) substances never will be distributed evenly over the population and the week, a safety factor of four was assumed at the time. This means that the *fms* (fraction of the main source) = 0.002. This value is used in the emission tables of the TGD. In this case the nds (number of emission days) is equal to 365.
There may be other applications where a point source is considered such as a hospital. In Van der Poel (2001) the *fms* for the model hospital has been estimated to be 0.007. This fraction was calculated as from the average number of beds in a region per hospital and the total number of beds in that region. The nds may be less than 365 in specific cases.

2. Emission scenario based on the consumption

This type of emission scenarios apply either the average consumption per inhabitant or the – estimated – use in a process. An example of the average consumption is the use of soaps and detergents for cleaning and washing ($l.cap^{-1}.d^{-1}$ or $g.cap^{-1}.d^{-1}$). The emission scenario is simple and applies an emission factor, the concentration of the substance in the product (in this report a disinfectant for which the notifier has to specify the value) and the penetration factor (i.e. the fraction of the product on the market containing the specific substance) Fpenetr.
For a point source like a hospital it may be also the use of this kind of products (usually known in $kg.y^{-1}$). The emission scenario is even more simple as there is no penetration factor needed. Only an emission factor and an amount of product used is needed besides the concentration of the substance in the product.
The *nds* (number of emission days) will be 365 days for consumption data for the public at large but may be less in specific cases as in the example of hospital applications.

3. Tonnage versus Consumption

When a substance with diffuse emissions is assessed the scenarios based on the tonnage will produce emissions directly related to the volume of the use. This is an advantage compared to scenarios that are based on consumptions.
There are, however, also some disadvantages in using scenarios based on the tonnage; there is an uncertainty in the regional tonnage if this is not known and another uncertainty in the fraction reaching the standard STP.

The use of average consumptions has several disadvantages. First, there is no direct relation with the actual quantity of the disinfectant for the application in the case of diffuse emissions. Second, the average consumptions are often not specifically for e.g.detergents with a biocide leading to an uncertainty and for many products no reliable data are known. Third, the average consumption in a region may be different from the EU average leading to an uncertainty (reason for the 'safety factor' of 4 applied in the STP calculations with tonnages). Last but not least, the factor for the market penetration has a considerable uncertainty.
For point sources the main disadvantage is the fact that calculations of the consumption may have considerable uncertainties because of lacking data impelling detours to obtain estimates.

Because of the complete different character the two types of scenarios will provide outcomes which may be quite different. The emission factor and concentration of the substances in the product will be the same. For the diffuse emissions, i.e. emissions caused by use by the public at large, the scenario with the average consumption will give a fixed value whereas the scenario with the tonnage will give the emission as a linear relation to the quantity. It may be assumed that the tonnage scenario is more realistic as the consumption per habitant determines the tonnage.
For the point sources there may be a situation that the use of the tonnage scenario is underestimating the emission. This is the case where the substance is not used in the product by all sources. For example, if we consider a cleaner with a disinfectant for sanitary purposes in hospitals the various manufacturers of that product may apply different active substances. So, one hospital will apply the disinfectant assessed but another applies a different substance. The tonnage scenario, however, will distribute the whole amount over all hospitals so to say by using the fraction of its relative size (0.007). So, there will be a break even point below which the consumption scenario will be better. The break-even point is found by matching the equations for emission calculation (ef = emission factor):

A) <u>Consumption per day per person for diffuse emissions collected at a point source (STP)</u>

Tonnage (10^3 kg.yr^{-1}): Emission I = Tonnage * 10^3 * fms * ef / nds
Consumption (kg.d^{-1}): Emission II = Npers * Fpers * Consumption * Concentration * ef* Fpenetr
(where:
Npers = numer of persons regarded
Fpers = fraction of persons using the product

Emission I = Emission II, So:
Tonnage * 10^3 * fms * ef / nds = Consumption * Concentration * ef
Tonnage = (Npers * Fpers * Consumption * Concentration * nds * Fpenetr) / (10^3 * fms)

Example for a fictious situation with the following data:

Numer of persons Npers (-)	10,000
Fraction of persons Fpers (-)	0.5
Number of emission days nds (y^{-1})	365
fraction for main point source (-)	0.005
Consumption point source (kg. d^{-1})	0.02
Concentration of substance (%)	10
Penetration factor (-)	1

Tonnage = (10,000 * 0.02 * 0.5 * 10/100 * 365 * 1) / (10^3 * 0.005) = 730 tonnes

B) <u>Consumption per day for a point source</u>

Tonnage (10^3 kg.yr^{-1}): Emission = Tonnage * 10^3 * fms * ef / nds
Consumption (kg.d^{-1}): Emission = Consumption * Concentration * ef

Tonnage * 10^3 * fms * ef / nds = Consumption * Concentration * ef
Tonnage at break-even = (Consumption * Concentration * nds) / (10^3 * fms)

Example for a fictious situation with the following data:

Number of emission days nds (y^{-1})	365
fraction for main point source (-)	0.005
Consumption point source (kg. y^{-1})	100
Concentration of substance (%)	10

Tonnage at break-even = (10 * 10/100 * 365) / (10^3 * 0.005) = 730 tonnes

C) <u>Consumption per year for a point source</u>

Tonnage (10^3 kg.yr^{-1}): Emission = Tonnage * 10^3 * fms * ef / nds
Consumption (kg.yr^{-1}):Emission = Consumption * Concentration * ef * / nds

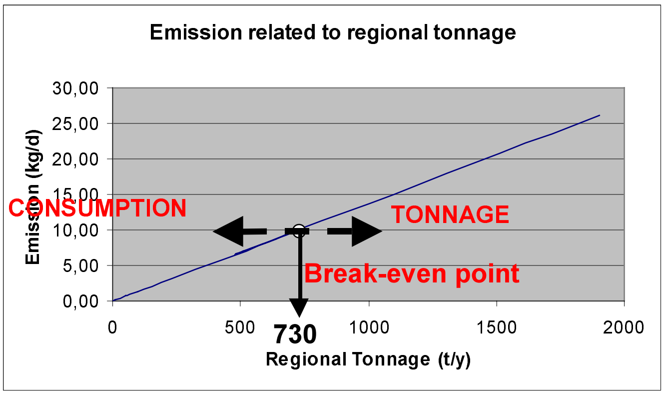
Tonnage at break-even = (Consumption * Concentration) / (10^3 * fms)

Example for a fictious situation with the following data:

fraction for main point source (-)	0.005
Consumption point source (kg. y^{-1})	36500
Concentration of substance (%)	10

Tonnage at break-even = (36500 * 10/100) / (10^3 * 0.005) = 730 tonnes

For a consumption pattern that yields 10 kg.d^{-1} for the point source the situation compared to the emission scenario based on the tonnage this has been illustrated in the figure below:



4. Number of inhabitants and area sizes in the TGD

In the TGD the area of the region is 200 x 200 km^2, which is more densely populated than the average region of that size elsewhere in the EU (total area of the EU $3.56 \cdot 10^6$ km^2). The number of inhabitants considered in the TGD is $2 \cdot 10^7$ in the region and $3 \cdot 7.10^8$ in the EU. So, the number of inhabitants per km^2 is 500 in the region and 104 in the EU. This means that the fraction of inhabitants in the region is $2 \cdot 10^7 / 3 \cdot 7.10^8 = 0.054$ and the fraction of the regional area $4 \cdot 10^4 / 3.56 \cdot 10^6 = 0.011$.