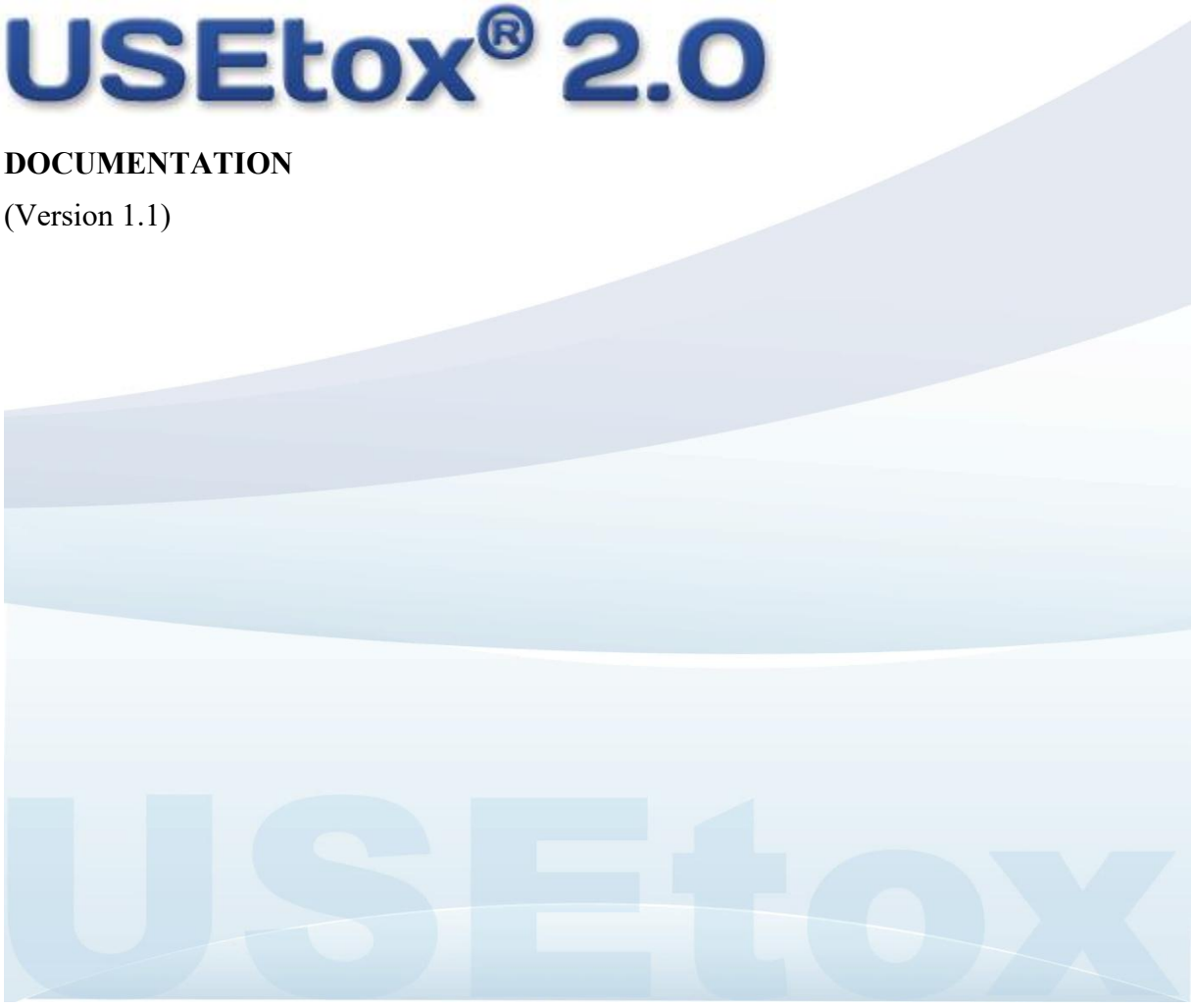
UNEP/SETAC scientific consensus model for characterizing human toxicological and ecotoxicological impacts of chemical emissions in life cycle assessment

USEtox® 2.0

DOCUMENTATION

(Version 1.1)



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USEtox® 2.0 Documentation (Version 1.1)

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PREFACE

This document represents the official **Documentation of USEtox**, the United Nations Environment Programme (UNEP) / Society of Environmental Toxicology and Chemistry (SETAC) **scientific consensus model** for characterizing human and ecotoxicological impacts of chemical emissions in life cycle assessment. Main output of USEtox is a database of **«recommended» and «indicative» characterization factors** for human toxicity and freshwater ecotoxicity, based on modelling of environmental fate, exposure, and effect parameters for the substances. Due to deficiencies in the model or the available substance data, the «indicative» factors are accompanied by a higher uncertainty than the «recommended» factors, which should be considered when applying the factors and interpreting the results.

USEtox is officially endorsed by the UNEP/SETAC Life Cycle Initiative, and recommended as assessment method by the European Commission (EC) in the Recommendations on the Use of Common Methods to Measure and Communicate the Life Cycle Environmental Performance of Products and Organisations, 2013/179/EU, by the European Commission's Joint Research Centre – Institute for Environment and Sustainability (JRC-IES) in the International Reference Life Cycle Data System (ILCD) Handbook – Recommendations for Life Cycle Impact Assessment in the European context, EUR 24571 EN, by the World Business Council for Sustainable Development (WBCSD) in the Life Cycle Metrics for Chemical Products – A Guideline by the Chemical Sector to Assess and Report on the Environmental Footprint of Products, Based on Life Cycle Assessment, and by the United States Environmental Protection Agency in the Tool for the Reduction and Assessment of Chemical and other Environmental Impacts (TRACI) User's Manual, S-10637-OP-1-0.

The **latest official release version of USEtox** is available at http://usetox.org.

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ABBREVIATIONS AND ACRONYMS

AGPP	Above-ground plant parts
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BGPP	Below-ground plant parts
BTF	Biotransfer factor
CF	Characterization factor
CPDB	Carcinogenic potency database
CDU	Comparative damage unit
CDUe	Comparative damage unit (ecosystem quality damage potential)
CDUh	Comparative damage unit (human health damage potential)
CTU	Comparative toxic unit
CTUe	Comparative toxic unit (ecotoxicity potential)
CTUh	Comparative toxic unit (human toxicity potential)
DALY	Disability-adjusted life year
DOC	Dissolved organic carbon
EC50	Effective concentration affecting 50% of the exposed population for a defined endpoint
ED50	Effective dose affecting 50% of exposed individuals for a defined endpoint
EF	Effect factor
FF	Fate factor
HC50	Hazardous concentration affecting 50% of the exposed species at their EC50 level
HSDB	Hazardous substances data bank
I	Intake
iF	Human intake fraction
IR	Intake rate
ISO	International Organization for Standardization
LAI	Leaf area index
LC50	Lethal concentration killing 50% of the exposed individuals
LCA	Life cycle assessment
LCI	Life cycle inventory
LCIA	Life cycle impact assessment

LOEL	Lowest observed effect level
MCI	Molecular connectivity index
MRDD	Maximum recommended daily dose
MRTD	Maximum recommended therapeutic dose
MTC	Mass transfer coefficient at the air-leaf interface, air-to-leaf conductance
NOEL	No-observed effect level
OECD	Organization for Economic Co-Operation and Development
PAF	Potentially affected fraction of species
PBDE	Polybrominated diphenyl ether
PDF	Potentially disappeared fraction of species
PM	Particulate matter
POC	Particulate organic carbon concentration
ppb	Parts per billion
ppm	Parts per million
q*	Low-dose slope factor for carcinogenic effects
QSAR	Quantitative structure-activity relationship
Quan-Tox	Extending, disseminating, and harmonizing the quantification of human and ecosystem toxicity impacts when assessing the sustainability of products and services over their life cycle
RCF	Root concentration factor
SD	Standard deviation
SETAC	Society of Environmental Toxicology and Chemistry
SSD	Species Sensitivity Distribution
SVOC	Semi-volatile organic compound
TD50	Tumorigenic dose affecting 50% of the exposed individuals
TF	Task force
Tox-Train	Toxicity assessment tool for practical evaluation of life-cycle impacts of technologies
TSCF	Transpiration stream concentration factor
UNEP	United Nations Environment Programme
US-EPA	United States Environmental Protection Agency
VOC	Volatile organic compound
WHO	World Health Organization
XF	Exposure factor

READERS GUIDE

Document status

The present document is the official documentation of USEtox, the UNEP/SETAC scientific consensus model for characterizing human and ecotoxicological impacts of chemical emissions in life cycle assessment (LCA) and other comparative toxicity assessments including product environmental footprinting (PEF).

Document contents

USEtox is a combined multimedia box model (to predict fate and exposure to chemicals)/impact assessment model (to quantify potential impacts at estimated exposures) that has been developed to calculate characterization factors for human toxicity and freshwater ecotoxicity. As shown in Figure 1, assessing the human toxicological or ecotoxicological effects of a chemical emitted into the environment implies the analysis of a cause-effect chain that links chemical emissions to impacts on humans and/or freshwater ecosystems through four assessment steps: environmental fate, (human and freshwater ecosystem) exposure, (human toxicological and freshwater ecotoxicological) effects, and damages on human health and ecosystem quality.

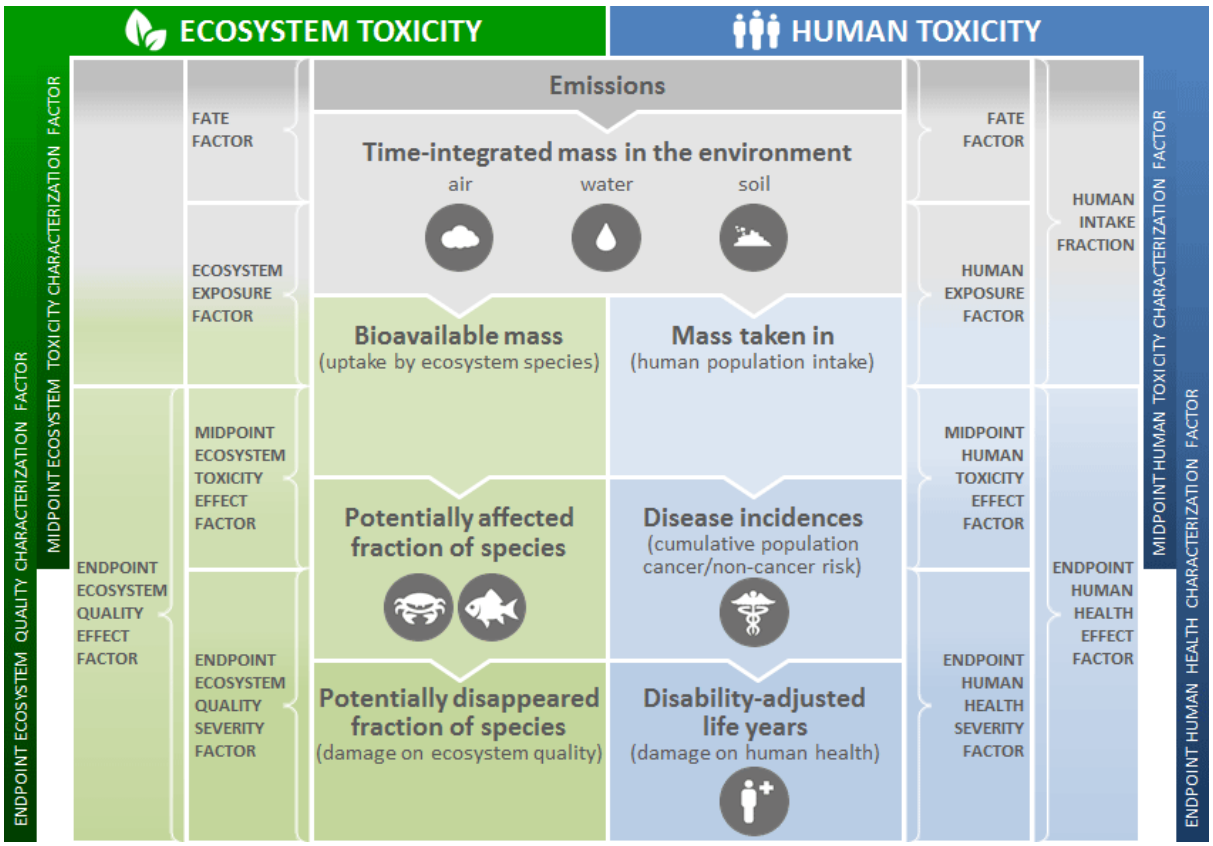

Figure 1: Framework for characterizing toxicity impacts with USEtox 2.0 with a set of factors (e.g. fate factor) linking different indicators (e.g. emissions and time-integrated mass in the environment) to characterize human toxicity and ecosystem toxicity of chemical emissions.

Chapter contents

In Chapter 1, the model presentation, the USEtox team and the updates in USEtox 2.0 are summarized. Chapter 2 describes the context, model concept and overall mathematical modeling framework of USEtox, Chapter 3 describes how to run the USEtox model and interpret its data and results, and Chapter 4 describes the underlying model input data. In Chapter 5, the environmental fate compartments and processes formulae are documented. The framework and its formulae are documented in Chapter 6 for human exposure and in Chapter 7 for indoor fate and human exposure. Chapter 8 documents the human toxicological effects framework and its formulae. In Chapter 9, the freshwater ecosystem exposure framework and its formulae are documented and Chapter 10 documents the freshwater ecotoxicological effects framework and its formulae. In Chapter 11, model application, limitations and recommendations are given.

Appendix

Explanations of symbols and indices are given in Appendix A and corresponding parameters in USEtox are given in Appendices B to E.

1. INTRODUCTION

1.1 Context

Life cycle assessment (LCA) is a standardized instrument to assess the environmental impacts connected with the life cycle of products, processes and activities. LCA consists of four elements: (1) goal and scope, to define the intended use of LCA and set boundaries for the product system under study, (2) life cycle inventory (LCI) analysis, to collect input (resources and materials use) and output (chemical emissions and waste) data for all processes in the considered product system aggregated over the life cycle, (3) life cycle impact assessment (LCIA), to characterize inventory data in terms of the considered product system's impacts on human, ecosystems, and resources, and (4) interpretation, to evaluate all LCA results according to the goal of a study (Hauschild & Huijbregts 2015). In the LCIA phase, different impact categories are included (e.g. climate change, acidification, toxicity, water use, and land use) to characterize the implications of chemical emissions and resources use. The characterization commonly serves in the comparative context of LCA: "is the environmental performance of product or product system A better than that of B?". Specifically, the characterization of human toxicity and ecotoxicity impacts commonly implies widely differing emission flows of many hundred or even thousand chemicals associated with a product system and different toxicity characterization models exist to address these impacts. This poses a special challenge compared to other impact categories, where typically much less emission or resources use flows need to be considered.

Addressing the challenge of harmonizing different existing toxicity characterization models, USEtox has been developed as a scientific consensus model under the auspices of the UNEP/SETAC Life Cycle Initiative for the characterization of human toxicity and ecotoxicity impacts in LCA and other comparative assessment frameworks.

In its current version 2.0x, USEtox covers three impact categories, namely human cancer toxicity, human non-cancer toxicity and freshwater aquatic ecotoxicity. For each of these impact categories, USEtox follows the whole impact pathway from a chemical emission to the final impact on humans and ecosystems. This includes modeling the environmental distribution and fate, human and ecosystem population exposure, and toxicity-related effects associated with the exposure. Combining fate, exposure and effects yields characterization factors for human toxicity and ecotoxicity. These factors serve as characterization results at the midpoint level in LCA. They can be combined with a damage factor translating human toxicity and ecotoxicity impacts into damages on human health and ecosystem quality, respectively, to arrive at a damage (endpoint) level in LCA. Further details about the general LCA midpoint-damage characterization framework are given in Hauschild and Huijbregts (2015). Thereby, uncertainty in all steps is explicitly taken into account in USEtox, allowing for a comparative assessment of the environmental impacts of chemicals to provide insights on "best in class" products in product comparisons regarding the environmental performance of products in terms of human toxicity and ecotoxicity related to chemical emissions.

Due to vast differences across chemicals in amounts produced, emitted, distribution processes in the environment and residual masses across different compartments, fractions taken up by humans and/or ecosystem species, and differences in species sensitivity to chemical exposure, USEtox characterization factors can vary by more than 12 orders of magnitude across chemicals (Rosenbaum et al. 2008). This is not a strange or unexpected outcome,

given all relevant amounts and processes considered; this output instead allows especially for factoring out those chemicals for which human or ecological impacts can be considered negligible in the context of a selected product system, thus highlighting those compounds for which choices in the life cycle matter most with respect to human health and ecosystem damage. Hence, USEtox provides a particular form of utility for decision making by ranking chemicals associated to products or product systems from negligible to higher toxicity impact potentials, even when hundreds or thousands of chemicals are involved.

1.2 USEtox model presentation

The USEtox model is an environmental model for characterization of human toxicological and ecotoxicological life cycle impacts in LCA. It has been developed by a team of researchers from the Task Force on Toxic Impacts under the UNEP-SETAC Life Cycle Initiative (Hauschild et al. 2008, Rosenbaum et al. 2008). The mission of developing USEtox is to improve the assessment and management of chemicals in the global environment. This is substantiated by further developing, evaluating, applying and disseminating the USEtox model, which describes the fate, exposure and effects of chemicals (Westh et al. 2015). Expanding on the original release version 1.01, this documentation describes the second official release version of USEtox (USEtox 2.0x), which is a version that has accommodated a suite of theoretical improvements as well as a broader coverage of assessment situations through a wider array of required input data and model extensions.

In Life cycle impact assessment (LCIA), the chemical emissions and resource uses which occur along the life cycle of a product or system are translated (characterized) into their potential impacts on the environment. These characterizations range in type from local impacts from land use, over regional impacts due to e.g. toxic substances, acidification or photochemical oxidants to global climate change. For each category of impacts (like global warming or photochemical ozone formation), the impact assessment framework applies substance-specific characterization factors (CFs) which represent the substance's potency to contribute to a specific type of impacts. Focusing on the impact categories “human toxicity” and “ecotoxicity”, emission inventories for the life cycle of a product often results in the need to consider the potential impacts of hundreds or thousands of substances. It has been estimated that more than 30,000 different chemicals are frequently used in the life cycle of products on the market (Judson et al. 2009, Wambaugh et al. 2013). Many of these substances have the potential to damage humans or ecosystems when released to the environment. There is thus the need to derive and use characterization factors for the human toxicity and ecotoxicity impact categories for potentially all relevant chemicals.

The need for developing toxicity-related characterization factors has been addressed over the last 15 years by deriving a number of characterization models, which vary in their scope, applied modeling principles and not least in terms of the resulting proposed characterization factors including definition, units and magnitudes (Hauschild et al. 2008). These characterization models did all cover a limited number of substances. Prior to USEtox, the situation for the LCA practitioner, who wished to include chemical-related impacts in the impact assessment was thus that (a) there were many substances in the LCI phase for which no characterization factor is available from any of the models, (b) for some substances several of the models may have published characterization factors, but these often vary substantially between the models.

This unsatisfactory situation was the background on which a Task Force on Toxic Impacts under the UNEP-SETAC Life Cycle Initiative launched a comparison and harmonization of existing characterization models in order to:

1. Identify which differences in the old characterization models cause the observed differences in their characterization factors;
2. Develop a scientific consensus about good modeling practice based on the identified influential differences;
3. Harmonize the old characterization models removing unintended but influential differences; and
4. Develop a scientific consensus model based on the learnings from the comparison of the characterization models with the following characteristics:
   a. Being parsimonious (as simple as possible, as complex as needed) containing only the model elements which were identified as the most influential in the comparison of the existing characterization models;
   b. Being transparent and well documented;
   c. Falling within the range of existing characterization models, i.e. not differing more from other characterization models than these differ among themselves;
   d. Being endorsed by the developers behind all involved models.

The result of the scientific consensus model development is the USEtox model and its associated set of characterization factors (http://usetox.org). A complete overview of the consensus process is given in Figure 2 and detailed in Hauschild et al. (2008) and Westh et al. (2015). Microsoft Excel® has been used to implement the consensus model. Continued conceptual and technical developments as well as increased availability of data has resulted in the current update to USEtox 2.0x.

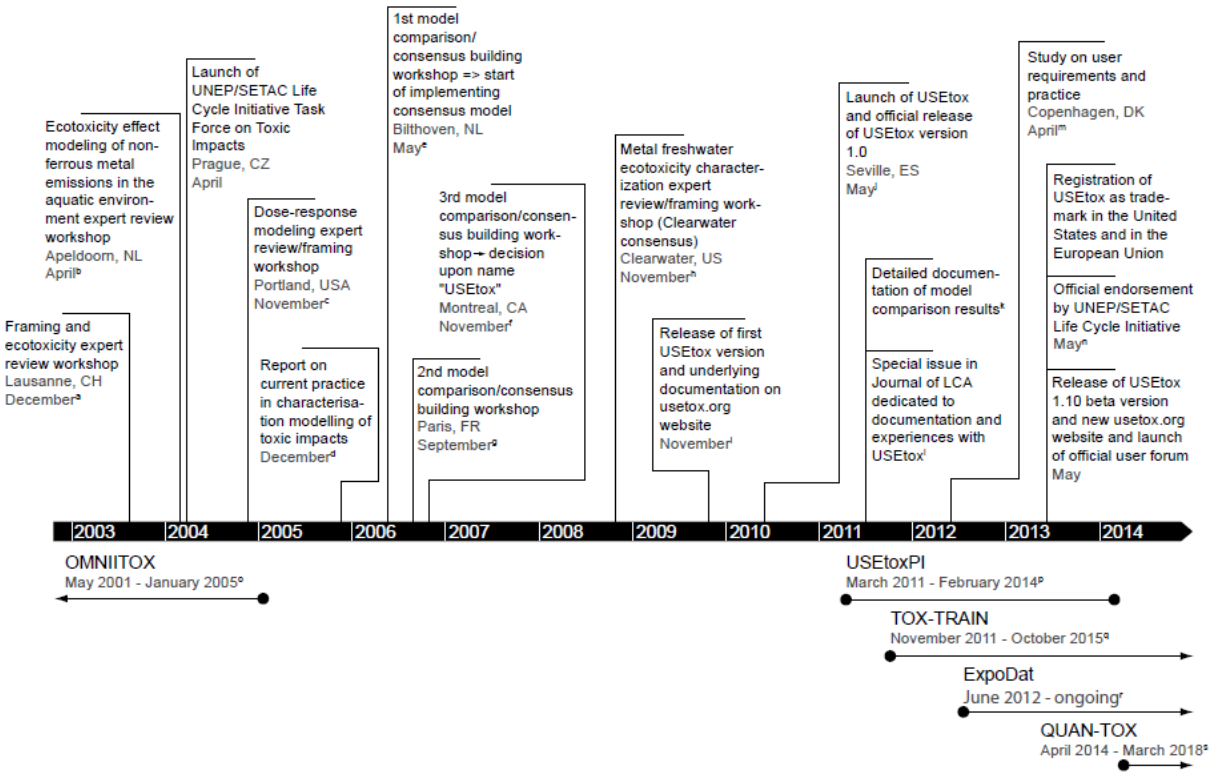

Figure 2: USEtox scientific development and dissemination timeline (Westh et al. 2015).

1.3 USEtox Team and USEtox model status

The USEtox Team is a core team of international researchers from the Task Force on Toxic Impacts (TF LCIA 3) under the auspices of UNEP/SETAC Life Cycle Initiative (Hauschild et al. 2008, Westh et al. 2015). The aim of the USEtox Team is to provide and maintain a scientific and technical rationale as basis for the comparative assessment of chemicals based on their impacts on human health and on ecosystems (as applied in life cycle assessment and comparative risk assessment).

The USEtox Team aims at:

- Creating and maintaining a model for calculating characterization factors for human toxicity and ecotoxicity impacts,
- Increasing the availability and quality of characterization factors for use in life cycle impact assessment and other comparative assessment contexts for all kinds of chemicals,
- Disseminating the developed USEtox model and characterization factors through the organization of user workshops, training courses, and demonstration projects, and
- Contributing to create international consensus on the principles for comparative assessment of chemicals.

The USEtox Team is part of the USEtox Centre, a non-for-profit organization. The USEtox Team is further described at http://usetox.org/team.

USEtox is officially endorsed by the UNEP/SETAC Life Cycle Initiative. It is officially recommended as assessment method by the European Commission in the Recommendations on the Use of Common Methods to Measure and Communicate the Life Cycle Environmental Performance of Products and Organisations, by the European Commission's Joint Research Centre in the International Reference Life Cycle Data System Handbook, by the World Business Council for Sustainable Development in the Life Cycle Metrics for Chemical Products, and by the United States Environmental Protection Agency in the Tool for the Reduction and Assessment of Chemical and other Environmental Impacts.

Models like USEtox accrue credibility through ongoing model performance testing and evaluation. There is testing of both model algorithms and overall model performance. The USEtox approach to model performance testing and evaluation includes both model specific evaluations that test the overall soundness of USEtox as well as scenario specific evaluations that need to be performed on a case-by-case basis to explore the relevance or usefulness of the model for chemical class or decision questions.

USEtox model algorithm auditing: All USEtox model algorithms are tested first using hand calculations and simple spreadsheet calculations to ensure that the mathematical model works as intended. We next conduct and audit the model by having at least one other group/individual independently test the same algorithm on another computer system. The two tests are compared against each other and all differences are resolved before the algorithm is determined to be acceptable for USEtox. To further assure the reliability of the algorithms, the documentation for the algorithm and the spreadsheet are submitted for publication in peer-reviewed journals. This adds a second layer of audit and quality assurance.

USEtox model performance evaluation: Model performance evaluation is an ongoing, iterative process that is expected to continue for the life of USEtox. Among the key elements of this process are publications on the basic model evaluation framework and on specific details related to identifying and reducing various types of uncertainty. Another key element

is continued participation in model evaluation workshops as well as inter-agency and multinational model evaluation exercises. A first approach for model performance evaluation is benchmark testing with similar models developed independently by other investigators. The USEtox model was developed as a result of a multi-year exercise to build a consensus model from a range of existing and well-vetted life-cycle impact models. Its performance has been tested against and among all of these models. Sensitivity and uncertainty analysis are fully integrated into the model development, performance testing, and evaluation process. We anticipate that this framework will lead to a reduced but informative set of model relationships. Sensitivity and uncertainty analyses are powerful tools for assessing the performance and reliability of models. As the USEtox model evolves and addresses a broader range of chemical substances, this type of rigorous model performance evaluation will continue.

USEtox peer review: The USEtox peer-review process began early in the model development process. The peer review process involves SETAC, UNEP, the academic community, scientists from private sector for-profit entities, and scientists from non-government non-profit research organizations. The peer review is based on information exchanges with and contributions from professional societies, government entities, industry groups, and NGOs. Conceptual model evaluation was initiated in the early stages of model development. During the process of framing the problem and designing the conceptual model, the appropriate level of modeling complexity (e.g., what to include and what to exclude), the availability and quality of information needed to run the model (i.e., input data), and the theoretical basis for the model were evaluated. A literature review was used to identify and evaluate the state-of-the-science for processes to be included in the model, as well as to compile and document the initial set of values that will be used as model inputs. Confidence is further enhanced if the user can easily inspect or verify the operation of the algorithms and data transformations and determine whether the model is internally consistent and contains no logical flaws or technical errors, such as incorrect code implementation. Easy access to the raw data used as inputs, transformed data and the steps of data transformations used in the calculation, and the computer coded algorithms underlying these data transformations will thus enhances user confidence in the model. The availability of clear documentation for model structure, and the possibility of performing calibration against an external standard (test data sets) or an internal standard (parallel algorithms to perform the same calculation) all increase user confidence in a model. The USEtox team maintains an ongoing effort to evaluate model outcomes using both internal evaluation exercises and peer review publication.

USEtox quality assurance and vetting of model inputs: USEtox does not have its own process for data development. All data used for this effort are obtained from existing databases and the peer review literature. The USEtox team reviews all data for consistency and reliability before entering these data as USEtox inputs. Inputs to USEtox include basic chemical properties data, landscape/climate data, exposure factors, human toxicity, and ecotoxicity data. The data used for these inputs have been reviewed and assessed in the peer review literature, reviewed and assessed by credible entity such as the US EPA, or reviewed for use by the USEtox team with adequate vetting or publication.

USEtox formal update process: Documented suggestions for progress-based updating, made by any party, will be considered by the USEtox team. When judged worthwhile, the USEtox team will ask the review chair of the UNEP/SETAC life cycle initiative to invite at least two external experts to review the proposal and advise on possible implementation. The USEtox team can suggest potential reviewers. The external experts should be knowledgeable of the specific elements to be updated (substance classes, modeling, regions, etc.) and at least

one should be familiar with the USEtox model, its purpose, and its underlying principles or with toxicity assessment in LCA. The external experts will carry out a peer review of the submitted/proposed updates with respect to the following criteria (defined by the USEtox team and based on the USEtox development criteria in Rosenbaum et al. (2008)):

- Scientific quality/viability (Is the method/data published in peer-reviewed literature?)
- Level of parsimony (What is the added complexity and is it justified?)
- Level of evaluation
- Level of transparency (documentation)
- Level of scientific acceptance/consensus in the community (Is the method/data already used in published methods?)
- Level of consistency with the data selection hierarchy (for previously published CFs and databases) as published in the official USEtox papers in IJLCA.
- Feasibility/influence in application (Is this possible to consider in practice?)
- Meaningfulness/added value (Is this meaningful to consider in practice? What is the improvement from a practical point of view? Does it entail an additional effort and is it worth it?)

An external review panel can also take on the form of a workshop, organized by the USEtox team. The USEtox team will consider the recommendations made by the review panel and decide whether and how to implement the proposed changes. If the USEtox team decides not to implement a proposal that was recommended for implementation by the review panel, the reasoning shall be published (e.g. on the USEtox website).

USEtox update proposals by any party can be submitted and the update process description can be found at http://www.usetox.org/update.

1.4 Updates in USEtox 2.0

Since USEtox release version 1.01, the basis of which is described in detail in Rosenbaum et al. (2008), a series of additional features, substances, exposure pathways and regionalized landscape data have been introduced and implemented in USEtox according to the official update process described in Section 1.3. All updates are available in the official release version of USEtox and are summarized in Table 1. The present documentation was completely updated to cover all changes made in USEtox 2.0.

Table 1: New USEtox 2.0 model components and features, and scientific publications related to the updated components.

Differences of USEtox 2.0x compared to USEtox 1.01	**References**
Residential and occupational indoor environments (This update adds an indoor air compartment with several parameter sets to the USEtox model, which allows calculating characterization factors for potential human toxicity impacts (cancer and non-cancer) of pollutants emitted indoors and inhaled by people present in the room.)	Hellweg et al. (2009) Wenger et al. (2012) Rosenbaum et al. (2015)
Ionizing organic chemicals (In this update, USEtox is adapted to estimate partition coefficients of (partly) ionized substances from known physical-chemical substance properties.)	Franco and Trapp (2008) Franco and Trapp (2010) van Zelm et al. (2013)
Exposure to pesticide residues via food crop consumption and pesticide physicochemical property data (This update integrates human exposure to pesticides via food crop consumption. This update further adds and corrects the USEtox substance database according to state-of-the-art knowledge for pesticides.)	Fantke et al. (2011a) Fantke et al. (2011b) Fantke et al. (2012) Fantke et al. (2014) Fantke and Jolliet (2016)
Generic freshwater ecotoxicity for metals (This update includes new CFs for 15 cationic metals in freshwater, taking metal speciation and bioavailability into account for different freshwater chemistries.)	Gandhi et al. (2010) Dong et al. (2014)
Continent-specific landscape parameters (This update provides landscape-specific parameters for 8 continents as well as 17 sub-continental regions.)	Kounina et al. (2014)
New substances and updated substance data (This update includes different new organic substances including all relevant substance data to calculate characterization factors. This update further includes updated substance data for some existing substances.)	Li et al. (2015) Demeau project (demeau-fp7.eu)
New user interface wizard (This update introduces a new step-by-step user interface for guiding the user through all important calculation and substance selection steps.)	Tox-Train project (toxtrain.eu)

2. MODELING FRAMEWORK

This chapter defines how the USEtox modeling framework is set up to meet the needs for quantifying life-cycle impacts in the context of a life-cycle assessment (LCA). In contrast to the some modeling frameworks used for human health and ecological risk- and impacts research or for informing regulatory actions, life-cycle impacts models operate at a relatively high level of spatial scale. Contaminant emissions developed for LCA are typically defined by region and often the location of chemical release for an LCA can only be characterized generically as indoor, urban, or rural. Time scales are typically avoided in LCA by considering steady-state systems. The framework is primarily used for classification and relative statements ("product system A performs better than B") rather than for prediction of local impacts. In light of the modeling challenges and specifications typical for LCA, this Chapter introduces the USEtox modeling framework and provides details on the assumptions and information used to develop the specific algorithms included in USEtox. The chapter begins with a discussion of life-cycle impact assessment and its need for quantitative inputs. Next the chapter introduces characterization factors both in a qualitative and quantitative context.

2.1 Life cycle impact assessment

Life cycle assessment (LCA) has become an important tool for comparing the environmental profile of products, materials, and services based on the function that they provide and broadly encompassing impacts along the life cycle of the product or system. Life-cycle impact assessment (LCIA) is the phase of LCA aimed at quantifying and evaluating the magnitude and significance of the potential environmental impacts of a product system.

To meet its objective for supporting product life-cycle decisions, an LCIA aims to quantify the impacts of chemical emissions and resource uses collated in the inventory stage along the life cycle of a product system. The major inputs of an LCIA with respect to chemicals are the identification of a contaminant emission and of the environmental compartment(s) receiving these emissions. Base on the multimedia framework discussed below, the receiving compartments in USEtox are broadly defined as indoor air, ambient air (lower atmosphere in urban and/or rural areas), and continental freshwater and agricultural soils. An LCIA impact score for potential impacts is needed for each combination of substance released and receiving compartment. The LCIA impact score is estimated (modelled) using a weighted summation of the releases of pollutants from a product system and characterization factors for the potential damages associated with that release:

$$IS = \sum_i \sum_x CF_{x,i} \times M_{x,i} \quad (1)$$

where

IS is the impact score for human toxicity expressed at midpoint level as number of cancer or non-cancer disease cases [cases] and at endpoint level as number of disability-adjusted life years [DALY], and the impact score for ecotoxicity expressed at midpoint level as potentially affected fraction (PAF) of freshwater species integrated over exposed volume and time [PAF m^3 d] and at endpoint level as potentially disappeared

fraction (PDF) of freshwater species integrated over exposed volume and time [PDF m^3 d]

$CF_{x,i}$ is the characterization factor for the potential toxicity impacts of substance x released to compartment i [cases/kg emitted] for human toxicity impacts and [PAF m^3 d/kg emitted] for ecotoxicity impacts at midpoint level and the characterization factor for the potential human health damages [DALY/kg emitted] and for the potential ecosystem quality damages [PDF m^3 d/kg emitted]

$M_{x,i}$ is the emission of substance x to compartment i [kg emitted]

The USEtox model is currently constructed to provide characterization factors (CFs) for human health and freshwater ecological damages for contaminant emissions to indoor air, urban air, rural air, freshwater and agricultural soil. Combined with emitted mass, the CFs thus serve derivation of an Impact Score (IS) for all compounds for each product or product system in a comparative LCA-setting. The final impact scores are used as input for selecting the preferred product or product system. Human health damages include carcinogenic impacts, non-carcinogenic impacts, and total impacts (carcinogenic and non-carcinogenic). Ecological damages addressed in USEtox are freshwater ecotoxicity for a range of aquatic species.

2.2 Characterization factors: Quantification and units

In order to make USEtox output compatible with the needs of LCA, the research team established the units of the characterization factor for human toxicity as cumulative cases of either cancer or non-cancer health outcomes per kg of contaminant emission, cases per kg emitted, and for freshwater aquatic ecotoxicity impacts as the potentially affected fraction (PAF) of aquatic species integrated over the exposed water volume (m^3) and time (d), PAF m^3 d per kg emitted. Ultimately, the human health and ecotoxicity outcomes are summarized using a Comparative Toxic Unit (CTU) approach, to substantiate the comparative nature of the characterization factors. This approach is discussed in more detail below.

In order to quantify the characterization factors of contaminants as a CTU, the quantification process is divided into three calculation steps. These sequentially provide a fate factor (FF), quantifying how the contaminant is dispersed in the environment, an exposure factor (XF), quantifying human and/or ecological system contact with environmental media, and an effect factor (EF), quantifying effects per kg intake for humans or PAF of aquatic species integrated over the exposed water volume per kg bioavailable chemical in the aquatic environment. The resulting characterization factor (CF) that is required for the impact score for either human health or ecological impacts is generally defined as the combination of these three factors:

$$CF = FF \times XF \times EF \quad (2)$$

This formula covers two major aspects, related to the environmental fate and behavior of chemicals (FF and XF), and related to human or ecological effects (EF). Regarding fate and behavior, multimedia fate models are applied to determine contaminant environmental fate factors (FF). Multi-pathway exposure models linked to multiple environmental media are used to calculate contaminant exposure factors (XF). In this system, the impacted region is represented by a number of homogeneous compartments, each representing a specific part of the environment (i.e. atmosphere, water, soil). The fate factor and exposure factor of a contaminant in a certain compartment is calculated by solving a set of mass balance equations that describe processes such as degradation and inter-compartment transfer. The fate factor represents the persistence of a chemical in the environment (e.g. in days) as well as the

relative distribution and the exposure factor expresses the availability for human or ecosystem contact, represented by the fraction of the chemical transferred to the receptor population in a specific time period such as a day. For different chemicals, different processes are important in defining both fate and exposure. Which processes are the most important for a certain contaminant depends on the physical-chemical properties of the corresponding substance. Also the environmental conditions (temperature, rain intensity etc.) influence both fate and receptor contact.

For chemicals causing human toxicity the fate factor and exposure factor can generally be combined to reflect the intake fraction (iF) for a chemical:

$$iF = FF \times XF \tag{3}$$

The iF represents the fraction of the quantity emitted that enters the human population. Intake through inhalation and ingestion is commonly considered in iF calculations.

The FF is the same for ecotoxicity and human toxicity. For humans, an exposure model determines the XF, which describes the effective human intake of a specific environmental medium – air, water, soil – through inhalation and ingestion. For freshwater ecosystems, the XF dimensionless, applies only to the freshwater compartment, and expresses the fraction of the chemical within the freshwater compartment that is dissolved in water.

The modelling regarding the effect factors utilizes the outcomes of the previous steps. The human EF reflects the change in lifetime disease probability due to the change in lifetime intake of a pollutant (cases/kg). Effect factors are reported separately for carcinogenic and non-carcinogenic effects, as well as data for effects after inhalation and oral exposure. A set of three human-health characterization factors can be reported, namely "carcinogenic", "non-carcinogenic" and "total", of which the latter is the sum of carcinogenic and non-carcinogenic effects.

The **characterization factor for human toxicity impacts at midpoint level** (human toxicity potential) is expressed in comparative toxic units (CTU_h), providing the estimated increase in morbidity in the total human population per unit mass of a contaminant emitted, assuming equal weighting between cancer and non-cancer effects due to a lack of more precise insights into this issue.

Unit: [CTU_h per kg emitted] = [disease cases per kg emitted]

The ecotoxicological EF reflects the change in the Potentially Affected Fraction (PAF) of species due to change in concentration (PAF m^3 kg^{-1}). Characterization factors are reported for freshwater aquatic ecotoxicological impacts for respectively emissions to urban air, rural air, freshwater and agricultural soil.

The **characterization factor for aquatic ecotoxicity impacts at midpoint level** (ecotoxicity potential) is expressed in comparative toxic units (CTU_e) and provides an estimate of the potentially affected fraction of species (PAF) integrated over time and volume per unit mass of a chemical emitted.

Unit: [CTU_e per kg emitted] = [PAF m^3 d per kg emitted]

The approaches explained above illustrate the use of USEtox to calculate characterization factors for human toxicity and freshwater ecotoxicity at midpoint level. These USEtox characterization factors are not normalized to a reference substance. The USEtox model results can be extended to determine endpoint effects expressed as disability adjusted life

years (DALY) for human health impacts and potentially disappeared fraction of species (PDF) for ecotoxicological impacts.

Determining the magnitude of the DALY related to a chemical emission involves the application of a weighting factor or damage factor to the disease cases that accounts for years of life lost and years of life disabled associated with that disease. For cancer effects, the relationship for 1 case = 11.5 DALY applies, while for non-cancer effects, the relationship for 1 case = 2.7 DALY applies (Huijbregts et al. 2005).

From this, it follows that the **characterization factor for human health at damage (endpoint) level** associated with human toxicity impacts in USEtox is expressed in comparative damage units (CDU_h).

Unit: [CDU_h per kg emitted] = [DALY per kg emitted]

Determining the damage to aquatic ecosystems involves translation of the Potentially Affected Fraction (PAF) of species into a Potentially Disappeared Fraction (PDF) related to a chemical emission, in which the PDF represents the damage at endpoint level. The PDF has been defined as a linear fraction of the PAF, whereby Jolliet et al. (2003) proposed that PDF = 0.5 × PAF. In the derivation of this formula, the PAF was specifically defined on the basis of EC50-based PAF-estimation. That is, the PAF (specifically: the PEF_{EC50}) expresses the fraction of species for which the EC50 endpoint is exceeded in ecotoxicity tests. Note that other disciplines (e.g., Ecological Risk Assessment) may apply different PAF-estimates, such as PAF_{NOEC} in the context of deriving water-, soil- or sediment quality criteria for chemicals).

From this, it follows that the **characterization factor for ecosystem quality at damage (endpoint) level** associated with aquatic ecotoxicity impacts in USEtox is expressed in comparative damage units (CDU_e).

Unit: [CDU_e per kg emitted] = [PDF m^3 d per kg emitted]

2.3 Model concept

USEtox includes separate model components for calculating fate factors (FF), exposure factors (XF), and effect factors (EF). These components operate independently but their outputs are merged together to provide the characterization factors, CF, for human toxicity and freshwater ecotoxicity impacts, respectively. The FF component is a multimedia transport and transformation model, which is used to determine the dispersion of emitted contaminants among, indoor air, urban air, agricultural soil, natural soil, fresh water, coastal marine water, and oceans. The XF component translates these environmental media concentrations into estimates of freshwater ecosystem contacts and human contact and intake. The EF component translates human intake into cases of cancer or non-cancer and ecosystem exposure concentrations into a measure of the potentially affected fraction of exposed species.

2.3.1 Fate and exposure modeling: general assessment framework

USEtox represents environmental compartments as well-mixed boxes that contain and exchange contaminant mass. A compartment is described by its total mass, total volume, solid-phase mass, liquid-phase mass, and gas-phase mass. Contaminants move among and are transformed within compartments through a series of transport and transformation processes that can be represented mathematically as first-order losses, which depend on

physicochemical characteristics of the chemicals modelled in USEtox and the characteristics of the considered compartments.

In any specific compartment, a contaminant inventory is determined by the competing processes that determine whether a substance will (a) remain within the compartment where it is emitted, (b) be transported to other compartments by cross-media transfers that are dispersive (intermedia transfers) advective (imports and exports) (i.e., volatilization, precipitation, etc.), (c) be transformed by a physical, chemical, or biological degradation process within a specified compartment (i.e., by hydrolysis, oxidation, etc.), or (d) be irreversibly removed from a compartment by leaching and/or burial.

Compartments in USEtox that are used as input for emissions are:

- Household indoor air
- Occupational indoor air
- Urban air
- Continental rural air
- Continental freshwater (which includes emissions to groundwater as groundwater is not currently modeled as separate compartment)
- Continental sea water (representing coastal zones)
- Continental agricultural soil
- Continental natural soil (for e.g. industrial emissions)
- Crop residues (as multiplier for the human intake fraction matrix)

To assess fate, a mass balance equation has been applied for each compartment. These equations have the following general format:

$$\frac{\mathrm{d}\vec{m}_x(t)}{\mathrm{d}t} = EMIS_x + IMT_{y\to x} \times m_y - IMT_{x\to y} \times m_x - DEG_x \times m_x - OUT_x \times m_x \qquad (4)$$

with

m_x :	mass of the chemical in box x [kg]
t :	time [d]
$EMIS_x$:	emission rate of the chemical into box x [kg/d]
$IMT_{y\to x}$:	intermedia transfer rate of the chemical from box y into box x [d^{-1}]
$IMT_{x\to y}$:	intermedia transfer rate of the chemical from box x into box y [d^{-1}]
DEG_x:	degradation rate of the chemical from box x [d^{-1}]
OUT_x:	transfer rate of the chemical from box x to outside the system [d^{-1}]

The exposure model (for humans) further transfers the amount found in a given environmental compartment (i.e. the result of the fate model) to a chemical intake by humans. USEtox can distinguish direct intake (e.g. by breathing air and drinking water, etc.), indirect intake through bioconcentration processes in animal tissues (e.g. meat, milk and fish) and intake by dermal contact (the latter not (yet) implemented in USEtox).

2.3.2 Fate and exposure modeling: scales and mass balance

USEtox provides fate factor and exposure factor calculations at four different spatial scales – indoor, urban, continental and global. At each of these scales the model imposes mass

balance calculations based on emissions tracked against exchanges with adjacent compartments and transformation losses. The continental-scale model has the flexibility to represent a range of different continents and can be adjusted to represent smaller regions or countries. Exposure factors are determined based on the human consumption of air, water, and food from a specific compartment.

2.3.3 Fate and exposure modeling: indoor and urban compartments

The lowest level spatial scale is the indoor environment, embedded within the urban scale as illustrated in Figure 3. Both the indoor compartment and the urban compartment contain only an air phase combined with aerosols. The indoor environment exchanges air with the urban air compartment but also with the continental air compartment – allowing the consideration of indoor environments located outside of urban regions. The indoor air compartment has losses due to irreversible deposition, chemical reactions, cleaning, and air filtering.

The urban air compartment exchanges air with the indoor-air compartment as well as with continental air and has irreversible removal processes that include chemical transformations (degradation), losses to the stratosphere and deposition to paved and non-paved surfaces where some fraction of the substance leaches out of the system. Deposition to paved surfaces is transported in part to continental surface water as part of urban runoff. Exposure factors for urban air account for inhalation. Indoor inhalation is considered separately from outdoor inhalation.

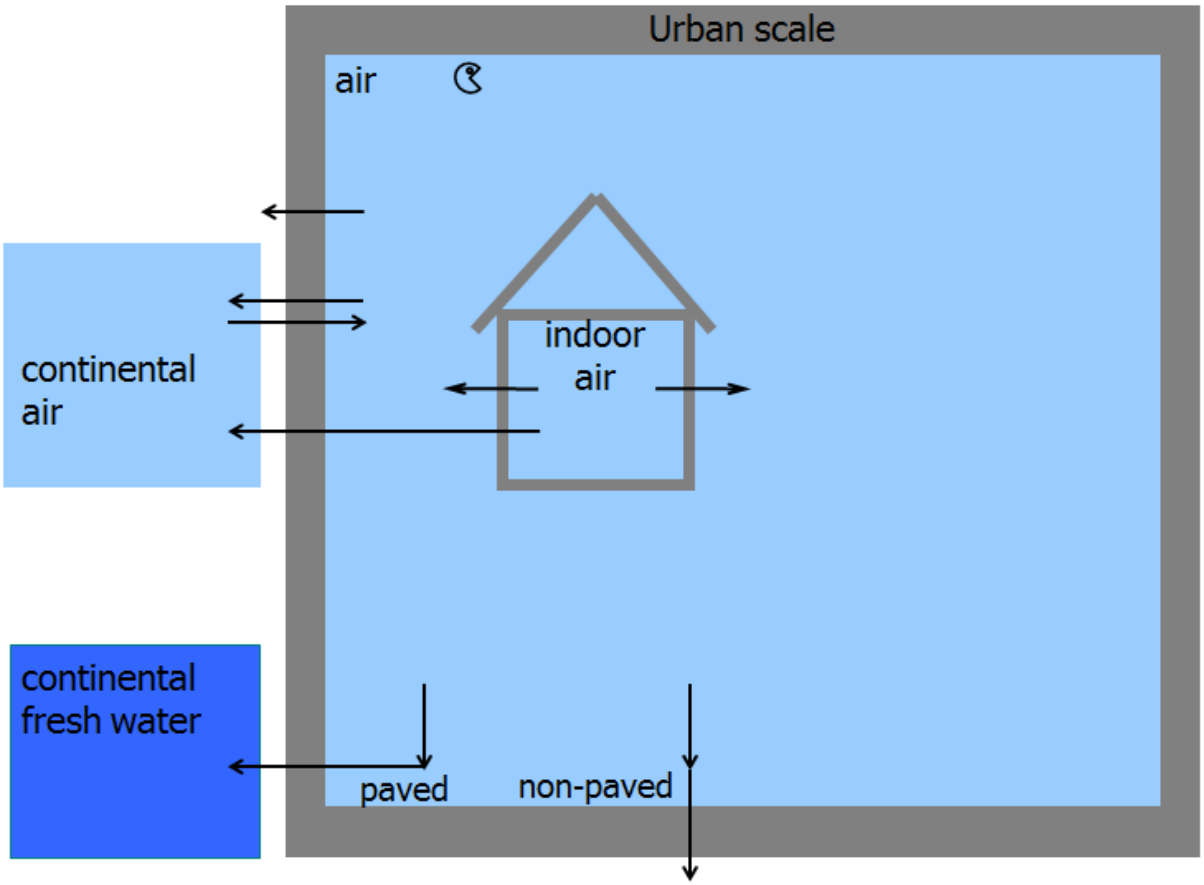

Figure 3: USEtox compartment setup for the indoor and urban scale. Arrows indicate flows of the substance in the system and the smiley indicates degradation.

2.3.4 Fate and exposure modeling: continental-scale compartments

The continental-scale compartments contain the urban-scale compartment and include an air compartment, freshwater, coastal marine water, agricultural soil, and natural soil. The continental-scale air compartment exchanges air with both the urban-air and global-air compartment and with the continental-scale agricultural soil, natural soil, freshwater, and coastal marine water. The continental-scale marine-water environment exchanges water with the global oceans. Within the continental scale system there are inter-media transfers as well as export and import by water/solid advection between the air compartment and agricultural soil, natural soil, freshwater and costal marine water. The runoff from both natural and agricultural soil goes to freshwater and freshwater flows into the coastal marine compartment. There is outflow from coastal marine water to the ocean compartment and air exchange between continental air and global-scale air. All compartments have chemical degradation as a removal process along irreversible advection removal processes – including removal to the stratosphere from air, leeching from soil to deeper layers, burial from fresh and coastal marine water. The USEtox mass balance on the continental scale is illustrated in Figure 4.

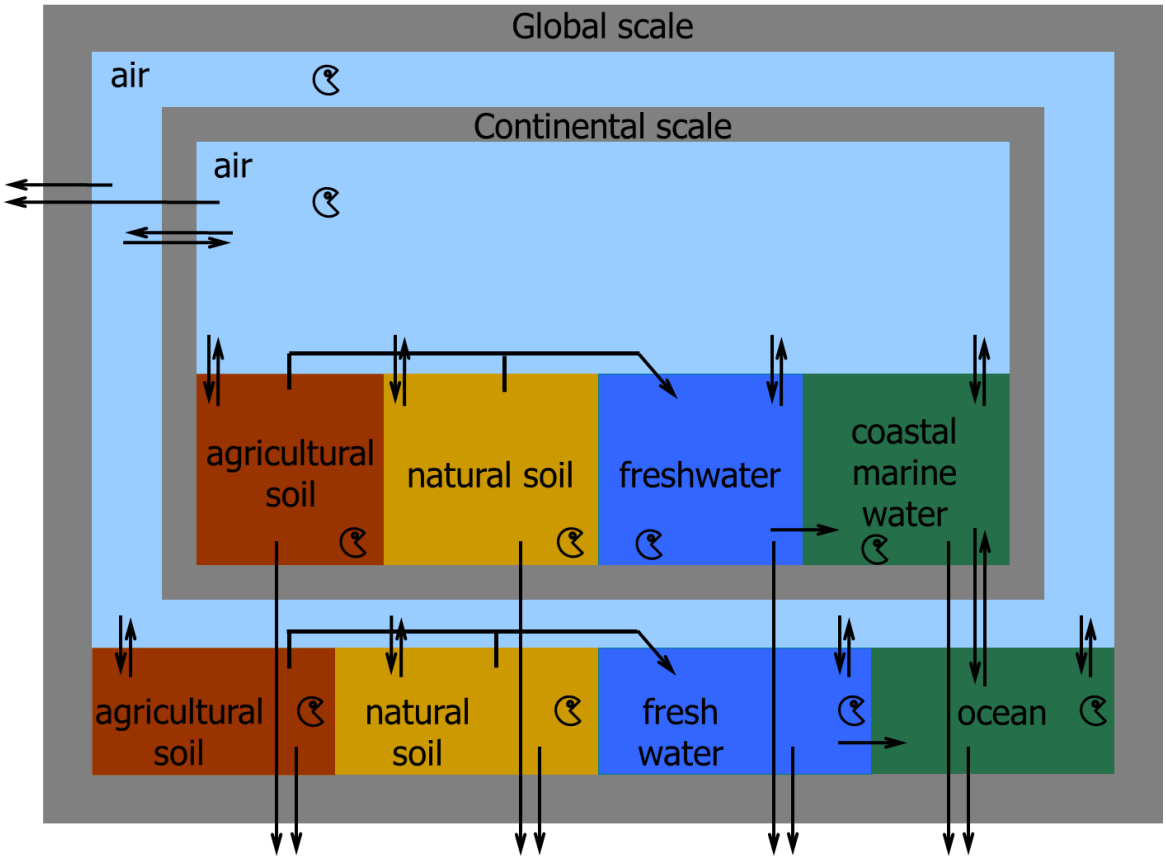

Figure 4: USEtox compartment setup for the continental and global scale. Arrows indicate flows of the substance in the system and the smiley indicates degradation.

2.3.5 Fate and exposure modeling: global-scale compartments

The global-scale compartments contain and exchange mass with the continental-scale compartments. The global-scale compartments include an air compartment, freshwater, ocean

water, agricultural soil, and natural soil. The global-scale air compartment exchanges mass with the continental-scale air compartment and with global-scale agricultural soil, natural soil, freshwater, and oceans. The global oceans exchange water with the continental-scale marine-water environment. Within the global-scale system there are inter-media transfers as well as export and import by water/solid advection between the air compartment and agricultural soil, natural soil, freshwater and oceans. All compartments have chemical degradation as a removal process along irreversible advection removal processes – including removal to the stratosphere from air, leeching from soil to deeper layers, burial from fresh and ocean waters. The USEtox mass balance on the continental scale is illustrated in Figure 4.

2.3.6 Effect modeling

The effect modeling for human toxicity is based on aggregated statistics for (a) cancer and (b) non-cancer effects based on Huijbregts et al. (2005).

The effect factor for ecotoxicity in the freshwater compartment is based on Species Sensitivity Distribution (SSD) modeling (Huijbregts et al. 2002, Posthuma et al. 2002). In the mid-1980's SSD-modeling has been founded in the observation in that the sensitivities of different species – expressed via toxicity test endpoints like NOECs and EC50s in laboratory tests with single species exposed to single chemicals – have the form of a bell-shaped distribution. Thereupon, ecotoxicity data have been compiled and used to derive SSD-models for different compounds following the concept of a Species Sensitivity Distribution model for a compound as derived from ecotoxicity data for a set of tested species (representing e.g. EC50 test endpoints for different species). The model has been used to underpin the derivation of water-, sediment- and soil quality criteria in the context of environmental protection policies, and for quantitative impact assessment. The latter format is basic to the LCIA of chemicals in USEtox. Databases have been compiled on various (sub)-groups of substances to support both forms of using SSD models. In the early stages of use, separate problem definitions resulted in a multitude of small data sets.

2.4 Model and input uncertainties

It should be recognized that the reliability of the USEtox output is limited by uncertainties that arise from both the model structure and form the lack of precision or accuracy of model inputs.

2.4.1 Model uncertainties

All models are approximations to the real world and thus can never be assured as providing fully accurate representations of the model output. However, in spite of potential uncertainties, models can be demonstrated as useful when the user recognizes key limitations and assumptions. In USEtox the model uncertainties arise from decisions that help making the model operational but may limit its reliability. Among these issues are the following for fate and exposure modelling:

- the assumption of homogenous compartments
- USEtox does not account for speciation or other potentially important specific processes for metals, metal compounds and certain types of organic chemicals
- no allowance for degradation of vegetation in exposure model

For the effect modelling, the model uncertainties for human health impacts are, amongst others related to the extrapolation from animal test studies to human toxicity effects and extrapolation between different exposure routes whenever route-specific data are missing.

For ecotoxicological impact modelling the uncertainties of the model relate to the statistical nature of the approach: an SSD describes a statistical pattern of across-species sensitivity variation, and neglects emergent characteristics of species assemblages in ecosystems. That is, e.g., species interactions are neglected, while those can modify ecological response to chemical exposure (e.g., when a chemical affects a predatory species, prey species may flourish).

2.4.2 Input uncertainties

Even with a fully reliable model structure, the output reliability of a model can be limited by lack of accuracy and/or precision of model inputs. There are a number of cases where there are questions about the precision and/or accuracy of USEtox inputs. Significant among these cases are the following:

- lack of accurate mechanistic quantitative structure-activity relationships (QSARs) for estimating chemical properties
- limited data on bioconcentration factors for fish
- lack of reliable data on chemical degradation rates
- uncertainties related to both human health and ecotoxicological effect data
    - use of chronic and acute data, route-to-route extrapolations
    - the application of a linear dose–response curve for both the human health and the aquatic ecotoxicity effect factors calculation
    - setting the human effect factor to zero if no toxicology information is available
    - the exclusion of an ecotoxicological effect factor when minimum data quality requirements could not be met.

2.5 Matrix-algebra calculation framework

The calculation framework for the derivation of characterization factors as given by Equation (2) provides a process by which the different intermediate results of the sub-models for fate, exposure and effects are linked to calculate a set of characterization factors for each chemical. The conceptual format of Equation (2) does not reveal that there are a large number of fate factors, exposure factors, and effects factors being combined in USEtox to calculate a full set of characterization factors for each chemical. USEtox does not perform these calculations sequentially, but simultaneously using a matrix-algebra-based calculation framework (Rosenbaum et al. 2007), transforming Equation (2) into a matrix equation of the following form:

$$\begin{aligned}\mathbf{CF} &= \mathbf{EF}\,\mathbf{XF}\,\mathbf{FF} \\ &= \mathbf{EF}\,\mathbf{iF} \quad \text{(for human toxicity)}\end{aligned} \tag{5}$$

This equation implies that the characterization factor matrix **CF** is obtained by multiplying a fate matrix (**FF**) by an exposure matrix (**XF**) and then by an effect factor matrix (**EF**). In the case of human health impacts the **XF FF** product produces the intake fraction matrix (**iF**). The elements of each matrix are calculated in the respective sub-models. The concept and interpretation of these matrices, their elements and their units as well as how to populate them is discussed in detail in Rosenbaum et al. (2007).

2.5.1 Human toxicity impacts matrix calculations

For human health, the unit of the elements in **FF** is [$kg_{in\ compartment}$ per $kg_{emitted}$/d], in **XF** [kg_{intake}/d per $kg_{in\ compartment}$], in **iF** [$kg_{intake}/kg_{emitted}$], in **EF** [disease cases/kg_{intake}], and in **CF** [disease cases/$kg_{emitted}$] or CTU_h. The matrix-algebra based calculation framework of USEtox allows for the straightforward integration of additional compartments and exposure pathways by simply adding the corresponding columns or rows to the respective fate and exposure matrices, for example as done for the implementation of the new indoor exposure model. The following section gives a brief overview of the respective matrices as implemented in the "Run" worksheet of USEtox.

The fate model links the quantity released into the environment to the chemical masses (or concentrations) in a given compartment. It accounts for multimedia and spatial transport between the environmental media (e.g. air, water, soil, etc.). It is quantified by the fate matrix **FF**, where a column denotes the source compartment *m* and a row denotes the destination compartment *i*, that is the compartment to where the chemical is transferred. The size of **FF** is determined by the number of environmental compartments n_i considered (n_i and the number of source compartments n_m are equal, since every destination compartment can also be a source compartment, hence $n_m = n_i$), and thus be ($n_i \times n_i$). The fate factor $FF_{i,m}$ [$kg_{in\ compartment}$ per $kg_{emitted}$/d] can be interpreted as the increase of chemical mass in compartment *i* [kg] due to an emission in compartment *m* [kg/d]. In case the emission and receiving compartment are the same, FF can be interpreted as the total residence time in that compartment with unit [d]. The fate matrix **FF** is calculated as the inverse of the exchange-rate matrix **K** [1/d]:

$$\mathbf{FF} = -\mathbf{K}^{-1} \tag{6}$$

The elements of the rate coefficient matrix **K** are the rate-constants *k* [1/d]. The off-diagonal elements $k_{i,j}$, reflect intermedia or advective transport from compartment i to j (e.g. air, water, soil) and the diagonal elements $-k_{i,tot}$ represent the negative of the total removal rate coefficient for compartment i including biotic/abiotic degradation, advective and intermedia removal. Chapter 5 provides further details on the fate model and the calculation of the various rate-constants *k*.

The exposure model (for humans) relates the amount of contaminant found in a given environmental compartment (i.e. the result of the fate model) to the chemical intake by humans. Human exposure is quantified by the exposure matrix $\mathbf{XF_{hum}}$ that contains exposure factors (or exposure rates) $XF_{hum,xp,i}$. In this matrix a column denotes a destination compartment i and a row denotes the exposure pathway xp (e.g. meat, milk and fish). The size of $\mathbf{XF_{hum}}$ is determined by the number of exposure routes n_{xp} and the number of environmental compartments n_i considered, and thus has size ($n_{xp} \times n_i$). The exposure factor $XF_{hum,xp,i}$ [1/d] is the equivalent rate of ingestion of the medium by humans. Chapter 6 provides further details on the human exposure model and the calculation of the various exposure factors XF_{hum}.

The fate and human exposure matrices **FF** and $\mathbf{XF_{hum}}$ can be aggregated into an intermediary matrix referred to as the intake-fraction matrix **iF**. In this matrix a column denotes an emission compartment *m* and a row denotes the exposure pathway xp (e.g. meat, milk and fish). The size of **iF** is determined by the number of exposure pathways n_{xp} and the number of compartments n_i considered, and will thus be ($n_{xp} \times n_i$). The intake fraction $iF_{xp,i}$ [$kg_{intake}/kg_{emitted}$] can be interpreted as the fraction of an emission into a source compartment m that is taken in by the overall population through a given intake pathway xp. *iF* is defined and interpreted by Bennett and coworkers (Bennett et al. 2002a, Bennett et al. 2002b). For further calculation, **iF** is aggregated by inhalation, ingestion, and (in case this route will be

implemented in future versions of USEtox) the dermal exposure routes via multiplication with a "pseudo-unitarian" matrix **U** and becomes $\mathbf{iF_{xr}}$.

The effects model (for humans) relates the quantity taken in by the human population via a given exposure route (i.e. the result of the combined fate and exposure models) to the adverse effects (or potential risk) of the chemical on the human population. It is quantified by the effect matrix $\mathbf{EF_{hum}}$ containing effect factors $EF_{\mathrm{hum,ef,xr}}$. In this matrix a column denotes an exposure route xr (e.g. inhalation, ingestion or dermal) and a row denotes an effect type ef (e.g. cancer, non-cancer). The size of $\mathbf{EF_{hum}}$ is determined by the number of effect types n_{ef} and the number of exposure routes n_{xr} considered, and thus is of size ($n_{\mathrm{ef}} \times n_{\mathrm{xr}}$). The effect factor $EF_{\mathrm{hum,ef,xr}}$ [disease cases/$\mathrm{kg_{intake}}$] can be interpreted as the increase in the number of cases of a given morbidity (e.g. cancer or non-cancer diseases) risk [dimensionless] in the exposed population per unit mass ingested or inhaled [$\mathrm{kg_{intake}}$] – itself due to an emission source in compartment m. Chapter 8 provides further details on the human toxicological effects and the calculation of the effect factors EF_{hum}.

The midpoint human toxicity potential matrix $\mathbf{CF_{hum}}$ combines all these steps and expresses the human health impact per unit mass emitted into the environment. In this matrix a row denotes the considered effect type (abbreviated in indices as "ef" for effect; e.g. cancer, non-cancer) and a column denotes the emission compartment m. The size of $\mathbf{CF_{hum}}$ is determined by the number of effect types n_{ef} and the number of environmental compartments n_{i} considered, and thus has size ($n_{\mathrm{ef}} \times n_{\mathrm{i}}$). The midpoint human toxicity potential [disease cases] or [$\mathrm{CTU_h}$] per kg chemical emitted can be interpreted as the increase in population risk of a morbidity effect due to an emission in a compartment.

The elements of the midpoint human toxicity potential matrix can be multiplied with a severity factor specific for each effect type in order to obtain the endpoint human toxicity potential matrix, expressing the human health damage per unit emitted into the environment. In this matrix a row denotes the considered effect and a column denotes the emission compartment m. The damage (endpoint) level human toxicity potential [DALY] or comparative damage unit [$\mathrm{CDU_h}$] per kg chemical emitted represents an increase in adversely affected life years as a consequence of an emission in a compartment. The severity (or damage) factor allows one to distinguish between differences in the severity of disabilities caused by a disease in terms of affected life years, e.g., discriminating between the severity of a lethal cancer and a reversible skin irritation.

2.5.2 Ecosystem toxicity impacts matrix calculations

For ecosystem impacts the link between a contaminant emission and its impact on ecosystems is established and modeled similarly to, but somewhat modified from the human-health consequences.

The fate model and resulting matrix **FF** is exactly the same as for human health impact characterization. The freshwater ecosystem exposure factor XF_{eco} for an organic chemical in freshwater equals the fraction of a chemical dissolved in water and is given in the freshwater ecosystem exposure factor matrix $\mathbf{XF_{eco}}$. Chapter 9 provides further details on the ecosystem exposure model and the calculation of the exposure factors XF_{eco}.

The ecotoxicological effect factor (EF_{eco}) quantifies the fraction of species in an ecosystem (related indices are abbreviated "es" for ecosystem) that is affected by a given level of exposure. It is quantified by the ecotoxicological effect matrix $\mathbf{EF_{eco}}$. In this matrix a row denotes the affected ecosystem (e.g. aquatic, marine or terrestrial) and a column denotes a exposure compartment *i*. The size of $\mathbf{EF_{eco}}$ is determined by the number of ecosystems n_{es}

and the number of environmental compartments n_i considered, and thus of size ($n_{es} \times n_i$). The ecotoxicological effect factor $EF_{eco,es,i}$, [PAF m^3 d/kg] can be interpreted as the time and volume integrated increase in affected fraction of species in an ecosystem [dimensionless] per unit of chemical mass increase in a compartment. Chapter 10 provides for further details on the ecotoxicological effect model and the calculation of the ecotoxicological effect factors EF_{eco}.

The midpoint ecotoxicity potential matrix $\mathbf{CF_{eco}}$ contains midpoint ecotoxicity potentials; a column denotes the emission compartment m and a row denotes the affected ecosystem (e.g. fresh water, marine water, terrestrial, etc. – currently only freshwater is implemented in USEtox). The size of $\mathbf{CF_{eco}}$ is determined by the number of affected ecosystems n_{es} and the number of environmental compartments n_i considered, and will thus be of size ($n_{es} \times n_i$). The midpoint ecotoxicity potential [PAF m^3 d] or [CTU_e] per kg chemical emitted represents an increase in the fraction of species potentially affected (for the specified test endpoint, e.g. PAF_{EC50} or PAF_{NOEC}, by a number of observable lethal and non-lethal effects) as a consequence of an emission in a compartment. The elements of the midpoint ecotoxicity potential matrix are multiplied with a severity factor specific for each affected ecosystem in order to obtain the endpoint ecotoxicity potential matrix, expressing the ecosystem damage per unit emitted into the environment; a row denotes the affected ecosystem and a column denotes the emission compartment.

The damage (endpoint) level ecotoxicity potential [PDF m^3 d] or comparative damage units [CDU_e] per kg chemical emitted represents an increase in the fraction of species potentially disappearing as a consequence of an emission in a compartment.

3. RUNNING THE USETOX MODEL

3.1 Model structure

The USEtox 2.0x model is developed as a Microsoft Excel® spreadsheet. The choice of platform was intentionally based on the rationale of transparency and accessibility using a widely available and broadly accessible system instead of more sophisticated and/or coding-language-based options.

The USEtox 2.0x model includes a number of worksheets. These are shortly explained in Table 2. To work with the consensus model in practice, substance-specific information for the chemical under consideration need to be gathered. This information should be stored in the sheet 'Substance data'.

Table 2: Explanation of USEtox 2.0x model worksheets.

Worksheet	Explanation
Version	Background information on the USEtox model and its developers
Agreement	License agreement that must be accepted to use the USEtox model, data, factors, and documentation files
Instructions	Instructions how to perform single substance calculations and series calculation of a list of chemicals
Run	Specification of the model runs and calculation routines for fate factors, exposure factors, intake fractions, effect factors and characterization factors for human toxicity and freshwater aquatic ecotoxicity including additional matrix output and figures
Results	Presentation of outcomes of USEtox for multiple chemical runs
Substance data	Substance-specific information required to calculate characterization factors with USEtox
Landscape & indoor data	Default and regionalized landscape and indoor data applied in USEtox
Fate	Background data and equations required for the calculation of fate factors and environmental exposure factors
Human exposure	Background data and equations required for the calculation of human exposure factors including crop residues
Indoor exposure	Background data and equations required for the calculation of indoor exposure factors
Ecotox effect	Background data and equations required for the calculation of ecotoxicological effect factors
Human tox effect	Background data and equations required for the calculation of human effect factors (carcinogenic and non-carcinogenic)
Lists	Lists and conversion numbers used in user forms and models for auto-conversion (e.g. exposure duration thresholds, allometric factors, midpoint-to-endpoint conversion factors

Worksheet	Explanation
avlogEC50	Output sheet from the user interface used for storing pre-calculated HC50 values for ecotoxicity effect factor calculations
Human tox ED50	Output sheet from the user interface used for storing pre-calculated ED50 values for human toxicity effect factor calculations
Conversion table	Hidden sheet containing unit conversion factors (e.g. for mass units)
Code inputs	Hidden sheet containing inputs for user forms or VBA code

3.1.1 System requirements

USEtox 2.0x works with Microsoft Windows® as operating system and is implemented in Microsoft Excel®. USEtox 2.0x was tested and runs under Windows 32 bit and 64 bit versions and Excel 32 bit and 64 bit. The USEtox 2.0x main model file (USEtox2.0x.xlsm) is saved as Excel Open XML Macro-Enabled Spreadsheet, which is a spreadsheet containing worksheets and embedded macros programmed in Visual Basic for Applications (VBA), saved in the Open XML format introduced in Microsoft Office 2007. To use macros in USEtox 2.0x, macros need to be enabled in the macro settings of Excel: go to the FILE tab, then OPIONS, then TRUST CENTER, click on TRUST CENTER SETTINGS button, and select under MACRO SETTINGS the entry "Enable all macros (not recommended, potentially dangerous code can run)".

USEtox 2.0x currently might not be fully operational on other operating systems (e.g. Apple OS X or Linux and its variants).

3.1.2 Definitions and input

For characterizing chemical emissions in terms of human and/or ecosystem toxicity impacts, USEtox requires input data for substances, compartments, and exposure scenarios. Data for compartments at different spatial scales and exposure scenarios are predefined in USEtox, while for substances the specific input data – related to the products or product systems of interest, such as chemical identities and masses involved – are required from the user.

In Table 3, an overview of required USEtox 2.0x substance data is given. In this overview, input data are referred to as mandatory in all cases where a substance cannot be fully characterized (i.e. characterization factors cannot be calculated, although some intermediate factors like fate, exposure and/or effect factors might be available from the given input data). If input parameters are not required, but used in USEtox, this means that when user input is not given for these parameters, they will be set to specific values, such as "neutral" for pKa chemical class, or calculated internally in USEtox from other (mandatory) input parameters, such as for Koc that can be estimated from Kow in case that Koc is not specified by the user.

Table 3: Requirements of USEtox 2.0x substance input data. "n/a" indicates that a parameter is not applicable for this substance group.

Parameter	Symbol in USEtox	Unit	Mandatory for organic substances	Mandatory for inorganic substances*
Chemical abstract service registry number	CAS RN	-	yes	yes
Chemical common name	Name	-	no	no

Parameter	Symbol in USEtox	Unit	Mandatory for organic substances	Mandatory for inorganic substances*
Target class for pesticides (e.g. herbicides)	PesticideTargetClass	-	no	n/a
Chemical class for pesticides (e.g. triazoles)	PesticideChemClass	-	no	n/a
Molecular weight	MW	g/mol	yes	yes
pKa chemical class	pKaChemClass	-	no	n/a
pKa base reaction	pKa.gain	-	no	n/a
pKa acid reaction	pKa.loss	-	no	n/a
Partitioning coefficient between *n*-octanol and water	K_{OW}	L/L	yes	n/a
Partitioning coefficient between organic carbon and water	K_{OC}	L/kg	no	n/a
Henry law coefficient (at 25°C)	K_{H25C}	Pa m^3/mol	no	no
Vapor pressure (at 25°C)	P_{vap25}	Pa	yes	no
Solubility (at 25°C)	Sol_{25}	mg/L	yes	no
Partitioning coefficient between dissolved organic carbon and water	Kp_{DOC}	L/kg	n/a	yes
Partitioning coefficient between suspended solids and water (for metals only)	Kp_{SS}	L/kg	n/a	yes
Partitioning coefficient between sediment particles and water (for metals only)	Kp_{Sd}	L/kg	n/a	yes
Partitioning coefficient between soil particles and water (for metals only)	Kp_{Sl}	L/kg	n/a	yes
Degradation rate in air	k_{degA}	1/s	yes	no
Degradation rate in water	k_{degW}	1/s	yes	no
Degradation rate in sediment	k_{degSd}	1/s	yes	no
Degradation rate in soil	k_{degSl}	1/s	yes	no
Dissipation rates in above-ground plant tissues	k_{dissP}	1/s	no	n/a
Dissipation rates in wheat	$k_{dissWheat}$	1/s	no	n/a
Dissipation rates in rice	$k_{dissRice}$	1/s	no	n/a
Dissipation rates in tomato	$k_{dissTomato}$	1/s	no	n/a
Dissipation rates in apple	$k_{dissApple}$	1/s	no	n/a
Dissipation rates in lettuce	$k_{dissLettuce}$	1/s	no	n/a
Dissipation rates in potato	$k_{dissPotato}$	1/s	no	n/a
Effect concentration (the average of the log-values of the species-specific eco-toxicity data)	$avlog_{EC50}$	mg/L	no	no
Human-equivalent lifetime dose per	$ED50_{inh,non-cancer}$	kg/lifetime	no	no

Parameter	Symbol in USEtox	Unit	Mandatory for organic substances	Mandatory for inorganic substances*
person that causes a non-cancer disease probability of 50% after inhalation				
Human-equivalent lifetime dose per person that causes a non-cancer disease probability of 50% after ingestion	$ED50_{ing,non\text{-}cancer}$	kg/lifetime	no	no
Human-equivalent lifetime dose per person that causes a cancer disease probability of 50% after inhalation	$ED50_{inh,cancer}$	kg/lifetime	no	no
Human-equivalent lifetime dose per person that causes a cancer disease probability of 50% after ingestion	$ED50_{ing,cancer}$	kg/lifetime	no	no
Bioaccumulation factor in root crops	BAF_{root}	kg_{soil}/kg_{veg}	no	no
Bioaccumulation factor in leaf crops	BAF_{leaf}	kg_{soil}/kg_{veg}	no	no
Biotransfer factor for meat	BTF_{meat}	d/kg_{meat}	no	no
Biotransfer factor for milk	BTF_{milk}	d/kg_{milk}	no	no
Bioaccumulation factor in fish	BAF_{fish}	L/kg_{fish}	no	no

*In USEtox, inorganic substances are currently only referring to metal ions.

Databases of chemical-specific properties are available for organic and inorganic (i.e. currently restricted to metal ions) substances in Microsoft Excel® format (file names «USEtox_substance_data_organics.xlsx» and «USEtox_substance_data_inorganics.xlsx»). The data are embedded in USEtox, so that the user is transparently and reproducibly provided with (a) a consistent set of data (b) of a certain minimum quality (c) for as many substances as possible for which characterization factors can be computed. This includes three types of datasets: (1) physicochemical properties, (2) toxicological effect data on laboratory animals as a surrogate to humans, and in rare cases effect data on humans, and (3) ecotoxicological effect data for freshwater organisms. We focused our effort on identifying and collecting existing reviewed databases for which scientific judgement was already made in selecting and recommending values from a large range of values collected from the literature. For each of the three types of datasets, we (1) identified the existing databases, (2) defined a selection scheme and criteria for data gathering and (3) compiled the databases for organic and inorganic substances for which physicochemical properties and effect data for aquatic ecosystems or humans were found.

A full description of required substance input data for USEtox is given in the USEtox manuals for organic and inorganic substances, respectively that can be downloaded at http://usetox.org.

3.1.3 Steady-state computation

The computation of the steady-state solution is performed in the 'Run' sheet in the table of mass balance rate constants. The mass balance rate constant (d^{-1}) is given for each emission compartment and receiving compartment combination. The indoor air mass balance rate

constants are gathered from the ‘indoor exposure’ sheet and the urban, continental and global mass balance rate constants are from the ‘Fate’ sheet.

3.1.4 Recommended and indicative characterization factors

Characterization factors for ‘inorganics’ (i.e. metal ions) and ‘dissociating substances’ without pKa information were all flagged as ‘indicative’ due to the relatively high uncertainty of addressing fate and human exposure for all chemicals within these substance groups. Dissociative substances were identified using a systematic procedure, based on the dissociation constant (pKa). More specifically, the acids and bases have been dealt with for all substances for which pKa values were available. First, chemicals characterized as acidic were labelled "a" and chemicals characterized as basic were labelled "b". Then, using the Henderson-Hasselbach equation, the fraction of the substance to be in the neutral (undissociated acid, unprotonated base) form in water of pH 7 is calculated. Substances were then flagged if the neutral fraction was expected to fall below 10%.

For human health effects, recommended characterization factors were based on chronic or subchronic effect data, whilst characterization factors based on sub-acute data were classified as indicative. Furthermore, if route-to-route extrapolation was applied to obtain ingestion or inhalation human health effect factors, a subdivision was made between recommended and indicative characterization factors. Human health characterization factors based on route-to-route extrapolation from animal data were considered indicative if the primary target site is specifically related to the route of entry. In addition, characterization factors based on extrapolation from the ingestion to inhalation route of entry were also considered indicative if the expected fraction absorbed via inhalation was a factor of 1,000 higher compared to the fraction absorbed via ingestion. This factor of 1,000 indicates that exposure by inhalation may be far more toxic than by ingestion for a few chemicals. In these cases, the indicative characterization factor would underestimate the potential impact by inhalation.

Consensus has been reached that recommended aquatic ecotoxicological characterization factors must be based on effect data of at least three different species covering at least three different trophic levels (or taxa) in order to ensure a minimum variability of biological responses necessary to quantify a fraction of those species potentially affected.

In USEtox, characterization factors can be specified as ‘indicative’, reflecting the level of reliability of the calculations in a qualitative way. Due to the relatively high uncertainty of addressing fate and human exposure, the following substance groups were classified as ‘indicative’:

- Ionizing compounds with pKa or Kow value that fall outside the range for which the Koc regressions applied in USEtox are applicable. The regressions used for calculating the Koc for the electrolytes are suited for acids within the pKa range 0–12 and with a log Kow between -2.18 and 8.50. For bases the pKa needs to be above 2 and log Kow is between -1.66 and 7.03 (Franco & Trapp 2008, van Zelm et al. 2013).
- Organo-metallic chemicals.
- Metals. Inorganics are all specified as ‘indicative’, reflecting the relatively high uncertainty associated with estimates of fate, exposure and effects for this substance group. In contrast to organic compounds, for which the substance-to-substance variations in transport properties can be attributable to basic chemical properties such as solubility ratios, variations in transport properties for inorganic substances depend in complex ways on a range of media properties. The solid/liquid partitioning of inorganic substances in soil can depend on several mineral components as well as the pH, redox potential (EH) and cation-exchange capacity. As a result, there can be significant

variations of chemical mobility over very small geographic scales. Hence, it is difficult to identify the appropriate regional "bulk" transport properties for metals, as is done for organic chemicals. In addition, inorganic species are not "removed" by chemical reactions in the same way that most organic chemicals are transformed by actions such as biodegradation, photolysis, and hydrolysis. The biodegradation of an organic chemical in soil, water, or sediment effectively removes it from the system, but species such as lead, cadmium, and arsenic can only be truly removed from water, soil, or sediment by advection and tend to persist for very long time periods. However, many inorganic species can be effectively removed by sequestration in a chemical form that is chemically and biologically unavailable. The magnitude and variability of this process is often difficult to quantify, but can be very important for both fate and exposure assessment. Finally, relative to organic chemicals there are large uncertainties in determining how the variations in observed bioaccumulation and bioavailability come about (in both aquatic and terrestrial food webs). There have not been sufficient experiments to provide the data needed to address the nature and mechanism of the variations of these processes for inorganic species.

- For human health effects, characterization factors are specified as «indicative» if effect factors are based on sub-acute data. Furthermore, if route-to-route extrapolation is applied to obtain ingestion or inhalation human health effect factors, a subdivision should be made between recommended and «indicative» characterization factors. First, human health characterization factors based on route-to-route extrapolation should be considered «indicative» when the primary target site is specifically related to the route of entry. In addition, characterization factors based on extrapolation from the ingestion to inhalation route of entry should be considered «indicative» if the expected fraction absorbed via inhalation is much higher than the fraction absorbed via ingestion, e.g. a factor of 1,000. This factor of 1,000 is rare but indicates that exposure by inhalation may be far more toxic than by ingestion. With the Kow-based QSARs applied to calculate the expected fraction absorbed via inhalation, it appears that this factor of 1,000 applies for organic substances with Kow smaller than 2.5×10^{-2} or Kow larger than 4.5×10^{9}. In these cases, the «indicative» characterization factor can underestimate the potential impact by inhalation. Fractions absorbed for inorganic substances were taken from Owen (1990). This factor of 1,000 indicates that exposure by inhalation may be far more toxic than by ingestion. In these cases, the «indicative» characterization factor can underestimate the potential impact by inhalation. This is the case for Hg(II).
- Aquatic ecotoxicological characterization factors are specified as «indicative», if effect factors are based on ecosystem species toxicity data covering less than three different trophic levels. This is to ensure a minimum variability of biological responses.

The "indicative" USEtox characterization factors should always be used together with the "recommended" factors, as otherwise the substances concerned would be characterized with zero impact as no characterization factor is applied to their emissions. The flag "indicative" means a higher uncertainty of the characterization factor compared to the flag "recommended", because not all the minima requirements are met for the calculation. Therefore, when an emission characterized with indicative characterization factors is dominating the overall impact, it implies that the associated results have to be interpreted as having a lower level of confidence. A sensitivity study might be performed by applying only the recommended characterization factors to see if and how the results (and the conclusions) change.

3.2 Executing the model

The USEtox model is implemented as a Microsoft Excel® spreadsheet and comes with several additional files for substance data, results, templates and documentation. All files are packed in a ZIP file named "USEtox_2.0x.zip". After unpacking the ZIP archive at the location that the user can specify, the following files and directories are available as part of USEtox:

- **USEtox2.0x.xlsm** (USEtox model file; version 2.0 or higher)
- USEtox2.0x_ChangeLog.txt (Log file of all changes since USEtox 2.0)
- Readme.txt (Introduction to the USEtox directory and file structure)
- \Documentation sub-folder (contains USEtox manuals and documentation files)
- \InputData sub-folder (contains substance input data files)
- \Results sub-folder (contains USEtox results files)
- \Templates sub-folder (contains USEtox template files that should not be modified by the user)

To use USEtox, please conduct the following steps:

- In Microsoft Windows, start Excel 2007 or higher.
- Unpack the "USEtox_2.0x.zip" archive at any location.
- In the unpacked directory, open the "USEtox_2.0x.xlsm" model file.
- Click "I agree" on the license/collaboration agreement form that pops up upon loading the model file. Note, when you do disagree to the license/agreement, USEtox will not open and cannot be used.
- You are now able to use the USEtox model either via the user interface (by clicking on "Create or customize substance data" or "Set up calculations with USEtox" on the welcome form or without the user interface by clicking "Use USEtox without the user interface wizard" on the welcome form.

To use the USEtox substance input data, please conduct the following steps:

- In Microsoft Windows, start Excel 2007 or higher.
- Unpack the "USEtox_2.0x.zip" archive at any location.
- In the unpacked directory, open the sub-directory "\InputData"
- In the sub-directory, open the "USEtox_substance_data_organics.xlsx" and/or "USEtox_substance_data_inorganics.xlsx" files.
- Alternatively, you can load the substance data into the USEtox model by opening the "USEtox_2.0x.xlsm" model file as described above, go to sheet "Substance data", click on the button "Import a database" and follow the instructions for specifying a substance data file to load.

To use the USEtox pre-calculated results, please conduct the following steps:

- In Microsoft Windows, start Excel 2007 or higher.
- Unpack the "USEtox_2.0x.zip" archive at any location.
- In the unpacked directory, open the sub-directory "\Results"
- In the sub-directory, open the "USEtox_results_organics.xlsx" and/or "USEtox_results_inorganics.xlsx" files.

3.3 Interpretation of USEtox intermediate and final results

3.3.1 Interpreting the matrices

In the USEtox model, special attention was paid to allow for a comprehensive interpretation also of the intermediate results, in order to support the interpretation and understanding of the final results. The goal was to avoid a "black-box model" and allow the user to see and understand "what's going on", why a characterization factor is high or low and what drives that. The "Run" worksheet contains a number of additional information and interpretations besides the **FF**, **XF**, **EF**, and **CF** matrices.

All matrices in USEtox, whether intermediate (**FF**, **XF**, **EF**) or final (**CF**) result are independent of the emission compartment or the amount of mass emitted. Contrary to what you would find in many environmental fate and exposure models, they do not directly represent environmental concentrations, intake doses and the like. As required in LCA, they represent fate, exposure and effects *per unit emitted* and only after multiplication with an actual quantity of emission (or rather an emission vector) the user obtains an impact score representing the toxicity potential of the amount(s) emitted. In more technical terms, the actual intermediate results environmental mass (or concentration) per compartment, human intake, etc. are dependent on the source vector, which defines the release compartment(s) and amount(s). The advantage of this approach is that no re-run of the model is required if amount or place of an emission changes. As long as the matrices are stored the emission vector can be modified and its multiplication with the respective matrices yields the corresponding result.

The following sections will directly refer to where a respective interpretation table can be found in the "Run" worksheet. The interpretation of the matrices in USEtox, their elements and their units is discussed in detail in Rosenbaum et al. (2007), therefore the following sections are a summary and directly taken from this publication but with some modifications.

3.3.1.1 Interpreting the rate coefficient matrix **K**

Fraction removed: Dividing the off diagonal element by the diagonal element of the respective column, one can readily measure the fraction of removal towards each compartment. They are given explicitly in a table at range W36:AI49 ("Run" worksheet).

3.3.1.2 Interpreting the fate factor matrix **FF**

Residence time: The main diagonal elements $FF_{m,m}$ describe the effective residence time in the respective compartments m, i.e. the inverse of the effective rate constant introduced by Bennett et al. (1998). These are given explicitly in a table at range W58:AI58 ("Run" worksheet).

Mass in the environment: A column of **FF** describes the mass in the environment resulting from a unit emission flow in the corresponding compartment. Hence, dividing each element by the sum of the respective column indicates the repartition of the resulting mass between all destination compartments due to the emission compartment represented by this column. Thus revealing, e.g., into which compartment(s) a chemical mainly partitions. This is given explicitly in a table at range W91:AI104 ("Run" worksheet).

Inter-compartment transfer fraction: Each non-diagonal element of **FF** can be expressed as a fraction transferred from the source compartment i multiplied by the effective residence time in the destination compartment. This means that dividing each element in a row by the residence time (the diagonal element) provides the transferred fractions from media i to j:

$f_{i,j}=FF_{j,i}/FF_{i,i}$ for an equal emission into all compartments. The transferred fractions already include the sum of all possible transfer pathways through a third media. They are given explicitly in a table at range W124:AI136 ("Run" worksheet).

Feedback fraction: The feedback fraction, which is the product of the corresponding diagonal elements of **K** and **FF**, yields the fraction of a chemical being transferred back into the compartment of origin (Margni et al. 2004). They are given explicitly in a table at range W53:AI53 ("Run" worksheet).

3.3.1.3 Interpreting the exposure matrix **XF**

Direct exposure: The top rows constitute a direct exposure square matrix in which off-diagonal elements are equal to zero and the diagonal elements are the direct exposure factor for the respective pathway. For direct intake of freshwater for example, the direct exposure rate corresponds to the fraction of the total mass of drinking water, ingested daily by humans. The inverse of this coefficient therefore represents the equivalent time required by the population to inhale or ingest the whole mass in the medium. The direct intake of soil and sediment is assumed to be zero. For inaccessible media like underground soil the diagonal element will be zero too. All pathways starting from second row and column are representing ingestion pathways and should be kept separate from inhalation as the dose-response differs according to the exposure route.

Indirect exposure: The bottom rows (i.e. only rows added) represent the indirect exposure pathways, each row corresponding to a different exposure substrate (e.g. meat, dairy produce, vegetables, and fish) polluted by a respective compartment (column). The indirect intake rate can be interpreted as the equivalent intake rate of a polluted medium due to the consumption of an exposure substrate. This means that the coefficients within the same column (i.e. for a given compartment) can be directly compared, thereby enabling the identification of the most significant exposure pathways. The sum of all elements per column represents the total transfer rate to the population per increment of mass in the respective compartment. The **XF** matrix also enables the comparison of direct and indirect exposure contribution.

3.3.1.4 Interpreting the intake fraction matrix **iF**

The difference with the exposure matrix is that the column refers here to the emission compartment (not the destination compartment) and already takes into account the multi-media transfers between compartments. The following analysis and interpretation of the intake fraction matrix applies:

Intake fraction for individual pathways: Each element represents an actual intake fraction, e.g., the fraction of one kg emitted which is taken in by the human population, for a given release compartment (column) and the exposure pathway (row).

Pathway contributions: The ratio of each element in a column with the sum of all elements of the same exposure route (e.g. inhalation, ingestion) within this column yields the contribution of this pathway to the corresponding route (e.g. the contribution of exposure via fish consumption relative to overall ingestion exposure). They are given explicitly in a table at range W141:AJ148 ("Run" worksheet).

Comparison of exposure routes: iF needs to be multiplied with an emission vector (which can be found in range W18:W31, "Run" worksheet), to yield the overall amount taken in by the whole population. This enables to determine which emission in which compartment contributes dominantly to each exposure route.

3.3.2 Interpretation and use of USEtox characterization factors

The following recommendations have been published (Rosenbaum et al. 2008) and are re-iterated here with some minor updates and modifications. The toxicity potentials, i.e. characterization factors, must be used in a way that reflects the large variation of more than 15 orders of magnitude (i.e. a factor of 10^{15} between the lowest – least toxic – and the highest – most toxic – characterization factor) between chemical characterization factors of all substances currently covered in USEtox as well as the 3 orders of magnitude uncertainty (see Rosenbaum et al. 2008) on the individual factors. This means that contributions of 1%, 5% or 90% to the total toxicity score can be interpreted as essentially equal, but significantly larger than those of a chemical contributing to less than 1 per thousand or less than 1 per million of the total score. Disregarding the fact that the orders of magnitude of predicted impacts far outranges the orders of magnitude of the uncertainty analysis has been a major cause of complaints about the variability of these factors across impact assessment methods, whereas the most important chemicals were often the same within a factor 1000 across those methods.

In practice, this means that for LCA practitioners these toxicity potentials are very useful to identify the 10 or 20 most important chemicals pertinent for their comparative applications, while implying a motive to disregard hundreds of other substance emissions whose impacts are by far less significant (and likely of negligible importance for comparative decision-making) for the considered products. Toxicity impact scores thus enable the identification of all chemicals contributing more than e.g. $1/1000^{th}$ to the total score. In this context it is usually more meaningful and thus recommended to plot and compare toxicity impact scores on logarithmic scales, avoiding the over-interpretation of small differences of a factor <10 that may appear large on a linear scale.

Once these most important substances have been identified, further analysis can be carried out on the life cycle phase, or individual processes responsible for these emissions, and the respective importance of fate, exposure and effect in determining the impacts of this chemical. Due to its transparent matrix format, USEtox will also allow identification of the main exposure pathways, (e.g. inhalation, water ingestion, various food ingestion) as well as the relative importance of potential carcinogenic and non-carcinogenic effects in the overall score. The inclusion of an urban area as a sub-compartment and emission scenario implies that the life cycle inventory should accommodate a distinction between air emissions in high and low population-density areas.

The distinction between “indicative” and “recommended” characterization factors only refers to their uncertainty, not in any way to their usefulness or whether or not they should be applied at all. There has been a number of confusing interpretations to these two terms which did not always lead to their application as intended originally. The following describes the correct use of these two classes of characterization factors:

1. Always use both “indicative” and “recommended” characterization factors in any LCA study, without any exception whatsoever! In fact, excluding the indicative characterization factors implicitly applies a “zero-impact” hypothesis to the respective emissions as their impact will not be characterized at all (i.e. emission multiplied with a 0 as characterization factor). The uncertainty of this hypothesis is most certainly always much higher than the uncertainty of the indicative characterization factors. Therefore, higher uncertainty of characterization factors is not a valid argument to exclude them and characterize emissions with zero-impact.
2. If the toxicity impact score of a study is dominated by substances characterized with indicative factors, it may be useful – and only then – to conduct a sensitivity study by excluding the indicative factors in order to see if the conclusions of the study are

affected or not. Attention, the numerical results (impact scores) of the study will certainly change by doing so, but the conclusions of the study may or may not be affected by that, which is what such a sensitivity study will reveal.

3. If the toxicity impact scores are dominated by indicative factors, but your conclusions are not affected by the exclusion of indicative characterization factors, one should interpret the toxicity impact scores with a larger uncertainty as given in Rosenbaum et al. (2008), i.e. as a rough expert-judgement-based estimate use a factor of 10^5 instead of 10^3 for human health and 10^4 instead of 10^2 for freshwater ecotoxicity.
4. If the conclusions change when excluding indicative factors it may be justified to exclude those emissions that dominate but are characterized by indicative factors from a study. In that case, one needs to clearly state that these emissions where excluded/not characterized but may still contribute significantly to the toxicity impact score. This exclusion then also needs to be considered when interpreting the results.

3.3.3 Are toxicity results still too uncertain or immature?

The principle "It is better to be vaguely right than exactly wrong" (Read 1920) is well worth considering here. (Eco)-toxicity is frequently excluded from LCA studies based on the argument that with uncertainty factors in the range of 10^2 to 10^5 it is still too uncertain (or even immature) and deemed not useful (at first sight) to proceed with the comparative analyses, as the output is considered not to provide information in a meaningful way. Besides the recommendations for their specific interpretation as given above, there is, however, another argument that is largely ignored in this kind of discussion, while playing a central role. Toxicity is very different from any other (non-toxicity) impact category when it comes to the number of potentially relevant elementary flows. Current LCIA models cover around 2500 to 3000 substances for aquatic ecotoxicity and about 1000 substances for human toxicity (Rosenbaum et al. 2008). No other (non-toxicity) impact category – with the exception of photochemical ozone formation perhaps – exceeds 100 contributing different elementary flows (i.e. different characterization factors), while both toxicity categories are "facing" the challenge of having to characterize several tens to hundreds of thousands of chemicals (= different elementary flows) with a coherent characterization model. As examples of the characteristics underlying LCIA for potentially (eco)-toxic chemicals:

- The CAS registry currently contains more than 101,000,000 unique organic and inorganic substances (www.cas.org/about-cas/cas-fact-sheets),
- of which roughly 100,000 may play an important industrial role as reflected e.g. by the:
    - 143,000 pre-registered and >13,250 (as of 21 July 2015) fully registered substances in the European Commission's REACH database (Registration, Evaluation, Authorisation and Restriction of Chemical substances), and the
    - >120,000 substances registered in the European Commission's Classification and Labelling (C&L) Inventory, which contains information on notified and registered substances received from manufacturers and importers.

There is no doubt that LCIA (eco)-toxicity models will become more precise and with lower uncertainty for some substances while covering more substances as more (eco)-toxicity test data become available. There is however also no doubt that given this vast amount of chemicals to be characterized and the inherent variability between those substances, however well they may be modelled, the toxicity impact category will always come with the aforementioned typical variability and uncertainty characteristics attached to its results. This leaves us with essentially two options: 1) exclude toxicity from LCA in order to avoid its

uncertainty, or 2) interpret toxicity impact scores considering their uncertainty (see recommendations above). Option 1) would leave us with the risk of selecting a potentially toxic product or product system without even realizing it. Option 2) allows for an explicit evaluation of the (eco)-toxicities as far as known. Furthermore, what is often overlooked in these discussions is the fact that not considering a potentially contributing impact pathway also comes with very large uncertainty, but which is rather unconscious and not quantified. Just because there are large numbers quantifying an uncertainty for toxicity characterization does not mean that there is no or lower uncertainty when ignoring an entire impact category, just because nobody has quantified that yet. Option 2) recognizes that it is not possible or meaningful to interpret the impact scores of all impact categories in LCA in the same way without considering their specific limitations and inherent properties.

As discussed above, the uncertainties of different impact categories are not directly comparable and thus a questionable argument to exclude an impact category. For example, the Global Warming Potential for a 100 years' time horizon (GWP_{100}) covers around 50 different substances (called greenhouse gases) that are considered relevant contributors to climate change. Their characterization factors from lowest to highest GWP_{100} range by a factor of about 10^4 and come with an uncertainty of less than factor 10. Toxicity potentials are currently available for 3000 different substances (a constantly rising number) with characterization factors ranging between a factor 10^{15} to 10^{21} from lowest to highest (depending on emission compartment and whether it is human health or ecotoxicity). Even assuming a very high uncertainty of a factor 10^4, there is still plenty of variability between substances that can be identified in a range of $>10^{15}$, certainly not less than for GWP_{100}.

4. MODEL INPUT DATA

The USEtox model operates through the combination of chemical data specific for a given comparison context, and default input data (such as physicochemical properties of each compound modelled in USEtox). The default-types of data pertain to data on environmental compartments, and on substances. Separate databases are used for the landscape data and the substance data, described in Sections 4.1 and 4.2, respectively.

4.1 Landscape data

4.1.1 Introduction

Landscape- and human-exposure relevant environmental characteristics are described for the default USEtox setting, and in addition for 8 continental landscapes and for 16 sub-continental landscapes. The landscape data in Table 4 and Table 5 contain values for the default continental and global systems as well as for the parameterized (sub)continental and global systems, namely: land area with the fraction of freshwater, natural and agricultural soil, sea area, the temperature, wind speed, rain rate, fresh water depth, fraction of freshwater discharge from the continental to the global system, fractions of the rain rate that run off and respectively infiltrate the soil, soil erosion and irrigation. Table 6 provides urban landscape data containing the urban area and the fractions of non-paved and paved area, the human population of world, continental and urban scales, the human breathing rate and water ingestion rate for both default USEtox setting, and in addition for 8 continental landscapes and for 16 sub-continental landscapes. Finally, Table 7 contains the production-based intake rates for default USEtox setting, and in addition for 8 continental landscapes and for 16 sub-continental landscapes.

Note that a user can select any of the regions belonging to the sub-continental or continental level instead of the USEtox default continent. Parameters of the selected region will automatically overwrite the USEtox default parameters. One could define its own region with specific parameters by adding a line on the “Landscape and indoor data” sheet. Global parameters should also be recalculated considering the difference between the new region and the world values.

These parameters are described for the default USEtox setting (Rosenbaum et al. 2008), for 16 sub-continental landscapes (Shaked 2011) and 8 continental landscapes as per Humbert et al. (2011). The parameterized landscape data are detailed in Kounina et al. (2014).

Table 4: Continental landscape parameters for the USEtox default continent model setting (Rosenbaum et al. 2008) and for the parameterized (sub)continents (Kounina et al. 2014).

Parameter name	Area	Area	Areafrac	Areafrac	Areafrac	Temp
USEtox variable						
Compartment	land	sea	fresh water	nat soil	agr soil	
Unit	km^2	km^2	[-]	[-]	[-]	°C
Detail	Area of land in the continental /global box	Area of sea in the continental /global box	Fraction of freshwater in the continental /global box	Fraction of natural soil in the continental /global box	Fraction of agricultural soil in the continental /global box	Mean temperature in the continental /global box
Default landscape value	9.01E+06	9.87E+05	3.00E-02	4.85E-01	4.85E-01	12
Default landscape reference	Calculated average continental area	Calculated based on average continental shelf width of 60 km	Calculated average fresh water area	Estimated value	Estimated value	Default
Continental and sub-continental value	Area of land including natural and agricultural soil, freshwater area and urban area	Area of coastal region (1)	Ratio of the area of freshwater on $Area_{land}$	$= 1 - areafrac_{agr\ soil} - areafrac_{freshwater} - areafrac_{othersoil}$	0.1	12
Continental and sub-continental reference	GIS computation made in IMPACT World (Shaked 2011)			Calculated	(Shaked 2011)	Default landscape data

(1) 33 coastal regions are defined as the long and narrow regions between the continents and oceans (Shaked 2011). They are included in the model as a compartment to better capture pollutant transport to marine ecosystems and the resulting accumulation of pollutants within consumed fish. Due to river runoff and high coastal population density, much of the ocean pollution is concentrated in coastal areas, which are relatively shallow and contain up to 90% of the global fisheries catch (Schwartz 2005). GIS has been used to define coastal regions as the sections of ocean adjacent to land that are less than 150 m in depth, which includes most of the continental shelf. USEtox model has been parameterized to operate with 60 km coastal zone, which correspond to the average width of the continental shelf.

Parameter name	Wind speed	Rain rate	Depth	RiverFlow	Fraction	Fraction	Soil erosion	Irrigation
USEtox variable								
Compartment			fresh water	reg-cont	run off	infiltration		
Unit	$m.s^{-1}$	$mm.yr^{-1}$	m	[-]	[-]	[-]	$mm.yr^{-1}$	km^3
Detail	Mean wind speed above 10 m above the	Mean rainfall rate in the	Mean freshwater	Mean river flow in the continental	Mean runoff in the continental /global	Mean infiltration in the continental	Mean erosion in the continental	Mean irrigation in the

	ground surface	continental /global box	depth in the continental /global box	/global box	box	/global box	/global box	continental/global box
Default landscape value	6.65	700	2.5	0	0.25	0.25	3.00E-02	2720
Continental and sub-continental value	$= \sigma * \sqrt{Area_{land} + Area_{se}} * \frac{Outflow_{cont}}{(Area_{land} + Area_{sea}}$ With σ: 75 h_{wind}: 1000 m $Outflow_{cont}$: continental outflow based on IMPACTWorld	Rainfall rate from IMPACTWorld	Freshwater depth from IMPACTWorld	0	Runoff from IMPACTWorld	0.25	3.00E-02	421
Continental and sub-continental reference	Based on GEOSChem wind speeds for IMPACT World	Based on GIS computation for IMPACT World		Default landscape data	Based on GIS computation for IMPACT World	Default landscape data		agricultural water withdrawal based on Aquastat

Table 5: Global landscape parameters for the USEtox default continent model setting (Rosenbaum et al. 2008) and for the parameterized (sub)continents (Kounina et al. 2014).

Parameter name	Area	Area	Areafrac	Areafrac	Areafrac	Areafrac	Temp
USEtox variable							
Compartment	land	sea	fresh water	nat soil	agr soil	other soil	
Unit	km^2	km^2	[-]	[-]	[-]	km	°C
Detail	Area of land in the continental /global box	Area of sea in the continental /global box	Fraction of freshwater in the continental /global box	Fraction of natural soil in the continental /global box	Fraction of agricultural soil in the continental /global box	Fraction of other soil in the continental /global box	Mean temperature in the continental /global box
Default landscape value	1.41E+08	3.29E+08	3.00E-02	4.85E-01	4.85E-01	1E-20	12
Continental and sub-	Sum of all (sub)-	Sum of all (sub)-	Fraction of	Fraction of natural	Fraction of	Fraction of other	12

continental value	continental land areas excluding the land area of the considered landscape	continental sea areas excluding the sea area of the considered landscape	freshwater for all continental landscapes excluding the landscape considered	soil for all continental landscapes excluding the landscape considered	agricultural soil for all continental landscapes excluding the landscape considered	soil for all continental landscapes excluding the landscape considered	
Continental and sub-continental reference	Based on continental data computations						Default landscape data

Parameter name	Wind speed	Rain rate	Depth	RiverFlow	Fraction	Fraction	Soil erosion	Irrigation
USEtox variable								
Compartment			fresh water	reg-cont	run off	infiltration		
Unit	$m.s^{-1}$	$mm.yr^{-1}$	m	[-]	[-]	[-]	$mm.yr^{-1}$	km^3
Detail	Mean wind speed above 10 m above the ground surface	Mean rainfall rate in the continental /global box	Mean freshwater depth in the continental /global box	Mean river flow in the continental /global box	Mean runoff in the continental /global box	Mean infiltration in the continental /global box	Mean erosion in the continental /global box	Mean irrigation in the continental/global box
Default landscape value	3	700	2.5	0	0.25	0.25	3.00E-02	227
Continental and sub-continental value	3	700	2.5	0	0.25	0.25	3.00E-02	
Continental and sub-continental reference	Default landscape data							

Table 6: Urban scale, human population and exposure data for the USEtox default model setting (Rosenbaum et al. 2008) and for the parameterized (sub)continents (Kounina et al. 2014).

	Urban scale			**Human Population**			**Exposure**	
Parameter name	Area	Areafrac	Areafrac	Human pop	Human pop	Human pop	Human breathing rate	Water ingestion

USEtox variable	SYSTEMAREA.U	AREAFRAC.s1U	AREAFRAC.s3U	Pop.world	Pop.cont	Pop.urban	Breath.hum	Ing.water
Compartment	land	non-paved surface	paved surface	world	continent	urban	world + cont + urban	world + cont
Unit	km^2	[-]	[-]	[-]	[-]	[-]	m^3/(person*day)	l/(person*day)
Detail	Land area	non-paved surface fraction	paved surface fraction	Human population in the world	Human population in the continent	Human population living in an urban setting in the continental landscape	Human breathing rate	Water ingestion
Default landscape value	240	0.667	0.333	6.00E+09	9.98E+08	2.00E+06	13*	1.4*
Continental and sub-continental value	240	0.667	0.333	Total population excluding continental and urban population	Continental population based on IMPACT World		13*	1.4*
Continental and sub-continental reference	Default landscape data			Based on GIS computation for IMPACT World			Default landscape data	

*https://cfpub.epa.gov/ncea/risk/recordisplay.cfm?deid=236252

Table 7: Production-based intake rates for the USEtox default model setting (Rosenbaum et al. 2008) and for the parameterized (sub)continents based on regional populations and FAO food production statistics (Kounina et al. 2014).

Parameter name	Exposed produce	Exposed produce	Unexposed produce	Unexposed produce	Meat	Meat	Dairy products	Dairy products	Fish freshwater	Fish freshwater	Fish coastal marine water	Fish coastal marine water
USEtox variable	Int.exp_world	Int.exp_cont	Int.unexp_world	Int.unexp_cont	Int.meat_world	Int.meat_cont	Int.milk_world	Int.milk_cont	Int.fishf_world	Int.fishf_cont	Int.fishs_world	Int.fishs_cont
Compartment	world	continent	world	continent	world	continent	world	continent	world	continent	world	continent
Unit	kg/(day*c	kg/(day*c	kg/(day*c	kg/(day*c	kg/(day*c	kg/(day*c	kg/(day*c	kg/(day*c	kg/(day*c	kg/(day*c	kg/(day*c	kg/(day*c

	apita)	apita)	apita)	apita)	apita)	apita)	apita)	apita)	apita)	apita)	apita)	apita)
Detail	Exposed produce ingestion in the global box	Exposed produce ingestion in the continental box	Unexposed produce ingestion in the global box	Unexposed produce ingestion in the continental box	Meat ingestion in the global box	Meat ingestion in the continental box	Dairy product ingestion in the global box	Dairy product ingestion in the continental box	Freshwater fish ingestion in the global box	Freshwater fish ingestion in the continental box	Marine fish ingestion in the global box	Marine fish ingestion in the continental box
Default landscape value	1.36	1.36	1.12	1.12	0.0949	0.0949	0.237	0.237	0.0113	0.0113	0.036	0.036
Continental and sub-continental value	Total exposed produce consumption excluding continental consumption	Based on FAO data	Total exposed produce consumption excluding continental consumption	Based on FAO data	Total exposed produce consumption excluding continental consumption	Based on IMPACT World data	Total exposed produce consumption excluding continental consumption	Based on IMPACT World data	Total exposed produce consumption excluding continental consumption	Based on IMPACT World data	Total exposed produce consumption excluding continental consumption	Based on IMPACT World data
Continental and sub-continental reference	Based on continental data computations	FAO production data from 2001	Based on continental data computations	FAO production data from 2001	Based on continental data computations	FAO production data from 2001	Based on continental data computations	FAO production data from 2001	Based on continental data computations	FAO FishSTAT	Based on continental data computations	FAO FishSTAT

Table 8: Household indoor air model data (Rosenbaum et al. 2015).

Parameter name	Volume	Air exchange rate	Number of persons	Average daily time spent at home	Ventilation per person	Individual hourly inhalation rate at home
USEtox variable	VOLUME.a1I	kex.a1I	N.a1I	day_time_at_home	ventilation_at_home	breathing_rate_at_home
Unit	m^3	h^{-1}	[-]	$h \cdot d^{-1}$	$m^3 \cdot h^{-1} \cdot pers^{-1}$	$m^3 \cdot h^{-1}$
Default (OECD countries average)	117	15.6	4	14.0	456	0.542
Non-OECD countries average (non-airtight building)	117	0.79	4	14.0	23	0.542

Non-OECD countries average (airtight building)	236	0.79	2.5	14.0	75	0.542
Europe (EU-27) average	209	0.79	2.4	14.0	69	0.542
North America	277	0.79	2.6	14.0	84	0.542

Table 9: Occupational indoor air model data (adapted from Tox-Train, http://toxtrain.eu).

Parameter name	Volume	Air exchange rate	Number of persons	Average daily time spent at work		Ventilation per person	Individual hourly inhalation rate at work	
USEtox variable	VOLUME.a2I	kex.a2I	N.a2I	day_time_at_work		ventilation_at_work	breathing_rate_at_work	
Unit	m^3	h^{-1}	[-]	$h \cdot d^{-1}$	Comment	$m^3 \cdot h^{-1} \cdot pers^{-1}$	$m^3 \cdot h^{-1}$	Comment
Industry, OECD	350	12	1	4.8	1737 h/y, 365 d/y	4200	2.5	average for male worker
Office, OECD	20	4	1	4.8	1737 h/y, 365 d/y	80	0.542	average for resting adult
Industry, non-OECD	250	8	1	5.3	1945 h/y, 365 d/y	2000	2.5	average for male worker
Office, non-OECD	15	3	1	5.3	1945 h/y, 365 d/y	45	0.542	average for resting adult

4.2 Substance data

The substance data describes the physical-chemical characteristics, degradation rates, toxicity, ecotoxicity, bioaccumulation factors and biotransfer factors of a substance. For USEtox two substance databases are given; one for organic substances and one for inorganic substances. The organic database contains the substance data of 3073 organic substances and the inorganic database contains 27 metal substances.

4.2.1 Default constants

Environmental fate

Parameters used in USEtox for the calculation of fate factors are presented in Table 10. Explanations of symbols and indices are given in Appendix A and corresponding parameters in USEtox are given in Appendices B to E.

Table 10. Parameters descriptions and their default value as used in the USEtox model for the fate calculations. Default values without reference are assumed a generally accepted value for that parameter.

Parameter name	Description	Default value	Reference
$C_E_{ae[S]}$	aerosol collection efficiency representing the volume of air efficiently scavenged by rain of its aerosol content, per unit volume of rain.	200000	Mackay (2001)
$C_F_{fish,w[S]}$	fat content continental and global fresh and sea water fish	0.05	Mackay (1982); Mackay and Fraser (2000)
$C_{biota,w[S]}$	concentration biota in continental and global fresh and sea water	0.001 kg·m^{-3}	-
$cf_{DOC\|w,w}$	correction factor for octanol/water partitioning coefficient in order to predict the DOC/water partitioning coefficient	0.08	Burkhard (2000)
$cf_{\tau air[S]}$	correction factor of urban and continental air residence time	0.75	Humbert et al. (2011) (in supporting information)
$C_{DOC,w[S]}$	concentration of dissolved (colloidal) organic carbon in continental and global fresh and sea water	0.005 kg·m^{-3} for fresh water; 0.001 kg·m^{-3} for sea water	-
$C_{susp,w[S]}$	concentration suspended matter in continental and global fresh and sea water	0.015 kg·m^{-3} for fresh water	Asselman (1997)
		0.005 kg·m^{-3} for sea water	-
$fr_m_{Corg,sl[S]}$	mass fraction organic	0.02	den Hollander et al.

Parameter name	Description	Default value	Reference
	carbon in continental and global natural and agricultural soil		(2004)
$fr_m_{Corg,susp,w[S]}$	mass fraction organic carbon in continental and global fresh and sea water suspended matter	0.1	-
$fr_m_{Corg,wsd[S]}$	mass fraction organic carbon in continental and global fresh and sea water sediment	0.05	-
$fr_V_{gas,sl[S]}$	volume fraction gas in continental and global natural and agricultural soil	0.2	-
$fr_V_{water,air[S]}$	volume fraction water in urban, continental and global air	0.000000000000246	Hess et al. (1998)
$fr_V_{cldw,air[S]}$	volume fraction cloud water in urban, continental and global air	0.00000005555	Hess et al. (1998)
$fr_V_{water,sd[S]}$	volume fraction water in continental and global sediment	0.8	Paterson and Mackay (1995)
$fr_V_{water,sl[S]}$	volume fraction water in continental and global natural and agricultural soil	0.2	-
$h_{air[S]}$	mixed height of the continental and global air	1000 m	den Hollander et al. (2004)
$h_{air[U]}$	mixed height of the urban air	240 m	Humbert et al. (2011)
H_{diss}	enthalpy of dissolution	10000 J.mol^{-1}	-
$h_{sl[S]}$	depth continental and global natural and agricultural soil	0.1 m	Hollander et al. (2004)
H_{vap}	enthalpy of vaporization	50000 J.mol^{-1}	-
$h_{w[S]}$	mixed depth of continental and global fresh and sea water	2.5 m for the continental and global freshwater; 100 m for the continental sea water; 200 m for the global sea water	-
$h_{wsd[S]}$	mixed depth continental and global fresh and sea water sediment	0.03 m	-
$J_{susp,fw[C]}$	autochtonous production of suspended matter in continental fresh water	85.74 kg·s^{-1} for continental fresh water; 312.78 kg·s^{-1} for continental sea water; 1341.32 kg·s^{-1} for global fresh water	den Hollander et al. (2004)

Parameter name	Description	Default value	Reference
		50577.12 $kg \cdot s^{-1}$ for the global sea water	-
pH_{cloud}	pH aerosol water, average of pH of water in air before oxidation (6.5) and after oxidation (4.7)	5.6	Franco and Trapp (2010)
pH_{sl}	pH of soil	5 for the natural soil; 7 for the agricultural soil	Franco and Trapp (2010)
pH_{w}	pH of water	7 for the fresh water; 8 for the sea water	Franco and Trapp (2010)
pKa,loss	equilibrium constant proton loss from conjugated acid of parent compound (pKa of the acid dissociation reaction)	described in substance data, if not: 14	-
pKa,gain	equilibrium constant proton loss from parent compound (pKa of the base's conjugated acid dissociation reaction)	described in substance data, if not: 0	-
$\tau_{sw[C]}$	residence time of the continental sea water	365 d	-
ρ_{air}	density of air	1.29 $kg \cdot m^{-3}$	-
$\rho_{sd,sl}$	mineral density of sediment and soil	2166.3 $kg \cdot m^{-3}$	-
ρ_{w}	density of water	1000 $kg \cdot m^{-3}$	-
$\upsilon_{dep,air,ae[S]}$	aerosol deprate or deposition velocity of aerosol particles	0.001 $m \cdot s^{-1}$	Mackay (2001)
$\upsilon_{m,sd,w \mid sd[S]}$	partial mass transfer coefficient at the sediment side of water/sediment interface	0.00000002778 $m.s^{-1}$	Mackay (2001)
$\upsilon_{m,w,w \mid sd[S]}$	partial mass transfer coefficient at the water side of water/sediment interface	0.000002778 $m.s^{-1}$	Mackay (2001)
$\upsilon_{rain[U]}$	annual average precipitation on the urban scale	700 $m \cdot s^{-1}$	-
$\upsilon_{[U]}$	wind speed at the urban scale	$^{2.5}$ $m \cdot s^{-1}$	-

Human exposure

Parameters in USEtox for calculating human exposure factors are presented in Table 11. Explanations of symbols and indices are given in Appendix A and corresponding parameters in USEtox are given in Appendices B to E.

Table 11. Parameters descriptions and their default value as used in the USEtox model for the human exposure calculations. Default values without reference are assumed a generally accepted value for that parameter.

Parameter name	Description	Default value	Reference
λ_g	Growth dilution rate constant	0.035	EC (2004)
Q_{transp}	Area equivalent transpiration flow from soil through stems	0.001	Trapp and Matthies (1995)
MTC	Mass transfer coefficient at the air-leaf interface	86	Trapp and Matthies (1995)
LAI	Leaf area index, the one-sided area of plant leaf surfaces per unit land area	4	Nobel (2009)
	Leaf area index at herbicide application time for	$[m^2_{leaf\ area} \cdot m^{-2}_{soil\ area}]$	Fantke et al. (2011b)
$LAI_{H,wheat}$	Wheat	0.2	
$LAI_{H,paddy}$	Paddy rice	1.87	
$LAI_{H,tomato}$	Tomato	1.04	
$LAI_{H,apple}$	Apple	0.2	
$LAI_{H,lettuce}$	Lettuce	0.14	
$LAI_{H,potato}$	Potato	3.91	
	Leaf area index at non-herbicide application time for	$[m^2_{leaf\ area} \cdot m^{-2}_{soil\ area}]$	Fantke et al. (2011b)
$LAI_{NH,wheat}$	Wheat	4.86	
$LAI_{NH,paddy}$	Paddy rice	5.02	
$LAI_{NH,tomato}$	Tomato	3.11	
$LAI_{NH,apple}$	Apple	2.35	
$LAI_{NH,lettuce}$	Lettuce	0.88	
$LAI_{NH,potato}$	Potato	0.3	
	Fruit area index at herbicide application time for Wheat	$[m^2_{leaf\ area} \cdot m^{-2}_{soil\ area}]$	Fantke et al. (2011b)
$FAI_{H,wheat}$	Paddy rice	0.04	
$FAI_{H,paddy}$	Tomato	0.81	
$FAI_{H,tomato}$	Apple	0.17	
$FAI_{H,apple}$		0.04	
	Fruit area index at non-herbicide application time for	$[m^2_{leaf\ area} \cdot m^{-2}_{soil\ area}]$	Fantke et al. (2011b)
$FAI_{NH,wheat}$	Wheat	1.08	
$FAI_{NH,paddy}$	Paddy rice	2.18	
$FAI_{NH,tomato}$	Tomato	0.49	
$FAI_{NH,apple}$	Apple	0.49	
V_{plant}	Area equivalent volume of above ground plant tissues	0.0125 $m^3_{plant\ tissues}/m^2_{soil\ area}$ (assumed to be the sum of cuticle and leaf volumes)	Nobel (2009)

Parameter name	Description	Default value	Reference
ν_d	Deposition ratio accounting for both wet and dry particle deposition of particles from air to plant surfaces	500 mol/(m^2·d) per mol/m^3	Whicker and Kirchner (1987)
ρ_{plant}	Plant density	800 kg_{wwt}/m^3	Trapp and Mc Farlane (1995); Riederer (1990)
	Individual farm animal intake rate from vegetation for		Margni (2003) (Table 4, p. 44)
$Pork_{veg}$	Pork	8.85 kg FM/d	
$Beef_{veg}$	Beef	26.63 kg FM/d	
$Poultry_{veg}$	Poultry	0.37 kg FM/d	
$GoatSheep_{veg}$	Goat and sheep	4.77 kg FM/d	
	Individual farm animal intake rate from air for		Margni (2003) (Table 4, p. 44)
$Pork_{air}$	Pork	60 m^3/d	
$Beef_{air}$	Beef	80 m^3/d	
$Poultry_{air}$	Poultry	2.2 m^3/d	
$GoatSheep_{air}$	Goat and sheep	60 m^3/d	
	Individual farm animal intake rate from water for		Margni (2003) (Table 4, p. 44)
$Pork_{water}$	Pork	7 kg/d	
$Beef_{water}$	Beef	30 kg/d	
$Poultry_{water}$	Poultry	0.1 kg/d	
$GoatSheep_{water}$	Goat and sheep	7 kg/d	
	Individual farm animal intake rate from soil for		Margni (2003) (Table 4, p. 44)
$Pork_{soil}$	Pork	0.04 kg/d	
$Beef_{soil}$	Beef	0.3 kg/d	
$Poultry_{soil}$	Poultry	0.001 kg/d	
$GoatSheep_{soil}$	Goat and sheep	0.1 kg/d	
	Percentage of fat in		Supporting information of Pennington et al. (2005)
$Pork_{fat}$	Pork	23%	
$Beef_{fat}$	Beef	25%	
$Poultry_{fat}$	Poultry	6%	
$GoatSheep_{fat}$	Goat and sheep	14%	
	Percentage of average diet consisting of		FAO (2002)
$Pork_{diet}$	Pork	39%	
$Beef_{diet}$	Beef	24%	
$Poultry_{diet}$	Poultry	30%	
$GoatSheep_{diet}$	Goat and sheep	5%	
$Other_{diet}$	Other	2%	
	Time in days of pesticide application before harvest for herbicides on		Fantke et al. (2011b)
$\tau_{H,wheat}$	Wheat	150 d	
$\tau_{H,paddy}$	Paddy rice	100 d	
$\tau_{H,tomato}$	Tomato	85 d	
$\tau_{H,apple}$	Apple	150 d	

Parameter name	Description	Default value	Reference
$\tau_{H,lettuce}$	Lettuce	55 d	
$\tau_{H,potato}$	Potato	60 d	
	Time in days of pesticide application before harvest for non-herbicides on		Fantke et al. (2011b)
$\tau_{nH,wheat}$	Wheat	43 d	
$\tau_{nH,paddy}$	Paddy rice	27 d	
$\tau_{nH,tomato}$	Tomato	5 d	
$\tau_{nH,apple}$	Apple	14 d	
$\tau_{nH,lettuce}$	Lettuce	10 d	
$\tau_{nH,potato}$	Potato	4 d	
	Substance capture coefficient (fraction of applied mass intercepted by crop) for		Fantke et al. (2012)
$k_{wheat.sl}$	Wheat		
$k_{paddy.sl}$	Paddy rice	0.50 $(kg/m^2_{leaf})/(kg/m^2_{soil})$	
$k_{toamto.sl}$	Tomato	0.50 $(kg/m^2_{leaf})/(kg/m^2_{soil})$	
$k_{apple.sl}$	Apple	0.45 $(kg/m^2_{leaf})/(kg/m^2_{soil})$	
$k_{lettuce.sl}$	Lettuce	0.50 $(kg/m^2_{leaf})/(kg/m^2_{soil})$	
$k_{potato.sl}$	Potato	0.34 $(kg/m^2_{leaf})/(kg/m^2_{soil})$ 0.40 $(kg/m^2_{leaf})/(kg/m^2_{soil})$	
	Food processing factor for		Fantke and Jolliet (2016)
$fp_{wheat,bread}$	Wheat	0.33 $kg_{intake}/kg_{in,harvest}$	
$fp_{paddy,parb}$	Paddy rice	0.32 $kg_{intake}/kg_{in,harvest}$	
$fp_{tomato,wash}$	Tomato	0.59 $kg_{intake}/kg_{in,harvest}$	
$fp_{apple,wash}$	Apple	0.59 $kg_{intake}/kg_{in,harvest}$	
$fp_{lettuce,wash}$	Lettuce	0.59 $kg_{intake}/kg_{in,harvest}$	
$fp_{potato,cook}$	Potato	0.32 $kg_{intake}/kg_{in,harvest}$	
	Fraction of pesticide applied mass transferred to air for		Fantke and Jolliet (2016)
$fr_{air,wheat}$	Wheat	16.4667%	
$fr_{air,paddy}$	Paddy rice	16.4667%	
$fr_{air,tomato}$	Tomato	23.667%	
$fr_{air,apple}$	Apple	35.433%	
$fr_{air,lettuce}$	Lettuce	5%	
$fr_{air,potato}$	Potato	14.85%	

Indoor exposure

Parameters in USEtox related to human indoor exposure are presented in Table 12. Explanations of symbols and indices are given in Appendix A and corresponding parameters in USEtox are given in Appendices B to E.

Table 12. Parameters descriptions and their default value as used in the USEtox model for the indoor exposure calculations. Default values without reference are assumed a generally accepted value for that parameter.

Parameter name	Description	Default value	Reference
k_{O3}	Second order constant rate for O_3	0 $h^{-1}ppbv^{-1}$	Rosenbaum et al. (2015)
k_{NO3}	Second order constant rate	0 $h^{-1}ppbv^{-1}$	Rosenbaum et al.

Parameter name	Description	Default value	Reference
	for NO_3		(2015)
$k_{deg,wall,indoor}$	Degradation rate on room surfaces - $k_{deg\ wall}/k_{a\ indoor}$	0.1	Rosenbaum et al. (2015)
Out_{OH}	Outdoor OH	0.000061 ppbv	Rosenbaum et al. (2015)
$Mix_{[H]}$, $Mix_{[O]}$	Mixing factor	1	Rosenbaum et al. (2015)
$A_{carpet[H]}$	Area per volume carpet in households	0.41 $m^2 \cdot m^3$	Rosenbaum et al. (2015)
$A_{carpet[O]}$	Area per volume carpet at work	0 $m^2 \cdot m^3$	Rosenbaum et al. (2015)
$A_{total[H]}$	Area per volume total in households	3.1 $m^2 \cdot m^3$	Rosenbaum et al. (2015)
h_m	Mass transfer coefficient at wall surface	8.8 $m^3 \cdot m^{-2} \cdot h^{-1}$	Rosenbaum et al. (2015)
OH	OH radical concentration indoors	0.000003 ppbv	Rosenbaum et al. (2015)
O_3	Ozone radical concentration indoors	8 ppbv	Rosenbaum et al. (2015)
NO_3	Nitrate radical concentration indoors	0.001 ppbv	Rosenbaum et al. (2015)
$f_{ex[H]}$, $f_{ex[O]}$	Air exchange fraction to urban air	0.5	Rosenbaum et al. (2015)

Human and ecosystem effects

Parameters in USEtox describing the linear extrapolation of effects are presented in Table 13. Explanations of symbols and indices are given in Appendix A and corresponding parameters in USEtox are given in Appendices B to E.

Table 13. Parameters descriptions and their default value as used in the USEtox model for the human and ecosystem linear effect calculations.

Parameter name	Description	Default value	Remarks
f_{nc}	Multiplier for non-cancer human effect	0.5	Defined as the 50% of the ED_{50}
f_c	Multiplier for cancer human effect	0.5	Defined as the 50% of the ED_{50}
f_{eco}	Multiplier for ecosystem effect	0.5	Defined as the 50% of the HC_{50}

4.2.2 USEtox substance database

Databases of chemical properties were set up aiming to (a) have a consistent set of data (b) have data of a certain minimum quality (c) have data for as many chemicals as possible for which characterization factors can be computed. In this sub-chapter, it is outlined where the data from the USEtox database were taken from.

The database includes three types of datasets: (1) physicochemical properties, (2) toxicological effect data on laboratory animals as a surrogate to humans and (3) ecotoxicological effect data for freshwater organisms. We focused our effort on identifying and collecting existing reviewed databases for which scientific judgment was already made in selecting and recommending values from a large range of values collected from the literature.

Physico-chemical properties

Organic chemicals

For Molecular weight, Kow, Koc, vapour pressure, and solubility experimental data from Episuite were taken when available. Otherwise, estimated data from EPISuite were applied. The United States Environmental Protection Agency EPI (Estimation Programs Interface, Suite is a Windows®-based suite of physical/chemical property and environmental fate estimation programs developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC). EPI Suite requires only a single input, a representation of the chemical structure in SMILES notation. SMILES means "Simplified Molecular Information and Line Entry System." See also http://www.epa.gov/oppt/exposure/pubs/episuite.htm). The following estimation routines were applied:

1. Molecular weight (MW in g/mol): no estimation routine required;
2. Octanol-water partitioning coefficient (Kow): A "fragment constant" methodology to predict log Kow has been applied. In a "fragment constant" method, a structure is divided into fragments (atoms or larger functional groups).
3. Ionization: (pKa): empirical pKa values were taken from the EPISuite database for ionizing organic chemicals. If empirical values were not available, pKa-values were estimated with the software SPARC (http://www.archemcalc.com/sparc.html). SPARC also shows in the structure diagram to which group the pKa applies. Chemical insight and expert judgment was used to decide whether that means that the chemical reaction involved is a release of a proton from the original structure, or a release of a proton from the protonated form of the original structure and whether the substance is an acid, a base, or a zwitter ion.
4. Organic carbon-water partitioning coefficient (Koc in l/kg): Regression equations developed with the molecular connectivity index (MCI) were used. The regressions used in USEtox for calculating the Koc for the electrolytes are suited for acids within the pKa range 0–12 and with a log Kow between -2.18 and 8.50. For bases the pKa needs to be above 2 and log Kow is between -1.66 and 7.03 (Franco & Trapp 2008).
5. Vapour pressure ($P_{vap}25$ in Pa): For solids, the modified Grain estimate is the suggested VP. For liquids and gases, the suggested VP is the average of the Antoine and the modified Grain estimates. Both methods use the boiling point to estimate vapour pressure.
6. Solubility (Sol25 in mg/l): The water solubility is estimated with regression equations using the octanol-water partition coefficient (Kow) and the melting point of a chemical.

If no experimental values for the Henry coefficient (K_H25C in $Pa.m^3/mol$) were reported in Episuite, K_H was calculated by $P_{vap}25$*MW/ Sol25.

For the partitioning coefficient between dissolved and organic carbon (Kdoc) no experimental data were implemented in the database and no estimation routine in EPI Suite

was available. Therefore, the Kdoc was estimated by Kdoc = 0.08 * Kow in the log Kow range up to 7.5, based on Burkhard (2000).

Explanation of using pKa: The two pKa values required in USEtox are to indicate that the model takes three species into account: the (uncharged) 'original' species, the protonated (cationic) species, and the dissociated (anionic) species. Generally, only two of these chemical species (most often only one!) are present in significant amounts in the environment. The dominant species are lumped into two fractions, named original (in USEtox sheet "fate": ".orig") and alternate (in USEtox sheet "fate": ".alt"). Different physicochemical properties and different intermedia partition coefficients are assigned to these two fractions ('.orig' and '.alt'). Partitioning of the 'total' substance is modeled as the mass-weighted average of the partitioning of the two dominant fractions. This way, the model can calculate the fractions of a substance in its '.orig' and '.alt' forms (at ambient pH), and can calculate Kp and Kh values for the mixture, based given properties of the '.orig' form and model-derived properties of the '.alt' form. For each new substance, USEtox needs as input into a single row per substance (i) properties of the original, unionized form ('.orig'), (ii) the two pKa values (of 'gain' and 'loss' reactions), and (iii) the pH at which partition coefficients are needed in the mass balance calculation. Example: to do the mass balance calculation for an acid, in fresh water, it needs the pKa of the proton loss reaction, the pH of natural water (given in USEtox), plus vapor pressure, water solubility and octanol-water partition coefficient of the original, undissociated form. USEtox then 'knows' how to derive the fraction of original species in water at the corresponding pH, and 'knows' how to assemble the Kp of the mixture of original and alternate forms.

Metals

The physicochemical properties for metals were selected as follows:

1. Molecular weights (MW in g/mol) were taken from the periodic table;

2. The Henry coefficient (KH25C in Pa.m3/mol) was set at 1.10-20 Pa.m3.mol-1, indicating negligible transfer of inorganic species from soil and water to air via volatilization.

3. Partition coefficients for soil, sediment, suspended solids and dissolved organic carbon were taken from IAEA International Atomic Energy Agency (2010) and Allison and Allison (2005), prioritizing the IAEA-data. The average partitioning coefficients for soil from IAEA International Atomic Energy Agency (2010) were used and refer to 'all soils'. The average partitioning coefficients for suspended solids from IAEA International Atomic Energy Agency (2010) are preferably based on field data. The exception is for Ag(I) with an average partitioning coefficient for suspended solids derived with adsorption experiments in the lab (IAEA International Atomic Energy Agency 2010). In case IAEA-data are not reported for partitioning coefficients, the average partitioning coefficients reported by Allison and Allison (2005) were applied. This is the case for all metals in case of sediment and dissolved organic carbon partitioning, and for the majority of the metals in case of suspended solids partitioning.

Degradation in the environment

Organic chemicals

Degradation rates in air, water, soil and sediment are required for the USEtox calculations. To derive the degradation rate in air ($k_{deg}A$ in 1/s), the k_{OH} is multiplied with the [OH] (the hydroxyl radical concentration in units of molecules (or radicals) per cm^3). For air

degradation rates, experimental values for the k_{OH} (the hydroxyl radical rate constant in units of cm^3/molecule-sec) are for some chemicals available in EPI Suite. The default [OH] is set at 1.5×10^6 molecules (radicals)/cm^3 per 12h of daylight. Furthermore, experimental degradation data in air, water, soil and sediments were taken from Sinkkonen and Paasivirta (2000) for dioxins and PCBs.

When no experimental data were available in EPISuite, the following estimation routines in EPISuite were applied:

1. Degradation in air ($k_{deg}A$ in 1/s): The estimation methods for k_{OH} are based upon structure-activity relationship (SAR) methods using "fragment constants". The default [OH] is set at 1.5×10^6 molecules (radicals)/cm^3 per 12h of daylight. Whenever using EPISuite estimated degradation in air, there are two ways to obtain the degradation rate constant in air based on the hydroxyl radicals reaction: (a) start from the overall OH rate constant, multiply it by the OH concentration in air and divide by a factor of 2 to reflect degradation during a 12 hours/day period, or (b) start from the half-life and convert it to a rate constant including unit conversion from day to second.
2. Degradation in water, soil and sediment ($k_{deg}W$, $k_{deg}Sl$, $k_{deg}Sd$ in 1/s): specifically for estimating biodegradation half-lives with EPI Suite, the Biowin3 model is used for USEtox input to convert the ultimate biodegradation probability in half-lives for all chemicals in the database (Table 14).

Table 14**:** Relation between BIOWIN3 output and default biodegradation half-lives and biodegradation rates

BIOWIN3 Output	**Assigned Half-Life (days)**	**Biodegradation rate (1/s)**
Hours	0.17	$4.7.10^{-5}$
Hours to Days	1.25	$6.4.10^{-6}$
Days	2.33	$3.4.10^{-6}$
Days to Weeks	8.67	$9.3.10^{-7}$
Weeks	15	$5.3.10^{-7}$
Weeks to Months	37.5	$2.1.10^{-7}$
Months	60	$1.3.10^{-7}$
Recalcitrant	180	$4.5.10^{-8}$

In addition, division factors of 1:2:9 are suggested in EPI Suite to extrapolate biodegradation rates for water, soil and sediment compartments respectively.

Other degradation mechanisms, such as direct photolysis and hydrolysis, were not included in the chemical database of USEtox. The user could of course adjust the specific degradation rates in any environmental compartment considering that $k_{degradation,total} = k_{biodegradation} + k_{hydrolysis} + k_{photolysis}$, etc.

Metals

Degradation rates in air, water, soil and sediment of metals were set at 1E-20 s^{-1}, indicating no degradation of inorganic in the environment.

Human exposure

Organic chemicals

Experimental data for the bioaccumulation in fish are provided in EPI Suite which were favoured over estimated data. For biotransfer factors for milk and meat, experimental data was collected by Rosenbaum et al. (2009) and implemented in the USEtox database. When no experimental data were available in EPISuite, estimation routines for bioaccumulation factors for fish were selected from EPISuite following the recommendations above were followed. If experimental data are not available, the following estimation routines are included for bioaccumulation factors for fish: the Arnot and Gobas (2003) model for the upper trophic level in EPI Suite is selected to estimate steady-state bioaccumulation factors (*BAF*; l/kg) for non-dissociating chemicals and chemicals with log K_{ow} < 9. The model includes mechanistic processes for bioconcentration and bioaccumulation such as chemical uptake from the water at the gill surface and the diet, and chemical elimination at the gill surface, faecal egestion, growth dilution and metabolic biotransformation. The model requires the octanol-water partition coefficient (Kow) of the chemical and the estimated whole-body metabolic biotransformation rate constant (1/day) as input parameters to predict BAF values. In case the chemical is indicated as dissociating or the chemical has a log Kow larger than 9, the Arnot and Gobas (2003) model is not recommended. Instead we applied the log Kow-based Bioconcentration factor (*BCF*; l/kg) estimation routine in EPISuite for these chemicals.

Biotransfer factors (BTF) for milk and meat are estimated based on the Travis and Arms (1988) model, truncated at the maximum and minimum Kow used in the underlying data. This results in a constant BTF outside the Kow range of their training set, as recommended in the Technical Guidance Document (TGD) on Risk Assessment (EC European Commission 2003).

For bioaccumulation in roots and leaves, no experimental data are implemented in the USEtox database for organic chemicals. QSARs readily implemented in USEtox are applied for this purpose.

Data for degradation in plants are based on dissipation half-lives compiled by Fantke et al. (2014) for various pesticide and crop classes based on an extensive collection of measured plant dissipation half-live data (Fantke & Juraske 2013).

Metals

The human exposure data for metals were selected as follows:

1. Bioaccumulation factors (BAF) for fish were preferably taken from IAEA International Atomic Energy Agency (2010). For Beryllium and Cadmium no BAF information was provided for fish by IAEA International Atomic Energy Agency (2010). For these two metals, BAFs for fish were taken from US-EPA (2002).

2. Biotransfer factors for milk and meat were taken from IAEA International Atomic Energy Agency (2010) and RTI (2002) with a preference for the IAEA-data. For Copper, however, these two data sources did not provide a biotransfer factor for milk and meat. In this case, the biotransfer factor to milk and meat for Copper was taken from Ng (1982).

3. Bioconcentration factors for root crops were derived from IAEA International Atomic Energy Agency (2010) and US-EPA (2002) with a preference for the IAEA-data. Concerning

the IAEA-data, information for temperate regions was used. The bioconcentration factors specified as 'root crops' were taken from IAEA International Atomic Energy Agency (2010) and RTI (2002) and converted from dry weight to wet weight by dividing with a factor of 5. For Copper, however, these two data sources did not provide a bioconcentration factor for root crops. In this case, the bioconcentration factor in roots for Copper was derived from Versluijs and Otte (2001), also using a conversion factor of 5 to extrapolate from dry weight to wet weight.

4. Bioconcentration factors for leaf crops were derived from IAEA International Atomic Energy Agency (2010) and RTI (2002) with a preference for the IAEA-data. For leaf crops, the bioconcentration factors specified for 'cereals - grain' were taken from IAEA International Atomic Energy Agency (2010) and RTI (2002), as cereals dominantly contributes to the food consumption by humans within this category. The dry weight to wet weight conversion was set at a factor of 1, indicating approximately equal water content in the grains of cereals and soils. For Copper, however, these two data sources did not provide a bioconcentration factor for leaf crops. In this case, the bioconcentration factor in leaf crops for Copper was derived from Versluijs and Otte (2001). The bioconcentration factor for leaf crops in the review of Versluijs and Otte (2001) refer to leafy vegetables, using a factor of 10 for dry weight to wet weight conversion.

Note that for Tin – Sn(II) – no bioaccumulation factors were available, but also no human effect data were found, i.e. no human health characterization factors were calculated for this metal.

Human carcinogenic toxicity

The following order of preference in toxicity data has been used in the USEtox calculations of carcinogenic effect factors:

1. The carcinogenic effect factor takes as a point of departure the effect dose 50% (ED50) which is preferably estimated from the low-dose, slope factor (q*), based on human data. The slope factors for 1,3-butadiene, acrylonitrile, benzene, benzidine, beryllium, cadmium, chromium VI, nickel and arsenic for humans after inhalation and for arsenic after ingestion were available via the IRIS database (http://www.epa.gov/iris/). Low-dose, slope factors for inhalation are reported in units of m3/µg. The ED50 is derived by 0.8/q* where 0.8 is a 1/q*-to-ED50 conversion factor. After that, the unit was converted from µg/m3 to kg/person/lifetime, using a lifetime of 70 years and an inhalation rate of 13 m3/day.

2. In case no quantitative effect information on humans was available from the IRIS database, ED50s from the carcinogenic potency database were taken (CPDB; http://potency.berkeley.edu/). ED50s for ingestion and inhalation are reported in units of mg/kg/day and converted to kg/person/lifetime, using a lifetime of 70 years and a body weight of 70 kg. For cancer, the harmonic mean of all positive ED50s in the CPDB is retained for the most sensitive species of animal cancer tests after application of an allometric interspecies conversion factor proportional to bodyweight to the power of 0.25. Table 15 provides an overview of interspecies conversion factors applied in constructing the USEtox chemical database (Huijbregts et al. 2005). Experimental data in the CPDB are available for rats, mice, hamsters, dogs, monkeys.

3. In case no quantitative effect information was available from the CPDB, the carcinogenic ED50 has been estimated from the low-dose, slope factor (q*) by a 1/q*-to-ED50 conversion

factor of 0.8, based on animal data. The slope factors were again taken from the Integrated Risk Information System (IRIS) database (http://www.epa.gov/iris/).

4. In case no data was available for a specific exposure route, a route-to-route extrapolation has been carried out, assuming equal ED50 or slope factor between inhalation and ingestion route. Chemicals with all negative carcinogenic effect data were also included as true zero carcinogenic effect factors and distinguished from missing data.

Note that for the following metals the carcinogenic ED50s were not directly reported, but derived from closely related substances via molecular weight correction:

- the carcinogenic ED50s of Cd(II) for ingestion were derived from information available for cadmium chloride;
- the carcinogenic ED50 of Hg(II) for ingestion was derived from information available for mercuric chloride;
- the carcinogenic ED50 of Pb(II) for ingestion was derived from information available for lead acetate.

Non-cancer human toxicity

In the case of effects other than cancer, for most of the substances, insufficient data were available to recalculate an ED50 with dose–response models. For chemicals with no evidence of carcinogenicity, the ED50 has been estimated from no-observed effect level (NOEL) by a NOEL-to-ED50 conversion factor of 9. In case only a LOEL was available, a LOEL-to-ED50 conversion factor of 2.25 has been applied. NOELs and LOELs were derived from the IRIS database and from the World Health Organisation (WHO) with priority for data from the WHO. If relevant, conversion factors to extrapolate from sub-chronic to chronic exposure and sub-acute to chronic exposure were applied as well (see Huijbregts et al. 2005 for further details). Also for non-carcinogenic effects, the units were converted to kg/person/lifetime, using a lifetime of 70 years and a body weight of 70 kg for ingestion and an inhalation rate of 13 m^3/day and a lifetime of 70 years for inhalation. An allometric interspecies conversion factor proportional to bodyweight to the power of 0.25 has been applied to the ED50 for ingestion (Table 15). As for non-cancer effects for inhalation, the critical effect concentration is defined as the concentration in the air, the interspecies extrapolation factor for inhalation is in principle 1, assuming that inhalation rates between species scale proportionally to metabolic rates. For some toxicity data after inhalation, however, substance-specific interspecies differences were derived by the US-EPA via pharmacokinetic modelling. In these specific cases, the interspecies conversion factors reported by the US-EPA were applied. As for carcinogenic effects, in case no data is available for a specific exposure route, a route-to-route extrapolation has been carried out, assuming equal ED50 between inhalation and ingestion route.

Note that for the following metals the non-carcinogenic ED50s were not directly reported, but derived from closely related substances via molecular weight correction:

- the non-carcinogenic ED50 of Tl(I) for ingestion was derived from information available for thallium(I) chloride.
- the non-carcinogenic ED50 of V(V) for ingestion was derived from information available for vanadium penta-oxide (V2O5).

Table 15: Interspecies conversion factors to humans for various species (Vermeire et al. 2001).

Type	CF interspecies (-)	Average bodyweight (kg)
human	1.0	70
pig	1.1	48
dog	1.5	15
monkey	1.9	5
cat	1.9	5
rabbit	2.4	2
mink	2.9	1
guinea pig	3.1	0.750
rat	4.1	0.250
hamster	4.9	0.125
gerbil	5.5	0.075
mouse	7.3	0.025

Ecotoxicity

The modelling of the ecotoxicity in USEtox is based on EC50-data. It specifically focuses on the median log-EC50 from a sufficiently large set of EC50-data across species (at least three species were selected as minimum). This median is the inflection point of the sigmoidal species sensitivity distribution (SSD), which is shown in Figure 16. The median log-EC50 for a substance is derived in a transparent way from compilations of ecotoxicity data, the essences of which are embedded in USEtox.

Two databases with ecotoxicity effect data on average EC50 values (i.e. HC50s) were available for creating USEtox 2.0, covering, respectively, 3,498 (van Zelm et al. 2007, van Zelm et al. 2009) and 1,408 chemicals (Payet 2004). The first database is based on acute EC50 values from the National Institute for Public Health and the Environment (RIVM) e-toxBase (http://www.ru.nl/environmentalscience/research/themes-0/risk-assessment/e-toxbase/) and the second one on chronic and acute EC50-data mainly from ECOTOX (http://www.epa.gov/ecotox) and IUCLID (http://bookshop.europa.eu/en/iuclid-cd-rom-pbLBNA19559/).

In USEtox, chronic EC50-values from Payet (2004) have been prioritized for the modelling, as long as they represent measured EC50 values. Second priority was given to acute data from Payet (2004), applying a best estimate extrapolation factor as an acute-to-chronic ratio (ACR), e.g. 1.9 for organic substances and 2.2 for pesticides. In case Payet (2004) does not provide ecotoxicity information for a chemical, acute toxicity data from the RIVM e-toxBase was used, applying an acute-to-chronic ratio (ACR) of 2 as detailed in Müller et al. (2017).

5. ENVIRONMENTAL FATE

5.1 Introduction

Within the USEtox characterization framework, this chapter deals with the determination of the fate factor which describes the distribution of chemicals between the different environmental compartments after an emission into the environment (Figure 5).

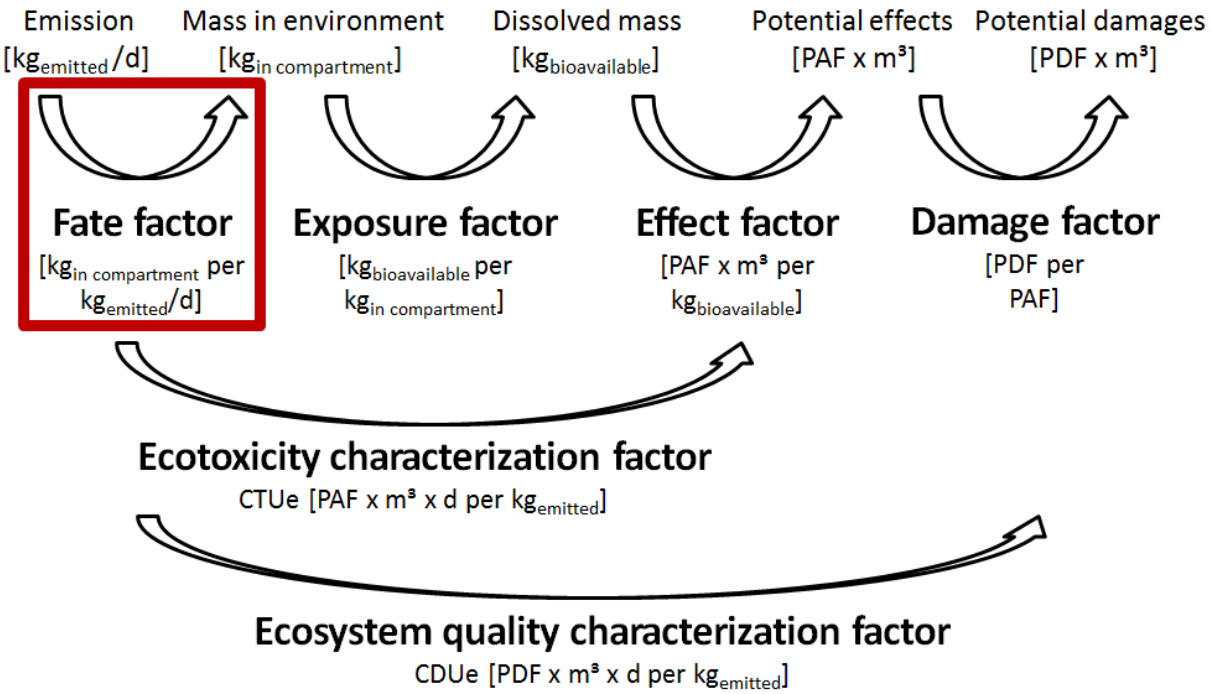

Figure 5: Symbolic description of the emission-to-damage framework for ecotoxicological impacts characterized with USEtox 2.0x.

The assessment framework of the environmental fate of a chemical consists of a continental and global scale and in addition, an urban air and indoor air phase (Figure 6). By default, USEtox uses generic landscape settings for all spatial scales. For regionalized calculations, specific values for landscape parameters can be set by users, or region specific landscape settings can be applied by selecting one of the 25 sets of landscape parameters described in Kounina et al. (2014). The compartments and their characteristics are described in Section 5.2 and the processes in the model in Sections 5.3-5.5.

In this chapter, the model calculations for all processes are described. The processes are divided into four subchapters, which describe the parameters and equations of the compartment characteristics, transformation processes, intermedia partition processes and intermedia transfer processes.

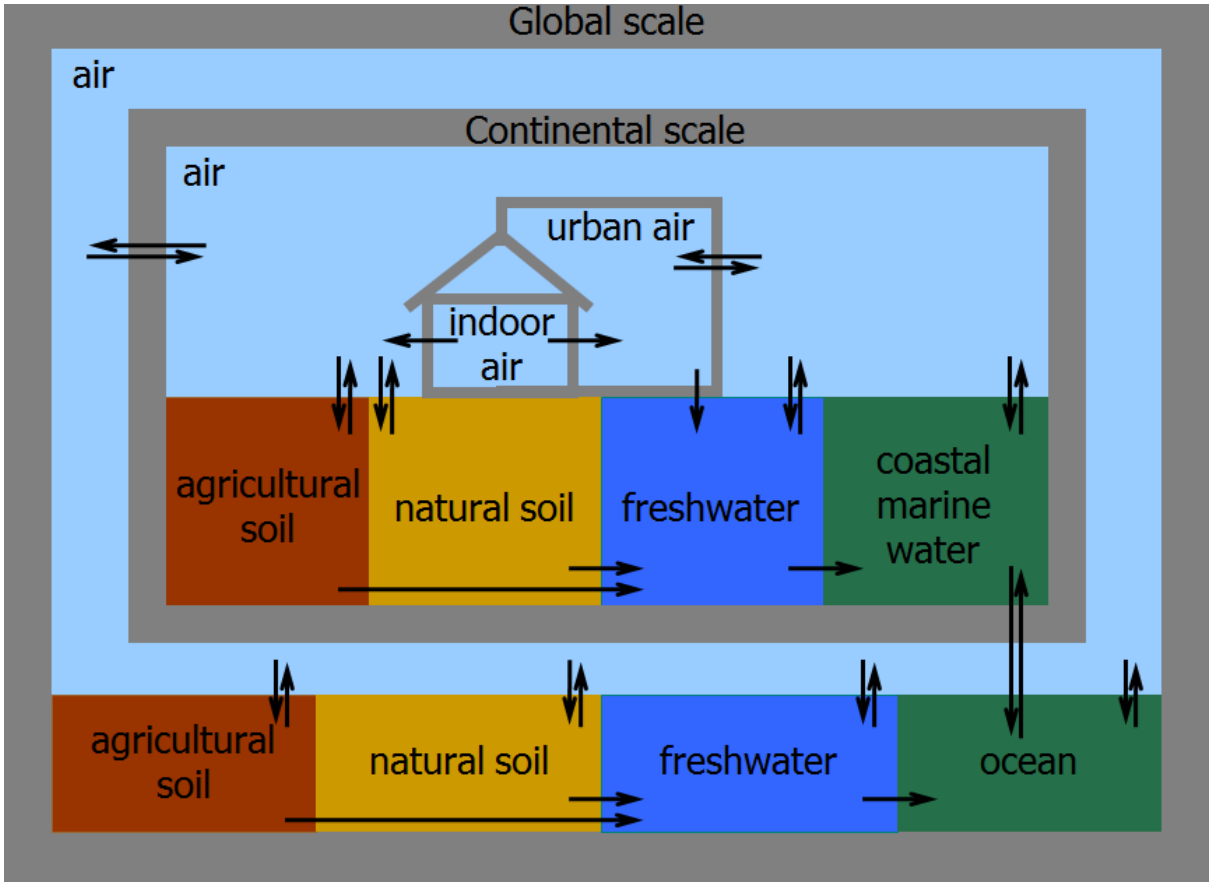

Figure 6. The scales and compartments used in the USEtox model.

5.2 Compartments

Explanations of symbols and indices are given in Appendix A and corresponding parameters in USEtox are given in Appendices B to E.

5.2.1 Air

Air is treated in USEtox as a homogeneous compartment, consisting of a gas phase, an aerosol phase and a rain water phase; the concentration in air is a total concentration. The air in the system is not stagnant; it is continuously being flushed. Wind blows air from a larger scale into the system and from the system to a larger scale. As the chemical is carried with these airstreams, this leads to "import" and "export" mass flows of the chemical to and from the system, see Figure 7. The refreshment rate is characterized by the atmospheric residence time.

The volume of the air compartment in the urban, continental and global scales may be obtained from:

$$V_{\mathrm{air[S]}} = A_{\mathrm{[S]}} \cdot h_{\mathrm{air[S]}} \qquad (7)$$

with

$V_{air[S]}$: volume of the urban, continental and global air [m^3]

$A_{[S]}$: urban, continental and global system area [m^2]

$h_{air[S]}$: mixed height of the urban, continental and global air [m]

Where the urban, continental and global system areas are described in Table 6, Table 4 and Table 5, respectively. The mixed height of the air is described in Table 10.

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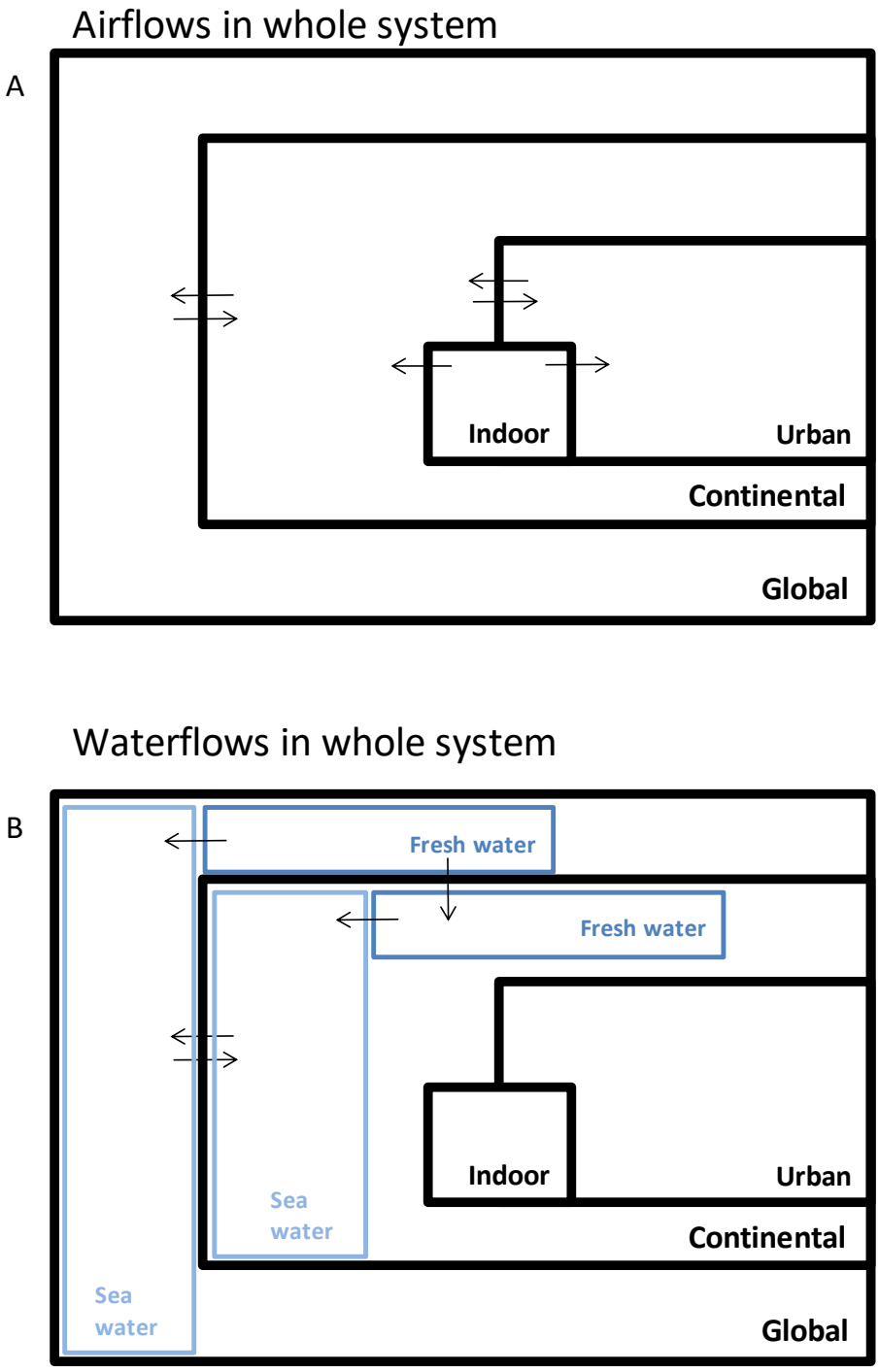

Figure 7: Air and water flows between the scales and compartments.

The mass fraction of the organic chemical present in the gas phase of the air compartment may be obtained from:

$$fr_m_{\text{gas,air[S]}} = \frac{1}{1 + \left(\frac{K_{\text{ow,app,pH7}}}{K_{\text{aw[S]}} \cdot fr_m_{\text{cldw}}}\right) \cdot fr_V_{\text{water,air[S]}}} \quad (8)$$

with

$fr_m_{\text{gas,air[S]}}$:	mass fraction of chemical in gas phase of urban, continental and global air [-]
$K_{\text{ow,app,pH7}}$:	apparent octanol/water partition coefficient at neutral pH [-]
$K_{\text{aw[S]}}$:	dimensionless urban, continental and global air/water partition coefficient of original species [-]
fr_m_{cldw}:	mass fraction original species in cloud water [-]
$fr_V_{\text{water,air[S]}}$:	volume fraction water in the air [-]

Where the $K_{\text{ow,app,pH7}}$ and the $K_{\text{aw[S]}}$ can be found in Section 5.4.2 and 5.4.1, respectively. The volume fraction water in the air is described in Table 10.

The mass fraction of original species in the cloud water may be obtained from:

When $pK_{a,loss} \leq pK_{a,gain}$:

$$fr_m_{\text{cldw}} = \frac{1}{1 + 10^{pKa_{loss} - pH_{\text{cloud}}} + 10^{pH_{\text{cloud}} - pKa_{gain}}} \quad (9)$$

When $pK_{a,loss} > pK_{a,gain}$:

$$fr_m_{\text{cldw}} = \frac{1}{1 + 10^{pKa_{gain} - pH_{\text{cloud}}} + 10^{pH_{\text{cloud}} - pKa_{loss}}} \quad (10)$$

with

fr_m_{cldw}:	mass fraction original species in cloud water [-]
pH_{cloud}:	pH cloud water [-]
pKa,loss:	equilibrium constant proton loss from conjugated acid of parent compound [-]
pKa,gain:	equilibrium constant proton loss from parent compound [-]

Where the pH of cloud water and the equilibrium constants proton loss from parent compound and from conjugated acid of the parent compound are described in Table 10.

Inorganic chemicals are non-volatile and therefore the mass fraction of chemical in gas phase is zero:

$$fr_m_{\text{gas,air[S]}} = 0 \quad (11)$$

with

$fr_m_{\text{gas,air[C]}}$: mass fraction of chemical in gas phase of urban, continental and global air [-]

5.2.1.1 Airflows

The airflows between the different scales can be found in Figure 7. The air flows from the urban scale to the continental scale, from the continental scale to the urban and global scale and back from the global to the continental scale. The airflows may be obtained from:

$$k_{air\,[U\rightarrow C]} = \frac{1}{\tau_{air[U]}} \quad (12)$$

with

$k_{\text{air[U→C]}}$: transfer rate of urban air to continental air [d^{-1}]

$\tau_{\text{air[U]}}$: residence time of air in urban air compartment [d]

$$k_{air\,[C\rightarrow U]} = \frac{\frac{V_{air[U]}}{\tau_{air[U]}}}{V_{air[C]}} \quad (13)$$

with

$k_{\text{air[C→U]}}$: transfer rate of continental air to urban air [d^{-1}]

$V_{\text{air[U]}}$: volume of the urban air [m^3]

$\tau_{\text{air[U]}}$: residence time of air in urban air compartment [d]

$V_{\text{air[C]}}$: volume of the continental air [m^3]

Where the volume of air is described in Equation (7) and the residence time in air in Equation (16).

$$k_{\text{air [C→G]}} = \frac{1}{\tau_{\text{air[C]}}} - k_{air[C\rightarrow U]} \quad (14)$$

with

$k_{air[C\rightarrow G]}$: transfer rate of continental air to global air [d^{-1}]

$\tau_{air[C]}$: residence time of air in continental air compartment [d]

$k_{air[C\rightarrow U]}$: transfer rate of continental air to urban air [d^{-1}]

Where the residence time in air is described in Equation (16) and the transfer rate of continental air to urban air in Equation (15).

$$k_{air\ [G\rightarrow C]} = \frac{\frac{V_{air[C]}}{\tau_{air[C]}} - \frac{V_{air[U]}}{\tau_{air[U]}}}{V_{air[G]}} \quad (15)$$

with

$k_{air[G\rightarrow C]}$: transfer rate of global air to continental air [d^{-1}]

$V_{air[C]}$: volume of the continental air [m^3]

$\tau_{air[C]}$: residence time of air in continental air compartment [d]

$V_{air[U]}$: volume of the urban air [m^3]

$\tau_{air[U]}$: residence time of air in urban air compartment [d]

$V_{air[G]}$: volume of the global air [m^3]

Where the volume of air is described in Equation (7) and the residence time in air in Equation (16).

In order to calculate the air flows, the residence times of air in the various air compartments should be known. To estimate such residence times, it is assumed that wind blows at a constant speed of 3 m/s through well-mixed cylindrical boxes.

For indoor:

The indoor air module consists of two indoor compartments which can be parameterized independently in order to (for example) represent household and occupational settings respectively. In both cases, the indoor air compartment is linked to outdoor air via the ventilation flow (which depends on the air-tightness of the building (windows, doors, sealing, wall-cracks, etc.) and the presence and use of active air ventilation systems). Based on the average distribution of the global population between urban and rural areas of about 50% respectively (UN United Nations 2012), half of the ventilation flow is directed to urban and continental rural air respectively for the household setting. For the occupational setting an assumption of 80% being ventilated into urban and 20% into rural continental air is used in the absence of representative global average data and the rationale that the predominant occupation in rural areas is related to agriculture mostly exercised outdoors.

For urban and continental scales:

$$\tau_{\text{air}[S]} = \left(\frac{cf_{\tau,\text{air}[S]} \cdot \frac{\sqrt{(A_{[S]})}}{u_{[S]}}}{(3600 \cdot 24)} \right) \quad (16)$$

with

$\tau_{\text{air}[S]}$:	residence times of air in urban and continental air compartments [d]
$cf_{\tau\text{air}[S]}$:	correction factor of urban and continental air residence time [-]
$A_{[S]}$:	urban and continental system area [m^2]
$u_{[S]}$:	urban and continental wind speed [$m \cdot s^{-1}$]
3600·24:	conversion factor [$s \cdot d^{-1}$]

Where the urban and continental system areas are described in Table 6 and Table 4, respectively. The correction factor of urban and continental air residence time is described in Table 10 as is the wind speed at the urban scale, which is assumed to be equal to the wind speed at the continental scale.

5.2.2 Water

At the urban scale no water compartments are present, while at the continental and global scale two water compartments are present; a fresh water and a sea water compartment. In USEtox the water compartments are treated as homogeneous boxes, consisting of a suspended matter phase, a dissolved (colloidal) organic carbon (DOC) phase and a biota phase. The presence of suspended matter, DOC and biota influences the fate of chemicals in a very similar way to that of aerosols and rain water in the atmosphere. These phases bind the chemical, thus inhibiting it from taking part in mass transfer and degradation processes that occur in the water phase. Suspended matter acts as a physical carrier of the chemical across the sediment-water interface. The DOC only causes the chemical to be inhibited from taking part in mass transfer and degradation processes. Concentration ratios among suspended matter, DOC, biota and water are often close to equilibrium. For multimedia fate modeling, the water compartment is treated the same way as the air, sediment and soil compartments: that is at all times equilibrium is assumed among water, suspended matter, DOC and biota. The water compartments at the continental and global scales are continuously flushed with water (and biota, suspended matter and DOC) from outside that scale.

The volume of the fresh and sea water compartments may be obtained from:

$$V_{\text{w}[S]} = A_{[S]} \cdot fr_A_{\text{w}[S]} \cdot h_{\text{w}[S]} \quad (17)$$

with

$V_{w[S]}$: volume of continental and global fresh and sea water [m^3]

$A_{[S]}$: continental and global system area [m^2]

$fr_A_{w[S]}$: area fraction continental and global fresh and sea water [-]

$h_{w[S]}$: mixed depth of continental and global fresh and sea water [m]

Where the continental and global system area are described in Table 4 and Table 5, respectively. The mixed depths of the waters are described in Table 10.

The area fraction freshwater may be obtained from:

$$fr_A_{fw[S]} = \frac{A_{land[S]} \cdot fr_A_{land,fw[S]}}{A_{[S]}} \quad (18)$$

with

$fr_A_{fw[S]}$: area fraction continental and global fresh water [-]

$A_{land[S]}$: continental and global area land [m^2]

$fr_A_{land,fw[S]}$: fraction continental and global fresh water [-]

$A_{[S]}$: continental and global system area [m^2]

Where the continental and global area land and system areas are described in Table 4 and Table 5, respectively.

The area fraction sea water may be obtained from:

$$fr_A_{sw[S]} = 1 - fr_A_{fw[S]} - fr_A_{nsl[S]} - fr_A_{asl[S]} \quad (19)$$

with

$fr_A_{sw[S]}$: area fraction continental and global sea water [-]

$fr_A_{fw[S]}$: area fraction continental and global fresh water [-]

$fr_A_{nsl[S]}$: area fraction continental and global natural soil [-]

$fr_A_{asl[S]}$: area fraction continental and global agricultural soil [-]

Where the area fraction continental and global fresh water is described in Equation (18) and the area fractions of natural and agricultural soil are described in Section 5.2.4.

The mass fraction of the chemical that is truly dissolved in the water compartments depends on the fraction of chemical in the dissolved phase, in the dissolved organic matter phase and in the biota phase. This may be obtained from:

$$fr_m_{\mathrm{diss,w[S]}} = \frac{1}{1 + K_{\mathrm{susp|w,w[S]}} \cdot \frac{C_{\mathrm{susp,w[S]}}}{1000} + K_{\mathrm{DOC|w,w[S]}} \cdot \frac{C_{\mathrm{DOC,w[S]}}}{1000} + BCF_{\mathrm{fish,w[S]}} \cdot \frac{C_{\mathrm{biota,w[S]}}}{1000}} \quad (20)$$

with

$fr_m_{\mathrm{diss,w[S]}}$: fraction of chemical dissolved in continental and global fresh and sea water [-]

$K_{\mathrm{susp\,|\,w,w\,[S]}}$: suspended solids/water partition coefficient in continental and global fresh and sea water [L·kg^{-1}]

$C_{\mathrm{susp,w[S]}}$: concentration suspended matter in continental and global fresh and sea water [kg·m^3]

$K_{\mathrm{DOC\,|\,w,w\,[S]}}$: dissolved (colloidal) organic carbon/water partition coefficient in continental and global fresh and sea water [L·kg^{-1}]

$C_{\mathrm{DOC,w[S]}}$: concentration of dissolved (colloidal) organic carbon in continental and global fresh and sea water [kg·m^3]

$BAF_{\mathrm{fish,w\,[S]}}$: bioaccumulation factor continental and global fresh and sea water fish [L·kg^{-1}]

$C_{\mathrm{biota,w\,[S]}}$: concentration biota in continental and global fresh and sea water [kg·m^3]

Where the default values of the concentration suspended matter, the concentration DOC, and the concentration biota are described in Table 10. The $K_{\mathrm{susp\,|\,w,w[S]}}$ and the $K_{\mathrm{DOC\,|\,w,w[S]}}$, and the bioconcentration factor can be found in Section 5.4.3, 5.4.7, 5.4.6, respectively.

The mass fraction of original species in the water may be obtained from:

When $\mathrm{pK_{a,loss}} \leq \mathrm{pK_{a,gain}}$:

$$fr_m_{\mathrm{w}} = \frac{1}{1 + 10^{pKa_{loss} - pH_{\mathrm{w}}} + 10^{pH_{\mathrm{w}} - pKa_{gain}}} \quad (21)$$

When $\mathrm{pK_{a,loss}} > \mathrm{pK_{a,gain}}$:

$$fr_m_{\mathrm{w}} = \frac{1}{1 + 10^{pKa_{gain} - pH_{\mathrm{w}}} + 10^{pH_{\mathrm{w}} - pKa_{loss}}} \quad (22)$$

with

fr_m_{w}: fraction original species in fresh and sea water [-]

pH_{w}: pH fresh and sea water [-]

pKa,loss: equilibrium constant proton loss from conjugated acid of parent compound [-]

pKa,gain: equilibrium constant proton loss from parent compound [-]

Where the pH of fresh, sea and the equilibrium constants proton loss from parent compound and from conjugated acid of the parent compound are described in Table 10.

5.2.2.1 Waterflows

The water flows from the freshwaters to the sea waters at the continental and global scale. The sea water from the continental scale flows to the sea water at the global scale and vice versa.

For continental and global freshwater to continental and global sea water:

$$k_{\mathrm{fw\rightarrow sw[S]}} = \frac{Q_{\mathrm{des,fw\rightarrow sw[S]}}}{V_{\mathrm{fw[S]}}} \cdot (3600 \cdot 24) \tag{23}$$

with

$k_{\mathrm{fw\rightarrow sw[S]}}$: transfer rate from continental and global freshwater to continental and global sea water [d^{-1}]

$Q_{\mathrm{des,fw\rightarrow sw[S]}}$: flow of continental and global fresh water to continental and global sea water [$m^3 \cdot s^{-1}$]

$V_{\mathrm{fw[S]}}$: volume of continental and global fresh water [m^3]

3600·24: conversion factor [$s \cdot d^{-1}$]

Where the volume of continental and global fresh water is described in Equation (17).

The flow of continental fresh water to continental sea water may be obtained from:

$$Q_{\mathrm{des,fw\rightarrow sw[C]}} = \left(Q_{\mathrm{rain,air\rightarrow fw[C]}} + Q_{\mathrm{runoff,water,nsl[C]}} + Q_{\mathrm{runoff,water,asl[C]}}\right) \cdot \left(1 - fr_M_{\mathrm{disc,fw[C\rightarrow G]}}\right) \tag{24}$$

with

$Q_{\mathrm{des,fw\rightarrow sw[C]}}$: flow of continental fresh water to continental sea water [$m^3 \cdot s^{-1}$]

$Q_{\mathrm{rain,air\rightarrow fw[C]}}$: rain input into continental fresh water [$m^3 \cdot s^{-1}$]

$Q_{\mathrm{runoff,water,nslC]}}$: water runoff from continental natural soil [$m^3 \cdot s^{-1}$]

$Q_{\mathrm{runoff,water,asl[C]}}$: water runoff from continental agricultural soil [$m^3 \cdot s^{-1}$]

$fr_M_{\mathrm{disc,fw[C\rightarrow G]}}$: fraction discharge continental fresh water to global scale [-]

Where the water runoff from natural and agricultural soil in Equation (26), the flow of global fresh water to the continental fresh water is zero and the fraction discharge from the continental fresh water to the global freshwater are described in Table 10.

The rain input into fresh water may be obtained from:

$$Q_{\text{rain,air}\rightarrow\text{w[S]}} = \upsilon_{\text{rain[S]}} \cdot fr_A_{\text{w[S]}} \cdot A_{\text{[S]}} \quad (25)$$

with

$Q_{\text{rain,air}\rightarrow\text{w[S]}}$:	rain input into continental and global fresh and sea water [$m^3 \cdot s^{-1}$]
$\upsilon_{\text{rain[S]}}$:	annual average precipitation on the continental and global scale [$m \cdot s^{-1}$]
$fr_A_{\text{w[S]}}$:	area fraction continental and global fresh and sea water [-]
$A_{\text{[S]}}$:	continental and global system area [m^2]

Where the area fraction water, volume fraction runoff from soil, the annual average precipitation and the system areas are described in Table 10 (urban), Table 4 (continental) and Table 5 (global).

The water runoff from continental and global natural and agricultural soil may be obtained from:

$$Q_{\text{runoff,water,sl[S]}} = fr_A_{\text{sl[S]}} \cdot fr_V_{\text{rain,runoff,sl[S]}} \cdot \upsilon_{\text{rain[S]}} \cdot A_{\text{[S]}} \quad (26)$$

with

$Q_{\text{runoff,water,sl[S]}}$:	water runoff from continental and global natural and agricultural soil [$m^3 \cdot s^{-1}$]
$fr_A_{\text{sl[S]}}$:	area fraction continental and global natural and agricultural water [-]
$fr_V_{\text{rain,runoff,sl[S]}}$:	volume fraction runoff continental and global natural and agricultural soil [-]
$\upsilon_{\text{rain[S]}}$:	annual average precipitation on continental and global scale [$m \cdot s^{-1}$]
$A_{\text{[S]}}$:	continental and global system area [m^2]

Where the area fraction water, volume fraction runoff from soil, the annual average precipitation and the system areas are described in Table 10 (urban), Table 4 (continental) and Table 5 (global).

For continental sea water to global sea water:

$$k_{\text{adv,sw[C}\rightarrow\text{G]}} = \frac{Q_{\text{adv,sw[C}\rightarrow\text{G]}}}{V_{\text{sw[C]}}} \cdot (3600 \cdot 24) \quad (27)$$

with

$k_{adv,sw[C→G]}$: transfer rate of continental sea water to global sea water [d^{-1}]
$Q_{adv,sw[C→G]}$: flow of continental sea water to the global sea water [$m^3 \cdot s^{-1}$]
$V_{sw[C]}$: volume of continental sea water [m^3]
3600·24: conversion factor [$s \cdot d^{-1}$]

Where the volume of continental fresh water is described in Equation (17).

The flow of continental sea water to the global sea water may be obtained from:

$$Q_{adv,sw[C→G]} = Q_{rain,air→sw[C]} + Q_{des,fw→sw[C]} + Q_{adv,sw[G→C]} \quad (28)$$

with

$Q_{adv,sw[C→G]}$: flow of continental sea water to the global ocean [$m^3 \cdot s^{-1}$]
$Q_{rain,air→sw[C]}$: rain input into continental sea water [$m^3 \cdot s^{-1}$]
$Q_{des,fw→sw[C]}$: flow of continental fresh water to continental sea water [$m^3 \cdot s^{-1}$]
$Q_{adv,sw[G→C]}$: flow of global sea water to continental scale [$m^3 \cdot s^{-1}$]

Where the rain input into water is described in Equation (25), the flow of continental fresh water to continental sea water in Equation (23) and the flow of global sea water to the continental scale is described in Equation (30).

The flow of global fresh water to global sea water may be obtained from:

$$Q_{des,fw→sw[G]} = \left(Q_{rain,air→fw[G]} + Q_{runoff,water,nsl[G]} + Q_{runoff,water,asl[G]}\right) \cdot \left(1 - fr_M_{disc,fw[G→C]}\right) \quad (29)$$

with

$Q_{des,fw→sw[G]}$: flow of global fresh water to global sea water [$m^3 \cdot s^{-1}$]
$Q_{rain,air→fw[G]}$: rain input into global fresh water [$m^3 \cdot s^{-1}$]
$Q_{runoff,water,nslG]}$: water runoff from global natural soil [$m^3 \cdot s^{-1}$]
$Q_{runoff,water,asl[G]}$: water runoff from global agricultural soil [$m^3 \cdot s^{-1}$]
$fr_M_{disc,fw[G→C]}$: fraction discharge global fresh water to continental scale [-]

Where the rain input into global fresh water is described in Equation (25); the water runoff from natural and agricultural soil is described in Equation (26) and the fraction discharge from the global fresh water to the continental freshwater is described in Table 5.

For global sea water to continental sea water:

$$k_{adv,sw[G\rightarrow C]} = \frac{Q_{adv,sw[G\rightarrow C]}}{V_{sw[G]}} \cdot (3600 \cdot 24) \quad (30)$$

with

$k_{adv,sw[G\rightarrow C]}$:	transfer rate from global sea water to continental sea water [d^{-1}]
$Q_{adv,sw[G\rightarrow C]}$:	flow of global sea water to continental sea water [$m^3 \cdot s^{-1}$]
$V_{sw[G]}$:	volume of global sea water [m^3]
3600·24:	conversion factor [$s \cdot d^{-1}$]

Where the volume of global sea water is described in Equation (17).

The flow of global sea water to the continental sea water may be obtained from:

$$Q_{adv,sw[G\rightarrow C]} = \left(\frac{V_{sw[C]}}{\tau_{sw[C]}}\right) - Q_{des,fw\rightarrow sw[C]} \quad (31)$$

with

$Q_{adv,sw[G\rightarrow C]}$:	flow of global sea water to continental scale [$m^3 \cdot s^{-1}$]
$V_{sw[C]}$:	volume continental sea water [m^3]
$\tau_{sw[C]}$:	residence time of continental sea water [s]
$Q_{des,fw\rightarrow sw[C]}$:	flow of continental fresh water to continental sea water [$m^3 \cdot s^{-1}$]

Where the volume of global sea water is described in Equation (17), the residence time of continental sea water is described in Table 10 and the flow of continental fresh water to continental sea water is described in Equation (23).

5.2.2.2 Suspended matter

In this context, "suspended matter" refers to all abiotic colloidal (except for DOC) or macromolecular materials (debris of organisms, "humic" material, "third phase", etc.) that is not truly dissolved. Suspended matter is treated as the dissolved fraction of the water compartment. The suspended matter in the continental fresh water can be “imported" to the continental coastal sea water. The suspended matter in the global fresh water can be “imported" to the global sea water. The suspended matter in the continental coastal sea water can be “imported” and “exported” to and from the global sea water. This transport is characterized by the flow of water and the concentrations of suspended matter in the incoming and outgoing water. Finally, there is continuous exchange of particles across the sediment-water interface by sedimentation and resuspension. The balance of these suspended matter mass flows determines the magnitude and the direction of the particle exchange

between sediment and water, and thus the mass flow of the chemical that is associated with the particles.

The settling velocity of the suspended particles in the water is by default 2.5 m·d^{-1} (Den Hollander & Van de Meent, 2004) and is conversed to s·d^{-1}:

$$\upsilon_{\text{sed,susp,w[S]}} = \frac{2.5}{(3600 \cdot 24)} \tag{32}$$

with

$\upsilon_{\text{sed,susp,w[S]}}$:	settling velocity suspended particles of the continental and global fresh and sea water [m·s^{-1}]
2.5:	settling velocity suspended particles of the continental and global fresh and sea water [m·d^{-1}]
3600·24:	conversion factor [s·d^{-1}]

The net sediment accumulation rate for the continental and global fresh water compartments may be obtained from:

$$\upsilon_{\text{sed,acc,fw[S]}} = \frac{\begin{pmatrix} \upsilon_{\text{nsl[S]}} \cdot fr_{A_{\text{nsl[S]}}} \cdot fr_{V_{\text{solid,nsl[S]}}} \\ +\upsilon_{\text{asl[S]}} \cdot fr_{A_{\text{asl[S]}}} \cdot fr_{V_{\text{solid,asl[S]}}} \end{pmatrix} \cdot A_{\text{[S]}} \cdot \rho_{\text{sd,sl}} + J_{\text{susp,fw[S]}} - C_{\text{susp,fw[S]}} \cdot \left(Q_{\text{des,fw}\rightarrow\text{sw[S]}}\right)}{fr_V_{\text{solid,sd[S]}} \cdot \rho_{\text{sd,sl}}} \Big/ A_{\text{[S]}} \cdot fr_A_{\text{fw[S]}} \tag{33}$$

with

$\upsilon_{\text{sed,acc,fw[S]}}$:	net sediment accumulation rate in continental and global fresh water [m·s^{-1}]
$\upsilon_{\text{nsl[S]}}$:	erosion of continental and global natural soil [m·s^{-1}]
$C_{\text{susp,fw[S]}}$:	concentration suspended matter in continental and global fresh water [kg·m^3]
$fr_A_{\text{nsl[S]}}$:	area fraction continental and global natural soil [-]
$fr_V_{\text{solid,nsl[S]}}$:	volume fraction solids in continental and global natural soil [-]
$\upsilon_{\text{asl[S]}}$:	erosion of continental and global agricultural soil [m·s^{-1}]
$fr_A_{\text{asl[S]}}$:	area fraction continental and global agricultural soil [-]
$fr_V_{\text{solid,asl[S]}}$:	volume fraction solids in continental and global agricultural soil [-]
$A_{\text{[S]}}$:	continental and global system area [m^2]
$\rho_{\text{sd,sl}}$:	mineral density of sediment and soil [kg·m^{-3}]
$J_{\text{susp,fw[S]}}$:	autochtonous production of suspended matter in continental and global fresh water [kg·s^{-1}]

$C_{susp,fw[S]}$: concentration suspended matter in continental and global fresh water [kg·m^3]

$Q_{des,fw→sw[S]}$: flow of continental and global fresh water to continental and global sea water [m^3·s^{-1}]

$fr_V_{solid,sd[S]}$: volume fraction solids in continental and global sediment [-]

$fr_A_{fw[S]}$: area fraction continental and global fresh water [-]

Where the default values of the concentration suspended matter in fresh water, the mineral density and the autochtonous production of suspended matter in continental and global fresh water are described in Table 10. The erosion rate of soil and the continental and global system area are described in Table 4. The volume fraction solids in sediment, the area fractions soil and the volume fraction solids in natural and agricultural soil are described in Sections 5.2.3 and 5.2.4. The area fraction fresh water is described in Equation (18).

The net sediment accumulation rate for the continental sea water compartments may be obtained from:

$$v_{sed,acc,sw[C]} = \frac{\frac{C_{susp,fw[C]} \cdot Q_{des,fw→sw[C]} + C_{susp,sw[G]} \cdot Q_{adv,sw[G→C]} + J_{susp,sw[C]} - C_{susp,sw[C]} \cdot Q_{adv,sw[C→G]}}{fr_V_{solid,sd[C]} \cdot \rho_{sd,sl}}}{A_{[C]} \cdot fr_A_{sw[C]}} \quad (34)$$

with

$v_{sed,acc,sw[C]}$: net sediment accumulation rate in continental sea water [m·s^{-1}]

$C_{susp,fw[C]}$: concentration suspended matter in continental fresh water [kg·m^3]

$Q_{des,fw→sw[C]}$: flow of continental fresh water to continental sea water [m^3·s^{-1}]

$C_{susp,sw[G]}$: concentration suspended matter in global sea water [kg·m^3]

$Q_{adv,sw[G→C]}$: flow of global sea water to continental scale [m^3·s^{-1}]

$J_{susp,sw[C]}$: autochtonous production of suspended matter in continental sea water [kg·s^{-1}]

$C_{susp,sw[C]}$: concentration suspended matter in continental sea water [kg·m^3]

$Q_{adv,sw[C→G]}$: flow of continental sea water to the global ocean [m^3·s^{-1}]

$fr_V_{solid,sd[C]}$: volume fraction solids in continental sediment [-]

$\rho_{sd,sl}$: mineral density of sediment and soil [kg·m^{-3}]

$A_{[C]}$: continental system area [m^2]

$fr_A_{sw[C]}$: area fraction continental sea water [-]

Where the default values of the concentration suspended matter in fresh water, the mineral density and the autochtonous production of suspended matter in continental fresh water are described in Table 10. The continental system area is described in Table 5. The volume

fraction solids in sediment is described in Section 5.2.3. The area fraction sea water is described in Equation (19).

The net sediment accumulation rate for the global sea water compartments may be obtained from:

$$\upsilon_{\text{sed,acc,sw[G]}} = \frac{C_{\text{susp,fw[G]}} \cdot Q_{\text{des,fw}\rightarrow\text{sw[G]}} + C_{\text{susp,sw[C]}} \cdot Q_{\text{adv,sw[C}\rightarrow\text{G]}} + J_{\text{susp,sw[G]}} - C_{\text{susp,sw[G]}} \cdot \left(Q_{\text{adv,sw[G}\rightarrow\text{C]}}\right)}{fr_V_{\text{solid,sd[G]}} \cdot \rho_{\text{sd,sl}}} \Big/ A_{\text{[G]}} \cdot fr_A_{\text{sw[G]}} \quad (35)$$

with

$\upsilon_{\text{sed,acc,sw[G]}}$: net sediment accumulation rate in global sea water [m·s^{-1}]

$C_{\text{susp,fw[G]}}$: concentration suspended matter in global fresh water [kg·m^3]

$Q_{\text{des,fw}\rightarrow\text{sw[G]}}$: flow of global fresh water to global sea water [m^3·s^{-1}]

$C_{\text{susp,sw[C]}}$: concentration suspended matter in continental sea water [kg·m^3]

$Q_{\text{adv,sw[C}\rightarrow\text{G]}}$: flow of continental sea water to the global ocean [m^3·s^{-1}]

$J_{\text{susp,sw[G]}}$: autochtonous production of suspended matter in global sea water [kg·s^{-1}]

$C_{\text{susp,sw[G]}}$: concentration suspended matter in global sea water [kg·m^3]

$Q_{\text{adv,sw[G}\rightarrow\text{C]}}$: flow of global sea water to continental scale [m^3·s^{-1}]

$fr_V_{\text{solid,sd[G]}}$: volume fraction solids in global sediment [-]

$\rho_{\text{sd,sl}}$: mineral density of sediment and soil [kg·m^{-3}]

$A_{\text{[G]}}$: global system area [m^2]

$fr_A_{\text{sw[G]}}$: area fraction global sea water [-]

Where the default values of the concentration suspended matter in fresh water, the mineral density and the autochtonous production of suspended matter in continental fresh water are described in Table 10. The global system area is described in Table 5. The volume fraction solids in sediment is described in Section 5.2.3. The area fraction sea water is described in Equation (19).

The gross sediment rate from the water compartment to the sediment compartment may be obtained from:

$$\text{If } \upsilon_{\text{sed,susp,w[S]}} \cdot \frac{C_{\text{susp,w[S]}}}{\rho_{\text{sd}}} > \upsilon_{\text{sed,acc,w[S]}} \text{, then:}$$
$$\upsilon_{\text{sed,w[S]}} = \upsilon_{\text{sed,susp,w[S]}} \cdot \frac{C_{\text{susp,w[S]}}}{\rho_{\text{sd}}} \text{, else:} \quad (36)$$

$$\upsilon_{\text{sed,w[S]}} = \upsilon_{\text{sed,acc,w[S]}}$$

with

$\upsilon_{\text{sed,susp,w[S]}}$: settling velocity suspended particles of the continental and global fresh and sea water [m·s^{-1}]

$C_{\text{susp,w[S]}}$: concentration suspended matter in continental and global fresh and sea water [kg·m^{3}]

ρ_{sd}: bulk density of continental and global sediment [kg·m^{-3}]

$\upsilon_{\text{sed,acc,w[S]}}$: net sediment accumulation rate in continental and global fresh and sea water [m·s^{-1}]

$\upsilon_{\text{sed,w[S]}}$: gross sedimentation rate from continental and global fresh and sea water [m·s^{-1}]

Where settling velocity of suspended particles is described in Equation (32) and the net sediment accumulation rate in Equations (33) until (35) The concentration suspended matter in water is described in Table 10 and the bulk density of sediment is described in Section 5.2.3.

5.2.3 Sediment

USEtox does not explicitly calculate concentrations in sediments. It does account for transport of substance between water and sediment via direct adsorption/desorption and by sedimentation/resuspension of suspended particulate matter, according to Margni et al. (2004). The sediment phase is treated as a homogeneous phase, consisting of a water sub-phase and a solid sub-phase. Equilibrium is assumed between the pore water and solid sub-phases of the sediment phase. The top layer of the sediment is considered to be well-mixed. If the sedimentation of particles from the water column is greater than the resuspension (net sedimentation), this top layer is continuously being refreshed. The older sediment layer, and the chemicals that are associated with the sediment with it, gets buried under the freshly deposited material. The fraction of the system area that is continental natural or agricultural soil may be obtained from:

$$V_{\text{wsd[S]}} = A_{\text{[S]}} \cdot fr_A_{\text{w[S]}} \cdot h_{\text{wsd[S]}} \qquad (37)$$

with

$V_{\text{wsd[S]}}$: volume of continental and global fresh and sea water sediment [m^{3}]

$A_{\text{[S]}}$: continental and global system area [m^{2}]

$fr_A_{\text{w[S]}}$: area fraction continental and global fresh and sea water [-]

$h_{\text{wsd[S]}}$: mixed depth continental and global fresh and sea water sediment [m]

Where the system areas and the area fractions water are described in Table 4 (continental) and Table 5 (global). The default mixed depths of the waters are described in Table 10.

The mass fraction of original species in the sediment may be obtained from:

When $pK_{a,loss} \leq pK_{a,gain}$:

$$fr_m_{\mathrm{wsd}} = \frac{1}{1 + 10^{pKa_{loss} - pH_{\mathrm{w}}} + 10^{pH_{\mathrm{w}} - pKa_{gain}}} \quad (38)$$

When $pK_{a,loss} > pK_{a,gain}$:

$$fr_m_{\mathrm{wsd}} = \frac{1}{1 + 10^{pKa_{gain} - pH_{\mathrm{w}}} + 10^{pH_{\mathrm{w}} - pKa_{loss}}} \quad (39)$$

with

fr_m_{wsd}:	fraction original species in fresh and sea water sediment [-]
pH_{w}:	pH fresh and sea water [-]
pKa,loss:	equilibrium constant proton loss from conjugated acid of parent compound [-]
pKa,gain:	equilibrium constant proton loss from parent compound [-]

Where the pH of fresh, sea and the equilibrium constants proton loss from parent compound and from conjugated acid of the parent compound are described in Table 10.

The volume fraction solids in the sediments may be obtained from:

$$fr_V_{\mathrm{solid,sd[S]}} = 1 - fr_V_{water,sd[S]} \quad (40)$$

with

$fr_V_{\mathrm{solid,sd[S]}}$:	volume fraction solids in continental and global sediment [-]
$fr_V_{\mathrm{water,sd[S]}}$:	volume fraction water in continental and global sediment [-]

Where the default volume fraction water in sediment is described in Table 10.

The bulk density of sediment may be obtained from:

$$\rho_{\mathrm{sd}} = fr_V_{\mathrm{water,sd[S]}} \cdot \rho_{\mathrm{w}} + fr_V_{\mathrm{solids,sd[S]}} \cdot \rho_{\mathrm{sd,sl}} \quad (41)$$

with

ρ_{sd}: bulk density of sediment [kg·m^{-3}]

$fr_V_{water,sd[S]}$: volume fraction water in continental and global sediment [-]

ρ_{w}: density of water [kg·m^{-3}]

$fr_V_{solid,sd[S]}$: volume fraction solids in continental and global sediment [-]

$\rho_{sd,sl}$: mineral density of sediment and soil [kg·m^{-3}]

Where the default values of the volume fraction water in sediment, the density of water and the mineral density are described in Table 10. The volume fraction solid in sediment is described in Equation (47).

The burial rate in continental and global fresh and sea water sediment may be obtained from:

$$\upsilon_{burial,wsd[S]} = \upsilon_{sed,acc,w[S]} \quad (42)$$

with

$\upsilon_{burial,wsd[S]}$: burial rate in continental and global fresh and sea water sediment [m·s^{-1}]

$\upsilon_{sed,acc,w[S]}$: net sediment accumulation rate in continental and global fresh and sea water [m·s^{-1}]

Where the net sediment accumulation rates in water are described in Equations (33) until (35).

5.2.4 Soil

Soil is the most stationary and, as a result, the most spatially inhomogeneous of all environmental compartments. There are many different soil types and differences in soil use. Unfortunately, the fate of chemicals is determined largely by just the characteristics that vary so much (porosity, water content, organic matter content). Also, soil use happens to be the key factor determining whether it may be loaded directly with a chemical. One soil compartment may not be sufficient to reflect the role of "soil" in the multimedia fate of chemicals. USEtox, therefore, comes with two separate soil compartments at the continental and global scale. The first soil compartment may be thought of as "natural soil". The second soil compartment may be thought of as "agricultural soil". At the urban scale area fraction of paved and non-paved surface are considered instead of soil compartment.

Chemical flow from the soil to the air is dependent of the penetration depth of the chemical into the soil. Soil is treated as a homogeneous compartment, consisting of a gas phase, a water phase and a solid phase; the concentration in soil is a total concentration. The different soil phases are assumed to be in equilibrium at all times.

The volumes of the soil compartments may be obtained from:

$$V_{sl[S]} = A_{[S]} \cdot fr_A_{sl[S]} \cdot h_{sl[S]} \quad (43)$$

with

$V_{sl[S]}$: volume of continental and global natural and agricultural soil [m^3]
$A_{[S]}$: continental and global system area [m^2]
$fr_A_{sl[S]}$: area fraction continental and global natural and agricultural soil [-]
$h_{sl[S]}$: depth continental and global natural and agricultural soil [m]

Where the system areas and the area fractions water are described in Table 4 (continental) and Table 5 (global). The default mixed depths of the soils are described in Table 10.

The fraction of the system area that is continental natural or agricultural soil may be obtained from:

$$fr_A_{sl[C]} = \frac{A_{land[C]} \cdot fr_A_{land,sl[C]}}{A_{[C]}} \quad (44)$$

with

$fr_A_{sl[C]}$: area fraction of continental natural and agricultural soil [-]
$A_{land[C]}$: continental area land [m^2]
$fr_A_{land,sl[C]}$: fraction continental natural and agricultural soil [-]
$A_{[C]}$: continental system area [m^2]

Where the area land, the fraction soil and the system areas are described in Table 4.

The fraction of the system area that is global natural or agricultural soil may be obtained from:

$$fr_A_{sl[G]} = \frac{\left(A_{land[G]} - A_{land[C]}\right) \cdot fr_A_{land,sl[G]}}{A_{[G]}} \quad (45)$$

with

$fr_A_{sl[G]}$: area fraction of global natural and agricultural soil [-]
$A_{land[G]}$: global area land [m^2]
$A_{land[C]}$: continental area land [m^2]
$fr_A_{land,sl[G]}$: fraction global natural and agricultural soil [-]
$A_{[G]}$: global system area [m^2]

Where the area land, the fraction soil and the system areas are described in Table 5.

The mass fraction of the chemical in solid phase of the natural and agricultural soil may be obtained from:

$$fr_m_{\text{solid,sl[S]}} = \frac{fr_V_{\text{solid,sl[S]}}}{fr_V_{\text{gas,sl[S]}} \cdot \frac{K_{\text{aw[S]}}}{K_{\text{solid,sl|w,sl[S]}} \cdot \frac{\rho_{\text{sd,sl}}}{1000}} + \frac{fr_V_{\text{water,sl[S]}}}{K_{\text{solid,sl|w,sl[S]}} \cdot \frac{\rho_{\text{sd,sl}}}{1000}} + fr_V_{\text{solid,sl[S]}}} \quad (46)$$

with

$fr_m_{\text{solid,sl[S]}}$: fraction of chemical in solid phase in continental and global natural and agricultural soil [-]

$fr_V_{\text{solid,sl[S]}}$: volume fraction solids in continental and global natural and agricultural soil [-]

$fr_V_{\text{gas,sl[S]}}$: volume fraction gas in continental and global natural and agricultural soil [-]

$K_{\text{aw[S]}}$: continental and global dimensionless air/water partition coefficient of original species [-]

$K_{\text{solid,sl | w,sl [S]}}$: soil/water partition coefficient of continental and global natural and agricultural soil [L·kg^{-1}]

$\rho_{\text{sd,sl}}$: mineral density of sediment and soil [kg·m^{-3}]

$fr_V_{\text{water,sl[S]}}$: volume fraction water in continental and global natural and agricultural soil [-]

1000: conversion factor [dm^3·m^{-3}]

Where the volume fraction gas in soil, the mineral density and the volume fraction water in soil are described in Table 10. The $K_{\text{aw[S]}}$ and the $K_{\text{solid,sl | w,sl[S]}}$ are described in section 5.4.1 and 5.4.4, respectively.

The volume fraction solids in the natural and agricultural soil may be obtained from:

$$fr_V_{\text{solid,sl[S]}} = 1 - fr_V_{gas,sl[S]} - fr_V_{water,sl[S]} \quad (47)$$

with

$fr_V_{\text{solid,sl[S]}}$: volume fraction solids in continental and global natural and agricultural soil [-]

$fr_V_{\text{gas,sl[S]}}$: volume fraction gas in continental and global natural and agricultural soil [-]

$fr_V_{water,sl[S]}$: volume fraction water in continental and global natural and agricultural soil [-]

Where the default values of the volume fraction gas in the soil and the volume fraction water in the soil are described in Table 10.

The mass fraction of the chemical in water phase of the natural and agricultural soil may be obtained from:

$$fr_m_{water,sl[S]} = \frac{fr_V_{water,sl[S]}}{fr_V_{gas,sl[S]} \cdot K_{aw[S]} + fr_V_{water,sl[S]} + fr_V_{solid,sl[S]} \cdot K_{solid,sl|w,sl[S]} \cdot \frac{\rho_{sd,sl}}{1000}} \quad (48)$$

with

$fr_m_{water,sl[S]}$: fraction of chemical in water phase of continental and global natural and agricultural soil [-]

$fr_V_{water,sl[S]}$: volume fraction water in continental and global natural and agricultural soil [-]

$fr_V_{gas,sl[S]}$: volume fraction gas in continental and global natural and agricultural natural soil [-]

$K_{aw[S]}$: dimensionless air/water partition coefficient of original species [-]

$fr_V_{solid,sl[S]}$: volume fraction solids in continental and global natural and agricultural soil [-]

$\rho_{sd,sl}$: mineral density of sediment and soil [kg·m^{-3}]

$K_{solid,sl\,|\,w,sl\,[S]}$: soil/water partition coefficient of continental and global natural and agricultural soil [L·kg^{-1}]

1000: conversion factor [dm^3·m^{-3}]

Where the volume fraction water in soil, the volume fraction gas in soil and the mineral density are described in Table 10. The $K_{aw[S]}$ and the $K_{solid,sl\,|\,w,sl[S]}$ are described in section 5.4.1 and 5.4.4, respectively. The volume fraction solid in soil is described in Equation (47).

The mass fraction of original species in the soil may be obtained from:

When $pK_{a,loss} \leq pK_{a,gain}$:

$$fr_m_{sl} = \frac{1}{1 + 10^{pKa_{loss} - pH_{sl}} + 10^{pH_{sl} - pKa_{gain}}} \quad (49)$$

When $pK_{a,loss} > pK_{a,gain}$: (50)

$$fr_m_{\mathrm{sl}} = \frac{1}{1 + 10^{pKa_{gain} - pH_{\mathrm{sl}}} + 10^{pH_{sl} - pKa_{loss}}}$$

with

fr_m$_{\mathrm{sl}}$: fraction original species in natural and agricultural soil [-]

pH_{sl}: pH natural and agricultural soil [-]

pKa,loss: equilibrium constant proton loss from conjugated acid of parent compound [-]

pKa,gain: equilibrium constant proton loss from parent compound [-]

Where the pH of natural and agricultural soil and the equilibrium constants proton loss from parent compound and from conjugated acid of the parent compound are described in Table 10.

The mass fraction of original species in the pore water of the soil may be obtained from:

When $pK_{a,loss} \leq pK_{a,gain}$:

$$fr_m_{\mathrm{sl,water}} = \frac{1}{1 + 10^{pKa_{loss} - pH_{\mathrm{sl}}} + 10^{pH_{\mathrm{sl}} - pKa_{gain}}} \quad (51)$$

When $pK_{a,loss} > pK_{a,gain}$:

$$fr_m_{\mathrm{sl,water}} = \frac{1}{1 + 10^{pKa_{gain} - pH_{\mathrm{sl}}} + 10^{pH_{\mathrm{sl}} - pKa_{loss}}} \quad (52)$$

with

fr_m$_{\mathrm{sl,water}}$: fraction original species in pore water of natural and agricultural soil [-]

pH_{sl}: pH natural and agricultural soil [-]

pKa,loss: equilibrium constant proton loss from conjugated acid of parent compound [-]

pKa,gain: equilibrium constant proton loss from parent compound [-]

Where the pH of natural and agricultural soil and the equilibrium constants proton loss from parent compound and from conjugated acid of the parent compound are described in Table 10.

The bulk density of the soil may be obtained from:

$$\rho_{\mathrm{sl}} = fr_V_{\mathrm{gas,sl[S]}} \cdot \rho_{\mathrm{air}} + fr_V_{\mathrm{water,sl[S]}} \cdot \rho_{\mathrm{w}} + fr_V_{\mathrm{solid,sl[S]}} \cdot \rho_{\mathrm{sd,sl}} \quad (53)$$

with

ρ_{sl}: bulk density of soil [kg·m^{-3}]

$fr_V_{gas,sl[S]}$: volume fraction gas in continental and global natural and agricultural soil [-]

ρ_{air}: density of air [kg·m^{-3}]

$fr_V_{water,sl[S]}$: volume fraction water in continental and global natural and agricultural soil [-]

ρ_{w}: density of water [kg·m^{-3}]

$fr_V_{solid,sl[S]}$: volume fraction solids in continental and global natural and agricultural soil [-]

$\rho_{sd,sl}$: mineral density of sediment and soil [kg·m^{-3}]

Where the volume fraction gas in soil, the volume fraction water in soil, the density of air and water, and the mineral density are described in Table 10. The volume fraction solid in soil is described in Equation (47).

5.2.4.1 Penetration depth

Chemicals tend to migrate vertically down into the soil, whereby processes of diffusion, absorption and degradation control the depth of migration (Brandes *et al.*, 1996; Thibodeaux, 1996).

The penetration depth in the continental and global natural and agricultural soil may be obtained from:

$$h_{sl,penetr[S]} = \frac{v_{eff,adv,sl[S]} + \sqrt{v_{eff,adv,sl[S]}^{2} + 4 \cdot \frac{k_{deg,sl[S]}}{(3600 \cdot 24)} \cdot D_{eff,sl[S]}}}{2 \cdot \frac{k_{deg,sl[S]}}{(3600 \cdot 24)}} \quad (54)$$

with

$h_{sl.penetr[S]}$: penetration depth of continental and global natural and agricultural soil [m]

$v_{eff,adv,sl[S]}$: effective advective transport in continental and global natural and agricultural soil [m·s^{-1}]

$D_{eff,sl[S]}$: effective diffusion coefficient in continental and global natural and agricultural soil [m^2·s^{-1}]

$k_{deg,sl[S]}$: degradation rate in continental and global natural and agricultural soil [d^{-1}]

3600·24: conversion factor [s·d^{-1}]

Where $k_{deg,sl[S]}$ is the described in section 5.3.4, if $k_{deg,sl[S]}$ is unknown, consider $1 \cdot 10^{-20}$ as default. The effective advective transport in soil and the effective diffusion coefficient in soil are described in Equations (55) and (57), respectively.

The effective advective transport in soil may be obtained from:

$$\upsilon_{eff,adv,sl[S]} = \left(\upsilon_{rain[S]} \cdot fr_V_{rain,inf,sl[S]}\right) \cdot \left(\frac{fr_m_{water,sl[S]}}{fr_V_{water,sl[S]}}\right) + \upsilon_{adv,solid,sl[S]} \cdot \left(\frac{fr_m_{solid,sl[S]}}{fr_V_{solid,sl[S]}}\right) \quad (55)$$

with

$\upsilon_{eff,adv,sl[S]}$: effective advective transport in continental and global natural and agricultural soil [$m \cdot s^{-1}$]

$\upsilon_{rain[S]}$: continental and global annual average precipitation [$m \cdot s^{-1}$]

$fr_V_{rain,inf,sl[S]}$: volume fraction of precipitation infiltrating into continental and global natural and agricultural soil [-]

$fr_m_{water,sl[S]}$: fraction of chemical in water phase continental and global natural and agricultural soil [-]

$fr_V_{water,sl[S]}$: volume fraction water continental and global natural and agricultural soil [-]

$\upsilon_{adv,solid,sl[S]}$: solid phase advection velocity continental and global natural and agricultural soil [$m \cdot s^{-1}$]

$fr_m_{solid,sl[S]}$: fraction of chemical in solid phase continental and global natural and agricultural soil [-]

$fr_V_{solid,sl[S]}$: volume fraction solids continental and global natural and agricultural soil [-]

Where the annual average precipitation and the volume fraction precipitation infiltrating into the soil are described in Table 4 (continental) and Table 5 (global). The volume fraction water in soil is described in Table 10. The mass fractions water and solid in soil are described in Equations (48) and (46). The solid phase advection velocity of soil is described in Equation (60) and the volume fraction solid in soil in Equation (47).

The solid phase advection velocity of the soil is by default 0.0002 $m \cdot yr^{-1}$ (Den Hollander & Van de Meent, 2004) and is conversed to $m \cdot s^{-1}$:

$$\upsilon_{adv,solid,sl[S]} = \frac{0.0002}{(3600 \cdot 24 \cdot 365)} \quad (56)$$

with

$\upsilon_{ad,solid,sl[S]}$: solid phase advection velocity continental and global natural and agricultural soil [m·s^{-1}]

0.0002: solid phase advection velocity continental and global natural and agricultural soil [m·yr^{-1}]

3600·24·365: conversion factor [s·yr^{-1}]

The effective diffusion in soil includes diffusion in the pore gas and the pore water phase, diffusion in the solid phase of the soil is negligible.

The effective diffusion coefficient in soil may be obtained from:

$$D_{\text{eff,sl[S]}} = D_{\text{gas}} \cdot fr_V_{\text{gas,sl[S]}}^{1.5} \cdot \frac{1 - fr_m_{aq,sl[S]} - fr_m_{solid,sl[S]}}{fr_V_{\text{gas,sl[S]}}} + D_{\text{water}} \cdot fr_V_{\text{water,sl[S]}}^{1.5} \cdot \frac{fr_m_{\text{water,sl[S]}}}{fr_V_{\text{water ,sl[S]}}} + D_{\text{solid,sl[S]}} \cdot \frac{fr_m_{\text{solid,sl[S]}}}{fr_V_{\text{solid,sl[S]}}} \quad (57)$$

with

$D_{\text{eff,sl[S]}}$: effective diffusion coefficient in continental and global natural and agricultural soil [m^2·s^{-1}]

D_{gas}: gas phase diffusion coefficient [m^2·s^{-1}]

$fr_V_{\text{gas,sl[S]}}$: volume fraction gas continental and global natural and agricultural soil [-]

$fr_m_{\text{water,sl[S]}}$: fraction of chemical in water phase continental and global natural and agricultural soil [-]

$fr_m_{\text{solid,sl[S]}}$: fraction of chemical in solid phase continental and global natural and agricultural soil [-]

D_{water}: water phase diffusion coefficient [m^2.s^{-1}]

$fr_V_{\text{water,sl[S]}}$: volume fraction water continental and global natural and agricultural soil [-]

$D_{\text{solid,sl[S]}}$: solid phase turbation coefficient continental and global natural and agricultural soil [m^2·s^{-1}]

$fr_V_{\text{solid,sl[S]}}$: volume fraction solids continental and global natural and agricultural soil [-]

Where the volume fractions gas and water in soil are described in Table 10. The gas phase diffusion coefficient and the water phase diffusion coefficient are described in Equation (58) and (59). The mass fraction of chemical in the water and solid phase of the soil are described in Equation (48) and (46). The solid phase turbation coefficient of soil is described in Equation (60) and the volume fraction solid in soil in Equation (47).

The gas phase diffusion coefficient is described by Schwarzenbach *et al.* (1993):

$$D_{\text{gas}} = 0.0000257 \cdot \frac{\sqrt{18}}{\sqrt{MW \cdot 1000}} \quad (58)$$

with

D_{gas}:	gas phase diffusion coefficient [$m^2 \cdot s^{-1}$]
0.0000257:	gas phase diffusion coefficient of water [$m^2 \cdot s^{-1}$]
18:	molar weight of water [$g \cdot mol^{-1}$]
MW:	molar weight of the chemical [$kg \cdot mol^{-1}$]
1000:	conversion factor [$g \cdot kg^{-1}$]

Where the molar weight of the chemical is described in the substance data.

The water phase diffusion coefficient is described by Schwarzenbach *et al.* (1993):

$$D_{\text{water}} = 0.000000002 \cdot \frac{\sqrt{32}}{\sqrt{MW \cdot 1000}} \quad (59)$$

with

D_{water}:	water phase diffusion coefficient [$m^2 \cdot s^{-1}$]
0.000000002:	water phase diffusion coefficient of oxygen gas [$m^2 \cdot s^{-1}$]
32:	molar weight of oxygen gas [$g \cdot mol^{-1}$]
MW:	molar weight of the chemical [$kg \cdot mol^{-1}$]
1000:	conversion factor [$g \cdot kg^{-1}$]

Where the molar weight of the chemical is described in the substance data.

The solid phase turbation coefficient is by default 0.00000055 $m^2 \cdot d^{-1}$ (McLachlan *et al.* (2002) and is conversed to $m^2 \cdot s^{-1}$:

$$D_{\text{solid,sl[S]}} = \frac{0.00000055}{3600 \cdot 24} \quad (60)$$

with

$D_{\text{solid,sl[S]}}$:	solid phase turbation coefficient continental and global natural and agricultural soil [$m^2 \cdot s^{-1}$]
0.00000055:	solid phase turbation coefficient continental and global natural and agricultural soil [$m^2 \cdot d^{-1}$]
3600·24:	conversion factor [$s \cdot d^{-1}$]

5.3 Transformation processes

5.3.1 Degradation in air

The transfer from air by degradation may be obtained from:

$$k_{\text{deg,air[S]}} = fr_{m_{\text{gas,air[S]}}} \cdot k_{\text{deg,air25°C}} \cdot (3600 \cdot 24) \quad (61)$$

with

$k_{\text{deg,air[S]}}$:	degradation in urban, continental and global air [d^{-1}]
$fr_m_{\text{gas,air[S]}}$:	fraction of chemical in gas phase of urban, continental and global air [-]
$k_{\text{deg,air25°C}}$:	gas phase degradation rate constant at 25°C, in air [s^{-1}]
3600·24:	conversion factor [$s \cdot d^{-1}$]

Where the fraction of chemical in the gas phase of air is described in Section 5.2.1 and the gas phase degradation rate constant in air is described in the substance data.

The transfer from air by escape to stratosphere is described by Den Hollander & Van de Meent (2004) and may be obtained from:

$$k_{\text{adv,air}\rightarrow\text{strat[S]}} = \frac{ln(2)}{60 \cdot 365} \quad (62)$$

with

$k_{\text{adv,air}\rightarrow\text{strat[S]}}$:	escape from urban, continental and global air to stratosphere [d^{-1}]
60:	half life time in the air [yr]
365:	conversion factor [$d \cdot yr^{-1}$]

5.3.2 Degradation in water

The transfer from water by degradation may be obtained from:

$$k_{\text{deg,w[S]}} = k_{\text{deg,w}} \cdot (3600 \cdot 24) \quad (63)$$

with

$k_{\text{deg,w[S]}}$:	degradation in continental and global fresh and sea water [d^{-1}]
$k_{\text{deg,w}}$:	bulk degradation rate constant at 25°C, in water [s^{-1}]
3600·24:	conversion factor [$s \cdot d^{-1}$]

Where the bulk degradation rate constant in water is described in the substance data.

5.3.3 Degradation in sediment

The transfer from sediment by degradation may be obtained from:

$$k_{\mathrm{deg,wsd[S]}} = k_{\mathrm{deg,sd}} \cdot (3600 \cdot 24) \quad (64)$$

with

$k_{\mathrm{deg,wsd[S]}}$:	degradation in continental and global fresh and sea water sediment [d^{-1}]
$k_{\mathrm{deg,sd}}$:	bulk degradation rate constant at 25°C, in sediment [s^{-1}]
3600·24:	conversion factor [$s \cdot d^{-1}$]

Where the bulk degradation rate constant in sediment is described in the substance data.

5.3.4 Degradation in soil

The transfer from soil by degradation may be obtained from:

$$k_{\mathrm{deg,sl[S]}} = k_{\mathrm{deg,sl}} \cdot (3600 \cdot 24) \quad (65)$$

with

$k_{\mathrm{deg,sl[S]}}$:	degradation in continental and global natural and agricultural soil [d^{-1}]
$k_{\mathrm{deg,sl}}$:	bulk degradation rate constant at 25°C, in soil [s^{-1}]
3600·24:	conversion factor [$s \cdot d^{-1}$]

Where the bulk degradation rate constant in soil is described in the substance data.

5.4 Intermedia partition processes

Intermedia equilibrium constants (air/water; air/soil; sediment/water; soil/water) or partition coefficients are required for various purposes, but principally for estimating intermedia mass transfer coefficients. The coefficients represent concentration ratios. Partition coefficients may be available from experimental data or field measurements. More often, however, this information is not available. If that is the case, the estimation methods described below may be used. It should be noted that, in general, the applicability of these estimation methods is limited to those classes of (organic) chemicals for which the relationships have been derived. Extrapolation beyond these limits may lead to errors of orders of magnitude. For metals, no generally applicable estimation methods are known.

5.4.1 Air-water

If Henry's constant ($KH_{25°C}$) is defined in substance data, the air/water partition coefficient may be obtained from:

$$K_{\text{gas|w}} = \frac{KH_{25°C}}{8.31 \cdot 298} \tag{66}$$

with

$K_{\text{gas}\,\vert\,\text{w}}$:	dimensionless gas/water partition coefficient of the original species [-]
$KH_{25°C}$:	Henry constant [Pa·m^3·mol^{-1}]
8.31:	gas constant [Pa·m^{-3}·mol^{-1}·K^{-1}]
298:	temperature [K]

Where the Henry constant is described in the substances data.

When Henry's constant is not defined in the substance data, the $KH_{25°C}$ may be derived from a QSAR. The estimation may be obtained with the temperature dependent ratio of vapor pressure and the water solubility of the chemical:

For $P_{vap,25°C} > 100000$:

$$K_{\text{gas|w}} = \frac{\frac{100000}{S_{\text{w,25°C}}}}{8.31 \cdot 298} \tag{67}$$

For $P_{vap,25°C} < 100000$:

$$K_{\text{gas}\,\vert\,\text{w}} = \frac{\frac{P_{\text{vap,25°C}}}{S_{\text{w,25°C}}}}{8.31 \cdot 298} \tag{68}$$

with

$K_{\text{gas}\,\vert\,\text{w}}$:	dimensionless gas/water partition coefficient of the original species [-]
$P_{\text{vap,25°C}}$:	vapor pressure of original species at 25°C [Pa]
$S_{\text{w,25°C}}$:	water solubility of original species at 25°C [mol·m^{-3}]
8.31:	gas constant [Pa·m^{-3}·mol^{-1}·K^{-1}]
298:	temperature [K]
100000:	maximum vapor pressure of original species at 25°C [Pa]

Where the vapor pressure and water solubility are described in the substance data.

The air/water partition coefficient differs across the different scales of the USEtox model. The scale specific air/water partition coefficient may be obtained from:

$$K_{\mathrm{aw[S]}} = K_{\mathrm{gas\,|\,w}} \cdot e^{\left(\left(\frac{H_{\mathrm{vap}}}{8.314}\right)\cdot\left(\frac{1}{298}-\frac{1}{T_{[S]}}\right)\right)} \cdot e^{\left(-\left(\frac{H_{\mathrm{diss}}}{8.314}\right)\cdot\left(\frac{1}{298}-\frac{1}{T_{[S]}}\right)\right)} \cdot \left(\frac{298}{T_{[S]}}\right) \quad (69)$$

with

$K_{\mathrm{aw[S]}}$: urban, continental and global dimensionless air/water partition coefficient of original species [-]

$K_{\mathrm{gas\,|\,w}}$: dimensionless gas/water partition coefficient of the original species [-]

H_{vap}: enthalpy of vaporization [J·mol^{-1}]

$T_{[S]}$: urban, continental and global temperature [K]

H_{diss}: enthalpy of dissolution [J·mol^{-1}]

8.31: gas constant [Pa·m^{-3}·mol^{-1}·K^{-1}]

298: temperature [K]

Where the $K_{\mathrm{gas\,|\,w}}$ is described in Equations (66) until (68). The enthalpy of vaporization and the dissolution are described in Table 10. The scale temperatures are described in Table 10 (urban), Table 4 (continental) and Table 5 (global).

5.4.2 Octanol-water

The octanol/water partition coefficient of the alternate form is described by Trapp & Horobin (2005) and may be obtained from:

$$K_{\mathrm{ow,alt}} = 10^{LOG(K_{\mathrm{ow}})-3.5} \quad (70)$$

with

$K_{\mathrm{ow,alt}}$: octanol/water partition coefficient of alternate form [-]

K_{ow}: octanol/water partition coefficient of the original species [-]

3.5: constant definition [-]

Where the K_{ow} is described in the substance data.

The apparent octanol/water partition coefficient may be derived by combining both the part of original species and the part in alternate form of the chemical:

When $pK_{a,loss} \leq pK_{a,gain}$:

$$K_{ow,app,pH7} = \left(\frac{1}{1 + 10^{pKa_{loss}-7} + 10^{7-pKa_{gain}}} \cdot K_{ow}\right) + \left(\frac{1}{1 + 10^{7-pKa_{loss}} + 10^{pKa_{gain}-7}} \cdot K_{ow,alt}\right) \quad (71)$$

When $pK_{a,loss} > pK_{a,gain}$:

$$K_{ow,app,pH7} = \left(\frac{1}{1 + 10^{pKa_{gain}-7} + 10^{7-pKa_{loss}}} \cdot K_{ow}\right) + \left(\frac{1}{1 + 10^{7-pKa_{gain}} + 10^{pKa_{loss}-7}} \cdot K_{ow,alt}\right) \quad (72)$$

with

$K_{ow,app,pH7}$:	apparent octanol/water partition coefficient at neutral pH [-]
7:	neutral pH [-]
pKa,loss:	equilibrium constant proton loss from conjugated acid of parent compound [-]
pKa,gain:	equilibrium constant proton loss from parent compound [-]
K_{ow}:	octanol/water partition coefficient of the original species [-]
$K_{ow,alt}$:	octanol/water partition coefficient of alternate form [-]

Where the equilibrium constants proton loss from parent compound and from conjugated acid of the parent compound are described in Table 10. The K_{ow} is described in the substance data and the $K_{ow,alt}$ in Equation (70).

5.4.3 Solids-water

The chemical can partition between the suspended solids phase in the water and the water phase (this section) and between the solid phase and the porewater phase of the soil or sediment (Sections 5.4.4 and 5.4.5).

If the suspended solids/water partition coefficient is defined in substance data, it may be considered for $K_{susp|w,w[S]}$.

If the suspended solids/water partition coefficient is not defined in substance data, the $K_{susp|w,w[S]}$ may be obtained from:

$$K_{susp|w,w[S]} = \left(fr_m_{w} \cdot K_{d} + (1 - fr_m_{w}) \cdot K_{d,alt}\right) \cdot \frac{1000}{\rho_{sd,sl}} \cdot \frac{fr_m_{Corg,susp,w[S]}}{fr_m_{Corg,std,sl|sd}} \quad (73)$$

with

$K_{susp\,|\,w,w\,[S]}$:	suspended solids/water partition coefficient, continental and global fresh and sea water [L·kg^{-1}]

fr_m_{w}:	fraction original species in fresh and sea water [-]
K_{d}:	dimensionless solids/water partition coefficient of the original species [-]
$K_{d,alt}$:	dimensionless solids/water partition coefficient of the alternate form [-]
1000:	conversion factor [$dm^3 \cdot m^{-3}$]
$\rho_{sd,sl}$:	mineral density of sediment and soil [$kg \cdot m^{-3}$]
$fr_m_{Corg,susp,w[S]}$:	mass fraction organic carbon in continental and global fresh and sea water suspended matter [-]
$fr_m_{Corg,std,sl\|sd}$:	standard mass fraction organic carbon in soil/sediment [-]

Where the fraction original species in water is described in Section 5.2.2, the K_{d} in Equations (74) until (78) and the $K_{d,alt}$ in Equations (79) until (82). By default the mineral density, the mass fraction organic carbon in water suspended matter and the standard mass fraction of organic carbon in sediment and soil are described in Table 10.

If the organic carbon/water partition coefficient is defined in substance data, the solids/water partition coefficient of the original species may be obtained from:

$$K_{d} = (K_{OC}) \cdot fr_m_{Corg,std,sl|sd} \cdot \frac{\rho_{sd,sl}}{1000} \quad (74)$$

with

K_{d}:	dimensionless solids/water partition coefficient of the original species [-]
K_{OC}:	organic carbon/water partition coefficient of the original species [$L \cdot kg^{-1}$]
$fr_m_{Corg,std,sl\|sd}$:	standard mass fraction of organic carbon in sediment and soil [-]
$\rho_{sd,sl}$:	mineral density of sediment and soil [$kg \cdot m^{-3}$]
1000:	conversion factor [$dm^3 \cdot m^{-3}$]

Where the K_{OC} is described in the substance data. By default the standard mass fraction of organic carbon in sediment and soil and the mineral density are described in Table 10.

If the organic carbon/water partition coefficient is not defined in substance data, it may be derived from a QSAR (Franco & Trapp, 2008). The organic carbon/water partition coefficient described for the original species and the alternate form of the chemical differ for ionizable compounds. The solids/water partition coefficient of the original species may be obtained from:

For neutral substances

$$K_{\mathrm{d}} = (1.26 \cdot \mathrm{Kow}^{0.81}) \cdot fr_m_{Corg,std,sl|sd} \cdot \frac{\rho_{\mathrm{sd,sl}}}{1000} \quad (75)$$

For acid substances

$$K_{\mathrm{d}} = \left(10^{0.54 \cdot \log(K_{\mathrm{ow}}) + 1.11}\right) \cdot fr_m_{Corg,std,sl|sd} \cdot \frac{\rho_{\mathrm{sd,sl}}}{1000} \quad (76)$$

For basic substances

$$K_{\mathrm{d}} = \left(10^{0.37 \cdot \log(K_{\mathrm{ow}}) + 1.7}\right) \cdot fr_m_{Corg,std,sl|sd} \cdot \frac{\rho_{\mathrm{sd,sl}}}{1000} \quad (77)$$

For amphoters

$$K_{\mathrm{d}} = (10.47 \cdot \mathrm{Kow}^{0.52}) \cdot fr_m_{Corg,std,sl|sd} \cdot \frac{\rho_{\mathrm{sd,sl}}}{1000} \quad (78)$$

with

K_{d}:	dimensionless solids/water partition coefficient of the original species [-]
$fr_m_{\mathrm{Corg,std,sl\,|\,sd}}$:	standard mass fraction organic carbon in soil/sediment [-]
$\rho_{\mathrm{sd,sl}}$:	mineral density of sediment and soil [kg·m^{-3}]
K_{ow}:	octanol/water partition coefficient of the original species [-]
1000:	conversion factor [kg·m^{-3}]
1.26:	constant definition
0.81:	constant definition
0.54:	constant definition
1.11:	constant definition
0.37:	constant definition
1.7:	constant definition
10.47:	constant definition
0.52:	constant definition

Where by default the standard mass fraction of organic carbon in sediment and soil and the mineral density are described in Table 10. The K_{ow} is described in the substance data.

The solids/water partition coefficient of the alternate form may be obtained from:

For neutral substances

$$K_{\mathrm{d,alt}} = \left(1.26 \cdot {K_{ow}}^{0.81}\right) \cdot fr_m_{Corg,std,sl|sd} \cdot \frac{\rho_{\mathrm{sd,sl}}}{1000} \quad (79)$$

For acid substances

$$K_{\mathrm{d,alt}} = \left(10^{0.11\cdot\log(K_{\mathrm{ow}})+1.54}\right) \cdot fr_m_{Corg,std,sl|sd} \cdot \frac{\rho_{\mathrm{sd,sl}}}{1000} \quad (80)$$

For basic substances the $K_{d,alt}$ depends on the $pK_{a,gain}$
When $pK_{a,gain} \leq 0$, $K_{d,alt}$ is 1

When $pK_{a,gain} > 0$,

$$K_{\mathrm{d,alt}} = 10^{pKa^{0.65\cdot\left(\frac{K_{\mathrm{ow}}}{(1+K_{\mathrm{ow}})}\right)^{0.14}}} \cdot fr_m_{Corg,std,sl|sd} \cdot \frac{\rho_{\mathrm{sd,sl}}}{1000} \quad (81)$$

For amphoters the $K_{d,alt}$ depends on the pH_{fw}

When $pH_{fw} \leq$ the average of $pK_{a,gain} + pK_{a,loss}$ and
$pK_{a,gain} \leq 0$, $K_{d,alt}$ is 1
$pK_{a,gain} > 0$,

$$K_{\mathrm{d,alt}} = 10^{pK_{a,gain}^{0.65\cdot\left(\frac{K_{\mathrm{ow}}}{(1+K_{\mathrm{ow}})}\right)^{0.14}}} \cdot fr_m_{Corg,std,sl|sd} \cdot \frac{\rho_{\mathrm{sd,sl}}}{1000}$$

When $pH_{fw} >$ the average of $pK_{a,gain} + pK_{a,loss}$,

$$K_{\mathrm{d,alt}} = \left(10^{0.11\cdot\log(K_{\mathrm{ow}})+1.54}\right) \cdot fr_m_{Corg,std,sl|sd} \cdot \frac{\rho_{\mathrm{sd,sl}}}{1000} \quad (82)$$

with

$K_{\mathrm{d,al}}$	dimensionless solids/water partition coefficient of the original species [-]
$fr_m_{\mathrm{Corg,std,sl\,|\,sd}}$:	standard mass fraction organic carbon in soil/sediment [-]
$\rho_{\mathrm{sd,sl}}$:	mineral density of sediment and soil [kg·m^{-3}]
K_{ow}:	octanol/water partition coefficient of the original species [-]
pH_{fw}:	pH of fresh water[-]
1000:	conversion factor [kg·m^{-3}]
pKa,loss:	equilibrium constant proton loss from conjugated acid of parent compound [-]
pKa,gain:	equilibrium constant proton loss from parent compound [-]
1.26:	constant definition
0.81:	constant definition
0.11:	constant definition
1.54:	constant definition
0.65:	constant definition
0.14:	constant definition

Where by default the standard mass fraction of organic carbon in sediment, soil and the mineral density, the pH of fresh water, the equilibrium constant proton loss from conjugated acid and parent compound are described in Table 10. The K_{ow} is described in the substance data.

5.4.4 Soil-water

The dimensionless soil/water partition coefficient may be obtained from:

$$K_{\mathrm{sl|w,sl[S]}} = fr_V_{\mathrm{gas,sl[S]}} \cdot K_{\mathrm{aw[S]}} + fr_V_{\mathrm{water,sl[S]}} + fr_V_{\mathrm{solid,sl[S]}} \cdot K_{\mathrm{solid,sl|w,sl[S]}} \cdot \frac{\rho_{\mathrm{sd,sl}}}{1000} \quad (83)$$

with

$K_{\mathrm{sl\,|\,w,sl\,[S]}}$: dimensionless soil/water partition coefficient continental and global natural and agricultural soil [-]

$fr_V_{\mathrm{gas,sl[S]}}$: volume fraction gas continental and global natural and agricultural soil [-]

$K_{\mathrm{aw[S]}}$: dimensionless air/water partition coefficient of original species [-]

$fr_V_{\mathrm{water,sl[S]}}$: volume fraction water continental and global natural and agricultural soil [-]

$fr_V_{\mathrm{solid,sl[S]}}$: volume fraction solids continental and global natural and agricultural soil [-]

$K_{\mathrm{solid,sl\,|\,w,sl\,[S]}}$: soil/water partition coefficient at the continental and global natural and agricultural soil [L·kg^{-1}]

$\rho_{\mathrm{sd,sl}}$: mineral density of sediment and soil [kg·m^{-3}]

1000: conversion factor [dm^3·m^{-3}]

Where the volume fraction gas and water in soil and the mineral density of sediment and soil are described in Table 10. The K_{aw} and the $K_{\mathrm{solids,sl\ |\ w,sl[S]}}$ are described in Section 5.4.1 and 5.4.3, respectively. The volume fraction solid in soil is described in Section 5.2.4.

If the soil/water partition coefficient is defined in substance data, it may be considered for $K_{\mathrm{solid,sl|w,sl[S]}}$. If the soil/water partition coefficient is not defined in substance data, the $K_{\mathrm{solid,sl|w,sl[S]}}$ may be obtained from:

$$K_{\mathrm{solid,sl|w,sl[S]}} = \left(fr_m_{\mathrm{sl}} \cdot K_{\mathrm{d}} + (1 - fr_m_{\mathrm{sl}}) \cdot K_{\mathrm{d,alt}}\right) \cdot \frac{1000}{\rho_{\mathrm{sd,sl}}} \cdot \frac{fr_m_{\mathrm{Corg,sl[S]}}}{fr_m_{\mathrm{Corg,std,sl|sd}}} \quad (84)$$

with

$K_{\mathrm{solid,sl\,|\,w,sl\,[S]}}$: soil/water partition coefficient at the continental and global natural and agricultural soil [L·kg^{-1}]

fr_m_{sl}: fraction original species in natural and agricultural soil [-]

K_d:	dimensionless solids/water partition coefficient of the original species [-]
$K_{d,alt}$:	dimensionless solids/water partition coefficient of the alternate form [-]
1000:	conversion factor [$dm^3 \cdot m^{-3}$]
$\rho_{sd,sl}$:	mineral density of sediment and soil [$kg \cdot m^{-3}$]
$fr_m_{Corg,sl[S]}$:	mass fraction organic carbon in continental and global natural and agricultural soil [-]
$fr_m_{Corg,std,sl\|sd}$:	standard mass fraction organic carbon in soil/sediment [-]

Where the fraction original species in soil is described in Section 5.2.4, the K_d and the $K_{d,alt}$ are described in Section 5.4.3. By default the mineral density, the mass fraction organic carbon in water suspended matter and the standard mass fraction of organic carbon in sediment and soil are described in Table 10.

5.4.5 Sediment-water

The dimensionless sediment/water partition coefficient may be obtained from:

$$K_{sd|w,w[S]} = fr_V_{water,sd[S]} + fr_V_{solid,sd[S]} \cdot K_{solid,sd|w[S]} \cdot \frac{\rho_{sd,sl}}{1000} \quad (85)$$

with

$K_{sd\|w,w[S]}$:	dimensionless sediment/water partition coefficient continental and global fresh and sea water [-]
$fr_V_{water,sd[S]}$:	volume fraction water in continental and global sediment [-]
$fr_V_{solid,sd[S]}$:	volume fraction solids in continental and global sediment [-]
$K_{solid,sd\|w,w[S]}$:	sediment/water partition coefficient continental and global fresh and sea water [$L \cdot kg^{-1}$]
$\rho_{sd,sl}$:	mineral density of sediment and soil [$kg \cdot m^{-3}$]
1000:	conversion factor [$dm^3 \cdot m^{-3}$]

Where the volume fraction water in soil and the mineral density of sediment and soil are described in Table 10. The $K_{solids,sl\ |\ w,sl[S]}$ is described in Equation (84), and the volume fraction solid in soil is described in Section 5.2.4.

If the sediment particles/water partition coefficient is defined in substance data, it may be considered for $K_{solid,sd|w,sd[S]}$. If the sediment particles/water partition coefficient is not defined in substance data, the $K_{solid,sd|w,sd[S]}$ may be obtained from:

$$K_{solid,sd|w,w[S]} = \left(fr_m_{wsd} \cdot K_d + (1 - fr_m_{wsd}) \cdot K_{d,alt}\right) \cdot \frac{1000}{\rho_{sd,sl}} \cdot \frac{fr_m_{Corg,wsd[S]}}{fr_m_{Corg,std,sl|sd}} \quad (86)$$

with

$K_{solid,sd\|w,w\,[S]}$:	sediment/water partition coefficient continental and global fresh and sea water [$L \cdot kg^{-1}$]
fr_m_{wsd}:	fraction original species in fresh and sea water sediment [-]
K_d:	dimensionless solids/water partition coefficient of the original species [-]
$K_{d,alt}$:	dimensionless solids/water partition coefficient of the alternate form [-]
1000:	conversion factor [$dm^3 \cdot m^{-3}$]
$\rho_{sd,sl}$:	mineral density of sediment and soil [$kg \cdot m^{-3}$]
$fr_m_{Corg,wsd[S]}$: water sediment [-]	mass fraction organic carbon in continental and global fresh and sea
$fr_m_{Corg,std,sl\|sd}$:	standard mass fraction organic carbon in soil/sediment [-]

Where the fraction original species in sediment is described in Section 5.2.3, the K_d and the $K_{d,alt}$ are described in Section 5.4.3. By default the mineral density, the mass fraction organic carbon in water suspended matter and the standard mass fraction of organic carbon in sediment and soil are described in Table 10.

5.4.6 Biota-water

Concentrations of chemical in organisms can exceed the concentrations in the surrounding environment as a result of various, simultaneously operating routes of uptake. This is a well-studied phenomenon, which is referred to in various scientific texts and policy contexts in slightly different ways, using different terms: bioconcentration, bioaccumulation, biomagnification. In USEtox, we adopt the terminology defined in Arnot and Gobas (2006) and refer to the combined uptake pathways as "bioaccumulation", the result of which is typically obtained from field observations. The extent of chemical bioaccumulation is usually expressed in the form of a bioaccumulation factor *BAF*, which is the ratio of a chemical concentration in the organism C_B ($mg.kg^{-1}$) and in the water C_W ($mg.L^{-1}$) at steady state. In USEtox, this terminology is used throughout, i.e. both for calculating fate (this section) and for calculating human exposure (Section 6.4.3). For the purpose of calculating LCA characterization factors, USEtox makes use of measured *BAF* values where available, or uses QSARs where necessary. A good read for more in-depth information is the related paper by Arnot and Gobas (2006).

For use in USEtox, bioaccumulation factors for fish may be obtained from measurement represented by measured BAF when these measurements are available in literature. Otherwise, the Arnot and Gobas (2003) model in EPISuite for the upper trophic level is used to estimate directly the steady-state *BAF* [l/kg] for non-dissociating chemicals and chemicals with log $K_{ow} < 9$. This model includes mechanistic processes for bioconcentration and bioaccumulation such as chemical uptake from the water at the gill surface and the dietary inputs, and chemical elimination at the gill surface, faecal egestion, growth dilution and metabolic biotransformation. Input parameters to predict *BAF* values are the K_{ow} of the chemical and the estimated whole-body metabolic biotransformation rate constant [1/day].

The *BAF*-values for fish calculated by the Arnot and Gobas (2003) model refer to the total concentration in water, while *BAF*-values related to the dissolved phase are required in USEtox. We therefore recalculated the Arnot-Gobas $BAF_{\text{total.fish}}$-values for fish by dividing them by the fraction dissolved following the default settings in EPISuite:

$$BAF_{\text{dissolved.fish}} = \frac{BAF_{\text{total.fish}}}{1 + 0.08 \cdot DOC \cdot K_{\text{ow}} + 0.35 \cdot POC \cdot K_{\text{ow}}} \quad (87)$$

where *DOC* is the dissolved organic carbon concentration and *POC* the particulate organic carbon concentration that both equal 5.10^{-7} kg/l in EPISuite. In case the chemical is indicated as dissociating or has a log $K_{ow} > 9$, the Arnot and Gobas (2003) regression results should be applied with care, since this is outside the model's fitting domain. Generally, whenever available, *BAF* values have been used in priority and may be significantly higher (especially around log Kow between 5 and 7) than *BCF*, where the latter is determined without considering the dietary uptake into fish. Note also that the Arnot-Gobas model is meant for non-dissociating chemicals. However, we currently also apply the Arnot-Gobas model here, as for ionizing organic substances, we have currently no model available to predict BAF in fish and also apply the model by Arnot and Gobas (2003).

5.4.7 Dissolved organic carbon-water

If the DOC/water partition coefficient is defined in the substance data, the partitioning of the chemical between the DOC phase and the water phase may be considered for $K_{\text{DOC|w,w[S]}}$. If the DOC/water partition coefficient is not defined in the substance data, the $K_{\text{DOC|w,w[S]}}$ may be obtained as described by Burkhard (2000):

$$K_{\text{DOC|w,w[S]}} = cf_{\text{DOC | w,w}} \cdot K_{\text{ow,app,pH7}} \quad (88)$$

For global fresh water:

$$K_{\text{DOC|w,fw[G]}} = cf_{\text{DOC | w,w}} \cdot K_{ow} \quad (89)$$

with

$K_{\text{DOC | w,w [S]}}$:	dissolved (colloidal) organic carbon/water partition coefficient of the continental fresh and sea water, and the global sea water [L·kg^{-1}]
$K_{\text{DOC | w,fw [G]}}$:	dissolved (colloidal) organic carbon/water partition coefficient of the global fresh water [L·kg^{-1}]
$K_{\text{ow,app,pH7}}$:	apparent octanol/water partition coefficient at neutral pH
K_{ow}:	octanol/water partition coefficient
$cf_{\text{DOC | w,w}}$:	proportionality constant

Where the $K_{\text{ow,app,pH7}}$ and the K_{ow} are described in Section 5.4.2 and the correction factor is described in Table 10.

5.5 Intermedia transfer processes

5.5.1 Deposition

The deposition pattern exists out of dry and wet periods of dry and wet deposition, respectively. The dry deposition contains dry deposition from the aerosol phase of the air and gas absorption from the air to the soil and water compartments. The wet deposition contains chemical washout from the aerosol and gas phase of the air and gas absorption from the air to the soil and water compartments.

The mean urban atmospheric deposition rate is described in Section 5.5.5 as deposition to the unpaved compartment of the urban scale causes removal of the substance.

The mean continental and global atmospheric deposition rate may be obtained from:

$$k_{\mathrm{dep,air[S]}} = k_{\mathrm{mean,air[S]}} - \frac{\upsilon_{\mathrm{abs,gas,air\rightarrow fw[S]}} \cdot fr_{\mathrm{A_{fw[S]}}} + \upsilon_{\mathrm{abs,gas,air\rightarrow sw[S]}} \cdot fr_{\mathrm{A_{sw[S]}}} + \upsilon_{\mathrm{abs,gas,air\rightarrow nsl[S]}} \cdot fr_{\mathrm{A_{nsl[S]}}} + \upsilon_{\mathrm{abs,gas,air\rightarrow asl[S]}} \cdot fr_{\mathrm{A_{asl[S]}}}}{h_{\mathrm{air[S]}}} - \frac{k_{\mathrm{deg,air[S]}}}{(3600 \cdot 24)} \quad (90)$$

with

$k_{\mathrm{dep,air[S]}}$:	mean continental and global atmospheric deposition rate [s^{-1}]
$k_{\mathrm{mean,air[S]}}$:	mean rate constant removal from continental and global air [s^{-1}]
$\upsilon_{\mathrm{abs,gas,air\rightarrow w[S]}}$:	gas absorption velocity to continental and global fresh or sea water [$m \cdot s^{-1}$]
$fr_A_{\mathrm{fw[S]}}$:	area fraction continental and global fresh water [-]
$fr_A_{\mathrm{sw[S]}}$:	area fraction continental and global sea water [-]
$\upsilon_{\mathrm{abs,gas,air\rightarrow sl[S]}}$:	gas absorption velocity to continental and global soil [$m \cdot s^{-1}$]
$fr_A_{\mathrm{nsl[S]}}$:	area fraction continental and global natural soil [-]
$fr_A_{\mathrm{asl[S]}}$:	area fraction continental and global agricultural soil [-]
$h_{\mathrm{air[S]}}$:	mixed height continental and global air [m]
$k_{\mathrm{deg,air[S]}}$:	degradation in continental and global air [d^{-1}]
3600·24:	conversion factor [$s \cdot d^{-1}$]

Where the mean rate constant removal from air is described in Equation (91). The gas absorption velocities are described in Section 5.5.2, the area fractions of water in Section 5.2.2, the area fraction of soil in Section 5.2.4, the mixed height of the air compartment in Section 5.2.1 and the degradation in the air in Section 5.3.1.

The mean rate constant removal from continental and global air may be obtained from:

$$k_{\text{mean,air[S]}} = \left(\left(\frac{1}{k_{\text{tot,dry,air[S]}}} \right) \cdot \frac{t_{\text{dry[S]}}}{t_{\text{dry[S]}} + t_{\text{wet[S]}}} + \left(\frac{1}{k_{\text{tot,wet,air[S]}}} \right) \cdot \frac{t_{\text{wet[S]}}}{t_{\text{dry[S]}} + t_{\text{wet[S]}}} - \left(\frac{\left(\frac{1}{k_{\text{tot,wet,air[S]}}} - \frac{1}{k_{\text{tot,dry,air[S]}}} \right)^2}{t_{\text{dry[S]}} + t_{\text{wet[S]}}} \right) \cdot \left(1 - e^{-k_{\text{tot,dry,air[S]}} \cdot t_{\text{dry[S]}}}\right) \cdot \frac{1 - e^{-k_{\text{tot,wet,air[S]}} \cdot t_{\text{wet[U]}}}}{1 - e^{-k_{\text{tot,dry,air[S]}} \cdot t_{\text{dry[S]}} - k_{\text{tot,wet,air[S]}} \cdot t_{\text{wet[S]}}}} \right)^{-1} \quad (91)$$

with

$k_{\text{mean,air[S]}}$: mean rate constant removal from atmosphere [s^{-1}]

$k_{\text{tot,dry,air[S]}}$: total rate constant removal from atmosphere during dry episodes [s^{-1}]

$t_{\text{dry[S]}}$: average duration of dry episodes [s]

$t_{\text{wet[S]}}$: average duration of wet episodes [s]

$k_{\text{tot,wet,air[S]}}$: total rate constant removal from atmosphere during wet episodes [s^{-1}]

Where the total rate constants removal from atmosphere during dry episodes are described in Equation (92) and (93), the average duration of dry episodes in (99) and of wet episodes in Equation (100). The total rate constants removal from atmosphere during wet episodes are described in Equation (95) and (96).

The total rate constant removal from urban atmosphere during dry episodes may be obtained from:

$$k_{\text{tot,dry,air[U]}} = \frac{\upsilon_{\text{dep,dry,ae[U]}} + \upsilon_{\text{abs,gas,air→npav[U]}}}{h_{\text{air [U]}}} \cdot fr_A_{\text{npav[U]}} + \frac{k_{\text{deg,air[U]}}}{(3600 \cdot 24)} \quad (92)$$

with

$k_{\text{tot,dry,air[U]}}$: total rate constant removal from urban atmosphere during dry episodes [s^{-1}]

$\upsilon_{\text{dep,dry,ae[U]}}$: urban dry aerosol deposition rate [$m \cdot s^{-1}$]

$\upsilon_{\text{abs,gas,air→npav[U]}}$: gas absorption velocity to urban non-paved surface [$m \cdot s^{-1}$]

$fr_A_{\text{fnpav[U]}}$: area fraction urban non-paved surface [-]

$k_{deg,air[U]}$: degradation in urban air [d^{-1}]

$h_{air\ [U]}$: mixed height of the urban air [m]

3600·24: conversion factor [$s \cdot d^{-1}$]

Where the dry aerosol deposition rate is described in Equation (94). The gas absorption velocity is described in Section 5.5.2, the area fraction urban non-paved surface in Table 6, the degradation in urban air in Section 5.3.1 and the mixed height of the urban air in Section 5.2.1.

The total rate constant removal from continental and global atmosphere during dry episodes may be obtained from:

$$k_{tot,dry,air[S]} = \frac{\upsilon_{dep,dry,ae[S]} + \begin{pmatrix} \upsilon_{abs,gas,air\rightarrow fw[S]} \cdot fr_{A_{fw[S]}} + \upsilon_{abs,gas,air\rightarrow sw[S]} \\ \cdot fr_{A_{sw[S]}} + \upsilon_{abs,gas,air\rightarrow nsl[S]} \cdot fr_{A_{nsl[S]}} \\ + \upsilon_{abs,gas,air\rightarrow asl[S]} \cdot fr_{A_{asl[S]}} \end{pmatrix}}{h_{air[S]}} + \frac{k_{deg,air[S]}}{(3600 \cdot 24)} \quad (93)$$

with

$k_{tot,dry,air[S]}$: total rate constant removal from continental and global atmosphere during dry episodes [s^{-1}]

$\upsilon_{dep,dry,ae[S]}$: continental and global dry aerosol deposition rate [$m \cdot s^{-1}$]

$\upsilon_{abs,gas,air\rightarrow w[S]}$: gas absorption velocity to continental and global fresh and sea water [$m \cdot s^{-1}$]

$fr_A_{fw[S]}$: area fraction continental and global fresh water [-]

$fr_A_{sw[S]}$: area fraction continental and global sea water [-]

$\upsilon_{abs,gas,air\rightarrow sl[S]}$: gas absorption velocity to continental and global natural and agricultural soil [$m \cdot s^{-1}$]

$fr_A_{nsl[S]}$: area fraction continental and global natural soil [-]

$fr_A_{asl[S]}$: area fraction continental and global agricultural soil [-]

$h_{air[S]:}$ mixed height of continental and global air [m]

$k_{deg,air[S]}$: degradation in continental and global air [d^{-1}]

3600·24: conversion factor [$s \cdot d^{-1}$]

Where the dry aerosol deposition rate is described in Equation (94). The gas absorption velocities are described in Section 5.5.2, the area fractions of water in Section 5.2.2, the area fractions of soil in Section 5.2.4, the mixed height of the continental and global air in Section 5.2.1 and the degradation in continental and global air in Section 5.3.1.

The urban, continental and global dry aerosol deposition rate may be obtained from:

$$\upsilon_{\text{dep,dry,ae[S]}} = \upsilon_{\text{dep,air,ae[S]}} \cdot \left(1 - fr_m_{\text{gas,air[S]}}\right) \quad (94)$$

with

$\upsilon_{\text{dep,dry,ae[S]}}$: urban, continental and global dry aerosol deposition rate [m·s^{-1}]

$\upsilon_{\text{dep,air,ae[S]}}$: urban, continental and global deposition velocity of aerosol particles [m·s^{-1}]

$fr_m_{\text{gas,air[S]}}$: urban, continental and global fraction of chemical in the gas phase of air [-]

Where the default value of the deposition velocity of aerosol particles is described in Table 10 and the fraction of chemical in the gas phase of the air is described in Section 5.2.1.

The total rate constant removal from urban atmosphere during wet episodes may be obtained from:

$$k_{\text{tot,wet,air[U]}} = \frac{\upsilon_{\text{wash,ae[U]}} + \upsilon_{\text{wash,gas[U]}} + \upsilon_{\text{abs,gas,air→npav[U]}}}{h_{\text{air[U]}}} \cdot fr_A_{npav[U]} + \frac{k_{\text{deg,air[U]}}}{(3600 \cdot 24)} \quad (95)$$

with

$k_{\text{tot,wet,air[U]}}$: total rate constant removal from urban atmosphere during wet episodes [s^{-1}]

$\upsilon_{\text{wash,ae[U]}}$: urban aerosol washout [m·s^{-1}]

$\upsilon_{\text{wash,gas[U]}}$: urban gas washout [m·s^{-1}]

$h_{\text{air[S]}}$: mixed height of urban air [m]

$\upsilon_{\text{abs,gas,air→npav[U]}}$: gas absorption velocity to urban non-paved surface [m·s^{-1}]

$fr_A_{\text{npav[U]}}$: area fraction urban non-paved surface [-]

$k_{\text{deg,air[U]}}$: degradation in urban air [d^{-1}]

3600·24: conversion factor [s·d^{-1}]

Where the gas washout and the aerosol washout are described in Equations (97) and (98), respectively. The mixed height of urban air is described in Section 5.2.1, the gas absorption velocity to urban non-paved surface in Section 5.5.2, the area fraction of urban non-paved surface in Table 6 and the degradation in urban air in Section 5.3.1.

The total rate constant removal from continental and global atmosphere during wet episodes may be obtained from:

$$k_{\text{tot,wet,air[S]}} = \frac{\upsilon_{\text{wash,ae[S]}} + \upsilon_{\text{wash,gas[S]}} + \left(\begin{matrix}\upsilon_{\text{abs,gas,air→fw[S]}} \cdot fr_{\text{A}_{\text{fw[S]}}} + \upsilon_{\text{abs,gas,air→sw[S]}} \cdot fr_{\text{A}_{\text{sw[S]}}} + \\ \upsilon_{\text{abs,gas,air→nsl[S]}} \cdot fr_{\text{A}_{\text{nsl[S]}}} + \upsilon_{\text{abs,gas,air→asl[S]}} \cdot fr_{\text{A}_{\text{asl[S]}}}\end{matrix}\right)}{h_{\text{air[S]}}} + \frac{k_{\text{deg,air[S]}}}{(3600 \cdot 24)} \quad (96)$$

with

$k_{\text{tot,wet,air[S]}}$: total rate constant removal from continental and global atmosphere during wet episodes [s^{-1}]

$\upsilon_{\text{wash,ae[S]}}$: continental and global aerosol washout [$m \cdot s^{-1}$]

$\upsilon_{\text{wash,gas[S]}}$: continental and global gas washout [$m \cdot s^{-1}$]

$\upsilon_{\text{abs,gas,air→fw[S]}}$: gas absorption velocity to continental and global fresh water [$m \cdot s^{-1}$]

$\upsilon_{\text{abs,gas,air→sw[S]}}$: gas absorption velocity to continental and global sea water [$m \cdot s^{-1}$]

$fr_A_{\text{fw[S]}}$: area fraction continental and global fresh water [-]

$fr_A_{\text{sw[S]}}$: area fraction continental and global sea water [-]

$\upsilon_{\text{abs,gas,air→nsl[S]}}$: gas absorption velocity to continental and global natural soil [$m \cdot s^{-1}$]

$\upsilon_{\text{abs,gas,air→asl[S]}}$: gas absorption velocity to continental and global agricultural soil [$m \cdot s^{-1}$]

$fr_A_{nsl[S]}$: area fraction continental and global natural soil [-]

$fr_A_{\text{fasl[S]}}$: area fraction continental and global agricultural soil [-]

$h_{\text{air[S]}}$: mixed height continental and global air [m]

$k_{\text{deg,air[S]}}$: degradation in continental and global air [d^{-1}]

3600·24: conversion factor [$s \cdot d^{-1}$]

Where the gas washout and the aerosol washout are described in Equations (97) and (98), respectively. The gas absorption velocities are described in Section 5.5.2, the area fractions of water in Section 5.2.2, the area fractions of soil in Section 5.2.4, the mixed height of the continental and global air in Section 5.2.1 and the degradation in continental and global air in Section 5.3.1.

The urban, continental and global gas washout may be obtained from:

$$\upsilon_{\text{wash,gas[S]}} = fr_m_{\text{gas,air[S]}} \cdot \frac{t_{\text{dry[S]}} + t_{\text{wet[S]}}}{t_{\text{wet[S]}}} \cdot \frac{\upsilon_{\text{rain[S]}}}{K_{\text{aw[S]}} \cdot fr_m_{\text{cldw}} + 0.00000005555} \quad (97)$$

with

$\upsilon_{\text{wash,gas[S]}}$: urban, continental and global gas washout [$m \cdot s^{-1}$]

$fr_m_{\text{gas,air[S]}}$: urban, continental and global fraction of chemical in gas phase of the air [-]

$t_{\text{dry[S]}}$: urban, continental and global average duration of dry episodes [s]

$t_{wet[S]}$: urban, continental and global average duration of wet episodes [s]

$\upsilon_{rain[S]}$: urban, continental and global annual average precipitation [m·s^{-1}]

$K_{aw[S]}$: urban, continental and global dimensionless air/water partition coefficient of original species [-]

fr_m_{cldw}: urban, continental and global fraction original species in cloud water [-]

0.00000005555: constant description [-]

Where the fraction of chemical in gas phase of the air is described in Section 5.2.1, the annual average precipitation is described in Table 10, the $K_{aw[S]}$ in Section 5.4.1, the fraction original species in cloud water in Section 5.2.1 and the constant is described in Table 10. The average duration of dry episodes is described in Equation (99) and of wet episodes in Equation (100).

The urban, continental and global aerosol washout may be obtained from:

$$\upsilon_{wash,ae[S]} = \left(1 - fr_m_{gas,air[S]}\right) \cdot \frac{t_{dry[S]} + t_{wet[S]}}{t_{wet[S]}} \cdot \upsilon_{rain[S]} \cdot CE_{ae[S]} \quad (98)$$

with

$\upsilon_{wash,ae[S]}$: urban, continental and global aerosol washout [m·s^{-1}]

$fr_m_{gas,air[S]}$: fraction of chemical in gas phase of the urban, continental and global air [-]

$t_{dry[S]}$: urban, continental and global average duration of dry episodes [s]

$t_{wet[S]}$: urban, continental and global average duration of wet episodes [s]

$\upsilon_{rain[S]}$: urban, continental and global annual average precipitation [m·s^{-1}]

$CE_{ae[S]}$: urban, continental and global aerosol collection efficiency [-]

Where the fraction of chemical in the gas phase of the air is described in Section 5.2.1, the annual average precipitation and the aerosol collection efficiency are described in Table 10. The average duration of dry episodes is described in Equation (99) and of wet episodes in Equation (100).

The urban, continental and global average duration of dry episodes is described by Jolliet & Hauschild (2005) and may be obtained from:

$$t_{dry[S]} = \left(\frac{80}{24}\right) \cdot \left(1 - \frac{\upsilon_{rain[S]}}{\frac{0.0013}{3600}}\right) \quad (99)$$

with

$t_{dry[S]}$: urban, continental and global average duration of dry episodes [d]

$\upsilon_{rain[S]}$: urban, continental and global annual average precipitation [m·s^{-1}]

80: constant definition [h]

24: conversion factor [h·d^{-1}]

0.0013: constant definition [m·h^{-}1]

3600: conversion factor [s·h^{-1}]

Where the annual average precipitation is described in Table 10.

The urban, continental and global average duration of dry episodes is described by Jolliet & Hauschild (2005) and may be obtained from:

$$t_{\text{wet[S]}} = \left(\frac{80}{24}\right) \cdot \left(\frac{\upsilon_{\text{rain[S]}}}{\frac{0.0013}{3600}}\right) \quad (100)$$

with

$t_{\text{wet[S]}}$: urban, continental and global average duration of wet episodes [d]

$\upsilon_{\text{rain[S]}}$: urban, continental and global annual average precipitation [m·s^{-1}]

80: constant definition [h]

24: conversion factor [h·d^{-1}]

0.0013: constant definition [m·h^{-}1]

3600: conversion factor [s·h^{-1}]

Where the annual average precipitation is described in Table 10.

5.5.2 Air to water and soil

The deposition flow from the air to water and soils exists out of a deposition and gas absorption of the chemical. At the urban scale, no water and soil compartments are considered. The deposition flow from urban air is considered to go to the paved surface of the urban scale, from which it will runoff to the continental fresh water. The overall mass transfer coefficient for gas absorption may be estimated using the classical two-film resistance model (Schwarzenbach *et al.,* 1993). In the case of transport across the air/water interface, the overall transfer coefficients follow from summation of the resistances at the water- and air sides of the interface. In the case of transport across the air/soil interface, the soil-side of the interface is treated as a pair of parallel resistances (air phase and water phase of the soil).

The deposition flow from the urban air to the continental freshwater may be obtained from:

$$\text{k}_{\text{air}\rightarrow\text{fw [U}\rightarrow\text{C]}} = \left(k_{dep,air[U]} + \frac{\upsilon_{abs,gas,air\rightarrow pav[U]}}{h_{air[U]}}\right) \cdot fr_{A_{pav[U]}} \cdot (3600 \cdot 24) \quad (101)$$

with

$\text{k}_{\text{air}\rightarrow\text{fw[U}\rightarrow\text{C]}}$: transfer rate urban air to continental fresh water [d^{-1}]

$K_{dep,air[U]}$:	mean urban atmospheric deposition rate [s^{-1}]
$v_{abs,gas,air→pav[U]}$:	velocity of urban air to urban paved surface [$m \cdot s^{-1}$]
$fr_A_{pav[U]}$:	area fraction urban paved [-]
$h_{air[U]}$:	mixed height of urban air [m]
3600·24:	conversion factor [$s \cdot d^{-1}$]

Where the mean atmospheric deposition rate is described in Section 5.5.1, the area fraction unpaved in Table 6, and the mixed height of the urban air in Section 5.2.1. The velocity of urban air to urban paved surface is described in Equation (102).

The velocity of urban air to urban paved or non-paved surface may be obtained from:

$$v_{abs,gas,air→pav[U]} = fr_m_{gas,air[U]} \cdot \frac{v_{m,air,air|sl[U]} \cdot v_{m,sl,air|sl[U]}}{v_{m,air,air|sl[U]} \cdot \left(\frac{K_{aw[U]} \cdot fr_m_{nsl}}{K_{sl|w,nsl[G]}}\right) + v_{m,sl,air|sl[U]}} \quad (102)$$

with

$v_{abs,gas,air→pav[U]}$: [$m \cdot s^{-1}$]	gas absorption velocity to paved and unpaved surface, urban
$fr_m_{gas,air[U]}$:	fraction of chemical in gas phase air, urban [-]
$v_{m,air,air\|sl[U]}$:	partial mass transfer coefficient air side of air/soil interface, urban [$m \cdot s^{-1}$]
$v_{m,sl,air\|sl[U]}$:	partial mass transfer coefficient soil side of air/soil interface, urban [$m \cdot s^{-1}$]
$K_{aw[U]}$:	dimensionless air/water partition coefficient of original species, urban [-]
fr_m_{nsl}:	fraction original species in natural soil [-]
$K_{sl\|w,nsl[G]}$:	dimensionless soil/water partition coefficient other soil, global [$m \cdot s^{-1}$]

Where the fraction of chemical in the gas phase of urban air is described in Section 5.2.1, the $K_{aw[U]}$ is described in Section 5.4.1, the fraction original species in natural soil is described in Section 5.2.4 and the $K_{sl\ |\ w,\ nsl}$ is described in Section 5.4.4. The partial mass transfer coefficients at air/soil interface are described in Equations (103) till (105).

Diffusive transport between air and soil occurs using the two-film resistance model as described by Schwarzenbach *et al.* (1993), where the constants are set by Mackay (2001). The urban partial mass transfer coefficient at the air side of the air/soil interface may be obtained from:

$$v_{m,air,air|sl[S]} = \frac{0.43}{\frac{3600 \cdot 24}{0.00475}} \quad (103)$$

with

$\upsilon_{m,air,air|sl[S]}$: partial mass transfer coefficient air side of air/soil interface [m·s^{-1}]

0.43: constant definition [m·d^{-1}]

3600·24: conversion factor [s·d^{-1}]

0.00475: constant definition [-]

The urban partial mass transfer coefficient at the soil side of the air/soil interface may be obtained from:

$$\upsilon_{m,sl,air|sl[U]} = \upsilon_{m,sl,air|sl[C]} \quad (104)$$

with

$\upsilon_{m,sl,air|sl[U]}$: partial mass transfer coefficient soil side of air/soil interface, urban [m·s^{-1}]

$\upsilon_{m,sl,air|sl[C]}$: partial mass transfer coefficient soil side of air/soil interface, coefficient [m·s^{-1}]

Where the continental partial mass transfer coefficient at the soil side of air/soil interface may be obtained from:

$$\upsilon_{m,sl,air|sl[S]} = \upsilon_{eff,adv,sl[S]} + \frac{D_{eff,nsl[S]}}{h_{nsl,penetr[S]}} \quad (105)$$

with

$\upsilon_{m,sl,air|sl[S]}$: partial mass transfer coefficient soil side of air/soil interface [m·s^{-1}]

$\upsilon_{eff,adv,sl[S]}$: effective advective transport in natural soil [m·s^{-1}]

$D_{eff,nsl[S]}$: effective diffusion coefficient in natural soil [m^2·s^{-1}]

$h_{nsl.penetr[S]}$: penetration depth natural soil [m]

Where the effective advective transport in, the effective diffusion coefficient and the penetration depth of the continental and global natural and agricultural soil are described in Section 5.2.4.

The deposition flow from the continental and global airs to the continental and global natural and agricultural soils may be obtained from:

$$k_{air\rightarrow sl[S]} = \left(k_{dep,air[S]} + \frac{\upsilon_{abs,gas,air\rightarrow sl[S]}}{h_{air[S]}}\right) \cdot fr_A_{sl[S]} \cdot (3600 \cdot 24) \quad (106)$$

with

$k_{air\rightarrow sl[S]}$: transfer rate continental and global air to continental and global natural and agricultural soil [d^{-1}]

$K_{dep,air[S]}$: mean continental and global atmospheric deposition rate [s^{-1}]

$\upsilon_{abs,gas,air\rightarrow sl[S]}$:	velocity of continental and global air to continental and global natural and agricultural soil [m·s^{-1}]
$fr_A_{sl[S]}$:	area fraction continental and global natural and agricultural soil [-]
$h_{air[S]}$:	mixed height of continental and global air [m]
3600·24:	conversion factor [s·d^{-1}]

Where the mean continental and global atmospheric deposition rate is described in Section 5.5.1, the area fraction continental and global natural and agricultural soil is described in Section 5.2.4 and the mixed height of continental and global air in Section 5.2.1. The velocity of continental and global air to soil is described in Equation (107).

The velocity of continental and global air to continental and global natural and agricultural soil may be obtained from:

$$\upsilon_{abs,gas,air\rightarrow sl[S]} = fr_m_{gas,air[S]} \cdot \frac{\upsilon_{m,air,air|sl[S]} \cdot \upsilon_{m,sl,air|sl[S]}}{\upsilon_{m,air,air|sl[S]} \cdot \left(K_{aw[S]} \cdot \frac{fr_m_{sl}}{K_{sl|w,sl[S]}}\right) + \upsilon_{m,sl,air|sl[S]}} \quad (107)$$

with

$\upsilon_{abs,gas,air\rightarrow sl[S]}$:	gas absorption velocity to continental and global natural and agricultural soil [m·s^{-1}]
$fr_m_{gas,air[S]}$:	fraction of chemical in gas phase of continental and global air [-]
$\upsilon_{m,air,air\,|\,sl[S]}$:	partial mass transfer coefficient air side of continental and global air/soil interface [m·s^{-1}]
$\upsilon_{m,sl,air\,|\,sl[S]}$:	partial mass transfer coefficient soil side of continental and global air/soil interface [m·s^{-1}]
$K_{aw[S]}$:	dimensionless air/water partition coefficient of continental and global original species [-]
fr_m_{sl}:	fraction original species in continental and global natural and agricultural soil [-]
$K_{sl\,|\,w,sl\,[S]}$:	dimensionless soil/water partition coefficient continental and global natural and agricultural soil [m·s^{-1}]

Where the fraction of chemical in the gas phase of continental and global air is described in Section 5.2.1, the $K_{aw[S]}$ is described in Section 5.4.1, the fraction original species in continental and global natural and agricultural soil is described in Section 5.2.4 and the $K_{sl\,|\,w,sl[S]}$ is described in Section 5.4.4. The partial mass transfer coefficients at air/soil interface are described in Equations (103) till (105).

The deposition flow from the continental and global airs to the continental and global fresh and sea waters may be obtained from:

$$k_{\text{air}\rightarrow\text{w [S]}} = (k_{\text{dep,air[S]}} + \frac{\upsilon_{\text{abs,gas,air}\rightarrow\text{w[S]}}}{h_{\text{air[S]}}}) \cdot fr_\text{A}_{\text{w[S]}} \cdot (3600 \cdot 24) \quad (108)$$

with

$k_{\text{air}\rightarrow\text{w[S]}}$:	transfer rate continental and global air to continental and global fresh and sea water [d^{-1}]
$K_{\text{dep,air[S]}}$:	mean continental and global atmospheric deposition rate [s^{-1}]
$\upsilon_{abs,gas,air\rightarrow w[S]}$:	velocity of continental and global air to continental and global fresh and sea water [$m \cdot s^{-1}$]
$fr_A_{w[S]}$:	area fraction continental and global fresh and sea water [-]
$h_{air[S]}$:	mixed height of continental and global air [m]
3600·24:	conversion factor [$s \cdot d^{-1}$]

Where the mean continental and global atmospheric deposition rate is described in Section 5.5.1, the area fraction continental and global fresh and sea water is described in Section 5.2.2 and the mixed height of continental and global air in Section 5.2.1. The velocity of continental and global air to soil is described in Equation (107).

The velocity of continental and global air to continental and global fresh and sea water may be obtained from:

$$\upsilon_{\text{abs,gas,air}\rightarrow\text{fw[S]}} = fr_{m_{\text{gas,air[S]}}} \cdot \left(\frac{\upsilon_{\text{m,air,air|w[S]}} \cdot \upsilon_{\text{m,w,air|w[S]}}}{\upsilon_{\text{m,air,air|w[S]}} \cdot K_{\text{aw[S]}} \cdot fr_{m_{\text{fw}}} + \upsilon_{\text{m,w,air|w[S]}}} \right) \quad (109)$$

with

$\upsilon_{\text{abs,gas,air}\rightarrow\text{w[S]}}$:	gas absorption velocity to continental and global fresh and sea water [$m \cdot s^{-1}$]
$fr_m_{\text{gas,air[S]}}$:	fraction of chemical in gas phase of continental and global air [-]
$\upsilon_{\text{m,air,air}\,|\,\text{w[S]}}$:	partial mass transfer coefficient air side of continental and global air/water interface [$m \cdot s^{-1}$]
$\upsilon_{\text{m,w,air}\,|\,\text{w[S]}}$:	partial mass transfer coefficient water side of continental and global air/water interface [$m \cdot s^{-1}$]
$K_{\text{aw[S]}}$:	dimensionless air/water partition coefficient of continental and global original species [-]
fr_m_{w}:	fraction original species in continental and global fresh and sea water [-]

Where the fraction of chemical in the gas phase of continental and global air is described in Section 5.2.1, the $K_{\text{aw[S]}}$ is described in Section 5.4.1 and the fraction original species in

continental and global fresh and sea water is described in Section 5.2.2. The partial mass transfer coefficients at air/water interface are described in Equations (110) and (111).

Diffusive transport between air and water occurs using the two-film resistance model as described by Schwarzenbach *et al.* (1993), where the constants are set by Mackay (2001). The continental and global partial mass transfer coefficient at the air side of the air/water interface may be obtained from:

$$\upsilon_{\mathrm{m,air,air|w[S]}} = 0.01 \cdot \left(0.3 + 0.2 \cdot u_{[S]}\right) \cdot \frac{0.018^{(0.67 \cdot 0.5)}}{MW} \quad (110)$$

with

$\upsilon_{\mathrm{m,air,air|w[S]}}$: continental and global partial mass transfer coefficient air side of air/water interface [m·s^{-1}]

MW: molecular weight [kg·mol^{-1}]

$u_{[S]}$: urban, continental and global wind speed [m·s^{-1}]

0.01: constant definition

0.3: constant definition

0.2: constant definition

0.018: constant definition

0.67: constant definition

0.5: constant definition

Where the molecular weight is described in the substance data and the wind speed is described in Table 10 (urban), Table 4 (continental) and Table 5 (global).

The continental and global partial mass transfer coefficient at the water side of the air/water interface may be obtained from:

$$\upsilon_{\mathrm{m,w,air|w[S]}} = 0.01 \cdot \left(0.0004 + 0.00004 \cdot {u_{[S]}}^2\right) \cdot \frac{0.032^{(0.5 \cdot 0.5)}}{MW} \quad (111)$$

with

$\upsilon_{\mathrm{m,w,air|w[S]}}$: continental and global partial mass transfer coefficient water side of air/water interface [m·s^{-1}]

$u_{[S]}$: continental and global wind speed [m·s^{-1}]

MW: molecular weight [kg·mol^{-1}]

0.01: constant definition

0.0004: constant definition

0.00004: constant definition

2: constant definition

0.032: constant definition

0.5: constant definition

Where the molecular weight is described in the substance data and the wind speed is described in Table 10 (urban), Table 4 (continental) and Table 5 (global).

5.5.3 Water and soil to air

The overall mass transfer coefficient for volatilization may be estimated using the classical two-film resistance model. In the case of transport across the air/water interface, the overall transfer coefficients follow from summation of the resistances at the water- and air sides of the interface. In the case of transport across the air/soil interface, the soil-side of the interface is treated as a pair of parallel resistances (air phase and water phase of the soil).

The transfer rate from the continental and global natural and agricultural soil may be obtained from:

$$k_{\mathrm{sl}\rightarrow\mathrm{air}\,[\mathrm{S}]} = \frac{v_{\mathrm{volat,sl[S]}}}{h_{\mathrm{sl[S]}}} \cdot (3600 \cdot 24) \tag{112}$$

with

$k_{\mathrm{sl}\rightarrow\mathrm{air[S]}}$: transfer rate from continental and global natural and agricultural soil to air [d^{-1}]

$v_{\mathrm{volat,sl[S]}}$: volatilization velocity from continental and global natural and agricultural soil to air [$m \cdot s^{-1}$]

$h_{\mathrm{sl[S]}}$: depth of continental and global natural and agricultural soil [m]

3600·24: conversion factor [$s \cdot d^{-1}$]

Where the volatilization velocity from soil to air is described in Equation (113) and the depth of soil is described in Section 5.2.4.

The volatilization velocity from continental and global natural and agricultural soil to air may be obtained from:

$$v_{\mathrm{volat,sl}\rightarrow\mathrm{air[S]}} = \frac{v_{\mathrm{m,air,air|sl[S]}} \cdot v_{\mathrm{m,sl,air|sl[S]}}}{v_{\mathrm{m,air,air|sl[S]}} + \frac{v_{\mathrm{m,sl,air|sl[S]}}}{K_{\mathrm{aw[S]}} \cdot \frac{fr_m_{\mathrm{sl}}}{K_{\mathrm{sl|w,sl[S]}}}}} \tag{113}$$

with

$v_{\mathrm{volat,sl}\rightarrow\mathrm{air[S]}}$: volatilization velocity from continental and global natural and agricultural soil [$m \cdot s^{-1}$]

$v_{\mathrm{m,air,air\,|\,sl[S]}}$: continental and global partial mass transfer coefficient air side of air/soil interface [$m \cdot s^{-1}$]

$\upsilon_{m,sl,air|sl[S]}$: continental and global partial mass transfer coefficient soil side of air/soil interface [m·s^{-1}]

$K_{aw[S]}$: continental and global dimensionless air/water partition coefficient of original species [-]

fr_m_{sl}: fraction original species in natural and agricultural soil [-]

$K_{sl|w,sl[S]}$: dimensionless soil/water partition coefficient continental and global natural and agricultural soil [m·s^{-1}]

Where partial mass transfer coefficients of the air/soil interface are described in Section 5.5.2, the $K_{aw[S]}$ in Section 5.4.1, the fraction original species in soil in Section 5.2.4 and the $K_{sl|w,sl[S]}$ in Section 5.4.4.

The transfer rate from the continental and global fresh and sea water may be obtained from:

$$k_{w\rightarrow air[S]} = \frac{\upsilon_{volat,w[S]}}{h_{w[S]}} \cdot (3600 \cdot 24) \quad (114)$$

with

$k_{w\rightarrow air[S]}$: transfer rate from continental and global fresh and sea water to air [d^{-1}]

$\upsilon_{volat,wl[S]}$: volatilization velocity from continental and global fresh and sea water to air [m·s^{-1}]

$h_{w[S]}$: mixed depth of continental and global fresh and sea water [m]

3600·24: conversion factor [s·d^{-1}]

Where the volatilization velocity from soil to air is described in Equation (113) and the depth of soil is described in Section 5.2.2.

The volatilization velocity from continental and global fresh and sea water to air may be obtained from:

$$\upsilon_{volat,w\rightarrow air[S]} = \left(\cdot \frac{\upsilon_{m,air,air|w[S]} \cdot \upsilon_{m,w,air|w[S]}}{\upsilon_{m,air,air|w[S]} \cdot K_{aw[S]} \cdot fr_m_{w} + \upsilon_{m,w,air|w[S]}} \right) \cdot K_{aw[S]} \cdot fr_m_{w} \cdot fr_m_{diss,w[S]} \quad (115)$$

with

$\upsilon_{volat,w\rightarrow air[S]}$: volatilization velocity from continental and global fresh and sea water [m·s^{-1}]

$\upsilon_{m,air,air|w[S]}$: continental and global partial mass transfer coefficient air side of air/soil interface [m·s^{-1}]

$\upsilon_{m,w,air|w[S]}$: continental and global partial mass transfer coefficient water side of air/water interface [m·s^{-1}]

$K_{aw[S]}$: continental and global dimensionless air/water partition coefficient of original species [-]

fr_m_{w}: fraction original species in fresh and sea water [-]

$fr_m_{diss,w[S]}$: fraction of chemical dissolved in continental and global fresh and sea water [-]

Where partial mass transfer coefficients of the air/water interface are described in Section 5.5.2, the $K_{aw[S]}$ in Section 5.4.1, the fraction original species in water and the fraction of chemical dissolved in water in Section 5.2.2.

5.5.4 Soil to water transfer

The transfer of a chemical from the natural and agricultural soil to the freshwater occurs only at the continental and global scale. At the urban scale, the chemical will flow from the air to the paved surface and non-paved surface. From the paved surface, it will be transferred to the continental freshwater as described in Equation (101) from Section 5.5.2. While from the non-paved surface the chemical will be removed as described in Equation (119) from Section 5.5.5.

The transfer rate from the continental and global natural and agricultural soil to the freshwater may be obtained from:

$$k_{sl\rightarrow fw\,[S]} = \frac{\left(\frac{v_{rain[S]} \cdot fr_V_{rain,runoff,sl[S]}}{K_{sl|w,sl[S]}} + v_{sl[S]}\right)}{h_{sl[S]}} \cdot (3600 \cdot 24) \quad (116)$$

with

$k_{sl\rightarrow fw[S]}$: transfer rate continental and global natural and agricultural soil to fresh water [d^{-1}]

$v_{rain[S]}$: annual average precipitation [$m \cdot s^{-1}$]

$fr_V_{rain,runoff,sl[S]}$: volume fraction of precipitation running off from continental and global natural and agricultural soil [-]

$v_{sl[S]}$: erosion of continental and global natural and agricultural soil [$m \cdot s^{-1}$]

$k_{sl|w,sl[S]}$: partition coefficient continental and global natural and agricultural soil/water [-]

$h_{sl[S]}$: depth of continental and global natural and agricultural soil [m]

3600·24: conversion factor [$s \cdot d^{-1}$]

Where the annual average precipitation is described in Table 10, the volume fraction of precipitation running off and the erosion of soils in Table 4 (continental) and in Table 5 (global), the $K_{sl\,|\,w,sl[S]}$ in Section 5.4.4 and the depth of the soils in Section 5.2.4.

5.5.5 Water to soil transfer

The transfer rate from the continental and global fresh water to agricultural soil may be obtained from:

$$k_{\mathrm{fw}\rightarrow\mathrm{asl\,[S]}} = \frac{v_{\mathrm{fw[S]}} \cdot fr_A_{\mathrm{asl[S]}}}{h_{\mathrm{fw[S]}} \cdot fr_A_{\mathrm{fw[S]}}} \cdot (3600 \cdot 24) \qquad (117)$$

with

$k_{\mathrm{fw}\rightarrow\mathrm{asl[S]}}$:	transfer rate continental and global fresh water to agricultural soil [d^{-1}]
$v_{\mathrm{fw[S]}}$:	irrigation from continental and global fresh water to agricultural soil [$m \cdot s^{-1}$]
$fr_A_{asl[S]}$:	area fraction continental and global agricultural soil [-]
$h_{\mathrm{fw[S]}}$:	depth of continental and global fresh water [m]
$fr_A_{fw[S]}$:	area fraction continental and global fresh water [-]
3600·24:	conversion factor [$s \cdot d^{-1}$]

Where the area fraction agricultural soil and continental and global fresh water are described in Equations (18), (44) and (45), respectively. The depth of the fresh water is described in Table 10.

The irrigation from continental and global fresh water to agricultural soil may be obtained from:

$$v_{\mathrm{fw[S]}} = \frac{v_{\mathrm{[S]}}}{A_{[C]} \cdot fr_{A_{\mathrm{asl[C]}}} + A_{[G]} \cdot fr_{A_{\mathrm{asl[G]}}}} \cdot \frac{0.6}{(3600 \cdot 24 \cdot 365)} \qquad (118)$$

with

$v_{\mathrm{fw[S]}}$:	irrigation from continental and global fresh water to agricultural soil [$m \cdot s^{-1}$]
$v_{\mathrm{[S]}}$:	irrigation at continental and global scale [km^3]
$A_{[S]}$:	continental and global system area [km^2]
$fr_A_{asl[S]}$:	area fraction continental and global agricultural soil [-]
0.6:	constant [y]
3600·24·365:	conversion factor [$s \cdot y^{-1}$]

Where the irrigation and the system areas are described in Table 4(continental) and Table 5 (global). The area fractions agricultural soil are described in Equation (44) (continental) and (45) (global).

5.5.6 Removal by deposition, burial and leaching

Removal of the chemical from the system occurs through deposition from the urban air to the non-paved surface, by burial from the fresh and sea water through the sediment phase and by leaching from the natural and agricultural soils.

The transfer rate form the urban air to the non-paved surface may be obtained from:

$$k_{\mathrm{air[U]\rightarrow npav[U]}} = \left(k_{\mathrm{mean,air[U]}} + \frac{\upsilon_{\mathrm{abs,gas,air\rightarrow npav[U]}}}{h_{\mathrm{air[U]}}}\right) \cdot fr_{\mathrm{A_{npav[U]}}} \cdot (3600 \cdot 24) \quad (119)$$

with

$k_{\mathrm{mean,air[U]}}$: mean rate constant removal from urban atmosphere [s^{-1}]

$\upsilon_{\mathrm{abs,gas,air\rightarrow npav[U]}}$: gas absorption velocity to urban non-paved surface [$m \cdot s^{-1}$]

$fr_A_{\mathrm{npav[U]}}$: area fraction urban non-paved surface [-]

$h_{\mathrm{air[U]}}$: mixed height urban air [m]

3600·24: conversion factor [$s \cdot d^{-1}$]

Where the mean rate constant removal from atmosphere is described in Section 5.5.1, the area fraction non-paved surface in Table 6, and the mixed height of air in Section 5.2.1. The gas absorption velocity to urban non-paved surface is described in Equation (120).

The gas absorption velocity to urban non-paved surface may be obtained from:

$$\upsilon_{\mathrm{abs,gas,air\rightarrow npav[U]}} = \frac{fr_m_{\mathrm{gas,air[U]}} \cdot \upsilon_{\mathrm{m,air,air|sl[U]}} \cdot \upsilon_{\mathrm{m,sl,air|sl[U]}}}{\upsilon_{\mathrm{m,air,air|sl[U]}} \cdot \left(\frac{K_{\mathrm{aw[U]}} \cdot fr_m_{\mathrm{nsl}}}{K_{\mathrm{sl|w,nsl[G]}}}\right) + \upsilon_{\mathrm{m,sl,air|sl[U]}}} \quad (120)$$

with

$\upsilon_{\mathrm{abs,gas,air\rightarrow npav[U]}}$: gas absorption velocity to urban non-paved surface [$m \cdot s^{-1}$]

$fr_m_{\mathrm{gas,air[U]}}$: fraction of chemical in gas phase urban air [-]

$\upsilon_{\mathrm{m,air,air|sl[U]}}$: urban partial mass transfer coefficient air side of air/soil interface [$m \cdot s^{-1}$]

$\upsilon_{\mathrm{m,sl,air|sl[U]}}$: urban partial mass transfer coefficient soil side of air/soil interface [$m \cdot s^{-1}$]

$K_{\mathrm{aw[U]}}$: urban dimensionless air/water partition coefficient of original species [-]

fr_m_{nsl}: fraction original species in natural soil [-]

$K_{\mathrm{sl|w,nsl[G]}}$: dimensionless soil/water partition coefficient of natural soil [$m \cdot s^{-1}$]

Where the fraction of chemical in gas phase of air is described in Section 5.2.1, the partial mass transfer coefficients of air/soil interface in Section 5.5.2, the $K_{\mathrm{aw[S]}}$ in Section 5.4.1, the fraction original species in natural soil in Section 5.2.4 and the $K_{\mathrm{sl|w,nsl[S]}}$ in Section 5.4.4.

The transfer rate from fresh and sea water by sedimentation and burial may be obtained from:

$$k_{w\rightarrow wsd[S]} = \left(\left(\frac{\upsilon_{ads,w\rightarrow wsd[S]} + \upsilon_{sed,w\rightarrow wsd[S]}}{h_w} \right) - \frac{\left(\frac{\upsilon_{ads,w\rightarrow wsd[S]} + \upsilon_{sed,w\rightarrow wsd[S]}}{h_w} \right) * \left(\frac{\upsilon_{res,wsd\rightarrow w[S]} + \upsilon_{des,wsd\rightarrow w[S]}}{h_{wsd}} \right)}{\left(\frac{\upsilon_{res,wsd\rightarrow w[S]} + \upsilon_{des,wsd\rightarrow w[S]} + \upsilon_{burial,wsd[S]}}{h_{wsd}} + \frac{k_{deg,wsd[S]}}{(3600 \cdot 24)} \right)} \right) \cdot (3600 \cdot 24) \quad (121)$$

with

$k_{w\rightarrow wsd[S]}$: transfer rate continental and global fresh and sea water to continental and global fresh and sea water sediment [d^{-1}]

$\upsilon_{ads,w\rightarrow wsd[S]}$: adsorbtion velocity from continental and global fresh and sea water to continental and global fresh and sea water sediment [$m \cdot s^{-1}$]

$\upsilon_{sed,w\rightarrow wsd[S]}$: sedimentation velocity from continental and global fresh and sea water to continental and global fresh and sea water sediment [$m \cdot s^{-1}$]

$h_{w[S]}$: mixed depth of continental and global fresh and sea water [m]

$\upsilon_{res,wsd\rightarrow w[S]}$: resuspension velocity from continental and global fresh and sea water sediment to continental and global fresh and sea water [$m \cdot s^{-1}$]

$\upsilon_{des,wsd\rightarrow w[S]}$: desorbtion velocity from continental and global fresh and sea water sediment to continental and global fresh and sea water [$m \cdot s^{-1}$]

$h_{wsd[S]}$: height of continental and global fresh and sea water sediment[m]

$\upsilon_{burial,wsd[S]}$: burial velocity from continental and global fresh and sea water sediment [$m \cdot s^{-1}$]

$k_{deg,wsd[S]}$: degradation rate in continental and global fresh and sea water sediment [d^{-1}]

3600·24: conversion factor [$s \cdot d^{-1}$]

Where the mixed depth of waters is described in Section 5.2.2, the height of the sediments and the burial velocities in Section 5.2.3 and the degradation rates of sediments in Section 5.3.3. The adsorbtion velocity is described in Equation (122), the sedimentation velocity in Equation (123), the desorption velocity in Equation (124) and the resuspension velocity in Equation (125).

The adsorbtion velocity from continental and global fresh and sea water to continental and global fresh and sea water sediment may be obtained from:

$$\upsilon_{\mathrm{ads,w\rightarrow wsd[S]}} = \frac{\upsilon_{\mathrm{m,w,w|sd[S]}} \cdot \upsilon_{\mathrm{m,sd,w|sd[S]}}}{\upsilon_{\mathrm{m,w,w|sd[S]}} + \upsilon_{\mathrm{m,sd,w|sd[S]}}} \cdot fr_m_{\mathrm{diss,w[S]}} \quad (122)$$

with

$\upsilon_{\mathrm{ads,w\rightarrow wsd[S]}}$: adsorption velocity to continental and global fresh and sea water sediment [m·s^{-1}]

$\upsilon_{\mathrm{m,w,w\,|\,sd[S]}}$: continental and global partial mass transfer coefficient water side of water/sediment interface [m·s^{-1}]

$\upsilon_{\mathrm{m,sd,w\,|\,sd[S]}}$: continental and global partial mass transfer coefficient sediment side of water/sediment interface [m·s^{-1}]

$fr_m_{\mathrm{diss,w[S]}}$: fraction of chemical dissolved in continental and global fresh and sea water [-]

Where the partial mass transfer coefficients water/sediment interface are described in Table 10 and the fraction of chemical dissolved in the water is described in Section 5.2.2.

The sedimentation velocity from continental and global fresh and sea water to continental and global fresh and sea water sediment may be obtained from:

$$\upsilon_{\mathrm{sed,w\rightarrow wsd[S]}} = \left(\upsilon_{\mathrm{sed,w[S]}} \cdot fr_{\mathrm{V_{solid,sd[S]}}} \cdot \frac{\rho_{\mathrm{sd,sl}}}{C_{\mathrm{susp,w[S]}}}\right) \cdot \left(\left(\frac{K_{\mathrm{susp\,|\,w[S]}} \cdot C_{\mathrm{susp,w[S]}}}{1000}\right) \cdot fr_m_{\mathrm{diss,w[S]}}\right) \quad (123)$$

with

$\upsilon_{\mathrm{sed,w\rightarrow wsd[S]}}$: sedimentation velocity to continental and global fresh and sea water sediment [m·s^{-1}]

$\upsilon_{\mathrm{sed,w[S]}}$: gross sedimentation rate from continental and global fresh and sea water [m·s^{-1}]

$fr_V_{\mathrm{solid,sd[S]}}$: volume fraction solids in continental and global sediment [-]

$\rho_{\mathrm{sd,sl}}$: mineral density of sediment and soil [kg·m^{-3}]

$C_{\mathrm{susp,w[S]}}$: concentration suspended matter in continental and global fresh and sea water [kg·m^{-3}]

$K_{\mathrm{susp\,|\,w\,[S]}}$: continental and global fresh and sea water suspended solids/water partition coefficient [L·kg^{-1}]

1000: conversion factor [dm^3·m^{-3}]

$fr_m_{\mathrm{diss,w[S]}}$: fraction of chemical dissolved in continental and global fresh and sea water [-]

Where the gross sedimentation rate from water and the concentration suspended matter in the water are described in Section 5.2.2, the volume fraction solids in the sediment in Section 5.2.3, the mineral density of sediment and soil are described in Table 10, the $K_{susp\ |\ w[S]}$ in Section 5.4.3 and the fraction of chemical dissolved in the water in Section 5.2.2.

The desorption velocity from continental and global fresh and sea water sediment to continental and global fresh and sea water may be obtained from:

$$\upsilon_{des,wsd\rightarrow w[S]} = \frac{\left(\frac{\upsilon_{m,w,w\,|\,sd[S]} \cdot \upsilon_{m,sd,w\,|\,sd[S]}}{\upsilon_{m,w,w\,|\,sd[S]} + \upsilon_{m,sd,w\,|\,sd[S]}}\right)}{K_{sd\,|\,w[S]}} \quad (124)$$

with

$\upsilon_{des,wsd\rightarrow w[S]}$: desorption velocity from continental and global fresh and sea water sediment [m·s^{-1}]

$\upsilon_{m,w,w\,|\,sd[S]}$: continental and global partial mass transfer coefficient water side of water/sediment interface [m·s^{-1}]

$\upsilon_{m,sd,w\,|\,sd[S]}$: continental and global partial mass transfer coefficient sediment side of water/sediment interface [m·s^{-1}]

$K_{sd\,|\,w,w[S]}$: dimensionless sediment/water partition coefficient continental and global fresh and sea water [-]

Where the partial mass transfer coefficients water/sediment interface are described in Table 10 and the $K_{sd\ |\ w,w[S]}$ in Section 5.4.4.

The resuspension velocity from continental and global fresh and sea water sediment to continental and global fresh and sea water may be obtained from:

$$\upsilon_{res,wsd\rightarrow w[S]} = \upsilon_{sed,w[S]} - \upsilon_{sed,acc,w[S]} \quad (125)$$

with

$\upsilon_{res,wsd\rightarrow w[S]}$: resuspension rate from continental and global fresh and sea water sediment [m·s^{-1}]

$\upsilon_{sed,w[S]}$: gross sedimentation rate from continental and global fresh and sea water [m·s^{-1}]

$\upsilon_{sed,acc,w[S]}$: net sediment accumulation rate continental and global fresh and sea water [m·s^{-1}]

Where the gross sedimentation rate from water and the net sedimentation rate from water are described in Section 5.2.2.

The transfer rate from continental and global natural and agricultural soil by leaching may be obtained from:

$$k_{leach,sl[S]} = \frac{\left(\frac{v_{rain[S]} \cdot fr_V_{rain,inf,sl[S]}}{K_{sl|w,sl[S]}}\right)}{h_{sl[S]}} \cdot (3600 \cdot 24) \quad (126)$$

with

$k_{leach,sl[S]}$: leach rate from continental and global natural and agricultural soil [d^{-1}]

$v_{rain[S]}$: continental and global annual average precipitation [$m \cdot s^{-1}$]

$fr_V_{rain,inf,sl[S]}$: volume fraction of precipitation infiltrating to continental and global natural and agricultural soil [-]

$K_{sl\ |\ w,sl[S]}$: partition coefficient continental and global natural and agricultural soil/water [-]

$h_{sl[S]}$: depth of continental and global natural and agricultural soil [m]

Where the annual average precipitation and the volume fraction of precipitation infiltrating to soil are described in Table 10, $K_{sl\ |\ w,sl[S]}$ in Section 5.4.4 and the depth of the soil in Section 5.2.4.

6. HUMAN EXPOSURE

6.1 Introduction

Within the USEtox characterization framework, this chapter deals with the determination of the human exposure factor which describes the uptake of chemicals into humans from the different environmental compartments via different exposure pathways (Figure 8). Explanations of symbols and indices are given in Appendix A and corresponding parameters in USEtox are given in Appendices B to E.

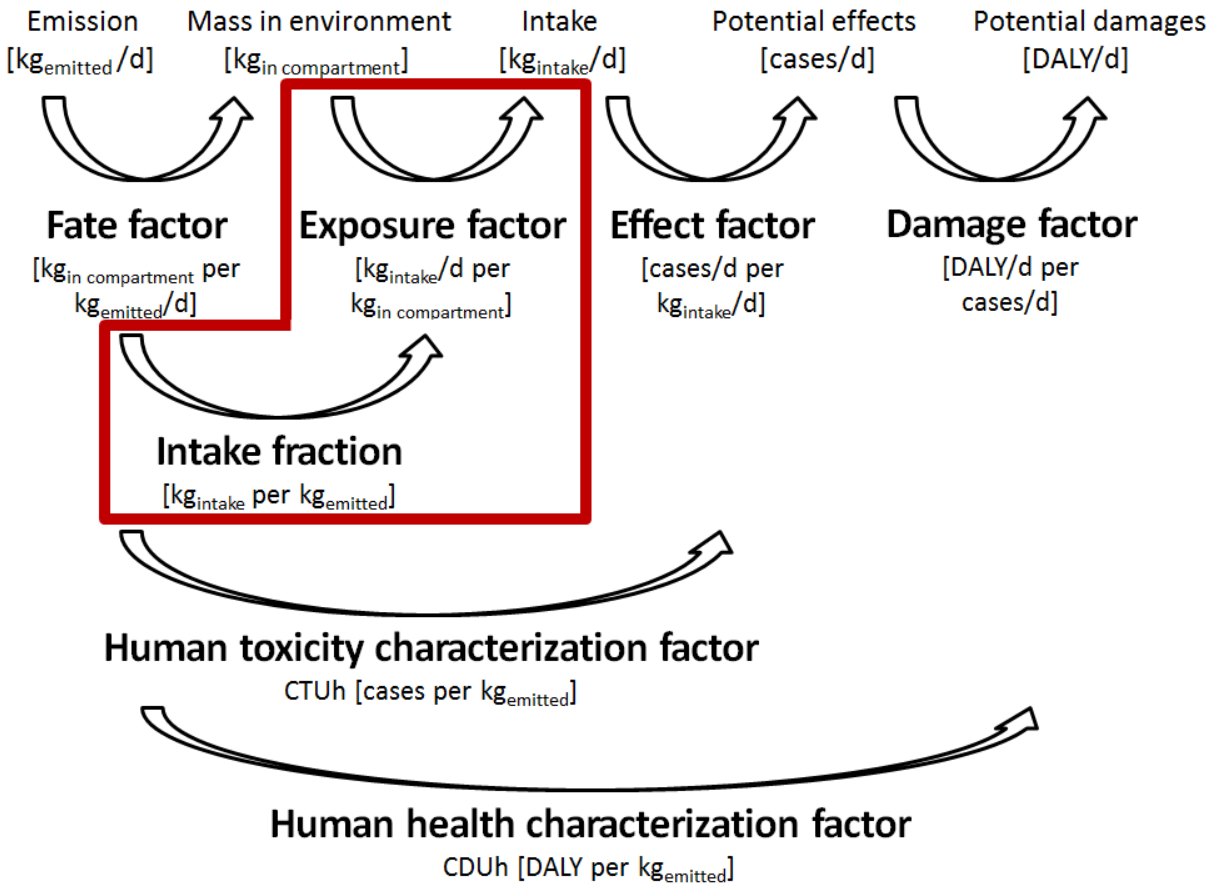

Figure 8: Symbolic description of the emission-to-damage framework for human toxicological impacts characterized with USEtox 2.0x.

The human exposure model of USEtox 1.01 was documented and published in Rosenbaum et al, 2011 and has not been modified in USEtox 2.0 (except for the addition of an indoor exposure model and exposure to crop residues, but these additions do not affect the general exposure model), therefore the following sections (except for indoor exposure and exposure to crop residues) are directly taken from this publication with some small modifications, while indoor air exposure is detailed in Chapter 7 and exposure to crop residues in Section 6.5.

The human exposure assessment of a chemical emitted into the environment (indoor or outdoor) is based on a cause-effect-chain linking the (time-integrated) chemical mass in the

environmental compartments (estimated in the fate model) to the substance intake by the total population via various exposure pathways. In USEtox this is modelled as a matrix product (Rosenbaum et al. 2007):

$$\mathbf{iF} = \mathbf{XF}\ \mathbf{FF} \tag{127}$$

where the fate factor *FF* [$kg_{in\ compartment}$ per $kg_{emitted}$/d] (i.e. the elements of the fate matrix **FF**) links the substance emission into the environment $\vec{s}$ [$kg_{emitted}$/d] to the chemical mass increase in a given compartment [$kg_{in\ compartment}$] and is the main result of the fate model. The human exposure factor *XF* [kg_{intak}/d per $kg_{in\ compartment}$] (i.e. the elements of the exposure matrix **XF**) relates the chemical mass in a given environmental compartment [$kg_{in\ compartment}$] to the chemical intake rate by humans [kg_{intake}/d]. It represents the equivalent rate of ingestion of the environmental medium by humans. Finally, the intake fraction *iF* [dimensionless: $kg_{intake}/kg_{emitted}$] (i.e. the elements of the intake fraction matrix **iF**) expresses the fraction of a pollutant emission that is eventually taken in by the human population via various exposure pathways (Bennett et al. 2002b). Due to the difficulty of linking a specific substance molecule (found in a population sample) to a specific emission source, **iF** is difficult to measure or monitor, unless traced from emission to intake using markers.

Human exposure factors *XF* corresponding to specific pathways xp can be distinguished into direct (e.g. direct consumption of an environmental compartment such as drinking water, or inhalation of air) and indirect (e.g. via food such as meat, dairy produce, vegetables, and fish) exposure factors

Each exposure pathway represents a contaminant transport mechanism from an environmental compartment into the human population. For indirect exposures, a food substrate can be contaminated from various environmental compartments. For example, a cow breathes air, drinks water, and eats forage (plants) and soil, any of which might contain a contaminant that can be subsequently transferred to the milk or meat obtained from that cow. Similar to fate factors in **FF** that quantify the transfer from one environmental compartment to another, the exposure factors in **XF** quantify the contaminant transfer from an environmental compartment into the human population via each exposure pathway.

The human exposure model currently differentiates the exposure routes inhalation and ingestion, which are represented by the exposure pathways:

- Inhalation of air,
- Ingestion of drinking water,
- Ingestion of meat and milk products,
- Ingestion of agricultural produce (distinguishing above-ground and below-ground),
- Ingestion of fish.

6.2 Key assumptions and landscape parameters

The USEtox exposure model is based on a set of necessary assumptions to address factors that are difficult to measure or that involve decision variables. There are a large number of assumptions deployed in USEtox, but only a small number that are over-arching and important for interpreting model results. Listed below are key assumptions in USEtox that must be considered when interpreting the characterization factors generated by this model:

- Population densities are assumed to be $2*10^6$ / 240 km^2 = 8333 persons/km^2 (Humbert et al. 2011) for the urban scale, $9.98*10^8$ / 9013369.37 km^2 = 111 persons/km^2 for the continental, and $6*10^9$ / $1.41*10^8$ km^2 = 43 persons/km^2 for the global scale.

- For the inhalation pathway, the urban exposure is considered separately from the rural exposure to better estimate the higher *iF* for emissions in areas with higher population densities.
- No distinction is made between sub-populations (e.g. age groups or gender), with averaging applied over the entire population.
- The *BAF* for direct exposure to environmental media is equal to one as the medium is directly taken in and no transfer modelling between medium and food substrate is required.
- For exposure pathways that relate to concentrations in fresh or marine water (e.g. drinking water and fish), only the dissolved chemical fraction is considered (relevant) instead of total concentration.
- Modelled and measured input data are assumed to represent steady-state values.
- We consider a production-based intake scenario where the contaminant levels in food and drinking water are associated with where food is produced (and contaminated) and not necessarily the location of where the population lives. This differs from a subsistence scenario, which is more often adopted in chemical screening and reflects exposure for an individual who eats, drinks, and lives within the region of an emission (Pennington et al. 2005).
- Exposure pathways that are only relevant for a small fraction of the population (e.g. breast milk) or that have been demonstrated as negligible contributors to total exposure (e.g. eggs) for most contaminants have been neglected following the USEtox development principle of parsimony (Hauschild et al. 2008).

The models and parameters used to calculate *XF* in USEtox are specific for each exposure pathway and are discussed below.

6.3 General direct exposure pathways

The exposure factor *XF* for direct exposure pathways can generally be expressed as (Rosenbaum et al. 2007):

$$XF_{\mathrm{xp,i}}^{\mathrm{direct}} = \frac{IR_{\mathrm{xp,i}} \cdot P}{\rho_{\mathrm{i}} \cdot V_{\mathrm{i}}} \tag{128}$$

Where $IR_{\mathrm{xp,i}}$ [kg/day] symbolizes the direct intake rate of an environmental medium i, polluted at a certain level, by the overall population via an exposure pathway xp, ρ_{i} is the bulk density of medium i [kg_i/m_i^3], and V_{i} [m_i^3] is the volume of medium i linked to the exposure pathway xp.

The inverse of $XF_{\mathrm{xp,i}}^{\mathrm{direct}}$ represents the equivalent time required by the population to inhale or ingest the whole chemical mass in the medium. Each exposure factor represents the increase in human exposure via pathway xp due to an increase in concentration in compartment/medium i (Rosenbaum et al. 2007).

6.3.1 Inhalation via air

The exposure factor for inhalation of air is calculated as:

$$XF_{\mathrm{inh}}^{\mathrm{direct}} = \frac{IR_{\mathrm{inh}} \cdot P}{V_{\mathrm{air}}} \tag{129}$$

where IR_{inh} [m^3/day] is the individual human inhalation rate (Breath.hum), P is the population (Pop.world, Pop.cont, Pop.urban, respectively), and V_{air} [m^3] is the volume of the global, continental, and urban air compartment, respectively. Inhalation through air depends on the individual's breathing rate ($IR_{inhalation,air}$), which is averaged over the entire population and assumed to be 13 m^3/day on an individual level (see Table 6).

6.3.2 Ingestion via drinking water

The exposure factor for ingestion of drinking water is calculated as:

$$XF_{ing,water}^{direct} = \frac{IR_{ing,water} \cdot P}{\rho_{water} \cdot V_{freshwater}} \quad (130)$$

where $IR_{ing,water}$ [l/day] is the individual daily drinking water ingestion rate (Ing.water), P is the population (Pop.world, Pop.cont, Pop.urban, respectively), ρ_{water} is the bulk density of water (RHO.water) [kg_i/m_i^3], and $V_{freshwater}$ [m^3] is the volume of the global and continental air compartment, respectively. Ingestion through drinking water is assumed to be 1.4 l/day of purified (particle filtered) surface water per person (see Table 6). The amount and source of ground water use for drinking are currently under research and thus not used as drinking water in the current version of USEtox.

6.4 General indirect exposure pathways

The exposure factor *XF* for indirect exposure pathways (via food) can be expressed as (Rosenbaum et al. 2007):

$$XF_{xp,i}^{indirect} = \frac{BAF_{xp,i} \cdot IR_{xp} \cdot P}{\rho_i \cdot V_i} \quad (131)$$

Where ρ_i is the bulk density of medium i [kg_i/m_i^3], and V_i [m_i^3] is the volume of medium i linked to the exposure pathway xp. IR_{xp} [kg/day] is the individual ingestion rate of a food substrate corresponding to exposure pathway xp, *P* is the population head count, and $BAF_{xp,i} = C_{xp}/C_i$ [kg_{xp}/kg_i] is the bioaccumulation factor (steady-state concentration ratio between food substrate corresponding to exposure pathway xp – such as meat or milk – and a specific compartment i). *BAF* represents the biotransfer from an environmental medium into a substrate and subsequent bioaccumulation within the substrate.

$XF_{xp,i}^{indirect}$ can be interpreted as the equivalent intake rate of the polluted medium i via the food substrate corresponding to exposure pathway xp. Each exposure factor represents the increase in human exposure via pathway xp due to an increase in concentration in compartment/medium i (Rosenbaum et al. 2007).

6.4.1 Ingestion via agricultural produce

The bioaccumulation factor *BAF,* needed to calculate the exposure factor *XF* for ingestion through agricultural produce, can be based on experimental data and measurements, or on model estimations. For inorganic chemicals, notably metals, only measured data are used. For organic chemicals *BAF* is estimated using a simple vegetation equilibrium model for plant-uptake that addresses both the soil-plant and air-plant transfer of chemicals. It has been developed to consolidate the significant differences in vegetation uptake algorithms used in multimedia fate/exposure models for toxic characterization in LCA as revealed during the

USEtox model comparison (Rosenbaum et al. 2008) and was developed by Thomas E. McKone (published in Rosenbaum et al., 2011).

Plant-uptake model summary

The plant-uptake model includes two components—the roots (or below-ground plant parts - bgpp) and the above-ground plant parts (agpp). The following section begins with consideration of the root concentration algorithm and then proposes the agpp model, which is more complex and includes transfer from both roots and air to edible plant parts.

Chemicals in soil enter plants primarily through the root system. Uptake of chemicals from soil into root tissues appears to be inversely proportional to water solubility and proportional to oil solubility (as represented by K_{ow}). However, as the molecules become large this relationship does not hold. Thus, studies on the bioconcentration of non-ionic organic chemicals have focused on correlations between partition factors and chemical properties that express relative solubility, such as K_{ow}. As a result there are a number of simple models that express plant uptake in terms of the octanol-water solubility ratio. (Briggs et al. 1982, Briggs et al. 1983) have developed an estimation equations based on K_{ow} for uptake of contaminants into a) roots, b) transpiration stream, and c) stems from soil solution. Based on a review of reported measurements of bioconcentration for 29 persistent organo-chlorines in plants, Travis and Arms (1988) have correlated plant-soil bioconcentration (on a dry-mass basis) in above-ground plant parts with K_{ow}. Dowdy et al. (1996) compared the precision and accuracy of the molecular connectivity index (MCI) and K_{ow} as predictors of bioconcentration from the soil matrix into above- or below- ground vegetation tissues. Attempts have been made to validate the uptake of chemicals by roots and leaves as estimated by a number of models and have empirically demonstrated need for and feasibility of more simple consensus models (Polder et al. 1995, 1998). The model includes both below-ground (i.e. root vegetables) and above-ground (i.e. grain, fruit, leafy vegetables, etc.) plant components. The below-ground plant-parts (bgpp) concentration for organics may be obtained from:

$$C_{sl-bgpp} = \frac{\rho_{sl}}{\rho_{plant}} \cdot RCF \cdot 0.8 \quad (132)$$

with

$C_{sl\text{-}bgpp}$:	below-ground plant-parts concentration due to transfer from soil to below-ground plant tissues [kg·L^{-1}]
ρ_{sl}:	bulk density of soil [kg·m^{-3}]
ρ_{plant}:	plant density [kg·m^{-3}]
RCF:	root concentration factor [kg_{FM}·L^{-1}]
0.8:	constant [-]

Where the bulk density of soil is described in Section 5.2.4 and the plant density is presented in Table 11.

The root concentration factor may be obtained from (when the RCF ≥ 200, then the RCF is 200):

$$RCF = 0.82 + 0.0303 \cdot K_{ow}^{0.77} \quad (133)$$

with

RCF: root concentration factor [$kg_{FM} \cdot L^{-1}$]

0.82: constant [-]

0.0303: constant [-]

K_{ow}: octanol/water partition coefficient of the original species [$L \cdot L^{-1}$]

0.77: constant [-]

Where the octanol/water partition coefficient of the original species is described in the substance data.

The above-ground plant-parts (agpp) concentration [$kg \cdot L^{-1}$] is the sum of the respective concentrations due to transfer from soil $C^{sw}_{plant-agpp}$, from air gas phase $C^{air}_{plant-agpp}$, and from particulate matter in air $C^{ap}_{plant-agpp}$ to above-ground plant tissues, which are calculated according to:

$$C^{sl}_{plant-agpp} = \frac{\frac{\rho_{sl}}{\rho_{plant}} \cdot 0.784^{-\frac{(\log K_{ow} - 1.78)^2}{2.44}} \cdot Q_{trans}}{\frac{MTC \cdot 2 \cdot LAI}{0.3 + \frac{0.65}{K_{ow}} + 0.015 \cdot \frac{K_{ow}}{K_{gas|w}}} + V_{plant} \cdot (\lambda_g + \lambda_t)} \quad (134)$$

$$C^{ap}_{plant-agpp} = \frac{\frac{\rho_{air}}{\rho_{plant}} \cdot v_d}{\frac{MTC \cdot 2 \cdot LAI}{0.3 + \frac{0.65}{K_{ow}} + 0.015 \cdot \frac{K_{ow}}{K_{gas|w}}} + V_{plant} \cdot (\lambda_g + \lambda_t)} \quad (135)$$

$$C^{air}_{plant-agpp} = \frac{\frac{\rho_{air}}{\rho_{plant}} \cdot MTC \cdot 2 \cdot LAI}{\frac{MTC \cdot 2 \cdot LAI}{0.3 + \frac{0.65}{K_{ow}} + 0.015 \cdot \frac{K_{ow}}{K_{gas|w}}} + V_{plant} \cdot (\lambda_g + \lambda_t)} \quad (136)$$

with

$C^{sl}_{plant-agpp}$: above-ground plant-parts concentration due to transfer from soil to above-ground plant tissues [$kg \cdot L^{-1}$]

$C^{ap}_{plant-agpp}$: above-ground plant-parts concentration due to transfer from particulate matter in air to above-ground plant tissues [$kg \cdot L^{-1}$]

$C^{air}_{plant-agpp}$: above-ground plant-parts concentration due to transfer from from air gas phase to above-ground plant tissues [$kg \cdot L^{-1}$]

ρ_{sl}: bulk density of soil [$kg \cdot m^{-3}$]

ρ_{plant}: plant density [$kg \cdot m^{-3}$]

ρ_{air}: density of air [$kg \cdot m^{-3}$]

K_{ow}: octanol/water partition coefficient of the original species [-]

Q_{trans}: area equivalent transpiration flow from soil through stems [$m^3_{transpiration} \cdot m^{-2}_{land\ area}$]

MTC: mass transfer coefficient at the air-leaf interface [$m \cdot d^{-1}$]

LAI: leaf area index, the one-sided area of plant leaf surfaces per unit land area [$m^2_{leaf\ surfaces} \cdot m^{-2}_{land\ area}$]

$K_{gas|w}$: dimensionless gas/water partition coefficient of the original species [-]

V_{plant}: area equivalent volume of above ground plant tissues [$m^3_{tissues} \cdot m^{-2}_{land\ area}$]

λ_g: growth dilution rate constant [d^{-1}]

λ_t: rate constant for elimination by chemical transformation (dissipation as proxy) within above-ground plant tissues [d^{-1}]

ν_d: deposition ratio accounting for both wet and dry particle deposition of particles from air to plant surfaces [$m \cdot d^{-1}$]

Where the bulk density of soil is described in section 5.2.4, the density of air is described in Table 10 and the plant density is presented in Table 11. The K_{ow} and the $K_{gas|w}$ are described in the substance data. The Q_{trans}, MTC, LAI, V_{plant}, ν_d and the λ_g are presented in Table 11.

If the rate constant for elimination by chemical transformation (dissipation as proxy) within above-ground plant tissues is given in the substance data, the following applies:

$$\lambda_t = k_{diss,p} \cdot (24 \cdot 3600) \quad (137)$$

with

λ_t: rate constant for elimination by chemical transformation (dissipation as proxy) within above-ground plant tissues [d^{-1}]

$k_{diss,p}$: overall dissipation as proxy for in/on-plant degradation [s^{-1}]

24·3600: conversion factor [$s \cdot d^{-1}$]

If the rate constant for dissipation from plants is not given in the substance data, this rate constant can be calculated following Equations (138) and (139), which are implemented in a freely accessible and user-friendly "Half-lives calculator" that is available for download on http://half-lives.dynamicrop.org. In this "Half-lives calculator", the crop, pesticide, growth conditions (field conditions or cold storage) and temperature are specified by the user, based on which a dissipation half-life and related dissipation rate constant $k_{diss[crop]}$ [s^{-1}] are calculated. The equations implemented in the "Half-lives calculator" are given in the following. For equations (138) and (139), the crop in cell D7 of the "Half-lives calculator" should be left blank to apply a generic crop and not correct for a specific crop species.

Whenever not available in the substance data, the rate constant for elimination by chemical transformation (dissipation as proxy) within above-ground plant tissues for an average crop (i.e. no factor required for correcting for a specific crop species) and $P_{vap,25°C} < 14.663$ reflecting the upper limit of the vapor pressure range for non-volatile pesticides that was used to build this regression model may be obtained from:

$$\lambda_t = \frac{\ln 2}{10^{1.345+\alpha-0.00039 \cdot MW+0.022 \cdot \log K_{ow}-0.092 \cdot P_{vap,25°C}}} \quad (138)$$

and for $P_{vap,25°C} > 14.663$ reflecting values above the upper limit of the vapor pressure range for non-volatile pesticides that was used to build this regression model, the rate constant for elimination by chemical transformation (dissipation as proxy) within above-ground plant tissues may be obtained from:

$$\lambda_t = \frac{\ln 2}{10^{1.345+\alpha-0.00039 \cdot MW+0.022 \cdot \log K_{ow}-0.092 \cdot 14.663}} \quad (139)$$

with

λ_t: rate constant for elimination by chemical transformation (dissipation as proxy) within above-ground plant tissues [d^{-1}]

α: pesticide chemical class regression coefficient for pesticide dissipation in plant [-]

MW: molar weight of the chemical [$kg \cdot mol^{-1}$]

$P_{vap,25°C}$: vapor pressure of original species at 25°C [Pa]

Where the overall dissipation as proxy for in/on-plant degradation, the molar weight and the vapor pressure of the chemical are described in the substance data. Alpha is chemical class dependent and may be obtained from Table 16.

Table 16: Pesticide chemical class regression coefficient for pesticide dissipation in plant

Pesticide chemical class	**α**	**Pesticide chemical class**	**A**
Anilinopyrimidine	0.176	Neonicotinoid	0.092
Benzoylurea	0.069	Organochlorine	-0.049
Botanical insecticide	-0.237	Organophosphate	-0.075
Carbamate	-0.191	Pyrethroid	-0.077
Dithiocarbamate	0.029	Strobilurin	0.201
Imidazole	0.305	Triazole	0.254
Morpholine	0.159	Other pesticide class	0.086

The bioaccumulation factor from air to above ground produce is calculated as:

$$BAF_{agp,a} = C^{ap}_{plant-agpp} + C^{air}_{plant-agpp} \quad (140)$$

with

$BAF_{agp,a}$: bioaccumulation factor from air to above ground produce [kg_{air}/kg_{veg}]

$C^{ap}_{plant-agpp}$: Above-ground plant-parts concentration due to transfer from particulate matter in air to above-ground plant tissues [kg·L^{-1}]

$C^{air}_{plant-agpp}$: Above-ground plant-parts concentration due to transfer from from air gas phase to above-ground plant tissues [kg·L^{-1}]

The bioaccumulation factor from soil to:

Above ground produce:

$$BAF_{agp,sl} = C^{sl}_{plant-agpp} \quad (141)$$

with

$BAF_{agp,sl}$: bioaccumulation factor from soil to above ground produce [kg_{soil}/kg_{veg}]

$C^{sl}_{plant-agpp}$: Above-ground plant-parts concentration due to transfer from soil to above-ground plant tissues [kg·L^{-1}]

Below ground produce:

$$BAF_{bgp,sl} = C_{sl-bgpp} \quad (142)$$

with

$BAF_{bgp,sl}$: bioaccumulation factor from soil to below ground produce [kg_{soil}/kg_{veg}]

$C_{sl-bgpp}$: below-ground plant-parts concentration due to transfer from soil to below-ground plant tissues [kg·L^{-1}]

More details including a complete description of the model can be found bellow.

The *BAF*, as the steady-state ratio of the concentrations in the respective plant part and the respective contact compartment, can then be calculated for all transfer pathways mentioned above. All *BAF* referring to above-ground plant-parts are used as *BAF* for exposed produce (i.e. grain, fruit, leafy vegetables, etc.), while the *BAF* for below-ground plant-parts represents the *BAF* for unexposed produce (i.e. root vegetables).

6.4.1.1 Background

Chemicals are transferred from air and soil to edible plant parts both through root uptake and through transfer from air through leave surfaces. The transfer from soil to edible plant parts has two stages. In the first stage the chemical can be transferred from soil to the vegetation via uptake through the roots. In the second stage the chemical moves from roots to the portion of the plant that is consumed (translocation). These stages are illustrated in Figure 9 where some common bioconcentration ratios are also illustrated. For many chemicals, the second stage is the dominant pathway by which chemicals are transferred from contaminated soil to edible plant parts. The transfer from air to above ground plant tissues involves transfer from air to the surface of the leaves and from there into other plant tissues.

It has long been recognized that vegetation can accumulate pollutants from air. Field studies have revealed that, for a whole range of semi-volatile chemicals, gas-phase transfer from the atmosphere is the dominant pathway for uptake of pollutants from air into above-ground vegetation. Field studies have also been used to estimate plant-atmosphere partition

coefficients. However, competing pathways, a large number of environmental variables, and the overall complexity of the soil/plant/air system make it difficult to use field studies alone to directly measure both the kinetic and the thermodynamic factors controlling pollutant uptake into plants. Experiments in exposure chambers have thus been used to measure plant uptake under controlled steady-state exposure conditions. These experiments have provided insight for the interpretation of field experiments, but have not provided sufficient information to interpret how transformation and translocation impact exposure. As a result, in spite of field and laboratory studies, the role of terrestrial vegetation in transferring chemicals from air into edible food commodities remains poorly understood. The inability of field studies to accurately link soil and air concentrations to human uptake has fostered the need for models to make the link from soil and air to food.

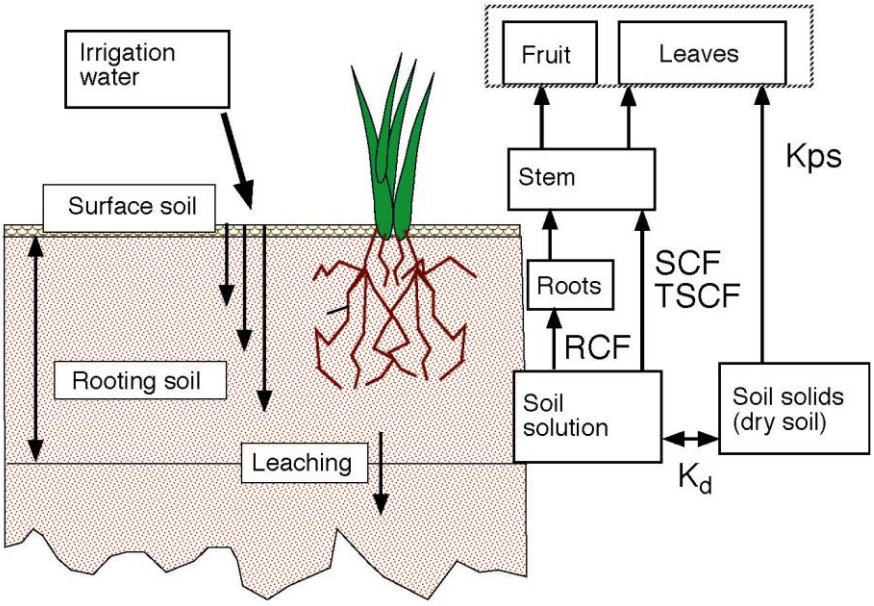

Figure 9. Illustration of the pathways by which chemical agents are transferred from irrigation water to soil and soil solution and then into roots, stems, leaves and edible plant tissues. The *RCF* refers to the root concentration factor. The *BCF* is the bioconcentration factor from dry soil solids to above-ground vegetation tissues.

6.4.2 Ingestion via meat and milk

Ingestion through meat and milk (substrate) is estimated using the Travis and Arms (1988) biotransfer factor models for cows:

$$BTF = C_{substrate}/I_{chemical} \quad (143)$$

where the biotransfer factor *BTF* [days/$kg_{substrate}$] is the steady-state ratio between the concentration $C_{substrate}$ in meat or milk respectively and the intake $I_{chemical}$ of a chemical by the animal) which were truncated to the corresponding constant value above the log-value of 6.5 of K_{ow} and below log K_{ow} = 3 following recommendations of the Technical Guidance Document on Risk Assessment (EC European Commission 2003), as these would otherwise overestimate chemical transfer into biota (Rosenbaum et al. 2009; Bennett et al. 2002a).

The bioaccumulation factor *BAF* for meat and milk exposure respectively is then the product of the respective *BTF* and the direct intake of the animal of the respective environmental

medium (air, water, vegetation, soil). It should be noted that improved biotransfer models with significantly reduced uncertainties have been published ((Birak et al. 2001, Dowdy et al. 1996, Hendriks et al. 2007, Rosenbaum et al. 2009), but scientific consensus has not yet been established. Biotransfer of chemicals into meat and milk has to be modelled due to availability of measured values being limited to 42 and 73 organic substances respectively (Rosenbaum et al. 2009) plus a few dissociating organics and some metals. This number cannot be expected to increase as feeding experiments on ruminants are very costly and rarely (if at all) conducted nowadays. These measured *BTF* data are all included in the USEtox substance database and used instead of the model for the respective chemicals.

Different types of meat have different contamination levels due to variation in fat content and feedstock intake rates of the respective animals. In USEtox this is accounted for by a correction of the (cow-based) BTF_{meat} for both fat content of meat types and respective animal intake rates (Margni 2003).

The resulting weighted average meat fat content is then 17.8%. The specific intake rates of vegetation, air, water, and soil for meat producing cattle were calculated similarly as an average weighted by the respective share of each meat type in the human population's meat diet. The vegetation, air, water, and soil intake rates of beef, pork, poultry, and goat/sheep meat producing farm animals can be found in Table 11. For inorganic chemicals, notably metals, only measured data are used, which are then included in the respective substance database.

The *BTF* for cattle milk and meat production is described in the substance data, or is indicated as not applicable (BTF_{meat}=0). If not then the BTF for cattle to meat may be obtained from:

For organics with Kow >6.5:

$$BTF_{meat} = 10^{6.5-5.6+\log\frac{Fat_{meat}}{MC_{veg}}} \quad (144)$$

For organics with Kow <3:

$$BTF_{meat} = 10^{3-5.6+\log\frac{Fat_{meat}}{MC_{veg}}} \quad (145)$$

For organics with Kow >3 & <6.5:

$$BTF_{meat} = 10^{\log K_{ow}-5.6+\log\frac{Fat_{meat}}{MC_{veg}}} \quad (146)$$

with

BTF_{meat}:	biotransfer factor from cattle intake to meat [$d \cdot kg^{-1}$]
6.5:	upper truncation constant [-]
5.6:	constant [-]
3:	lower truncation constant [-]
K_{ow}:	octanol/water partition coefficient of the original species [-]
Fat_{meat}:	weighted average meat fat content [-]
MC_{veg}:	weighted intake of meat cattle from vegetation [$kg_{FM} \cdot d^{-1}$]

Where the octanol-water partition coefficient is described in the substance data.

The weighted average meat fat content may be obtained from:

$$\mathrm{Fat_{meat}} = \mathrm{Beef_{fat}} \cdot \mathrm{Beef_{diet}} + \mathrm{Pork_{fat}} \cdot \mathrm{Pork_{diet}} + \mathrm{Poultry_{fat}} \cdot \mathrm{Poultry_{diet}} + \mathrm{GoatSheep_{fat}} \cdot (\mathrm{GoatSheep_{diet}} + \mathrm{Other_{diet}}) \quad (147)$$

with

$\mathrm{Fat_{meat}}$:	weighted average meat fat content [-]
Beef/Pork/Poultry/GoatSheep$_{fat}$:	beef, pork, poultry, goat and sheep fat content [%]
Beef/Pork/Poultry/GoatSheep$_{diet}$/Other$_{diet}$:	content of beef, pork, poultry, goat or sheep, and other meat types in human meat diet [%]

Where the fat contents and the content of different sorts of meat in diet are presented in Table 11.

The weighted intake of meat cattle from vegetation may be obtained from:

$$\mathrm{MC_{veg}} = \mathrm{Beef_{veg}} \cdot \mathrm{Beef_{diet}} + \mathrm{Pork_{veg}} \cdot \mathrm{Pork_{diet}} + \mathrm{Poultry_{veg}} \cdot \mathrm{Poultry_{diet}} + \mathrm{GoatSheep_{veg}} \cdot (\mathrm{GoatSheep_{diet}} + \mathrm{Other_{diet}}) \quad (148)$$

with

$\mathrm{MC_{veg}}$:	weighted intake of meat cattle from vegetation [$kg_{FM} \cdot d^{-1}$]
Beef/Pork/Poultry/GoatSheep$_{veg}$:	individual intake of beef, pork, poultry, goat and sheep cattle from vegetation [$kg_{FM} \cdot d^{-1}$]
Beef/Pork/Poultry/GoatSheep/Other$_{diet}$:	content of beef, pork, poultry, goat or sheep, and other meat types in human meat diet [%]

Where the individual intake of cattle from vegetation and the content of different sorts of meat in diet are presented in Table 11.

The biotransfer factor in cattle to milk may be obtained from:

For organics with Kow >6.5:

$$BTF_{milk} = 10^{6.5-8.1} \quad (149)$$

For organics with Kow <3:

$$BTF_{milk} = 10^{3-8.1} \quad (150)$$

For organics with Kow >3 & <6.5:

$$BTF_{milk} = 10^{\log K_{ow}-8.1} \quad (151)$$

with

BTF_{milk}:	biotransfer factor from cattle intake to milk [$d \cdot kg^{-1}$]
6.5:	upper truncation constant [-]
8.1:	constant [-]
3:	lower truncation constant [-]
K_{ow}:	octanol/water partition coefficient of the original species [-]

Where the octanol-water partition coefficient is described in the substance data.

The weighted intake of meat cattle from air may be obtained from:

$$MC_{air} = Beef_{air} \cdot Beef_{diet} + Pork_{air} \cdot Pork_{diet} + Poultry_{air} \cdot Poultry_{diet} + GoatSheep_{air} \cdot (GoatSheep_{diet} + Other_{diet}) \quad (152)$$

with

MC_{air}:	weighted intake of meat cattle from air [$m^3 \cdot d^{-1}$]
$Beef/Pork/Poultry/GoatSheep_{air}$:	individual intake of beef, pork, poultry, goat and sheep cattle from air [$kg_{FM} \cdot d^{-1}$]
$Beef/Pork/Poultry/GoatSheep/Other_{diet}$:	content of beef, pork, poultry, goat or sheep and other meat types in human meat diet [%]

Where the individual intake of cattle from air and the content of different sorts of meat in diet are presented in Table 11.

The weighted intake of meat cattle from water may be obtained from:

$$MC_{water} = Beef_{water} \cdot Beef_{diet} + Pork_{water} \cdot Pork_{diet} + Poultry_{water} \cdot Poultry_{diet} + GoatSheep_{water} \cdot (GoatSheep_{diet} + Other_{diet}) \quad (153)$$

with

MC_{water}:	weighted intake of meat cattle from water [$m^3 \cdot d^{-1}$]
$Beef/Pork/Poultry/GoatSheep_{water}$:	individual intake of beef, pork, poultry, goat and sheep cattle from water [$kg_{FM} \cdot d^{-1}$]
$Beef/Pork/Poultry/GoatSheep/Other_{diet}$:	content of beef, pork, poultry, goat or sheep and other meat types in human meat diet [%]

Where the individual intake of cattle from water and the content of different sorts of meat in diet are presented in Table 11.

The weighted intake of meat cattle from soil may be obtained from:

$$\mathrm{MC_{soil}} = \mathrm{Beef_{soil}} \cdot \mathrm{Beef_{diet}} + \mathrm{Pork_{soil}} \cdot \mathrm{Pork_{diet}} + \mathrm{Poultry_{soil}} \cdot \mathrm{Poultry_{diet}} + \mathrm{GoatSheep_{soil}} \cdot (\mathrm{GoatSheep_{diet}} + \mathrm{Other_{diet}}) \quad (154)$$

with

MC_{soil}:	weighted intake of meat cattle from soil [$m^3 \cdot d^{-1}$]
Beef/Pork/Poultry/GoatSheep$_{soil}$:	individual intake of beef, pork, poultry, goat and sheep cattle from soil [$kg_{FM} \cdot d^{-1}$]
Beef/Pork/Poultry/GoatSheep/Other$_{diet}$:	content of beef, pork, poultry, goat or sheep and other meat types in diet [%]

Where the individual intake of cattle from soil and the content of different sorts of meat in diet are presented in Table 11.

With the above described parameters the following human bioaccumulation factors may be obtained:

Air -> meat:

$$\mathrm{BAF_{meat,a}} = BTF_{meat} \cdot MC_{air} \cdot \rho_{air} \quad (155)$$

Air -> dairy products:

$$\mathrm{BAF}_{dairy,a} = BTF_{milk} \cdot DC_{air} \cdot \rho_{air} \quad (156)$$

Fresh or seawater -> meat:

$$BAF_{meat,w} = BTF_{meat} \cdot MC_{water} \quad (157)$$

Fresh or seawater -> dairy products:

$$BAF_{dairy,w} = BTF_{milk} \cdot DC_{water} \quad (158)$$

Soil -> meat:

$$BAF_{meat,sl} = BTF_{meat} \cdot MC_{soil} \quad (159)$$

Soil -> dairy products:

$$BAF_{dairy,sl} = BTF_{milk} \cdot DC_{soil} \quad (160)$$

Vegetation -> meat:

$$BAF_{meat,veg} = BTF_{meat} \cdot MC_{veg} \quad (161)$$

Vegetation -> dairy products:

$$BAF_{dairy,veg} = BTF_{milk} \cdot DC_{veg} \quad (162)$$

with

BAFmeat/dairy,a/w/sl/veg:	bioaccumulation factor from air, water, soil or vegetation to meat or dairy products [-]
BTFmeat:	biotransfer factor from cattle intake to meat [d·kg^{-1}]
BTFmilk:	biotransfer factor from cattle intake to milk [d·kg^{-1}]
MCair/water/soil/veg:	weighted intake of meat cattle from air, water, soil or vegetation [m^3·d^{-1}]
DCair/water/soil/veg:	weighted intake of dairy cattle from air, water, soil or vegetation [m^3·d^{-1}]
ρ_{air}:	density of air [kg·m^{-3}]

Where the density of air is described in Table 10.

6.4.3 Ingestion via fish

Ingestion through fish is represented by measured BAF when these measurements are available in literature. Otherwise, the Arnot and Gobas (2003) model in EPISuite for the upper trophic level is used to estimate directly the steady-state *BAF* [l/kg] for non-dissociating chemicals and chemicals with log K_{ow} < 9. This model includes mechanistic processes for bioconcentration and bioaccumulation such as chemical uptake from the water at the gill surface and the dietary inputs, and chemical elimination at the gill surface, faecal egestion, growth dilution and metabolic biotransformation. Input parameters to predict *BAF* values are the K_{ow} of the chemical and the estimated whole-body metabolic biotransformation rate constant [1/day]. Note that the *BAF*-values for fish calculated by the Arnot and Gobas (2003) model refer to the total concentration in water, while $BAF_{total.fish}$-values related to the dissolved phase are required in USEtox. We therefore recalculated the Arnot-Gobas $BAF_{total.fish}$-values for fish by dividing them by the fraction dissolved following the default settings in EPISuite:

$$BAF_{\text{dissolved.fish}} = \frac{BAF_{\text{total.fish}}}{1 + 0.08 \cdot DOC \cdot K_{\text{ow}} + 0.35 \cdot POC \cdot K_{\text{ow}}} \quad (163)$$

where *DOC* is the dissolved organic carbon concentration and *POC* the particulate organic carbon concentration that both equal 5.10^{-7} kg/l in EPISuite. In case the chemical is indicated as dissociating or has a log K_{ow} > 9, the Arnot and Gobas (2003) regression results should be applied with care, since this is outside the model's fitting domain. Generally, whenever available, *BAF* values have been used in priority and may be significantly higher (especially around log Kow between 5 and 7) than *BCF*, where the latter is determined without considering the dietary uptake into fish. Note also that the Arnot-Gobas model is meant for non-dissociating chemicals. However, we currently also apply the Arnot-Gobas model here,

as for ionizing organic substances, we have currently no model available to predict BAF in fish and also apply the model by Arnot and Gobas (2003).

6.5 Pesticide residue in crops

If the pesticide target class (e.g. herbicide, insecticide) and pesticide chemical class (e.g. triazole, carbamate) are defined in the substance data, the chemical is grouped either as herbicide (herbicide, herbicide safener, herbicide metabolite) or non-herbicide (all other pesticide target classes) with respect to average application time of pesticides to crops before crop harvest.

6.5.1 Crop harvest residues

For organic pesticides, the fraction of applied pesticide mass in crop harvest is pesticide target class dependent and may be obtained from:

$$\begin{aligned} fr_{harv[crop]} = {} & 10^{(-1.291-0.324\cdot\tau_{[crop]}\cdot Diss_{[crop]}-0.0029\cdot(MW-350)} \\ & + 10^{(-2.978-0.563\cdot\tau_{[crop]}\cdot Diss_{[crop]}-0.0029\cdot(MW-350)} \\ & + 10^{(-4.381-\frac{0.394\cdot\tau_{[crop]}}{\tau_{asl[C]}}-0.0029\cdot(MW-350)} \end{aligned} \quad (164)$$

with

$fr_{harv[crop]}$: fraction of applied chemical that is found in wheat, paddy rice, tomato, apple, lettuce or potato harvest [$kg_{in\ harvest}\ kg_{applied}^{-1}$]

$\tau_{[crop]}$: time between herbicide or non-herbicide application and wheat, paddy rice, tomato, apple, lettuce or potato harvest [d]

$Diss_{[crop]}$: overall rate constant for chemical dissipation from wheat, paddy rice, tomato, apple, lettuce or potato (proxy for degradation) [d^{-1}]

MW: molar weight of the chemical [kg mol^{-1}]

$\tau_{asl[C]}$: residence of chemical in soil [d]

Where the time until harvest is presented in Table 11, the dissipation rate constant is obtained from Equation (165), the molar weight of the chemical is given in the substance data, and the residence time in soil is calculated with USEtox.

If the rate constant for dissipation from a certain crop is given in the substance data:

$$Diss_{[crop]} = k_{diss[crop]} \cdot (24 \cdot 36000) \quad (165)$$

with

$Diss_{[crop]}$: overall rate constant for dissipation from wheat, paddy rice, tomato, apple, lettuce or potato [d^{-1}]

$k_{diss[crop]}$: dissipation rate from wheat, paddy rice, tomato, apple, lettuce or potato [s^{-1}]

24·3600: conversion factor [s d^{-1}]

If the rate constant for dissipation from a certain crop is not given in the substance data, this rate constant can be calculated following Equations (166) and (167), which are implemented in a freely accessible and user-friendly "Half-lives calculator" that is available for download on https://dynamicrop.org/Fantke_HalfLivesCalculator.xlsx. In this "Half-lives calculator", the crop, pesticide, growth conditions (field conditions or cold storage) and temperature are specified by the user, based on which a dissipation half-life and related dissipation rate constant $k_{diss[crop]}$ [s^{-1}] are calculated. The equations implemented in the "Half-lives calculator" are given in the following.

If not defined in the substance data file, the rate constant for dissipation from plant for $P_{vap,25°C}$ < 14.663 Pa reflecting the upper limit of the vapor pressure range for non-volatile pesticides that was used to build this regression model may be obtained from:

$$Diss_{[crop]} = \frac{\ln 2}{10^{1.345+\alpha-0.00039 \cdot MW+0.022 \cdot \log K_{ow}-0.092 \cdot P_{vap,25°C}+\beta}} \quad (166)$$

with

- $Diss_{[crop]}$: overall rate constant for dissipation from wheat, paddy rice, tomato, apple, lettuce or potato [d^{-1}]
- α: pesticide chemical class regression coefficient for pesticide dissipation in plant [-]
- MW: molar weight of the chemical [kg mol^{-1}]
- K_{ow}: octanol/water partition coefficient of the original species [-]
- $P_{vap,25°C}$: vapor pressure of original species at 25°C [Pa]
- β: plant species regression coefficient for pesticide dissipation in plant [-]

Where the molar weight, the octanol-water partition coefficient and the vapor pressure are described in the substance data. Alpha and beta may be obtained from Table 16 and Table 17, respectively.

When the $P_{vap,25°C}$ >14.663 Pa reflecting values above the upper limit of the vapor pressure range for non-volatile pesticides that was used to build this regression model, the rate constant for dissipation from plant may be obtained from:

$$Diss_{[crop]} = \frac{\ln 2}{10^{1.345+\alpha-0.00039 \cdot MW+0.022 \cdot \log K_{ow}-0.092 \cdot 14.663}} \quad (167)$$

with

- $Diss_{[crop]}$: overall rate constant for dissipation from wheat, paddy rice, tomato, apple, lettuce or potato [d^{-1}]
- α: pesticide chemical class regression coefficient for pesticide dissipation in plant [-]
- MW: molar weight of the chemical [kg·mol^{-1}]
- K_{ow}: octanol/water partition coefficient of the original species [-]
- $P_{vap,25°C}$: vapor pressure of original species at 25°C [Pa]

β: plant species regression coefficient for pesticide dissipation in plant [-]

Where the molar weight, the octanol-water partition coefficient and the vapor pressure are described in the substance data. Alpha and beta may be obtained from Table 16 and Table 17, respectively.

Table 17: Plant species regression coefficient for pesticide dissipation in plant

Plant species regression coefficient for pesticide dissipation in plant	β
Wheat	-0.175
Paddy rice	0.119
Tomato	-0.034
Apple	0.069
Lettuce	-0.330
Potato	-0.227

6.5.2 Transfer from crop to soil

If the substance is classified as herbicide or non-herbicide the fraction of applied pesticide mass transferred to the soil environment may be obtained from:

$$fr_{soil[crop]} = (1 - fr_{air[crop]}) \cdot (e^{-CSS_{crop} \cdot (LAI_{[crop]} + FAI_{[crop]})}) \quad (168)$$

with

$fr_{soil[crop]}$: fraction of pesticide applied mass transferred to soil for wheat, paddy rice, tomato, apple [$kg_{in\ soil} \cdot kg_{applied}^{-1}$]

$fr_{air[crop]}$: fraction of pesticide applied mass transferred to air for wheat, paddy rice, tomato, apple [$kg_{in\ air} \cdot kg_{applied}^{-1}$]

CSS_{crop}: substance capture coefficient for wheat, paddy rice, tomato, apple [$(kg \cdot m^{-2}leaf) \cdot (kg \cdot m^{-2}soil)$]

LAI[crop]: leaf area index of wheat, paddy rice, tomato, apple at herbicide or non-herbicide application time [m^2leaf area$\cdot m^{-2}$soil area]

FAI[crop]: fruit area index of wheat, paddy rice, tomato, apple at herbicide or non-herbicide application time [m^2leaf area$\cdot m^{-2}$soil area]

Where the fraction of pesticide applied mass transferred to air, the leaf and fruit area indices and the substance capture coefficient are presented in Table 11.

For the crops lettuce and potato the fraction of pesticide applied mass transferred to soil may be obtained from:

$$fr_{soil[crop]} = (1 - fr_{air[crop]}) \cdot (e^{-CSS_{crop} \cdot LAI_{[crop]}}) \quad (169)$$

with

$fr_{soil[crop]}$: fraction of pesticide applied mass transferred to soil for lettuce and potato [$kg_{in\ soil} \cdot kg_{applied}^{-1}$]

$fr_{air[crop]}$: fraction of pesticide applied mass transferred to air for lettuce and potato [$kg_{in\ air} \cdot kg_{applied}^{-1}$]

CSS_{crop}: substance capture coefficient for lettuce and potato [$(kg \cdot m^{-2}leaf) \cdot (kg \cdot m^{-2}soil)$]

LAI[crop]: leaf area index of lettuce and potato at herbicide or non-herbicide application time [m^2leaf area$\cdot m^{-2}$soil area]

Where the fraction of pesticide applied mass transferred to air, the leaf area indices and the substance capture coefficient are presented in Table 11.

The fraction harvest (Equation (164)), the fractions transferred from the crop to air (Table 11) and soil (Equations (168) and the factor from food processing (Table 11) are human exposure output values, used in the “run” matrix of the model.

7. INDOOR FATE AND EXPOSURE

7.1 Introduction

Within the USEtox characterization framework, this chapter deals with the determination of the fate factor and the human exposure factor for indoor environments which describe the distribution of chemicals between the different environmental compartments after an emission into the environment and the uptake of chemicals into humans from the indoor air compartments via different exposure pathways, respectively (Figure 10). Explanations of symbols and indices are given in Appendix A and corresponding parameters in USEtox are given in Appendices B to E.

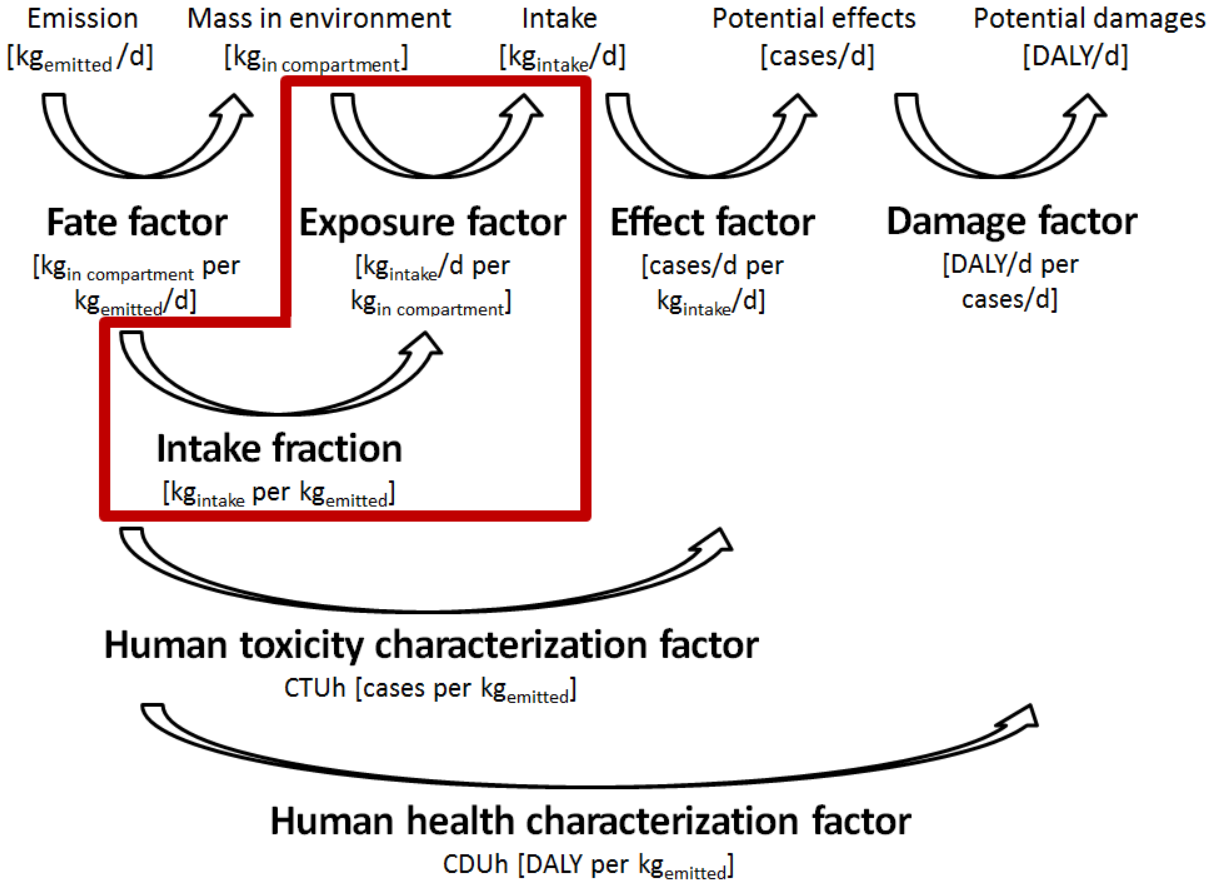

Figure 10: Symbolic description of the emission-to-damage framework for human toxicological impacts characterized with USEtox 2.0x.

The indoor air module consists of two indoor compartments which can be parameterized independently in order to (for example) represent household and occupational settings respectively. The indoor exposure model of USEtox 2.0 is based on the recommendations by Hellweg et al. (2009) and its implementation and parameterization (only for household settings) in USEtox was documented and published in Rosenbaum et al. (2015), therefore the following sections are essentially taken from this publication with some small modifications.

The one-box model recommended by Hellweg et al. (2009) for estimation of indoor air intake fraction is given as (Equation 1b in Hellweg et al. (2009)):

$$iF_{\text{inhalation,indoor}} = \frac{IR_{\text{inhalation,air}}}{V_{\text{indoor,air}} \cdot m \cdot k_{\text{ex}}} \cdot N \quad (170)$$

where $iF_{\text{inhalation,indoor}}$ is the population intake fraction of a chemical [-], $IR_{\text{inhalation,air}}$ is the daily inhalation rate of air of an individual [m^3/day], N is the number of people exposed [-], $V_{\text{indoor,air}}$ is the volume of the indoor air compartment [m^3], k_{ex} is the air exchange (or ventilation) rate of the volume in the indoor air compartment [-] and m is the mixing factor [-].

The following sections describe how this has been implemented into the matrix-algebra framework of the USEtox model.

7.2 Fate

The indoor environment is modeled as a separate air compartment, which is added to the existing 11 USEtox compartments. See Figure 11 for a schematic representation of this integration. Three removal mechanisms are considered, 1) air exchange according to Hellweg et al, 2009 and optionally (not used for the official USEtox indoor characterization factors, but instead implemented in in USEtox for conducting sensitivity studies only and by default set to zero) 2) gas-phase (g) air-degradation, and 3) surface adsorption, the latter two according to Wenger et al. (2012):

The total removal at home or work rate may be obtained from:

$$k_{total[I]} = k_{ex[I]} + k_{g,deg\,[I]} + k_{s[I]} \quad (171)$$

with

$k_{total[I]}$: total removal rate at home or work [h^{-1}]

$k_{ex[I]}$: Air exchange rate at home or work [h^{-1}]

$k_{g,deg[I]}$: removal rate due to indoor air degradation at home or work [h^{-1}]

$k_{s[I]}$: removal rate due to surface net adsorption and degradation at home or work [h^{-1}]

Where the air exchange rate at home or work can be found in Table 8 and Table 9, respectively.

1) The advective ventilation flow, parameterized as the air exchange rate k_{ex} [h^{-1}] (Table 8 (household) and Table 9 (occupational)). The air exchange rate does not depend on the substance, but on the building characteristics, such as type and size of windows and doors, type of walls, number of cracks in the façades, and presence and use of (active) ventilation systems. k_{ex} is not a loss, but an inter-media transport mechanism connecting indoor with outdoor compartments. Based on the average distribution of the global population between urban and rural areas of about 50% respectively (UN United Nations 2012), half of the ventilation flow is directed to urban and continental rural air respectively for the household setting. For the occupational setting an assumption of 80% being ventilated into urban and 20% into rural continental air is used in the absence of representative global average data and

the rationale that the predominant occupation in rural areas is related to agriculture mostly exercised outdoors. These advective inter-media airflows are taken into account in the model by a non-diagonal term from indoor to compartment i given as:

$$k_{\text{indoor,i}} = f_{\text{ex,i}} \cdot k_{\text{ex}} \quad (172)$$

with $f_{\text{ex,urban air}} = 0.5$ for the household setting, $f_{\text{ex,urban air}} = 0.8$ for the occupational setting, and $f_{\text{ex,continental rural air}} = 1 - f_{\text{ex,urban air}}$ for household and occupational settings respectively.

2) The gas-phase (g) air-degradation rate, $k_{g,deg}$ [h^{-1}] , that is used in USEtox as sensitivity study only and by default is set to zero, is mainly related to reactions with ozone, hydroxyl radicals, and nitrate radicals (gas-phase degradation). The overall degradation rate in the indoor air is calculated as the average radical concentration ([OH], [O_3], [NO_3]) multiplied by the corresponding second order degradation rate constant:

$$k_{g,deg[I]} = k_{OH} \cdot OH_{[I]} + k_{OH} \cdot O3_{[I]} + k_{NO3} \cdot NO3_{[I]} \quad (173)$$

with

$k_{g,deg[I]}$:	removal rate due to indoor air degradation at home or work [h^{-1}]
k_{OH}:	second order constant rate of OH [h^{-1} $ppbv^{-1}$]
$OH_{[I]}$:	concentration OH indoor at home or work [ppbv]
k_{O3}:	second order constant rate of O3 [h^{-1} $ppbv^{-1}$]
$O3_{[I]}$:	concentration O3 indoor at home or work [ppbv]
k_{NO3}:	second order constant rate of NO3 [h^{-1} $ppbv^{-1}$]
$NO3_{[I]}$:	concentration NO3 indoor at home or work [ppbv]

The second order constant rates of O_3 and NO_3 and the concentration of OH, O_3 and NO_3 can be found in Table 12.

The second order constant rate of hydroxide (OH) may be obtained from:

$$k_{\text{OH}} = \frac{k_{deg,air25°C}}{out_{OH}} \cdot 3600 \quad (174)$$

with

k_{OH}:	second order constant rate of OH [h^{-1} $ppbv^{-1}$]
$k_{deg,air25°C}$:	gas phase degradation rate constant at 25°C, in air [s^{-1}]
out_{OH}:	outdoor OH [ppbv]
3600:	conversion factor [$s \cdot h^{-1}$]

Where the gas phase degradation rate constant at 25°C, in air is described in the substance data and the outdoor OH in Table 12.

3) An equivalent removal rate by adsorption to indoor surfaces, k_s [h^{-1}], that is used in USEtox as sensitivity study only and by default is set to zero, can be calculated as a net removal rate from the air, assuming steady-state conditions between the air and room surface without adding a separate compartment (Wenger et al. 2012). This approach is similar to the net removal rate calculated in USEtox from the freshwater outdoor environment to the sediments, which are not considered as separate compartments to limit the model complexity. Since degradation on surfaces is not well characterized, this removal rate to surfaces is subject to high uncertainty. Surface removal in the current model is applied primarily to Semi-Volatile Organic Compounds (SVOCs), for which additional gaseous dermal exposure may also be relevant and may compensate this removal. If the model is eventually used for particulate matter (PM) and ozone, then surface removal could become more important and requires further assessment of the literature on indoor ozone and PM deposition including the work of Weschler and Nazaroff (Nazaroff 2004, Weschler 2000). We therefore do not include the sorption removal pathway in the default model, but as an option to allow users to conduct sensitivity studies together with the dermal gaseous exposure pathway. A more detailed description of the calculation of the equivalent removal rate to the surface k_s is given in the supporting information of Rosenbaum et al., 2015 (section S3).

The removal rate due to surface net adsorption and degradation at home or work when turned on may be obtained from:

$$K_{s[I]} = \frac{A_{carpet[I]}}{\frac{1}{h_{m[I]}} + \frac{1}{k_{deg,wall,indoor[I]}} \cdot k_{g,\deg[I]} \cdot k_{eq,carpet[I]}} + \frac{A_{total[I]}}{\frac{1}{h_{m[I]}} + \frac{1}{k_{deg,wall,indoor[I]}} \cdot k_{g,\deg[I]} \cdot k_{eq,wall[I]}} \quad (175)$$

with

$k_{s[I]}$:	removal rate due to surface adsorption and degradation at home or work [h^{-1}]
$A_{carpet[I]}$:	area per volume, carpet at home or work [m^2m^{-3}]
$h_{m[I]}$:	mass transfer coefficient at wall surface at home or work [$m^3m^{-2}h^{-1}$]
$k_{deg,wall,indoor[I]}$:	degradation rate on room surfaces at home or work [-]
$k_{g,deg[I]}$:	removal rate due to indoor air degradation at home or work [h^{-1}]
$k_{eq,carpet[I]}$:	partitioning coefficient indoor air - carpet at home or work [-]
$A_{total[I]}$:	area per volume, wall at home or work [m^2m^{-3}]
$k_{eq,wall[I]}$:	partitioning coefficient indoor air - wall at home or work [-]

Where the removal rate due to indoor air degradation is described in Equation (173), the partitioning coefficient indoor air (carpet) and (wall) in Equation (177) and (178), respectively. The area per volume of carpet and wall, the mass transfer coefficient at wall surface and the degradation rate on room surfaces are described in Table 12.

The area per volume of wall at work may be obtained from:

$$A_{total[O]} = \frac{A_{total[H]}}{1.5} \quad (176)$$

with

$A_{total[O]}$:	area per volume, wall at work [m^2m^{-3}]
$A_{total[H]}$:	area per volume, wall at home [m^2m^{-3}]
1.5:	constant [-]

Where the area per volume of wall at home is described in Table 12.

The partitioning coefficient indoor air - carpet may be obtained from:

$$K_{eq,carpet} = 10^{(-0.814842 \cdot \log\frac{P_{vap,25°C}}{101325} - 1.14928)} \quad (177)$$

with

$K_{eq,carpet}$:	partitioning coefficient indoor air - carpet [-]
0.814942:	constant (Wenger et al. 2012)
$P_{vap,25°C}$:	vapor pressure of original species at 25°C [Pa]
101325:	conversion factor [$Pa \cdot atm^{-1}$]
1.14928:	constant (Wenger et al. 2012)

Where the vapor pressure of original species is described in the substance data.

The partitioning coefficient indoor air – wall surface may be obtained from:

$$K_{eq,wall} = 10^{(-0.74299 \cdot \log\frac{P_{vap,25°C}}{101325} - 1.94003)} \quad (178)$$

with

$K_{eq,wall}$:	partitioning coefficient indoor air – wall surface [-]
0.74299:	constant (Wenger et al. 2012)
$P_{vap,25°C}$:	vapor pressure of original species at 25°C [Pa]
101325:	conversion factor [$Pa \cdot atm^{-1}$]
1.94003:	constant (Wenger et al. 2012)

Where the vapor pressure of original species is described in the substance data.

The gas-phase air-degradation rate $k_{g,deg}$ and the equivalent removal rate by adsorption to indoor surfaces k_s are directly added to the total air removal rate of the corresponding diagonal term of the **K** matrix.

Attention: as mentioned above, the removal processes 2) and 3) are not part of the default indoor air model in USEtox and thus also not considered in the official USEtox indoor characterization factors. They are deactivated in the default USEtox model setup but can be activated by the user via the "switches" in the "Indoor exposure" worksheet, cells G26 and G27 for the household indoor setting and cells G48 and G49 for the occupational indoor setting.

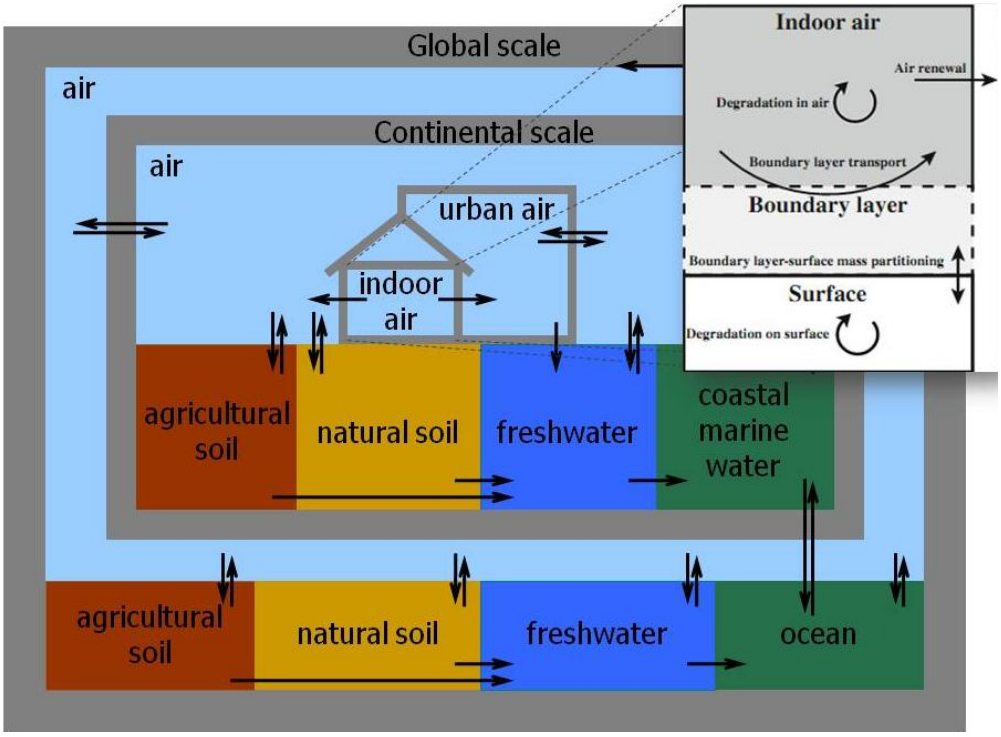

Figure 11: Schematic representation of the USEtox model with indoor compartment embedded (Rosenbaum et al. 2015)

7.3 Exposure

The relevant exposure route for indoor air emissions is inhalation. The exposure factor XF_{indoor} [1/d] for the indoor exposure setting is then calculated based on Equation (179) (with mixing factor m = 1, with complete mixing within the indoor volume being an inherent hypothesis of the indoor *iF* model):

$$XF_{indoor}^{direct} = \frac{IR_{inhalation,air}}{V_{building}} \cdot f_t \cdot N \qquad (179)$$

where $IR_{inhalation,air}$ is the individual daily inhalation (breathing) rate [m^3/d], N is the average number of people in the building [dimensionless], $V_{building}$ is the building volume [m^3], and f_t is the daily time fraction spent indoors f_t [dimensionless]. The latter is the quotient of the time spent indoors [h] and the total time of a day (24h). Recommendations, assumptions, and choices for these parameter values are further discussed below.

The calculated XF_{indoor} values are placed in the corresponding element of the exposure matrix **XF** in USEtox for household and occupation indoor respectively. For SVOCs the dermal

absorption of gas-phase chemicals may become important and means that the validity of equation (179) is restricted to VOCs (Gong et al. 2014, Weschler & Nazaroff 2012, Weschler & Nazaroff 2014), with higher uncertainty when applied to SVOCs. For further details on this issue in USEtox, Rosenbaum et al. (2015) investigated the potential influence of the dermal gaseous uptake pathway as a sensitivity study together with the influence of adsorption removal on indoor surfaces which competes with this exposure pathway.

7.4 Model Parameterization

In order to calculate characterization factors (and intake fractions) for indoor exposure, the parameters discussed above are needed in the USEtox model. In LCA, the exact situation where the indoor exposure takes place is seldom known. In order to calculate characterization factors for generic situations, regions can be defined, for each of which a characterization factor can be calculated using region-specific parameters. Regions can be defined as 1) countries or continents, 2) based on the level of economic development or urbanization, or 3) as a combination of 1) and 2). All parameters describing the indoor compartment and the resulting exposure are provided as recommended value sets for household settings and indicative values for occupational settings in different regions, but can also be modified freely by the user in the model to represent more site-specific conditions. As opposed to general environmental outdoor exposure, it is not meaningful to define parameter sets representing global averages for indoor exposure. Besides important differences in exposure conditions (which in fact also apply to outdoor exposure) indoor exposure is related to the use of a given product at home (household setting) or the production/provision of a product/service at a workplace (occupational setting) and thus not affecting the general population in the same way.

7.4.1 Household indoor exposure

Rosenbaum et al. (2015) defined four regions for the household indoor setting in USEtox: Europe (EU-27), North America (USA), OECD countries, and non-OECD countries. They assume that a population-weighted average from EU-27 countries is representative for Europe, that an average from the USA is representative for North America, that a population-weighted average from EU-27 countries and the USA is representative for OECD countries, and that a population-weighted average from China, India, Uganda, Brazil, and Guatemala is representative for non-OECD countries. The region-specific parameters considered are the building volume ($V_{building}$) and the number of people in the building (N). For the air exchange rate (k_{ex}) data availability is even less robust than for N and $V_{building}$. Therefore, a distinction has been made between houses with a low air exchange rate ($k_{ex} < 8\ h^{-1}$) named “airtight” and houses with higher air exchange rates ($k_{ex} > 8\ h^{-1}$, especially for houses with no windows and/or doors) named “non-airtight”. All houses in OECD countries were assumed as being relatively airtight, while in non-OECD countries, both airtight and non-airtight houses (e.g. houses with no glass in the windows) exist. In the absence of data for airtight houses in non-OECD countries, we assume the same value for k_{ex} as for OECD countries. In Table 18, the recommended values of the region-specific parameter sets are summarized. In the supporting information of Rosenbaum et al. (2015) (Table S1), the parameter values are given for the different countries within the regions.

Table 18: Recommended parameter values and standard deviations (SD) for the indoor exposure model per region, calculated as averages from the individual countries and weighted over the population of those countries (Rosenbaum et al. 2015).

Region	$V_{building}$ [m^3]		N [-]		k_{ex} [h^{-1}]		$IR_{inhalation,air}$ [m^3/d]	f_t [-]
	Average	SD	Average	SD	Average	SD		
Non-OECD countries (non-airtight building)	119	25.6	4.0	0.87	15.6	0.85	13	0.58
Non-OECD countries (airtight building)					0.64	0.08		
OECD countries	236	37.9	2.5	0.22				
Europe (EU-27)	209	22.9	2.4	0.26				
North America (USA)	277	[a]	2.6	[a]				

[a] single data point (US average) as we are using country averages and hence no variability assessed on sub-country level
See Table S1 in SI of Rosenbaum et al. (2015) for data per country and literature references

The average time spent indoors needs to be differentiated between time spent at work and time spent at home (which could even be further distinguished between private and public buildings such as shops, restaurants, etc.), where exposure conditions can be very different. As we are focusing here on household exposure, we assume a daily average of 14 hours spent at home. These can be complemented by 7-8 hours at work, leaving 2-3 hours outdoors. The time fraction spent indoors (at home) is then calculated as f_t = 14h/24h = 0.58.

Further details on parameters and justifications for value choices are discussed in Rosenbaum et al. (2015).

7.4.2 Occupational indoor exposure

The data availability for the parameterization of the occupational indoor exposure setting is even more limited and at the same time also more variable on a global scale and between economic sectors than for the household setting. As a preliminary starting point four archetypes were defined for occupational settings, differentiating industrial and office conditions in OECD and non-OECD countries respectively. Industrial settings should be used for manufacturing facilities, factories and warehouses. Office settings should be used for services. These archetypes are representative of average conditions at the workplace based on publically available data. The corresponding parameter values for each archetype are given in Table 19. The building volume is assumed proportional to the number of people in the building/room, which in consequence defines N = 1. The average daily time spent at work does not correspond to the average time spent at work per working day but to total time spent at work annually divided by 365 days. Country-specific values for this variable are provided by the International Labour Organization (ILO) and can be used to create customized archetypes. Due to lack of available data, non-OECD countries are assumed to have 30% less volume of room per person and 30% lower ventilation rate than OECD countries (rough assumption).

Table 19: Interim parameter values for archetypical occupational indoor exposure settings for OECD and non-OECD regions

	$V_{building}$/person [m^3]	k_{ex} [h^{-1}]	N^a	$IR_{inhalation,air}$ [m^3/d]	Daily time spent at work [h]

[a] With the volume being assumed proportional to the number of people in the building/room, this parameter is set to 1.

OECD	Industry	350	12	1	60	4.76
	Office	20	4		13	
Non-OECD	Industry	250	8		60	5.33
	Office	15	3		13	

The raw data used to calculate these values are given in Rosenbaum et al. (2015).

7.5 Model output

The population household indoor exposure intake fraction may be obtained from:

$$f_{intake[H]} = \frac{\mathrm{IR}_{a[H]}}{V_{[H]} \cdot mix_{[H]} \cdot k_{total[H]} \cdot 24} \cdot N_{[H]} \quad (180)$$

with

$f_{intake[H]}$: population household indoor exposure intake fraction [-]

$IR_{a[H]}$: individual daily inhalation rate at home [$m^3 \cdot d^{-1} \cdot pers^{-1}$]

$V_{[H]}$: building volume of house [m^3]

$mix_{[H]}$: mixing factor in house [-]

$k_{total[H]}$: total removal rate at home [h^{-1}]

24: conversion factor [$h \cdot d^{-1}$]

$N_{[H]}$: number of people in house [-]

Where the individual daily inhalation rate at home and the total removal rate from home are described in Equations (181) and (183), respectively. The building volume and the number of people in house are described in Table 8 and the mixing factor in Table 12.

Indoor air degradation and surface adsorption degradation can be turned on and off by the user by entering a 1 (on) or a 0 (off). The individual daily inhalation rate at home may be obtained from:

$$IR_{a[H]} = k_{IR[H]} \cdot t_{home} \quad (181)$$

with

$IR_{a[H]}$: individual daily inhalation rate at home [$m^3 \cdot d^{-1} \cdot pers^{-1}$]

$k_{IR[H]}$: individual hourly inhalation rate at home [$m^3 \cdot h^{-1} \cdot pers^{-1}$]

t_{home}: daily time at home [$h \cdot d^{-1}$]

Where the individual hourly inhalation rate at home and the daily time at home are described in Table 8.

The population occupational indoor exposure intake fraction may be obtained from:

$$f_{intake[O]} = \frac{\mathrm{IR}_{a[O]}}{V_{[O]} \cdot mix_{[O]} \cdot k_{total[O]} \cdot 24} \cdot N_{[O]} \quad (182)$$

with

$f_{intake[O]}$:	population occupational indoor exposure intake fraction [-]
$IR_{a[O]}$:	individual daily inhalation rate at work [$m^3 \cdot d^{-1} \cdot pers^{-1}$]
$V_{[O]}$:	building volume of house [m^3]
$mix_{[O]}$:	mixing factor in house [-]
$k_{total[O]}$:	total removal rate at work [h^{-1}]
24:	conversion factor [$h \cdot d^{-1}$]
$N_{[O]}$:	number of people in house [-]

Where the individual daily inhalation rate at work and the total removal rate from work are described in Equations (183) and (171), respectively. The building volume and the number of people at work are described in Table 9 and the mixing factor in Table 12.

Indoor air degradation and surface adsorption degradation can be turned on and off by the user by entering a 1 (on) or a 0 (off).

The individual daily inhalation rate at work may be obtained from:

$$IR_{a[O]} = k_{IR[O]} \cdot t_{work} \quad (183)$$

with

$IR_{a[O]}$:	individual daily inhalation rate at work [$m^3 \cdot d^{-1} \cdot pers^{-1}$]
$k_{IR[O]}$:	individual hourly inhalation rate at work [$m^3 \cdot h^{-1} \cdot pers^{-1}$]
t_{work}:	daily time at work [$h \cdot d^{-1}$]

Where the individual occupationally hourly inhalation rate and the daily time at work are described in Table 9.

8. HUMAN-TOXICOLOGICAL EFFECTS

8.1 Introduction

Within the USEtox characterization framework, this chapter deals with the determination of the human toxicological effect factor which relates human health effects to the mass taken in by humans via different exposure pathways (Figure 12). Explanations of symbols and indices are given in Appendix A and corresponding parameters in USEtox are given in Appendices B to E.

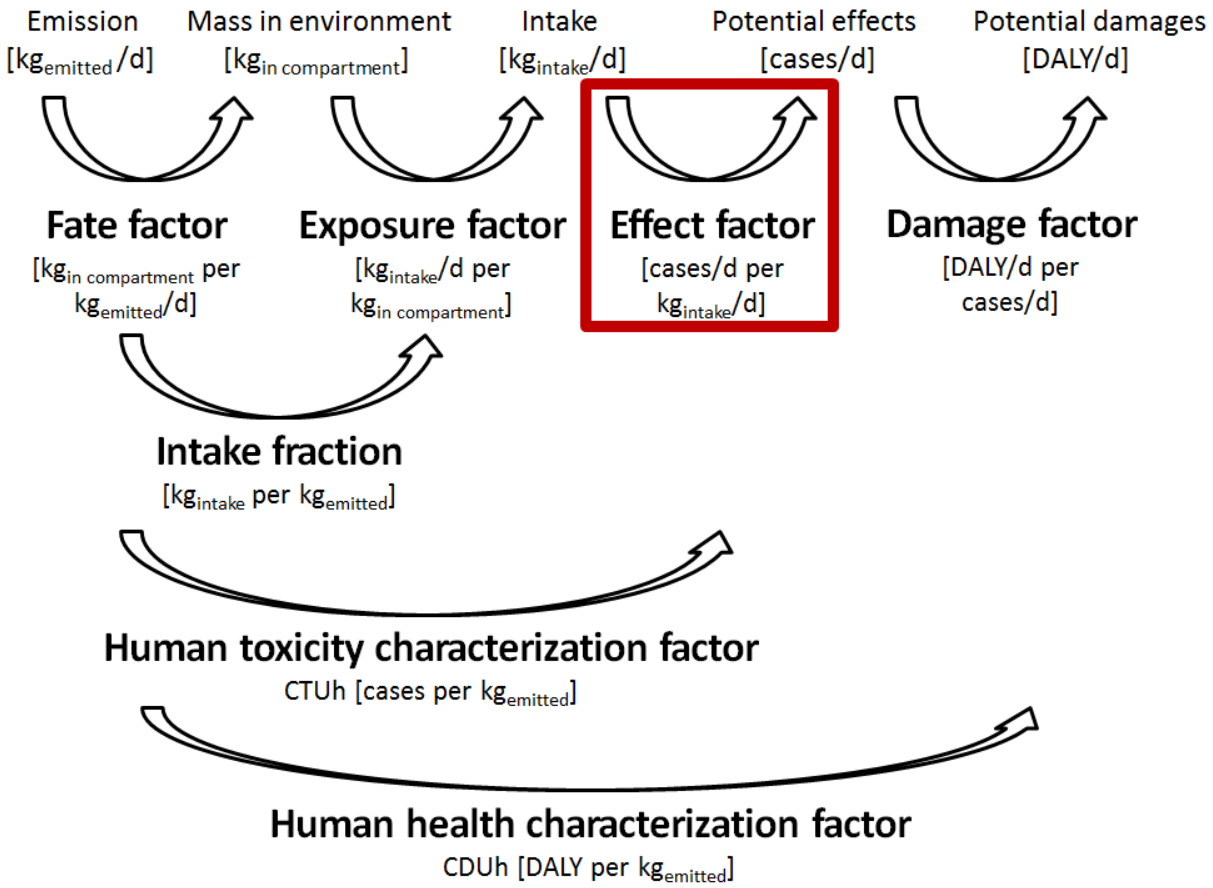

Figure 12: Symbolic description of the emission-to-damage framework for human toxicological impacts characterized with USEtox 2.0x.

Building on the recommendations of an expert workshop held within the UNEP-SETAC Life Cycle Initiative (McKone et al. 2006) and on several additional sources (Crettaz et al. 2002, Huijbregts et al. 2005, Pennington et al. 2006) the human toxicity potential can be expressed as a combination of the ratios of intake fractions to ED_{50}s, keeping inhalation and ingestion route separate and differentiating between the contributions of cancer and non-cancer impacts:

$$\begin{aligned} CF_{hum} &= CF_{hum,cancer} + CF_{hum,non-cancer} \\ &= iF^{inh}\left(\frac{\alpha}{ED50^{inh}_{hum,cancer}} + \frac{\alpha}{ED50^{inh}_{hum,non-cancer}}\right) \\ &+ iF^{oral}\left(\frac{\alpha}{ED50^{oral}_{hum,cancer}} + \frac{\alpha}{ED50^{oral}_{hum,non-cancer}}\right) \end{aligned} \quad (184)$$

Where $ED50^{route}_{hum}$ is the estimated lifetime dose for humans related to inhalation or oral exposure that causes an increase in disease probability of 50% [kg/person/lifetime]. This lifetime ED_{50} is calculated either in priority from human based data for a few substances for which such data are available or nearly always derived from animal cancer tests from the TD_{50} (Tumorigenic dose-rate in [mg/kg/d] for 50% of the animals over background in a standard lifetime). α is the slope factor that relates the inverse of the ED_{50} to a potential probability of getting a cancer. For example, a default value of $\alpha = 0.5$ assumes a linear effect with 50% additional chance to get cancer while ingesting a quantity equal to the ED_{50} over lifetime.

8.2 Cancer effects

Approach for comparing positivity and carcinogenic potency by route: To empirically test for route-to-route extrapolation, cancer potencies are compared by route using results in the Carcinogenic Potency Database (CPDB) of Gold et al. (http://potency.berkeley.edu), which includes 6540 experiments on 1547 chemicals tested in rats, mice, hamsters, dogs, and non-human primates. We identified 106 chemicals as having an experiment where the route of administration was inhalation (99 chemicals in rats, 79 in mice, and 12 in hamsters). Only 31% (33/106) of these also have an experiment in the CPDB in which the chemical was administered to the same species by an oral route, usually by gavage, and less frequently by water or diet. Nearly all are tested in rats by both routes (32), and only 18 in mice. In our analysis, if there is one positive cancer test by either an oral or inhalation route in a species, then the result is considered positive regardless of whether other inhalation tests or other oral tests are negative. These 33 chemicals have been tested more often than usual in the CPDB. Overall, 85% (28/33) are carcinogenic in at least one experiment, which compares to 52% in the CPDB overall.

The experimental comparison between inhalation and oral routes is carried out by comparing positivity by the two routes and by plotting the harmonic mean of TD_{50} for one route against the other. The results of the route comparison may reflect variation in factors other than route for each chemical, thus making conclusions difficult for this small number of chemicals, e.g. the power to detect a carcinogenic effect is greater when there are more experiments or when more strains are tested, or more animals are used in an experiment.

In our route analysis, harmonic means of TD_{50} in each species are calculated separately for positive experiments by the inhalation and oral routes of administration. In USEtox, for each exposure route, the lower (more potent) harmonic mean of TD_{50} in rats or mice is retained after application of an interspecies allometric factor (see Table S3 of Rosenbaum et al. (2011)). The CPDB reports the harmonic mean to summarize potency values from different experiments because it uses all of the experimental data and is more similar to the most potent site than other averaging measures (Gold et al. 1989). The use of harmonic mean is also consistent with the use of ED_{50} (as derived from the TD_{50}).

Complementary to the experimental approach, special attention is given to the few outliers in the potency comparison of routes by accounting for the following exclusion criteria: First, one can expect important variations in sensitivity if observed tumors are related to toxic

effects at the site of application for a given route, e.g. for nasal or lung tumors by inhalation or stomach tumors by gavage. Second, inhalation and oral doses in bioassays are based on maximum tolerated doses, which may differ by oral vs inhalation routes due to differences in absorption between the two routes. Physicochemical properties may influence the absorbed fraction by each route of intake. These properties, especially the different partition coefficients, may also affect the subsequent distribution of the dose to the target organs. Therefore, chemicals for which absorbed fraction by inhalation and by oral route differ greatly may also show important variations between TD_{50}s by different routes of exposure.

For **calculations of carcinogenicity effect factors**, the following order of preference in toxicity data has been used in the USEtox calculations:

1. In the few cases for which data from human studies were available from the IRIS database (US-EPA United States - Environmental Protection Agency 2011), the carcinogenic effect factor the 50% effect dose (ED_{50}) was estimated from the low-dose slope factor (q_1*) in humans (n = 9).
2. For carcinogenic potency values from animal cancer tests, ED_{50}s were derived from TD_{50} values in the CPDB (Gold 2011): n = 584).
3. In case no quantitative effect information was available from the CPDB, the carcinogenic ED_{50} has been estimated from the animal-based low-dose slope factor (q_1*) from the IRIS database (US-EPA United States - Environmental Protection Agency 2011), using a 1/ q_1*-to-ED_{50} conversion factor of 0.8 (n = 10).
4. If LD_{50} data are available, convert to chronic human ED_{50} based on the relationship ED_{50} = LD_{50}/129 building on Rosenbaum et al. (2011, Figure 7);
5. Chemicals with all negative carcinogenic effect data in the CPDB were also included as true zero carcinogenic effect factors and thus distinguished from missing data (n = 417).

8.3 Non-cancer effects

For effects other than cancer, insufficient data were available for most substances to recalculate an ED_{50} with dose–response models. For chemicals with no evidence of carcinogenicity, the ED_{50} has been estimated from no-observed effect level (*NOEL*) by a *NOEL*-to-ED_{50} conversion factor of 9 (Huijbregts et al. 2005). In case only a *LOEL* was available, a *LOEL*-to-ED_{50} conversion factor of 2.25 has been applied (Huijbregts et al. 2005). *NOEL*s and *LOEL*s were derived from the IRIS database (US-EPA United States - Environmental Protection Agency 2011) and from the World Health Organisation (WHO) (IPCS International Programme on Chemical Safety 2009, Lu 1995) with priority for data from the WHO.

Several knowledge gaps deserved particular attention in order to determine an extended list of ED_{50}s: a) Most of the available toxicity tests have been carried out for oral intake. This means that missing exposure routes need to be characterized using basic hypotheses. Thus, the route-to-route and interspecies extrapolations need to be further analyzed based on available bioassays and on theoretical pharmacokinetics knowledge in order to propose a recommendation for the extrapolation. b) Only chronic carcinogenicity data are presently used in USEtox and these are only available for about 1600 chemicals. To expand the number of chemicals in the future, there is a need to reassess the possibility of acute-to-chronic extrapolation. Methods developed to address and analyze these two main points are described below.

Acute-to-chronic extrapolation: At present, USEtox is based only on chronic data, which limits the number of substances covered. Previous extrapolations were often based on a limited number of chemicals and a limited range of toxicity values. We have used an alternative, approach to extend the chemical coverage: In order to cover the broadest range possible in cancer values, all positive chemicals with a cancer ED_{50} were selected in the USEtox database, excluding those that also have a *NOEL* or a non-cancer ED_{50} available in order to keep the analysis of cancer and non-cancer effects separate. We then checked if corresponding acute animal data (LD_{50} in mg/kg) were available in the Hazardous Substances Data Bank (HSDB) database (https://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB). The calculated ED_{50}s were then plotted against the lowest mouse or rat acute data from the HSDB database to study their correlation (n = 106). A similar approach was tested for the non-cancer data from the USEtox database against HSDB LD_{50}s, using all the human adjusted non cancer ED_{50} in the USEtox database as derived from *NOEL* and *LOEL*, for which HSDB data are also available (n = 207). Chemicals that also had positive carcinogenic effect data in USEtox were excluded to keep the analysis of cancer and non-cancer effects separate. The few substances for which non-cancer ED_{50}s are directly calculated from bioassays and are not extrapolated from *NOEL*s or *LOEL*s were all kept in the analysis since they provide more accurate estimate of the ED_{50} (n = 10). A regression and variance analysis was performed to test the adequacy of a fixed extrapolation ratio between chronic ED_{50} and acute LD_{50}.

For statistical reasons one expects to find that TD_{50} and LD_{50} are correlated, assuming that doses tested in acute and chronic experiments are related: Measured effects in bioassays are restricted to a narrow range around the maximum dose tested, whereas the doses tested for individual chemicals vary greatly and span a very wide range.

Creation of a full set of ED_{50} for use in USEtox: Finally, applying the above-described approach, a full set of ED_{50}s was derived on the basis of the full CPDB database. Resulting factors are differentiated between recommended and indicative factors for which uncertainty is high.

Effect factor for indoor exposure: The human health inhalation effect factor EF_{inh} for indoor exposure is the same as for general outdoor exposure in USEtox and independent of the exposure setting or region.

The effect factor non-cancer via inhalation may be obtained from:

$$EF_{inh,nc} = \frac{f_{nc}}{ED_{50,inh,nc}} \quad (185)$$

with

$EF_{inh,nc}$: effect factor non-cancer via inhalation [cases kg_{intake}^{-1}]

f_{nc}: multiplier non-cancer [-]

$ED_{50,inh,nc}$: lifetime inhalation dose inducing non-cancer disease in 50% of population [kg_{intake} $lifetime^{-1}$]

Where the multiplier non-cancer can be found in Table 13 and the lifetime inhalation dose inducing non-cancer disease in 50% of population is described in the substance data.

The effect factor non-cancer via ingestion may be obtained from:

$$EF_{ing,nc} = \frac{f_{nc}}{ED_{50,ing,nc}} \quad (186)$$

with

$EF_{ing,nc}$: effect factor non-cancer via ingestion [cases kg_{intake}^{-1}]

f_{nc}: multiplier non-cancer [-]

$ED_{50,ing,nc}$: lifetime ingestion dose inducing non-cancer disease in 50% of population [kg_{intake} $lifetime^{-1}$]

Where the multiplier non-cancer can be found in Table 13 and the lifetime ingestion dose inducing non-cancer disease in 50% of population is described in the substance data.

The effect factor cancer via inhalation may be obtained from:

$$EF_{inh,c} = \frac{f_c}{ED_{50,inh,c}} \quad (187)$$

with

$EF_{inh,c}$: effect factor cancer via inhalation [cases kg_{intake}^{-1}]

f_c: multiplier cancer [-]

$ED_{50,inh,c}$: lifetime inhalation dose inducing cancer disease in 50% of population [kg_{intake} $lifetime^{-1}$]

Where the multiplier cancer can be found in Table 13 and the lifetime inhalation dose inducing cancer disease in 50% of population is described in the substance data.

The effect factor cancer via ingestion may be obtained from:

$$EF_{ing,c} = \frac{f_c}{ED_{50,ing,c}} \quad (188)$$

with

$EF_{ing,c}$: effect factor cancer via inhalation [cases kg_{intake}^{-1}]

f_c: multiplier cancer [-]

$ED_{50,ing,c}$: lifetime inhalation dose inducing cancer disease in 50% of population [kg_{intake} $lifetime^{-1}$]

Where the multiplier cancer can be found in Table 13 and the lifetime inhalation dose inducing cancer disease in 50% of population is described in the substance data.

In above equations, the units were converted to kg/person/lifetime, using a default lifetime of 70 years and a default body weight of 70 kg for ingestion and a default inhalation rate of 13 m^3/day and a default lifetime of 70 years for inhalation, all per person. An allometric interspecies conversion factor proportional to body weight to the power of 0.25 has been applied to the ED_{50} for ingestion (see Table 20). As for non-cancer effects for inhalation, the critical effect concentration is defined as the concentration in the air, the interspecies extrapolation factor for inhalation is in principle 1, assuming that inhalation rates between species scale proportionally to metabolic rates. For some toxicity data after inhalation, however, substance-specific interspecies differences were derived by the US-EPA via pharmacokinetic modelling. In these specific cases, the interspecies conversion factors reported by the US-EPA were applied. As for carcinogenic effects, in case no data is available for a specific exposure route, a route-to-route extrapolation has been carried out, assuming equal ED_{50} between inhalation and ingestion route.

Table 20. Interspecies conversion factors (CF) to humans for various animal species.

Type	**CF interspecies (-)**	**Average body weight (kg)**
human	1.0	70
pig	1.1	48
dog	1.5	15
monkey	1.9	5
cat	1.9	5
rabbit	2.4	2
mink	2.9	1
guinea pig	3.1	0.750
rat	4.1	0.250
hamster	4.9	0.125
gerbil	5.5	0.075
mouse	7.3	0.025

In summary, the following **calculation steps of the human-equivalent ED_{50}** should be followed:

1. Gather experimental non-carcinogenic oral (ingestion exposure) ED_{50} or LD_{50} data and non-carcinogenic inhalation exposure ED_{50} or acute LD_{50} data;
2. Specify for every ED_{50} value whether it is chronic, subchronic or subacute exposure;
3. In case of subchronic or subacute ED_{50} data, derive the chronic-equivalent ED_{50} by respectively dividing by a factor of 2 and a factor of 5 (subchronic-to-chronic extrapolation factor and subacute-to-chronic extrapolation factor);
4. In case of non-human ED_{50} data, derive the human-equivalent ED_{50} by dividing by an extrapolation factor for interspecies differences (see Table 20);
5. In case only NOAEL-data or NOAEC-data are available, derive the non-carcinogenic ED_{50} via multiplication with the extrapolation factor for NOAEL to ED_{50}, which is a factor of 9;
6. In case only LOAEL-data or LOAEC-data are available, derive the non-carcinogenic ED_{50} via division by the extrapolation factor for LOAEL to NOAEL, which is a factor of 4, and multiply with the extrapolation factor for NOAEL to ED_{50}, which is a factor of 9;

7. If LD_{50} data (always acute) are available, convert to chronic human ED_{50} based on the relationship $ED_{50} = LD_{50}/26$ building on Rosenbaum et al. (2011, Figure 8);
8. If more than one human-equivalent ED_{50} are derived based on data available for more than one animal species, select the smallest human-equivalent ED_{50} per exposure route to reflect the animal that is closed to humans in terms of body size-to-shape relationship (see Table 20) – note that this is different than for ecotoxicity effects, where we use all available ecosystem species in the calculation of the ecotoxicity effect factor as we want to reflect the effect on the entire ecosystem, whereas for human toxicity effect factor calculation, we want to find the data most representative for humans;
9. Implement the human-equivalent ED_{50} values (maximum 4 values) in columns AE:AH of the sheet «Substance data» of USEtox model file or of the USEtox organic substances database file.
10. Always be careful with the units!

8.4 Damage

Within the USEtox characterization framework, this section deals with the determination of the human health damage factor related to human toxicological effects (Figure 13).

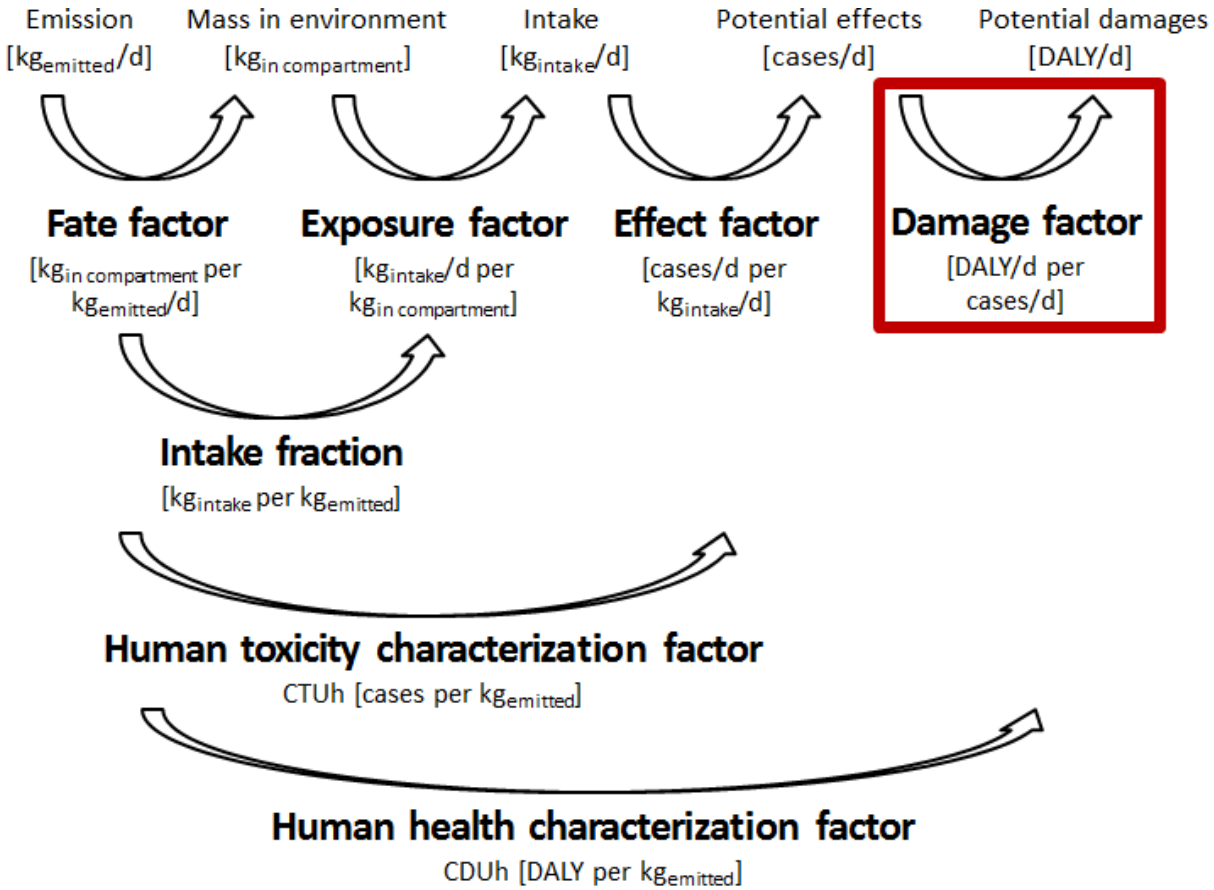

Figure 13: Symbolic description of the emission-to-damage framework for ecotoxicological impacts characterized with USEtox 2.0x.

The Effect Factor calculates the cumulative disease cases in a human population that is affected by an exposure via different exposure pathways. The area of protection in LCA that is relevant for human toxicity is Human Health, and damage to this area of protection is

typically expressed in LCA as a loss of healthy life years. In USEtox characterization modelling, the damage modelling thus consists of a translation of the number of disease cases for cancer and non-cancer effects into the disability-adjusted life years (DALY) metric. The translation from cancer and non-cancer cases to DALY in USEtox applies respectively a factor of 11.5 and 2.7 based on Huijbregts et al. (2005):

$$\mathrm{DF}_{\mathrm{human}} = \begin{cases} 11.5 \text{ for cancer effects} \\ 2.7 \text{ for non-cancer effects} \end{cases} \quad (189)$$

with

$\mathrm{DF}_{\mathrm{human}}$: damage factor for human toxicity [DALY/disease case]

9. FRESHWATER ECOSYSTEM EXPOSURE

9.1 Introduction

Within the USEtox characterization framework, this chapter deals with the determination of the ecosystem exposure factor, which describes the fraction of the chemicals in freshwater that is bioavailable for uptake into freshwater ecosystem species, and thus potentially causing impact and damage (Figure 14). Explanations of symbols and indices are given in Appendix A and corresponding parameters in USEtox are given in Appendices B to E.

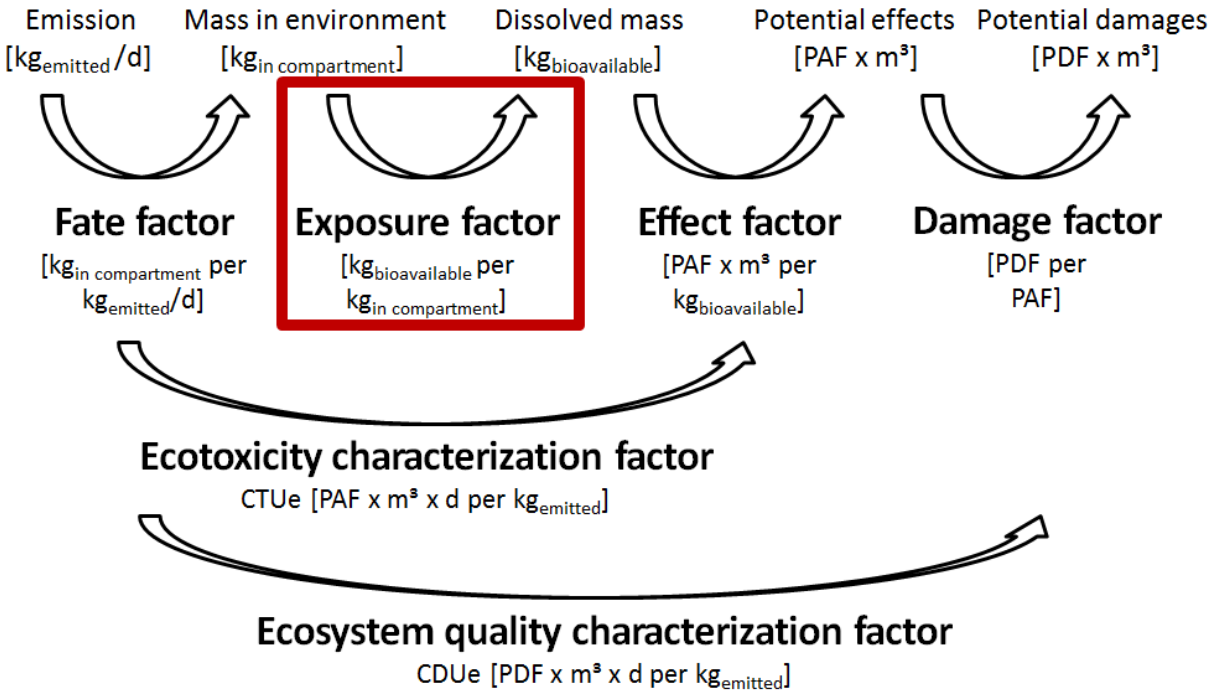

Figure 14: Symbolic description of the emission-to-damage framework for ecotoxicological impacts characterized with USEtox 2.0x.

The ecotoxicity effect factor is calculated from ecotoxicity test results expressed as a concentration of dissolved chemical to which the organism is exposed in the test. The freshwater ecosystem exposure factor for an organic chemical in freshwater therefore needs to equal the fraction of the chemical that is dissolved. To obtain this fraction the following approach is applied, based on Brandes et al. (1996):

$$\begin{aligned} \mathrm{XF}_{\mathrm{eco},x} &= \frac{m_{\mathrm{dissolved},x}}{m_{\mathrm{total},x}} \\ &= \frac{m_{\mathrm{dissolved},x}}{m_{\mathrm{dissolved},x} + m_{\mathrm{susp},x} + m_{\mathrm{doc},x} + m_{\mathrm{biota},x}} \\ &= \frac{C_{\mathrm{fw},x} \times V_{\mathrm{fw}}}{C_{\mathrm{fw},x} \times V_{\mathrm{fw}} + C_{\mathrm{susp},x} \times V_{\mathrm{susp}} + C_{\mathrm{doc},x} \times V_{\mathrm{doc}} + C_{\mathrm{biota},x} \times V_{\mathrm{biota}}} \end{aligned} \quad (190)$$

$$= \frac{1}{1 + \frac{C_{\text{susp},x} \times V_{\text{susp}}}{C_{\text{fw},x} \times V_{\text{fw}}} + \frac{C_{\text{doc},x} \times V_{\text{doc}}}{C_{\text{fw},x} \times V_{\text{fw}}} + \frac{C_{\text{biota},x} \times V_{\text{biota}}}{C_{\text{fw},x} \times V_{\text{fw}}}}$$

$$= \frac{1}{1 + \mathrm{K}_{\text{susp},x} \cdot \frac{\mathrm{C}_{\text{susp,fw}}}{1000} + \mathrm{K}_{\text{doc},x} \cdot \frac{\mathrm{C}_{\text{doc,fw}}}{1000} + \mathrm{BAF}_{\text{fish,fw},x} \cdot \frac{\mathrm{C}_{\text{biota,fw}}}{1000}}$$

where

$XF_{\text{eco},x}$ ecological exposure factor in freshwater of chemical x [dimensionless];
$m_{\text{dissolved},x}$ dissolved mass of chemical x in freshwater [kg]
$m_{\text{total},x}$ total mass of chemical x in freshwater [kg]
$m_{\text{susp},x}$ mass of chemical x associated with suspended matter in freshwater [kg]
$m_{\text{doc},x}$ mass of chemical x associated with dissolved organic carbon in freshwater [kg]
$m_{\text{biota},x}$ mass of chemical x associated with biota in freshwater [kg]
$C_{\text{fw},x}$ concentration of dissolved chemical in freshwater [kg/m^3]
$C_{\text{susp},x}$ concentration of chemical associated with suspended matter in freshwater [kg/m^3]
$C_{\text{doc},x}$ concentration of chemical associated with dissolved organic carbon in freshwater [kg/m^3]
$C_{\text{biota},x}$ the concentration of chemical associated with biota in freshwater [kg/m^3]
V_{fw} volume of freshwater compartment [m^3]
V_{susp} volume of suspended matter in freshwater compartment [m^3]
V_{doc} volume of dissolved organic carbon in freshwater compartment [m^3]
V_{biota} volume of biota in freshwater compartment [m^3]
$K_{\text{susp},x}$ suspended solids/water partitioning coefficient of chemical x [l/kg];
$C_{\text{susp,fw}}$ concentration suspended matter in freshwater [15 mg/m^3; taken from ECHA European Chemicals Agency (2012)]
$K_{\text{doc},x}$ dissolved (colloidal) organic carbon/water partition coefficient of chemical x [l/kg]
$C_{\text{doc,fw}}$ concentration of dissolved (colloidal) organic carbon in freshwater [5 mg/m^3, derived from Gandhi et al. (2010)]
$\mathrm{BAF}_{\text{fish,fw},x}$ bioaccumulation factor for freshwater fish of chemical x [l/kg]
$C_{\text{biota,fw}}$ concentration of biota in freshwater [1 mg/m^3, taken from Brandes et al. (1996)]

For metals the ecological exposure factor is derived similarly as:

$$\mathrm{XF}_{\text{eco},x} = \frac{m_{\text{truly dissolved},x}}{m_{\text{total},x}} \tag{191}$$

where

$m_{\text{truly dissolved},x}$ truly dissolved mass of metal x in freshwater calculated as the sum of the free ion and the inorganic complex-bound metal [kg]

The size of the different metal species fractions varies among the different metals and also depends on water chemistry parameters like pH and presence of anions and other cations. Following the approach suggested by Gandhi et al. (2010) and Dong et al. (2014), $K_{\text{susp,x}}$ and $K_{\text{doc,x}}$ are calculated using the geochemical model WHAM 7.0 (Tipping et al. 2011) assuming the water chemistry of EU freshwater archetype V in Dong et al. (2014) which has been found to be a good representative of the emission weighted average across all European freshwater archetypes for all metals investigated. Bioaccumulation factors (BAF) for fish are

preferably taken from IAEA International Atomic Energy Agency (2010). For Beryllium and Cadmium no BAF information was provided for fish by this source so for these two inorganic substances, BAFs for fish are taken from US-EPA United States - Environmental Protection Agency (2002).

9.2 Data selection and conversion

Chemical-specific data required are $K_{susp,x}$, $K_{doc,x}$ and $BAF_{fishfw,x}$. The selection or calculation of $K_{susp,x}$, $K_{doc,x}$ and $BAF_{fishfw,x}$ for a specific chemical is explained in Sections 5.4.3, 5.4.7, and 5.4.6, respectively.

10. FRESHWATER ECOTOXICOLOGICAL EFFECTS

10.1 Introduction

Within the USEtox characterization framework, this chapter deals with the determination of the freshwater ecotoxicological effect factor which relates effects on freshwater ecosystem species to the bioavailable fraction of chemicals in freshwater (Figure 15). Explanations of symbols and indices are given in Appendix A and corresponding parameters in USEtox are given in Appendices B to E.

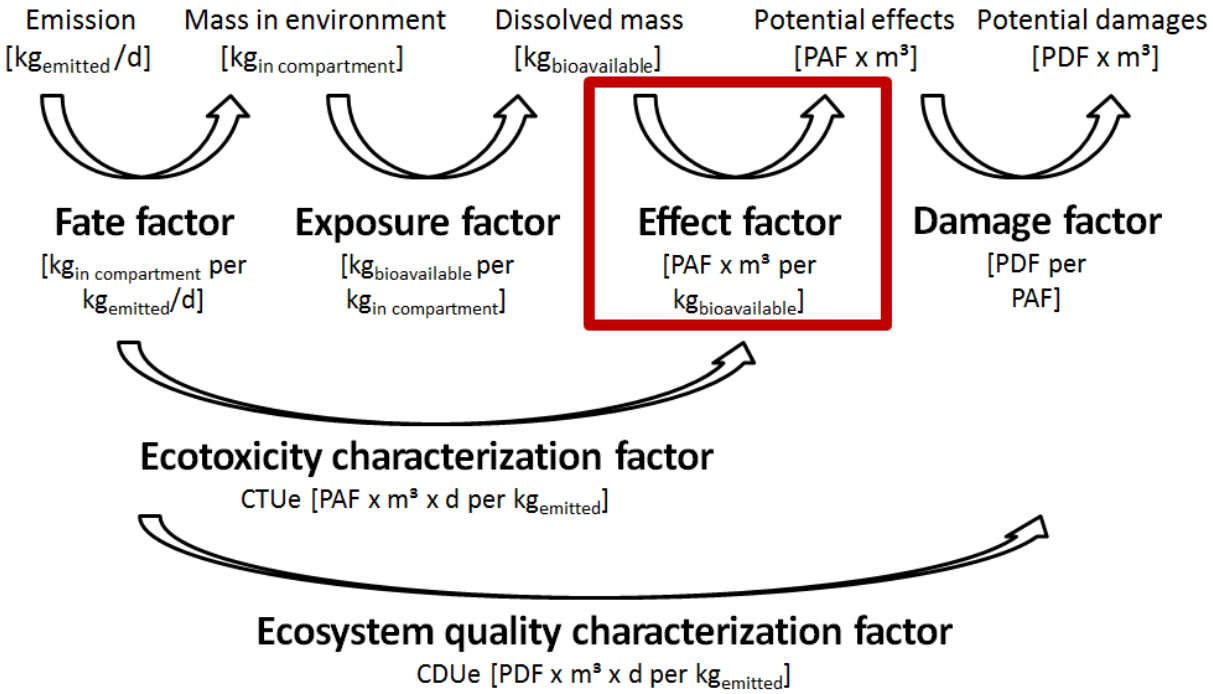

Figure 15: Symbolic description of the emission-to-damage framework for ecotoxicological impacts characterized with USEtox 2.0x.

The ecotoxicological effect factor represents the chronic toxicity of the substance to a freshwater ecosystem. The chronic toxicity is derived from observations on the sensitivities of a sample of the species of which an ecosystem can be composed. The approach is based on confirmation studies, in which it has been shown that an increase in the predicted fraction of species that is potentially affected (PAF based on SSD modeling) for a compound relates to an increased ecological effect (e.g. de Zwart 2005, Posthuma & de Zwart 2006, 2012, van den Brink et al. 2002).

The sensitivity observations that are needed to the derive the Effect Factor are composed of the set of available test results, which are commonly laboratory experiments exposing freshwater test organisms from different trophic levels in the ecosystem to the chemical under controlled and reproducible conditions in preferably standardized tests. A selection is made from the available toxicity data, which may represent acute or chronic exposures as compared to the life cycle of the organism (time aspect) or no-, low or median response endpoints, such as the NOEC (No Observed Effect Concentration), LOEC (Lowest Observed Effect

Concentration), EC10 (an Effect Concentration causing a 10% effect to a vital life history trait), or – often – the EC50 (*ibidem*, causing 50% effect to a vital life history trait). To reveal the possible chronic effects of a substance on the ecosystem, preference is given to results from chronic or sub-chronic tests at the EC50-level in the LCIA step (Jolliet et al. 2006, Larsen & Hauschild 2007). The motives for this are, amongst others, the statistical robustness of deriving the 50%-response level, and – not the least – the ecological interpretation of the EC50-endpoint in terms of impacts that are meaningful and can be observed in field-exposed ecosystems. Technically, this requires a definition of chronic exposures. Table 21 shows the USEtox exposure duration requirements to identify chronic and sub-chronic tests (de Zwart 2002, ECETOC European Centre for Ecotoxicology and Toxicology of Chemicals 1993, Embry et al. 2015, Müller et al. 2017, Payet 2004).

Table 21: Duration requirement for classification of a test as acute, sub-chronic or chronic.

	Acute	Sub-chronic	Chronic
Vertebrates	< 7 days	≥7 days; < 32 days	≥ 32 days
Invertebrates	< 7 days	≥7 days ; < 21 days	≥ 21 days
Plants	< 7 days	-	≥ 7 days
Algae	< 3 days	-	≥ 3 days

Ecotoxicity test results are reported as Effect Concentrations EC_x where the effect may be mortality, immobilization, reproduction or other endpoints and 'x' refers to the fraction of the test organisms showing the effect. EC_{50} results are determined at the middle of the concentration effect curve from the experiment and are hence more robust than test results for lower effect levels. Therefore they are used for determination of the ecotoxicological effect factor to minimize uncertainties in the effect factor.
Upon collation of the set of test results, the distribution of the test results for the chemical across different test organisms is shown in the Species Sensitivity Distribution (SSD) curve (Posthuma et al. 2002). An SSD of chronic EC50s ($SSD_{EC50,\ chronic}$) depicts the fraction of species in the ecosystem which are affected above their chronic EC50 value (Y) as a function of the bioavailable concentration (X) of the chemical. An example of an SSD curve is shown in Figure 16. The SSD-midpoint has been named the HC50, the Hazardous Concentration for 50% of the species. In USEtox the HC50 is thus specifically: the $HC50_{EC50}$[b]. This USEtox HC_{50}-value of the chemical indicates the concentration corresponding to 50% of the species being exposed above their EC_{50} value. In a series of chemicals it holds that the lower the HC50-value of a chemical, the higher the relative ecotoxicity of a compound. This principle is the basis for quantifying expected aquatic ecosystem impacts in USEtox, in combination with the exposure quantification (described in Chapter 9).

[b] Note that, in the derivation of water quality criteria for chemicals, the term HC5 is used, in that case with an SSD based on NOECs, that is: $HC5_{NOEC}$).

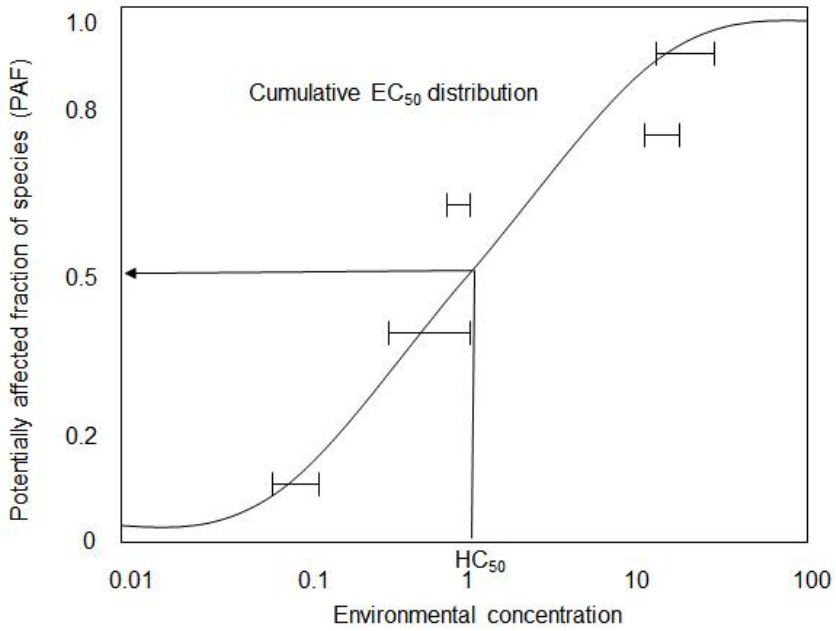

Figure 16: Species Sensitivity Distribution (SSD) curve showing the cumulative distribution of EC_{50} values across tested species for a chemical (ranges of test-EC50s represent variation between available data for a given species).

The purpose of LCA and hence also characterization modelling is to compare alternatives rather than to predict effects or absolute risk (Jolliet et al. 2006, Ligthart et al. 2004). Following previous work and recommendations on the choice of the LCIA ecotoxicity indicator, it is therefore chosen to give priority to the use of robust measures of toxicity rather than the lowest measures of toxicity, which are generally interpolated in the lower tail of the SSD-distribution. The effect factor in USEtox is thus based on the HC50 (here: geometric mean of EC50) level rather than the HC5 or the PNEC level used in regulatory chemical risk assessment, reflecting in fact the most likely estimate of sensitivity at the EC50-level rather than the most sensitive species.
As a formula, the Effect Factor for aquatic ecotoxicity has thus been defined by (Gandhi et al. 2010, Rosenbaum et al. 2008) as:

$$EF_{eco} = \frac{f_{eco}}{HC_{50}} \tag{192}$$

with

EF_{eco}: ecotoxicological effect factor for freshwater aquatic ecosystems [PAF m^3 kg^{-1}]
f_{eco}: multiplier for ecosystems [-]
HC_{50}: geometric mean of chronic EC50s for freshwater species [kg m^{-3}]

where the multiplier for ecosystems is given in Table 13.

The hazardous concentration at which 50% of the species in the freshwater ecosystem are exposed above their EC50 value is determined as the geometric mean of chronic aquatic EC50 values:

$$HC_{50} = \sqrt[n]{\prod_{i=1}^{n} EC_{50,i}} = 10^{\left[\frac{1}{n}\sum_{i=1}^{n}\log_{10}\left(\frac{EC_{50,i}}{1000}\right)\right]} \quad (193)$$

with

HC_{50}: geometric mean of chronic aquatic EC_{50}'s [kg m^{-3}]
$EC_{50,i}$: concentration at which 50% of test organisms of species *i* show effects [mg L^{-1}]
1000: conversion factor to convert from mg/L to g/L [mg g^{-1}]

The effect factor in USEtox must be based on effect data for at least three trophic levels (typically algae, crustacean and fish), which (when fulfilled) results in the USEtox characterization factor being classified as "recommended". As mentioned, preference is given to chronic or sub-chronic data in the calculation of the effect factor, but acute data may be more prevalent, and for many substances there will only be acute data available for one or maybe all trophic levels. If this is the case, chronic EC_{50} values are estimated from acute values dividing the latter by an acute-to-chronic ratio (ACR). This is possible, as various authors have delineated consistent patterns across the ecotoxicity data and/or the SSDs of compounds, e.g. when based on chronic *versus* acute data; see further below, starting with the SSD-pattern analysis of de Zwart (2002).

For metals (Al, Ba, Be, Cd, Co, Cr(III), Cs, Cu, Fe(II), Fe(III), Mn, Ni, Pb, Sr and Zn), the ecotoxicological effect factor is derived by the same method as described above. Note that metals exist in freshwater in different forms, including particulate forms, DOC complex-bound forms and truly dissolved forms. Due to the very limited bioavailability of the other species, only the truly dissolved metal species (sum of free ion and inorganic complex-bound forms) are considered toxic to the aquatic biota. For metals, the chronic EC_{50} in Equation (193) therefore represents the concentration of truly dissolved metals that is found to cause effects on 50% of a single species population. Truly dissolved metal EC_{50} is calculated from reported total EC_{50} in literatures by use of a geochemical speciation model. Details can be found in Gandhi et al. (2010) and Dong et al. (2014).

10.2 Data selection and conversion

The procedure for calculation of ecotoxicity effect factors can be summarized as follows:

1. Gather experimental EC_{50} data for the chemical of interest;
2. Specify for every EC_{50}-value whether it is based on chronic or acute exposure (see Table 21) and give preference to chronic EC_{50}-values;
3. Where chronic data is missing, use available acute EC_{50}-data to derive the chronic-equivalent EC_{50} per species by dividing by an ACR value of 2 (Rosenbaum et al. 2008) unless other information is available. For metals an ACR of 10 is applied for crustaceans, 20 for fishes (Dong et al. 2014) and 15 (average of crustaceans and fishes) for all other trophic levels.
4. When more than one EC_{50} data point is available for a species, eliminate possible outliers and calculate the representative EC_{50} value for the species as the geometric

mean of the rest of the available EC_{50} values (mg/L) for that species i ($EC_{50,i} = 10^{\left[\frac{1}{n}\sum_{j=1}^{n}\log_{10}(EC_{50,i,j})\right]}$ for $j \in \{1, \dots, n\}$ individual EC_{50} values for species i)

5. Following Equation (193), take the log of the geometric mean EC_{50} per species and calculate the average of the log-values. This average equals the $\log_{10}HC_{50}$ ($\log_{10}$ kg/m³). If as user you want to directly pre-calculate the $\log_{10}HC_{50}$ (which is denoted $avlogEC_{50}$ in the substances databases of USEtox) from various individual EC_{50} values $j \in \{1, \dots, m\}$ per species $i \in \{1, \dots, n\}$, the following equation directly applies after point (3), i.e. for all EC_{50} data points being or being converted to chronic values: $\log_{10}(HC_{50}) = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{m}\sum_{j=1}^{m}\log_{10}(EC_{50,i,j})$.
6. Implement this value in column AD of the sheet "Substance data" of the USEtox model file or substances database files.
7. Always be careful with the units!

In USEtox version 2.0x, two databases with ecotoxicity effect data on average EC_{50} values (i.e. HC_{50}s) were taken as a starting point, covering, respectively, 3,498 (van Zelm et al. 2007, van Zelm et al. 2009) and 1,408 chemicals (Payet 2004). The first one contains data based on acute EC_{50} values from the National Institute for Public Health and the Environment (RIVM) e-toxBase (http://www.ru.nl/environmentalscience/research/themes-0/risk-assessment/e-toxbase/). The second contains data on chronic and acute EC50-data mainly from the US-EPA ECOTOX database (http://www.epa.gov/ecotox) and IUCLID (http://bookshop.europa.eu/en/iuclid-cd-rom-pbLBNA19559/). Note that these three databases in part have a common origin, not only because of the collation of test data from literature sources (many original test data in all three databases), but also due to some decades of database contents exchanges (originally between US-EPA and RIVM, later expanded to Payet).

USEtox preferably applies chronic values from Payet (2004), as long as they represent measured EC50 values. Second priority is given to acute data from Payet (2004), applying a best estimate acute-to chronic ratio (ACR) of 2 as described above for organic substances and 2.2 for pesticides. In case Payet (2004) does not provide ecotoxicity information for a chemical, acute ecotoxicity data from the RIVM e-toxBase are used, applying an acute-to-chronic ratio (ACR) of 2 to estimate chronic EC_{50} per species. The EC_{50} data for metals are taken from three studies (Dong et al. 2014, Gandhi et al. 2011, Gandhi et al. 2010), all of which are based on chronic and acute EC_{50} values from the ECOTOX database (http://cfpub.epa.gov/ecotox/). First priority is given to chronic data. If chronic data is not available, acute data is used, applying ACR as described before.

10.3 Damage

Within the USEtox characterization framework, this section deals with the determination of the ecosystem quality damage factor related to ecosystem toxicological effects (Figure 17).

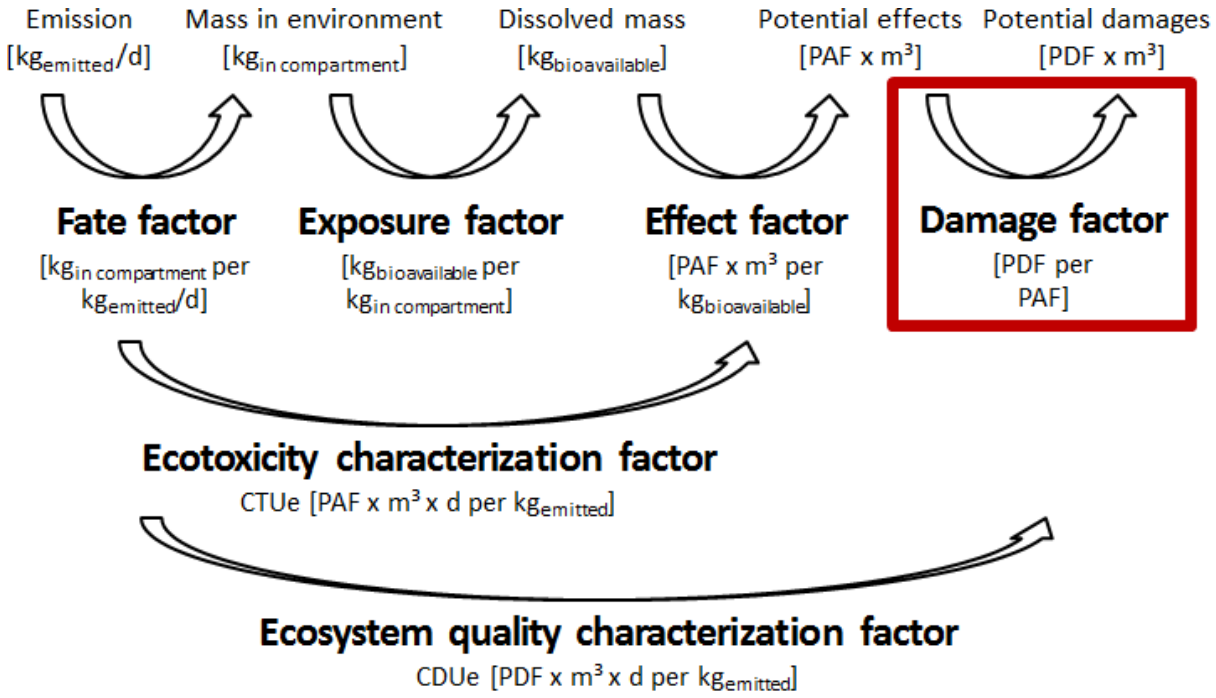

Figure 17: Symbolic description of the emission-to-damage framework for ecotoxicological impacts characterized with USEtox 2.0x.

The Effect Factor calculates the fraction of species in the ecosystem that is potentially affected by an exposure above the concentration that elicits chronic effects in 50% of the population. The area of protection in LCA that is relevant for ecotoxicity is Ecosystem Quality, and damage to this area of protection is typically expressed in LCA as a loss of biodiversity, represented by a change in species richness of the ecosystem. In USEtox characterization modelling, the damage modelling thus consists of a translation of the potentially affected fraction of species (PAF) into the potentially *disappeared* fraction of species (PDF). The translation from PAF to PDF in USEtox applies a factor of 0.5 based on Jolliet et al. (2003):

$$DF_{eco} = 0.5 \quad (194)$$

with

DF_{eco}: damage factor for freshwater ecotoxicity [PDF/PAF]

11. MODEL APPLICATION AND LIMITATIONS

Models are designed to carry out specific tasks and offer users both quantitative outcomes but also provide insight on how these results come about. The USEtox model has been developed specifically to assess potential impacts of toxic emissions in a comparative context such as life cycle assessment, providing characterization factors as substance-specific measures of relative impact potential. In this chapter we discuss when and how USEtox can be applied for comparative assessments. We also discuss the capabilities and limitations of USEtox—areas where it is applicable for supporting comparative assessments but also areas where it should be applied with caution.

USEtox is a comparative assessment tool and was not intended for risk assessment. We begin this chapter with a discussion of the differences between chemical risk assessment and comparative assessment to make clear the situations for which USEtox is relevant.

We next develop sections that provide guidance on the capabilities and limitations of USEtox in the field of comparative impact assessment. We first consider USEtox results and how they can be interpreted. For this we discuss the model's geographical scale, time scales, chemicals covered, exposure assessment, health endpoints, and effects calculations. We next consider interpretation of USEtox results in light of the model's capabilities as well as consideration of model performance uncertainties, knowledge gaps, incomplete data, and data gaps. We then discuss model limitations with regard to the scope and limitations of the fate model, exposure routes and pathways, chemical substances, and health endpoints.

11.1 Chemical risk assessment versus comparative impact assessment

In order to identify, characterize, and compare opportunities for increasing the sustainable use of energy, resources, chemicals, and materials, we need reliable and informative environmental, health and economic impact assessments. The USEtox model has specifically been developed to assess potential impacts of toxic emissions in a comparative context such as life cycle assessment, providing characterization factors as substance-specific measures of relative impact potential. Although LCA-type characterizations of impacts are inspired by human and ecological risk assessment (HERA), it is important to consider the fundamental differences that distinguish these two assessment approaches to better understand the underlying methodological choices of USEtox.

The goal of a risk assessment is to quantify the likelihood of harm in a format that assists decision makers who must act to tolerate, mitigate, or eliminate the potential harm. LCA has become an important tool for the environmental impact assessment of products and materials. Businesses are increasingly relying on it for their decision-making. The information obtained from an LCA can also influence environmental policies and regulations. Life-cycle impact assessment is the phase of LCA aimed at understanding and evaluating the magnitude and significance of the potential environmental impacts of environmental interventions (including toxic emissions) occurring throughout the whole life cycle of a product system. Both potential impact and risk relate to some measure of harm, such as number of deaths or diseases, financial loss, species loss, resource privation, etc.

The scope of LCA is relative to a functional unit, where only a fraction of the burdens associated to the activities within the product life cycle is attributable to it. LCA takes the "emitter perspective", assessing potential burdens of such emissions over space and time with

the ultimate aim to compare hundreds of life-cycle emissions against each other and allow a consistent summation of all effects into one impact score in the human toxicity or ecotoxicity impact categories--in the specific case of USEtox. In contrast, HERA adopts a conservative approach to evaluate a "safe" level for a chemical emission and the resulting exposure to a targeted population or ecosystem ("receptor perspective") with the ultimate aim of setting emission goals with respect to acceptable limits. The scope of the HERA is restricted to assess the risk of one or a few chemicals and a specific release location, activity or process (instead of the full life cycle), within limited time boundaries. Overall LCA indicates the desirability of a decrease in hazardous substances within a relative context ("less-is-better"), whereas HERA describes an absolute "only-above-threshold" approach (Udo de Haes et al. 2006).

In LCIA, the selection of a generic multimedia environment (air, freshwater, agricultural and natural soil and marine water) nested in a world box model accounts for the full fate and intermedia transfer and of chemical emissions and transboundary effects from a regional to a global environment, where location and the time of emissions along the life cycle chain are often unknown. Fate and exposure modeling approaches of HERA might be far more sophisticated accounting for site-specific conditions and exposure pathways as this information is generally known and environmental mechanisms can be adapted to the targeted chemical.

The most fundamental difference between risk assessment and comparative assessments in modeling fate, exposure and effect is to be found in the effect-characterization step and in the expression of the indicator. In regulatory risk assessment, such as REACH and other national regulations, risk characterization ratios (RCR or hazard quotients) such as PEC/PNEC, are traditionally used to assess whether the risk to a chemical exposure is acceptable (ratio < 1) or not (ratio > 1). PEC (predicted effect concentration) traditionally considers fate and exposure assessment, whereas PNEC (predicted no effect concentration) refers to regulatory thresholds. For ecotoxicity assessment PNECs are based on the conservative choice of selecting the most sensitive species among the available ecotoxicity effect data, then applying safety factors for less-known chemicals. A similar approach is applied for human reference doses selecting the most sensitive test results on animals. RCR are one of the several assessment techniques used by the ecological risk assessment community. Among the alternatives techniques, the species sensitivity distribution (SSD) is widely used to derive environmental quality criteria and has been adopted in various legal frameworks in US, Canada, The Netherlands and Scandinavian countries (Posthuma et al. 2002). It offers a common approach to extrapolate from single species toxicity test (the same used to determine RCR) results to biotic communities.

In order to avoid unwanted bias in chemical comparison, similarly to SSDs, USEtox relies on a multiple species approach adopting best estimate effect concentrations (EC50) to calculate the harmful concentration at which 50% of species [HC50 (or EC50)] are affected. This choice has been evaluated appropriate in a review workshop with the participation ecologists (Jolliet et al. 2006).

11.2 Applicability of USEtox for Comparative Impact Assessment

The USEtox model includes three linked model components—a multimedia transport and transformation model that translates emissions into environmental inventories, an exposure model that links environmental concentrations from the fate model to human intake and ecosystem exposures, and an effects model that links human intake to the incidence of health

effects and links ecosystem exposure to the fraction of potentially affected species in aquatic or terrestrial ecosystems.

A major objective of USEtox is to provide decision makers who seek comparative impact metrics with a more complete picture of both how potential human and ecosystem exposures come about and how the potential exposure pathways can be tracked and quantified. When USEtox was first released, its approach provided a major step forward in several areas. It is a consensus-based model that capture key aspects of number of multimedia exposure models worldwide available for comparative assessments. It is based on both conservation of mass and chemical equilibrium. USEtox addresses gains and losses and audits mass potential, thus eliminating the need to make assumptions that might implicitly "double count" the spread of contaminants. The model makes a distinction between environmental concentrations and exposure concentrations. Finally, the model provides methods for addressing a broad range of potential exposure pathways including highly uncertain, but sometimes significant, indirect exposures such as those through food.

11.2.1 Geographical scale

USEtox is a lumped systems course-dimension-scale model. This means that it includes compartments to represent various components of the environment, but that there are limited explicit vertical or horizontal dimensions in these compartments. The model has embedded urban, regional, and global environments but does not have detailed spatial resolution.

However, because of the nature of these compartments, and the way mass exchange is modeled among these compartments, there are implicit transport vectors within the model. In the atmosphere contaminants either move vertically back to the ground-surface soil or are blown by wind horizontally out of the landscape to the next level of spatial resolution. Transport from soil to surface water is implicitly horizontal and at the surface.

11.2.2 Time scale

The USEtox transport model was designed to be applied over long time periods--months to years--when seasonally and yearly-averaged partition factors apply. The exposure model is intended for situations in which the environmental media concentrations are constant over the exposure duration.

11.2.3 Chemicals classes covered

There are many classes of chemicals that must be addressed in comparative assessments, including nonionic organic chemicals, ionic organic chemicals, metals, and inorganic chemicals. These chemicals species can also be categorized according to the physical state in which they are introduced to the environment (gas, liquid, or solid), according to whether they dissociate in solution (ionic or nonionic) and according to the charge distribution on the molecule (polar or nonpolar). The traditional multimedia fate modeling approach of USEtox is most appropriate for nonionic, organic chemicals in a liquid or gaseous state. However, with modifications for condensation of solids on air particles, this approach can be made appropriate for solid-phase organic chemicals.

Additional adjustments make possible the treatment of inorganic species, metals, and partially or fully ionized organic species. Metals (such as mercury) and inorganic chemicals with a relatively large vapor pressure pose special problems, which are not yet fully addressed in USEtox. Special modeling problems also occur with mixed polarity, dissociating organic species, such as surfactants.

The USEtox model, in descending order of reliability, is capable of handling nonionic organic chemicals, fully dissociating organic and inorganic chemicals, and solid-phase metal species. With careful attention to inputs, the model can be used for partially dissociated organic and inorganic species. The model has not been designed to work with surfactants, inorganic chemicals species with high vapor-pressure-to-solubility ratios, and volatile metals such as mercury.

11.2.4 Exposure pathways

USEtox employs human-exposure assessments to translate contaminant sources into quantitative estimates of the amount of an emitted chemical that comes in contact with the human-environment boundaries, that is, the lungs, the gastrointestinal tract, and (potentially) the skin surface of individuals within a specified population. An assessment of intake requires that we determine how much crosses these boundaries. Exposure assessments often rely implicitly on the assumption that exposure can be linked by simple parameters to ambient concentrations in air, water, and soil. However, total exposure assessments that include time and activity patterns and micro-environmental data reveal that an exposure assessment is most valuable when it provides a comprehensive view of exposure pathways. This creates the need to address many types of "multiples" in the quantification of human exposure, such as multiple media (air, water, soil); multiple exposure pathways (or scenarios); multiple routes (inhalation, ingestion, dermal); multiple chemicals; multiple population subgroups; and multiple health endpoints. In order to address these issues USEtox was designed to be comprehensive and flexible. Potential dose by route is linked to contaminant-specific, multimedia dispersion in the environment.

11.2.5 Health effects

USEtox has two human-health effects metrics and makes use of the potentially affected fraction (PAF) of species for ecotoxicological impacts. Human health endpoints are classified as either cancer or non-cancer endpoints. Dose-response models based primarily on animal data are used to estimate expected incidence of human cancer or non-cancer diseases.

11.2.6 Summary points on applicability

Based on the approaches employed in USEtox for spatial/temporal resolution, for capturing chemical-property classes, for human/ecosystem exposure pathways, and health endpoints, we conclude that it is not appropriate for making absolute quantitative estimates of health and/or ecosystem impacts. Instead USEtox is most applicable for comparison and sorting chemicals with regard to their potential health and environmental impacts. While it has not been structured for applicability in higher tier quantitative impact assessments, it is well structured as a tool for reliably selecting chemicals that can be classified as low impact and chemicals that present potential concerns and thus require impact assessment and at a higher tier of resolution. Overall USEtox allows to sort out from a full life cycle inventory of several hundred chemicals those few ones of potentially higher concern for health and environmental impacts.

11.3 Interpreting USEtox results

11.3.1 Model outputs

The primary outputs of USEtox are characterization factors for human toxicity and freshwater ecotoxicity. Assessing the toxicological effects of a chemical emitted into the environment implies a cause–effect chain that is captured in different ways for humans and freshwater systems. For human toxicity, the cause-effect chain includes environmental fate, exposure and effects. For freshwater systems the chain includes fate and effects based only on freshwater concentrations. In both cases characterization factors are used to make quantitative rankings for chemicals with regard to either human toxicity or freshwater ecotoxicity. This approach gives toxicological comparisons of emission impacts in activities such as life-cycle impact assessment. In addition to toxicity characterization factors, USEtox provides the model user with three intermediate outputs in the form of matrices. The fate matrix reveals the steady-state distribution of an emission from any one environmental compartment (air, surface water, soil) to all other compartments in the global system. The exposure matrix reveals how much interaction (rate of consumption) humans have with each compartment through multiple exposure pathways. For humans the product of the fate matrix and the exposure matrix is the intake fraction matrix that shows what fraction of an emitted chemical mass enters the human population by any selected environmental/exposure pathway.

11.3.2 Reliability and uncertainty

The reliability of model outputs for supporting decisions on products and services is related to model performance and data uncertainty including knowledge and data gaps. Identifying, characterizing, and confronting uncertainties are among the foremost challenges for those who carry out life-cycle impact assessment (LCIA) as well as other types of technology assessments such as comparative risk assessment. There are many sources of uncertainty in the process of human-health and environmental impact assessment. Many of these uncertainties, which are associated with knowledge or data gaps, are not reducible. Effective decision making is possible under conditions of uncertainty, but such policies must confront the uncertainty not ignore it. There are well-established protocols for making decisions in the context of uncertainty, which have been described in Chernoff and Moses (1959), Lindley (1985), and Berger (1985), among others. These authors argue that the existence of uncertainty should not be an excuse for abandoning quantitative assessments. Instead they emphasize that uncertainty creates the need for flexibility to address margins of error; to consider reducible versus irreducible uncertainty; to separate variability from true scientific uncertainty; and to consider benefits, costs, and comparable risks in the decision-making process.

Here we consider the nature of and strategies for addressing uncertainties that arise in USEtox from data gaps, data quality, variability, and model performance. Identifying the sources of uncertainty can be a key starting point for confronting uncertainty, but in many cases more evaluation is needed. In most impact studies there are a range of options for addressing uncertainty ranging from single-value outcomes based on defaults to detailed probabilistic assessments. Some of the existing approaches used to characterize uncertainty include the use of simple defaults, expert elicitation, sensitivity analysis, and probabilistic methods (Krupnick et al. 2006, Morgan & Henrion 1990).

The collection and interpretation of input data give rise to many type of uncertainty in any quantitative impact assessment. A few such sources include variation in measured data, disagreement between alternate sources of information, natural heterogeneity, and

extrapolation errors (Krupnick et al. 2006). As noted by Krupnick et al. (2006) it is important to recognize that variability and parameter uncertainty apply to empirical quantities. In an assessment such as LCIA there are model variables that represent "measurable properties of the system being modeled" (Morgan & Henrion 1990). In this context, variability is the inherent heterogeneity of an empirical quantity across a population (of people or objects), space, or time, whereas parameter uncertainty is the lack of knowledge about an empirical quantity stemming from limitations of measurement, disagreement among measurements, or extrapolation errors.

Model uncertainty includes uncertainties about model structure, about how well the model captures key elements of the system or population being modeled, the selection of one model form over another, simplifications of model structure, and value judgments. Model performance uncertainty is commonly addressed by sensitivity analysis and/or expert evaluations.

11.4 Limitations of USEtox

Limitations arise by choice of modeling approach or by consequence of lack of knowledge, lack of data or lack of global consensus. USEtox allows the user to determine whether a substance will (a) remain or accumulate within the compartment of its origin, (b) be physically, chemically, or biologically transformed within the compartment of its origin (i.e., by hydrolysis, oxidation, etc.), or (c) be transported to another compartment by cross-media transfer that involves dispersion or advection (i.e., volatilization, precipitation, etc.). This approach is comprehensive but applied at a rather course scale of resolution. Among a very large number of pathways linking compartment concentrations to human contact there are some pathways that are considered as having limited contribution and other pathways for which there is not sufficient data to parameterize the pathway. These types of issues give rise to limitations in the USEtox output.

11.4.1 Compartment coverage and structure

The compartment structure of USEtox spans three spatial scales. At the lowest tier of resolution is the urban environment that includes outdoor-air and indoor-air compartments interacting with natural soil and freshwater. Next is the continental scale consisting of indoor air and six interconnected environmental compartments: urban air, rural air, agricultural soil, industrial soil, freshwater, and coastal marine water. The global scale has the same structure as the continental scale, but without the urban air, and accounts for impacts outside the continental scale. The USEtox structure provides for full mass balance but lacks a high level of spatial resolution. Currently chemicals that migrate below the surface soil are considered lost from the overall mass balance systems because there is currently no groundwater compartment in USEtox.

11.4.2 Exposure routes and pathways coverage

The USEtox exposure models encompass complex exposure pathways linking the environment to humans and/or ecological receptors. The human exposure assessment process consists of relating contaminant concentrations in the multimedia model compartments to contaminant concentrations in the media with which a human population has contact (personal air, tap water, foods, household dusts soils, etc.). The average intake fraction is the product of the exposure concentrations in the contact media and an intake or uptake factor that relates the concentrations to the distributions of potential dose within the population.

USEtox exposure media include outdoor air; food products including meat, milk/dairy products, above ground produce, below ground produce; and fish; and tap water. Current USEtox exposure routes include inhalation and ingestion.

It should be noted that several potentially important exposure pathways are excluded in USEtox due to lack of scientific consensus indicating further research needs. These are notably breast milk, indoor inhalation, exposure to directly applied pesticide residues, or increased exposure due to proximity to the source (e.g. workers handling chemicals), and dermal exposure. These can be dominant exposure pathways for specific sub-populations (e.g. babies, children, workers, consumers, etc.). The impact of neglecting important exposure pathways has been discussed by Franco et al. (2007). For chemicals with an important fish intake pathway, bioaccumulation modeling is an area of improvement, better considering the role of organisms in the food web living in sediments.

Another notable limitation is that the majority of the exposure equations are based on empirical regressions instead of mechanistic insight such as published by Czub and McLachlan (2004) for example. The problem of empirical vs. mechanistic exposure modeling has been discussed by Rosenbaum et al. (2009) who also demonstrated how empirical regressions may be used in conjunction with mechanistic models to increase understanding of the underlying processes. However, as shown by Smítková et al. (2005) mechanistic bioaccumulation models for fish may produce approximately the same result as an empirical regression. This type of work can be used to further underpin or adapt the use of other empirical regressions in human exposure models, such as USEtox.

11.4.3 Chemical substances

The USEtox exposure model is best suited to model non-dissociating and non-amphiphilic organic substances. However, meaningful value choices for important parameters enable the model to also cover chemicals with a more complex behavior, like metals, dissociating organics, or detergents. These are then flagged as interim characterization factors and their impact scores need to be interpreted cautiously as explained by Rosenbaum et al. (2008).

11.4.4 Human and ecosystem toxicological endpoints

USEtox was developed with comparative assertions regarding the variation of potential toxic impacts within a large range of potential impacts among thousands of chemicals. USEtox is applicable in any comparative toxicity impact assessment (e.g. comparative hazard assessment, ranking of chemicals according to their potential impact, or prioritization of chemicals in a policy context) and not limited to be used in the context of life cycle assessment only. Comparative assessments aim to estimate the impact of a chemical relative to other substances and establishing rankings that can be used as the basis for decisions, e.g. regarding choices of chemicals as product compounds with the least toxic impact, or in the context of chemical policy identifying priority substances for regulation, etc. Important assumptions commonly made in comparative models are for example 1) use of best estimates instead of conservative choices (i.e. often mean or median values instead of lowest/highest parameter values) (Barnthouse et al. 1997, Olsen et al. 2001, Owens 1997, Pennington et al. 2006, Udo de Haes et al. 2002); 2) consideration of large sets of chemical emissions instead of one substance at a time; 3) consideration of impacts integrated over time and space (global in the case of USEtox) at the population level instead of e.g. peak exposures of individuals or sub-populations at a specific site and point in time.

USEtox can support such comparisons but the endpoints used for this comparison are currently limited for both human toxicity and ecotoxicity. For human toxicity, comparisons are constrained by the aggregations of non-cancer effects into a single endpoint and aggregation of cancer effects to a single generic “cancer” outcome. For ecotoxicity, chemical comparisons are currently based on freshwater toxicity without consideration of terrestrial or marine toxicity.

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APPENDIX: MODEL PARAMETERS

A. Description of symbols and notation

General object and operator syntax

Symbol	Definition
$k, k_{ij}, K, K_{\mathrm{ow}}$	Scalar (italic), sometimes with indices (upright unless a counting index or vector/matrix element index). Matrix element k_{ij} is interpreted as the element of matrix **K** at row *i* and column *j* and can be interpreted as process from column *j* (input) to row *i* (output).
$V_{\mathrm{air[G]}}$	Separation of different indices: specification of variable (e.g. index "air") is separated from spatial context of variable (e.g. index "G" for global). Alternative notations would be (both not used): $V_{\mathrm{air}}^{\mathrm{G}}$ or $V_{\mathrm{air\|G}}$
$k_{\mathrm{air\rightarrow air\|sl}}$ $K_{\mathrm{air\|carpet}}$ $EF_{\mathrm{human,noncanc,inh}}$ $fr_M_{\mathrm{dis,C.fw\rightarrow G.fw[C\rightarrow G]}}$	Different separators between indices: Direction from e.g. compartment to another compartment is expressed by "→". Intersection for e.g. partition coefficients or compartments or phases is expressed by "|". Indices indicating different aspects (e.g. human tox/ecotox vs. cancer/non-cancer vs. inhalation/ingestion exposure) are separated by ",". Indices that belong together, but must be separated, are separated by ".".
$\vec{m} \in \mathbb{R}^n$	Vector (non-capital italic letters) containing elements (scalars) as in $\vec{m} = \begin{pmatrix} m_1 \\ \vdots \\ m_n \end{pmatrix} = (m_1, \ldots, m_n)^T$
$\mathbf{K} \in \mathbb{R}^{n \times m}$	Matrix (capital bold upright letters) containing elements (scalars) as in $\mathbf{K} = \begin{pmatrix} k_{11} & \cdots & k_{1m} \\ \vdots & \ddots & \vdots \\ k_{n1} & \cdots & k_{nm} \end{pmatrix}$
$\frac{\mathrm{d}\vec{m}(t)}{\mathrm{d}t} = \mathbf{K}\,\vec{m}(t) + \vec{s}$	Operators between matrices and vectors should not be "·" (vector dot product) or "×" (vector cross product). Between scalars, all operators are allowed.

Symbols for spatial scales

Symbol	Refers to
[C]	Continental scale
[G]	Global scale
[S]	Generic scale (refers to all spatial scales)
[U]	Urban scale

Symbols for indices of objects

Symbol	Refers to
acc	Accumulation
abs	Absorption
ads	Adsorption
adv	Advective
air	Air
app	Apparent
aq	Water phase
asl	Agricultural soil compartment
aw	Air water
beef	Beef
biota	Biota
burial	Burial
cattle	Cattle
Corg	Organic carbon
dairy	Dairy
deg	Degradation
dep	Deposition
des	Desorption
disc	Discharge
diss	Dissolution /dissolved
DOC	Dissolved organic carbon
drizzle	Drizzle
dry	Dry
dw	Drinking water compartment
eff	Effective
esc	Escape
exp	Exposed
fish	Fish
fw	Fresh water compartment
fwsd	Fresh water sediment compartment
gas	Gas
goat	Goat
growth	Growth
inf	Infiltration
land	Land
leach	Leaching
leaf	Leaf
m	Mass
meat	Meat
metab	Metabolism
milk	Milk
mixed	Mixed
npav	Unpaved surface compartment

Symbol	Refers to
nsl	Natural soil compartment
osl	Other soil compartment
other	In conjunction with “meat” it refers to “goat and sheep”.
ow	Octanol/water
part	Particles
pav	Paved surface compartment
penetr	Penetration
pork	Pork
rain	Rain
rain	Rain
res	Re-suspension
runoff	Run off
sd	Sediment compartment
sea	Sea
sed	Sedimentation
sheep	Sheep
sl	Soil
sl	Aerosol
solid	Solid phase
std	Standard
strat	Stratosphere
susp	Suspended matter
sw	Sea water compartment
tot	Total
unexp	Unexposed
vap	Vaporization/vapor
veg	Vegetation
vol	Volatilization
w	Water
wash	Washout
wet	Wet
τ	Residence time

B. Environmental fate (and ecosystem exposure)

USEtox variable	Symbol	Unit	Explanation	Equation
ADSORB.w1C.sd1C	$\upsilon_{ads,fw\rightarrow fwsd[C]}$	[m.s^{-1}]	ADSORPTION to sediment	eq. (122)
ADSORB.w1G.sd1G	$\upsilon_{ads,fw\rightarrow fwsd[G]}$	[m.s^{-1}]		
ADSORB.w2C.sd2C	$\upsilon_{ads,sw\rightarrow swsd[C]}$	[m.s^{-1}]		
ADSORB.w2G.sd2G	$\upsilon_{ads,sw\rightarrow swsd[G]}$	[m.s^{-1}]		
AEROSOLdeprate.C	$\upsilon_{dep,air,ae[C]}$	[m.s^{-1}]	DEPOSITION VELOCITY aerosol particles	Table 10
AEROSOLdeprate.G	$\upsilon_{dep,air,ae[G]}$	[m.s^{-1}]		
AEROSOLdeprate.U	$\upsilon_{dep,air,ae[U]}$	[m.s^{-1}]		

USEtox variable	Symbol	Unit	Explanation	Equation
AerosolWashout.C	$v_{wash,ae[C]}$	[m.s^{-1}]	Aerosol WASHOUT	eq. (98)
AerosolWashout.G	$v_{wash,ae[G]}$	[m.s^{-1}]		
AerosolWashout.U	$v_{wash,ae[U]}$	[m.s^{-1}]		
AREAFRAC.s1C	$fr_A_{nsl[C]}$	[-]	AREA FRACTION soil	eq. (44)
AREAFRAC.s1G	$fr_A_{nsl[G]}$	[-]		eq. (45)
AREAFRAC.s2C	$fr_A_{\alpha sl[C]}$	[-]		eq. (45)
AREAFRAC.s2G	$fr_A_{\alpha sl[G]}$	[-]		eq. (44)
AREAFRAC.s1U	$fr_A_{npav[U]}$	[-]	AREA FRACTION unpaved surface	Table 6
AREAFRAC.s3U	$fr_A_{pav[U]}$	[-]	AREA FRACTION paved surface	Table 6
AREAFRAC.w1C	$fr_A_{fw[C]}$	[-]	AREA FRACTION water	eq. (18)
AREAFRAC.w1G	$fr_A_{fw[G]}$	[-]		
AREAFRAC.w2C	$fr_A_{sw[C]}$	[-]		eq. (19)
AREAFRAC.w2G	$fr_A_{sw[G]}$	[-]		
AREAland.C	$A_{land[C]}$	[km^2]	Area land	Table 4
AREAland.G	$A_{land[G]}$	[km^2]		Table 5
AREAsea.C	$A_{sea[C]}$	[km^2]	Area sea	Table 4
AREAsea.G	$A_{sea[G]}$	[km^2]		Table 5
BAFfish1.C	$BAF_{dissolved.fish.fw[C]}$	[L.kg^{-1}]	BIOACCUMULATION FACTOR fish	eq. (87)
BAFfish1.G	$BAF_{dissolved.fish.fw[C]}$	[L.kg^{-1}]		
BAFfish2.C	$BAF_{dissolved.fish,sw[C]}$	[L.kg^{-1}]		
BAFfish2.G	$BAF_{dissolved.fish,sw[G]}$	[L.kg^{-1}]		
BIOmass.w1C	$C_{biota,fw[C]}$	[mg.L^{-1}]	CONCENTRATION biota in water	Table 10
BIOmass.w1G	$C_{biota,fw[G]}$	[mg.L-1]		
BIOmass.w2C	$C_{biota,sw[C]}$	[mg.L^{-1}]		
BIOmass.w2G	$C_{biota,sw[G]}$	[mg.L-1]		
BURIAL.sd1C	$v_{burial,fwsd[C]}$	[m.s^{-1}]	SEDIMENT BURIAL sediment	eq. (42)
BURIAL.sd1G	$v_{burial,fwsd[G]}$	[m.s^{-1}]		
BURIAL.sd2C	$v_{burial,swsd[C]}$	[m.s^{-1}]		
BURIAL.sd2G	$v_{burial,swsd[G]}$	[m.s^{-1}]		
C.aC	$cf_{\tau air[C]}$	[-]	Calibration constant	Table 10
C.aU	$cf_{\tau air[U]}$	[-]	Correction factor	Table 10
COLLECTeff.C	$CE_{ae[C]}$	[-]	Aerosol COLLECTION EFFICIENCY	Table 10

USEtox variable	Symbol	Unit	Explanation	Equation
COLLECTeff.G	$CE_{ae[G]}$	[-]		
COLLECTeff.U	$CE_{ae[U]}$	[-]		
CORG	$fr_m_{Corg,std,sl\|sd}$	[-]	Standard mass FRACTION organic carbon in soil/sediment	Table 10
CORG.s1C	$fr_m_{Corg,nsl[C]}$	[-]	Mass FRACTION organic carbon soil	
CORG.s1G	$fr_m_{Corg,nsl[G]}$	[-]		
CORG.s2C	$fr_m_{Corg,asl[C]}$	[-]		
CORG.s2G	$fr_m_{Corg,asl[G]}$	[-]		
CORG.sd1C	$fr_m_{Corg,fwsd[C]}$	[-]	Mass FRACTION organic carbon sediment	
CORG.sd1G	$fr_m_{Corg,fwsd[G]}$	[-]		
CORG.sd2C	$fr_m_{Corg,swsd[C]}$	[-]		
CORG.sd2G	$fr_m_{Corg,swsd[G]}$	[-]		
CORGsusp1.C	$fr_m_{Corg,susp,fw[C]}$	[-]	Mass FRACTION organic carbon in suspended matter	
CORGsusp1.G	$fr_m_{Corg,susp,fw[G]}$	[-]		
CORGsusp2.C	$fr_m_{Corg,susp,sw[C]}$	[-]		
CORGsusp2.G	$fr_m_{Corg,susp,sw[G]}$	[-]		
D	$K_{ow,app,pH7}$	[-]	Apparent octanol/water PARTITION COEFFICIENT at neutral pH	eqs. (71) - (72)
Deff.s1C	$D_{eff,nsl[C]}$	$m^2.s^{-1}$	Effective DIFFUSION coefficient in soil	eq. (57)
Deff.s1G	$D_{eff,nsl[G]}$	$[m^2.s^{-1}]$		
DEPTH.s1C	$h_{nsl[C]}$	[m]	DEPTH soil compartment	Table 10
DEPTH.s1G	$h_{nsl[G]}$	[m]		
DEPTH.s2C	$h_{asl[C]}$	[m]		
DEPTH.s2G	$h_{asl[G]}$	[m]		
DEPTH.sd1C	$h_{fwsd[C]}$	[cm]	Mixed DEPTH sediment compartment	
DEPTH.sd1G	$h_{fwsd[G]}$	[cm]		
DEPTH.sd2C	$h_{swsd[C]}$	[cm]		
DEPTH.sd2G	$h_{swsd[G]}$	[cm]		
DEPTH.w1C	$h_{fw[C]}$	[m]	Mixed DEPTH water compartment	
DEPTH.w1G	$h_{fw[G]}$	[m]		
DEPTH.w2C	$h_{sw[C]}$	[m]		
DEPTH.w2G	$h_{sw[G]}$	[m]		

USEtox variable	Symbol	Unit	Explanation	Equation
DESORB.sd1C.w1C	$\upsilon_{des,fwsd\rightarrow fw[C]}$	[m.s^{-1}]	DESORPTION from sediment	eq. (124)
DESORB.sd1G.w1G	$\upsilon_{des,fwsd\rightarrow fw[G]}$	[m.s^{-1}]		
DESORB.sd2C.w2C	$\upsilon_{des,swsd\rightarrow sw[C]}$	[m.s^{-1}]		
DESORB.sd2G.w2G	$\upsilon_{des,swsd\rightarrow sw[G]}$	[m.s^{-1}]		
DIFFgas	D_{gas}	[m^2.s^{-1}]	Gas phase DIFFUSION coefficient	eq. (58)
DIFFwater	D_{water}	[m^2.s^{-1}]	Water phase DIFFUSION coefficient	eq. (59)
DOC.w1C	$K_{DOC\mid w,fw\ [C]}$:	[mg.L^{-1}]	Concentration of dissolved (colloidal) organic carbon in water	eq. (89)
DOC.w1G	$K_{DOC\mid w,fw\ [G]}$:	[mg.L^{-1}]		
DOC.w2C	$K_{DOC\mid w,sw\ [C]}$:	[mg.L^{-1}]		eq. (88)
DOC.w2G	$K_{DOC\mid w,sw\ [G]}$:	[mg.L^{-1}]		
DRYDEPaerosol.C	$\upsilon_{dep,dry,ae[C]}$:	[m.s^{-1}]	Dry aerosol DEPOSITION rate	eq. (94)
DRYDEPaerosol.G	$\upsilon_{dep,dry,ae[G]}$:	[m.s^{-1}]		
DRYDEPaerosol.U	$\upsilon_{dep,dry,ae[U]}$:	[m.s^{-1}]		
EROSION.s1C	$v_{nsl[C]}$	[mm.yr^{-1}]	EROSION of soil	Table 4
EROSION.s1G	$v_{nsl[G]}$	[mm.yr^{-1}]		Table 5
EROSION.s2C	$v_{asl[C]}$	[mm.yr^{-1}]		Table 4
EROSION.s2G	$v_{asl[G]}$	[mm.yr^{-1}]		Table 5
FATfish1.C	$C_F_{fish,fw[C]}$	[-]	FAT CONTENT fish	Table 10
FATfish1.G	$C_F_{fish,fw[G]}$	[-]		
FATfish2.C	$C_F_{fish,sw[C]}$	[-]		
FATfish2.G	$C_F_{fish,sw[G]}$	[-]		
FRAC.w1C.w1G	$fr_M_{disc,fw[C\rightarrow G]}$	[-]	FRACTION discharge continental fresh water to global fresh water	Table 10
FRAC.w1G.w1C	$fr_M_{disc,fw[G\rightarrow C]}$	[-]	FRACTION discharge global fresh water to continental fresh water	
FRACa.s1C	$fr_V_{gas,nsl[C]}$	[-]	VOLUME FRACTION air in soil	Table 10
FRACa.s1G	$fr_V_{gas,nsl[G]}$	[-]		
FRACa.s2C	$fr_V_{gas,asl[C]}$	[-]		
FRACa.s2G	$fr_V_{gas,asl[G]}$	[-]		
FRACagsoil.C	$fr_A_{land,asl[C]}$:	[-]	Fraction agricultural soil	Table 4
FRACagsoil.G	$fr_A_{land,asl[G]}$:	[-]		Table 5
FRACfresh.C	$fr_A_{land,fw[C]}$:	[-]	Fraction fresh water	Table 4
FRACfresh.G	$fr_A_{land,fw[G]}$:	[-]		Table 5
FRACinf.s1C	$fr_V_{rain,inf,nsl[C]}$	[-]	VOLUME FRACTION of precipitation infiltrating into soil	Table 4
FRACinf.s1G	$fr_V_{rain,inf,nsl[G]}$	[-]		Table 5

USEtox variable	Symbol	Unit	Explanation	Equation
FRACinf.s2C	$fr_V_{rain,inf,asl[C]}$	[-]		Table 4
FRACinf.s2G	$fr_V_{rain,inf,asl[G]}$	[-]		Table 5
FRACnatsoil.C	$fr_A_{land,nsl[C]}$:	[-]	Fraction natural soil	Table 4
FRACnatsoil.G	$fr_A_{land,nsl[G]}$:	[-]		Table 5
FRACrun.s1C	$fr_V_{rain,runoff,nsl[C]}$	[-]	VOLUME FRACTION of precipitation on soil running off to surface water	Table 4
FRACrun.s1G	$fr_V_{rain,runoff,nsl[G]}$	[-]		Table 5
FRACrun.s2C	$fr_V_{rain,runoff,asl[C]}$	[-]		Table 4
FRACrun.s2G	$fr_V_{rain,runoff,asl[G]}$	[-]		Table 5
FRACs.s1C	$fr_V_{solid,nsl[C]}$	[-]	VOLUME FRACTION solids soil	Table 10
FRACs.s1G	$fr_V_{solid,nsl[G]}$	[-]		
FRACs.s2C	$fr_V_{solid,asl[C]}$	[-]		
FRACs.s2G	$fr_V_{solid,asl[G]}$	[-]		
FRACs.sdC	$fr_V_{solid,wsd[C]}$	[-]	VOLUME FRACTION solids in sediment	eq. (40)
FRACs.sdG	$fr_V_{solid,wsd[G]}$	[-]		
FRACw.s1C	$fr_V_{water,nsl[C]}$	[-]	VOLUME FRACTION water soil	Table 10
FRACw.s1G	$fr_V_{water,nsl[G]}$	[-]		
FRACw.s2C	$fr_V_{water,asl[C]}$	[-]		
FRACw.s2G	$fr_V_{water,asl[G]}$	[-]		
FRACw.sdC	$fr_V_{water,wsd[C]}$	[-]	VOLUME FRACTION water in sediment	
FRACw.sdG	$fr_V_{water,wsd[G]}$	[-]		
FRg.aC	$fr_m_{gas,air[C]}$	[-]	FRACTION of chemical in gas phase air	eq. (8)
FRg.aG	$fr_m_{gas,air[G]}$	[-]		
FRg.aU	$fr_m_{gas,air[U]}$	[-]		
FRorig.cldw	fr_m_{cldw}	[-]	Fraction original species in cloud water	eqs. (9)-(10)
FRorig.s1	fr_m_{nsl}	[-]	Fraction original species in soil	eqs. (49)-(50)
FRorig.s2	fr_m_{asl}	[-]		
FRorig.s1w	$fr_m_{nsl,water}$	[-]	Fraction original species in porewater of soil	eqs. (51)-(52)
FRorig.s2w	$fr_m_{asl,water}$	[-]		
FRorig.sd1	fr_m_{fwsd}	[-]	Fraction original species in sediment	eqs. (38)-(39)
FRorig.sd2	fr_m_{swsd}	[-]		
FRorig.w1	fr_m_{fw}	[-]	Fraction original species in water	eqs. (21)-(22)
FRorig.w2	fr_m_{sw}	[-]		

USEtox variable	Symbol	Unit	Explanation	Equation
FRs.s1C	$fr_m_{solid,nsl[C]}$	[-]	FRACTION of chemical in solid phase soil	eq. (46)
FRs.s1G	$fr_m_{solid,nsl[G]}$	[-]		
FRs.s2C	$fr_m_{solid,asl[C]}$	[-]		
FRs.s2G	$fr_m_{solid,asl[G]}$	[-]		
FRw.s1C	$fr_m_{water,nsl[C]}$	[-]	FRACTION of chemical in water phase soil	eq. (48)
FRw.s1G	$fr_m_{water,nsl[G]}$	[-]		
FRw.s2C	$fr_m_{water,asl[C]}$	[-]		
FRw.s2G	$fr_m_{water,asl[G]}$	[-]		
FRw.w1C	$fr_m_{diss,fw[C]}$	[-]	FRACTION of chemical dissolved in water	eq. (20)
FRw.w1G	$fr_m_{diss,fw[G]}$	[-]		
FRw.w2C	$fr_m_{diss,sw[C]}$	[-]		
FRw.w2G	$fr_m_{diss,sw[G]}$	[-]		
GASABS.aC.s1C	$v_{abs,gas,air→nsl[C]}$	[m.s^{-1}]	GAS ABSORPTION to soil	eq. (107)
GASABS.aC.s2C	$v_{abs,gas,air→asl[C]}$	[m.s^{-1}]		
GASABS.aG.s1G	$v_{abs,gas,air→sl[G]}$	[m.s^{-1}]		
GASABS.aG.s2G	$v_{abs,gas,air→sl[G]}$	[m.s^{-1}]		
GASABS.aC.w1C	$v_{abs,gas,air→fw[C]}$	[m.s^{-1}]	GAS ABSORPTION to water	eq. (109)
GASABS.aC.w2C	$v_{abs,gas,air→sw[C]}$	[m.s^{-1}]		
GASABS.aG.w1G	$v_{abs,gas,air→fw[C]}$	[m.s^{-1}]		
GASABS.aG.w2G	$v_{abs,gas,air→sw[G]}$	[m.s^{-1}]		
GASABS.aU.s1U	$v_{abs,gas,air→npav[U]}$	[m.s^{-1}]	GAS ABSORPTION to unpaved surface	eq. (102)
GASABS.aU.s3U	$v_{abs,gas,air→pav[U]}$	[m.s^{-1}]	GAS ABSORPTION to paved surface	
GasWashout.C	$v_{wash,gas[C]}$	[m.s^{-1}]	Gas WASHOUT	eq. (97)
GasWashout.G	$v_{wash,gas[G]}$	[m.s^{-1}]		
GasWashout.U	$v_{wash,gas[U]}$	[m.s^{-1}]		
GROSSSEDrate.w1C	$v_{sed,fw[C]}$	[m.s^{-1}]	GROSS SEDIMENTATION rate from water	eq. (36)
GROSSSEDrate.w1G	$v_{sed,fw[G]}$	[m.s^{-1}]		
GROSSSEDrate.w2C	$v_{sed,sw[C]}$	[m.s^{-1}]		
GROSSSEDrate.w2G	$v_{sed,sw[G]}$	[m.s^{-1}]		
H0sol	H_{diss}	[kJ.mol^{-1}]	ENTHALPY of dissolution	Table 10
H0vap	H_{vap}	[kJ.mol^{-1}]	ENTHALPY of vaporization	
HEIGHT.aC	$h_{air[C]}$	[m]	Mixed HEIGHT air compartment	
HEIGHT.aG	$h_{air[G]}$	[m]		
HEIGHT.aU	$h_{air[U]}$	[m]		
IRRIGATION.C	$v_{[C]}$	[km^3]	Irrigation	Table 4

USEtox variable	Symbol	Unit	Explanation	Equation
IRRIGATION.G	$u_{[G]}$	[km^3]		Table 5
IRRIGATION.w1C	$u_{fw[C]}$	[$m.s^{-1}$]	IRRIGATION from fresh water to soil	eq. (118)
IRRIGATION.w1G	$u_{fw[G]}$	[$m.s^{-1}$]		
k.aC.aG	$k_{air[C\rightarrow G]}$	[s-1]	TRANSFER air from continental to global scale	eq. (14)
k.aC.aU	$k_{air[C\rightarrow U]}$	[s-1]	TRANSFER air from continental to urban scale	eq. (13)
k.aC.s1C	$k_{air\rightarrow nsl[C]}$	[d^{-1}]	TRANSFER air to natural soil	eq. (106)
k.aC.s2C	$k_{air\rightarrow asl[C]}$	[d^{-1}]	TRANSFER air to agricultural soil	
k.aC.w1C	$k_{air\rightarrow fw[C]}$	[d^{-1}]	TRANSFER air to fresh water	eq. (108)
k.aC.w2C	$k_{air\rightarrow sw[C]}$	[d^{-1}]	TRANSFER air to seawater	
k.aG.aC	$k_{air[G\rightarrow C]}$	[d^{-1}]	TRANSFER air from global to continental scale	eq. (15)
k.aG.s1G	$k_{air\rightarrow nsl[G]}$	[d^{-1}]	TRANSFER air to natural soil	eq. (106)
k.aG.s2G	$k_{air\rightarrow asl[G]}$	[d^{-1}]	TRANSFER air to agricultural soil	
k.aG.w1G	$k_{air\rightarrow fw[G]}$	[d^{-1}]	TRANSFER air to fresh water	eq. (108)
k.aG.w2G	$k_{air\rightarrow sw[G]}$	[d^{-1}]	TRANSFER air to seawater	
k.aU.aC	$k_{air[U\rightarrow C]}$	[d^{-1}]	TRANSFER air from urban to continental scale	eq. (12)
k.aU.s3U	$k_{air\rightarrow fw[U\rightarrow C]}$	[d^{-1}]	TRANSFER urban air to continental fresh water	eq. (101)
k.s1C.aC	$k_{nsl\rightarrow air[C]}$	[d^{-1}]	TRANSFER natural soil to air	eq. (112)
k.s1C.w1C	$k_{nsl\rightarrow fw[C]}$	[d^{-1}]	TRANSFER natural soil to fresh water	eq. (116)
k.s1G.aG	$k_{nsl\rightarrow air[G]}$	[d^{-1}]	TRANSFER natural soil to air	eq. (112)
k.s1G.w1G	$k_{nsl\rightarrow fw[G]}$	[d^{-1}]	TRANSFER natural soil to fresh water	eq. (116)
k.s2C.aC	$k_{asl\rightarrow air[C]}$	[d^{-1}]	TRANSFER agricultural soil to air	eq. (112)
k.s2C.w1C	$k_{asl\rightarrow fw[C]}$	[d^{-1}]	TRANSFER agricultural soil to fresh water	eq. (116)
k.s2G.aG	$k_{asl\rightarrow air[G]}$	[d^{-1}]	TRANSFER agricultural soil to air	eq. (112)
k.s2G.w1G	$k_{asl\rightarrow fw[G]}$	[d^{-1}]	TRANSFER agricultural soil to fresh water	eq. (116)
k.w1C.aC	$k_{fw\rightarrow air[C]}$	[d^{-1}]	TRANSFER fresh water to air	eq. (114)
k.w1C.s2C	$k_{fw\rightarrow asl[C]}$	[d^{-1}]	TRANSFER fresh water to agricultural soil	eq. (117)
k.w1C.w2C	$k_{fw\rightarrow sw[C]}$	[d^{-1}]	TRANSFER fresh water to coastal seawater	eq. (23)
k.w1G.aG	$k_{fw\rightarrow air[G]}$	[d^{-1}]	TRANSFER fresh water to air	eq. (114)
k.w1G.s2G	$k_{fw\rightarrow asl[G]}$	[d^{-1}]	TRANSFER fresh water to agricultural soil	eq. (117)
k.w1G.w2G	$k_{fw\rightarrow sw[G]}$	[d^{-1}]	TRANSFER fresh water to ocean	eq. (23)
k.w2C.aC	$k_{sw\rightarrow air[C]}$	[d^{-1}]	TRANSFER seawater to air	eq. (114)
k.w2C.w2G	$k_{adv,sw[C\rightarrow G]}$	[d^{-1}]	TRANSFER coastal seawater to	eq. (27)

USEtox variable	Symbol	Unit	Explanation	Equation
			global scale	
k.w2G.aG	$k_{sw\rightarrow air[G]}$	[d^{-1}]	TRANSFER seawater to air	eq. (114)
k.w2G.w2C	$k_{adv,sw[G\rightarrow C]}$	[d^{-1}]	TRANSFER ocean water to continental scale	eq. (30)
kas.air.aC	$u_{m,air,air\|sl[C]}$	[$m.s^{-1}$]	PARTIAL MASS TRANSFER COEFFICIENT air side of air/soil interface	eq. (103)
kas.air.aG	$u_{m,air,air\|sl[G]}$	[$m.s^{-1}$]		
kas.air.aU	$u_{m,air,air\|sl[U]}$	[$m.s^{-1}$]		
kas.soil.sC	$u_{m,sl,air\|sl[C]}$	[$m.s^{-1}$]	PARTIAL MASS TRANSFER COEFFICIENT soil side of air/soil interface	eq. (105)
kas.soil.sG	$u_{m,sl,air\|sl[G]}$	[$m.s^{-1}$]		
kas.soil.sU	$u_{m,sl,air\|sl[U]}$	[$m.s^{-1}$]		eq. (104)
kaw.air.aC	$u_{m,air,air\|w[C]}$	[$m.s^{-1}$]	PARTIAL MASS TRANSFER COEFFICIENT air side of air/water interface	eq. (110)
kaw.air.aG	$u_{m,air,air\|w[G]}$	[$m.s^{-1}$]		
kaw.water.wC	$u_{m,w,air\|w[C]}$	[$m.s^{-1}$]	PARTIAL MASS TRANSFER COEFFICIENT water side of air/water interface	eq. (111)
kaw.water.wG	$u_{m,w,air\|w[G]}$	[$m.s^{-1}$]		
kdeg.aC	$k_{deg,air[C]}$	[d^{-1}]	TRANSFER from air by degradation	eq. (61)
kdeg.aG	$k_{deg,air[G]}$	[d^{-1}]		
kdeg.air	$k_{deg,air25°C}$	[s^{-1}]	Gas phase degradation RATE CONSTANT at 25 oC	Substance data
kdeg.aU	$k_{deg,air[U]}$	[d^{-1}]	TRANSFER from air by degradation	eq. (61)
kdeg.s1C	$k_{deg,nsl[C]}$	[d^{-1}]	TRANSFER from soil by degradation	eq. (65)
kdeg.s1G	$k_{deg,nsl[G]}$	[d^{-1}]		
kdeg.s2C	$k_{deg,asl[C]}$	[d^{-1}]		
kdeg.s2G	$k_{deg,asl[G]}$	[d^{-1}]		
kdeg.sd1C	$k_{deg,fwsd[C]}$	[d^{-1}]	TRANSFER from sediment by degradation	eq. (64)
kdeg.sd1G	$k_{deg,fwsd[G]}$	[d^{-1}]		
kdeg.sd2C	$k_{deg,swsd[C]}$	[d^{-1}]		
kdeg.sd2G	$k_{deg,swsd[G]}$	[d^{-1}]		
kdeg.sed	$k_{deg,sd}$	[s^{-1}]	Bulk degradation RATE CONSTANT standard sediment at 25 oC	Substance data
kdeg.soil	$k_{deg,sl}$	[s^{-1}]	Bulk degradation RATE CONSTANT standard soil at 25 oC	
kdeg.w1C	$k_{deg,fw[C]}$	[d^{-1}]	TRANSFER from water by degradation	eq. (63)
kdeg.w1G	$k_{deg,fw[G]}$	[d^{-1}]		
kdeg.w2C	$k_{deg,sw[C]}$	[d^{-1}]		
kdeg.w2G	$k_{deg,sw[G]}$	[d^{-1}]		
kdeg.water	$k_{deg,w}$	[s^{-1}]	Bulk degradation RATE CONSTANT at 25 oC	Substance data
k.aU.s1U	$k_{air[U]\rightarrow npav[U]}$	[d^{-1}]	TRANSFER from air to unpaved surface	eq. (119)
KDEPmean.C	$kdep,air[C]$	[s^{-1}]	MEAN atmospheric deposition rate	eq. (90)

USEtox variable	Symbol	Unit	Explanation	Equation
KDEPmean.G	$k_{dep,air[G]}$	[s^{-1}]		
KDEPmean.U	$k_{dep,air[U]}$	[s^{-1}]		
kdry.C	$k_{tot,dry,air[C]}$	[s^{-1}]	Total rate constant removal from atmosphere during dry episodes	eq. (93)
kdry.G	$k_{tot,dry,air[G]}$	[s^{-1}]		
kdry.U	$k_{tot,dry,air[U]}$	[s^{-1}]		eq. (92)
kesc.aC	$k_{adv,air\rightarrow strat[C]}$	[d^{-1}]	TRANSFER from air to stratosphere	eq. (62)
kesc.aG	$k_{adv,air\rightarrow strat[G]}$	[d^{-1}]		
Kh	$K_{gas\|w}$	[-]	Dimensionless gas/water PARTITION COEFFICIENT of the original species	eq. (66)
Kh.C	$K_{aw[C]}$	[-]	Dimensionless air/water PARTITION COEFFICIENT of original species	eq. (69)
Kh.G	$K_{aw[G]}$	[-]		
Kh.U	$K_{aw[U]}$	[-]		
kleach.s1C	$k_{leach,nsl[C]}$	[d^{-1}]	TRANSFER from soil by leaching	eq. (126)
kleach.s1G	$k_{leach,nsl[G]}$	[d^{-1}]		
kleach.s2C	$k_{leach,asl[C]}$	[d^{-1}]		
kleach.s2G	$k_{leach,asl[G]}$	[d^{-1}]		
Kow	K_{ow}	[-]	Octanol/water PARTITION COEFFICIENT of the original species	Substance data
Kow.alt	$K_{ow,alt}$	[-]	Octanol/water PARTITION COEFFICIENT of alternate form	eq. (70)
Kp	K_d	[-]	Dimensionless solids/water PARTITION COEFFICIENT of the original species	eqs. (74)-(78)
Kp.alt	$K_{d,alt}$	[-]	Dimensionless solids/water PARTITION COEFFICIENT of the alternate form	eqs. (79)-(82)
Kp.doc1C	$K_{DOC\|w,fw\ [C]}$	[$L.kg^{-1}$]	Dissolved (colloidal) organic carbon/water partition coefficient	eq.
Kp.doc1G	$K_{DOC\|w,fw\ [G]}$	[$L.kg^{-1}$]		eq.
Kp.doc2C	$K_{DOC\|w,sw\ [C]}$	[$L.kg^{-1}$]		eq.
Kp.doG2G	$K_{DOC\|w,sw\ [G]}$	[$L.kg^{-1}$]		eq.
Kp.s1C	$K_{solid,sl\|w,nsl\ [C]}$	[$L.kg^{-1}$]	Soil/water PARTITION COEFFICIENT soil	eq. (84)
Kp.s1G	$K_{solid,sl\|w,nsl\ [G]}$	[L.kg-1]		
Kp.s2C	$K_{solid,sl\|w,asl\ [C]}$	[$L.kg^{-1}$]		
Kp.s2G	$K_{solid,sl\|w,asl\ [G]}$	[L.kg-1]		
Kp.sd1C	$K_{solid,sd\|w,fw\ [C]}$	[$L.kg^{-1}$]	Sediment/water PARTITION COEFFICIENT water	eq. (86)
Kp.sd1G	$K_{solid,sd\|w,fw\ [G]}$	[L.kg-1]		
Kp.sd2C	$K_{solid,sd\|w,sw\ [C]}$	[$L.kg^{-1}$]		

USEtox variable	Symbol	Unit	Explanation	Equation
Kp.sd2G	$K_{solid,sd\|w,sw\ [G]}$	[L.kg-1]		
Kp.susp1C	$K_{susp\|w,fw\ [C]}$	[L.kg^{-1}]	Suspended solids/water PARTITION COEFFICIENT	eq. (73)
Kp.susp1G	$K_{susp\|w,fw\ [G]}$	[L.kg-1]		
Kp.susp2C	$K_{susp\|w,sw\ [C]}$	[L.kg^{-1}]		
Kp.susp2G	$K_{susp\|w,sw\ [G]}$	[L.kg-1]		
Ks1w.C	$K_{sl\|w,nsl\ [C]}$	[-]	Dimensionless soil/water PARTITION COEFFICIENT soil	eq. (83)
Ks1w.G	$K_{sl\|w,nsl\ [G]}$	[-]		
Ks2w.C	$K_{sl\|w,asl\ [C]}$	[-]		
Ks2w.G	$K_{sl\|w,asl\ [G]}$	[-]		
Ksdw1.C	$K_{sd\|w,fw\ [C]}$	[-]	Dimensionless sed/water PARTITION COEFFICIENT water	eq. (85)
Ksdw1.G	$K_{sd\|w,fw\ [G]}$	[-]		
Ksdw2.C	$K_{sd\|w,sw\ [C]}$	[-]		
Ksdw2.G	$K_{sd\|w,sw\ [G]}$	[-]		
ksed.w1C	$k_{w\rightarrow fwsd[C]}$	[d^{-1}]	TRANSFER from sediment by sedimentation + burial	eq. (121)
ksed.w1G	$k_{w\rightarrow fwsd[G]}$	[d^{-1}]		
ksed.w2C	$k_{w\rightarrow swsd[C]}$	[d^{-1}]		
ksed.w2G	$k_{w\rightarrow swsd[G]}$	[d^{-1}]		
ktot.C	$k_{mean,air[C]}$	[s^{-1}]	Mean rate constant removal from atmosphere	eq. (91)
ktot.G	$k_{mean,air[G]}$	[s^{-1}]		
ktot.U	$k_{mean,air[U]}$	[s^{-1}]		
kwet.C	$k_{tot,wet,air[C]}$	[s^{-1}]	Total rate constant removal from atmosphere during wet episodes	eq. (96)
kwet.G	$k_{tot,wet,air[G]}$	[s^{-1}]		
kwet.U	$k_{tot,wet,air[U]}$	[s^{-1}]		eq. (95)
kwsd.sed.sdC	$u_{m,sd,w\ \|sd[C]}$	[m.s^{-1}]	PARTIAL MASS TRANSFER COEFFICIENT sediment side of water/sed interface	Table 10
kwsd.sed.sdG	$u_{m,sd,w\ \|sd[G]}$	[m.s^{-1}]		
kwsd.water.wC	$u_{m,w,w\ \|sd[C]}$	[m.s^{-1}]	PARTIAL MASS TRANSFER COEFFICIENT water side of water/sed interface	
kwsd.water.wG	$u_{m,w,w\ \|sd[G]}$	[m.s^{-1}]		
Molweight	MW	[g.mol^{-1}]	MOLECULAR WEIGHT	Substance data
NETsedrate.w1C	$u_{sed,acc,fw[C]}$	[m.s^{-1}]	Net SEDIMENT ACCUMULATION rate water	eq. (33)
NETsedrate.w1G	$u_{sed,acc,fw[G]}$	[m.s^{-1}]		
NETsedrate.w2C	$u_{sed,acc,sw[C]}$	[m.s^{-1}]		eq. (34)
NETsedrate.w2G	$u_{sed,acc,sw[G]}$	[m.s^{-1}]		
PENdepth.s1C	$h_{sl.penetr[C]}$	m	PENETRATION DEPTH soil	eq. (54)

USEtox variable	Symbol	Unit	Explanation	Equation
PENdepth.s1G	$h_{sl.penetr[G]}$	[m]		
pH.aerw	pH_{cloud}	[-]	pH water aerosol	Table 10
pH.s1	pH_{nsl}	[-]	pH natural soil	
pH.s2	pH_{asl}	[-]	pH agricultural soil	
pH.w1	pH_{fw}	[-]	pH fresh water	
pH.w2	pH_{sw}	[-]	pH in sea water	
pKa.gain	*pKa,gain*	[-]	Equilibrium constant proton loss from parent compound (pKa of the base's conjugated acid dissociation reaction)	Table 10
pKa.loss	*pKa,loss*	[-]	Equilibrium constant proton loss from conjugated acid of parent compound (pKa of the acid dissociation reaction)	
PRODsusp.w1C	$J_{susp,fw[C]}$	[$g.m^{-2}.yr^{-1}$]	Autochtonous PRODUCTION of suspended matter in water	Table 10
PRODsusp.w1G	$J_{susp,fw[G]}$	[$g.m^{-2}.yr^{-1}$]		
PRODsusp.w2C	$J_{susp,sw[C]}$	[$g.m^{-2}.yr^{-1}$]		
PRODsusp.w2G	$J_{susp,sw[G]}$	[$g.m^{-2}.yr^{-1}$]		
Pvap25	$P_{vap,25°C}$	[Pa]	VAPOR PRESSURE of original species at 25 oC	Substance data
RAINflow.aC.w1C	$Q_{rain,air→fw[C]}$	[$m^3.s^{-1}$]	RAIN input into continental water	eq. (25)
RAINflow.aC.w2C	$Q_{rain,air→sw[C]}$	[$m^3.s^{-1}$]		
RAINflow.aG.w1G	$Q_{rain,air→fw[G]}$	[$m^3.s^{-1}$]		
RAINflow.aG.w2G	$Q_{rain,air→sw[G]}$	[$m^3.s^{-1}$]		
RAINrate.C	$u_{rain[C]}$	$mm.yr^{-1}$	Average precipitation	Table 4
RAINrate.G	$u_{rain[G]}$	$mm.yr^{-1}$		Table 5
RAINrate.U	$u_{rain[U]}$	[$mm.yr^{-1}$]	Annual PRECIPITATION	Table 10
RESUSPrate.sd1C	$u_{res,fwsd→fw[C]}$	[$m.s^{-1}$]	RESUSPENSION rate from sediment	eq. (125)
RESUSPrate.sd1G	$u_{res,fwsd→fw[G]}$	[$m.s^{-1}$]		
RESUSPrate.sd2C	$u_{res,swsd→sw[C]}$	[$m.s^{-1}$]		
RESUSPrate.sd2G	$u_{res,swsd→sw[G]}$	[$m.s^{-1}$]		
RHO.air	ρ_{air}	[$kg.m^{-3}$]	DENSITY of air	Table 10
RHO.sed	ρ_{sd}	[$kg.m^{-3}$]	Bulk DENSITY of sediment	eq. (41)
RHO.soil	ρ_{sl}	[$kg.m^{-3}$]	Bulk DENSITY of soil	eq. (53)
RHO.water	ρ_{w}	[$kg.m^{-3}$]	DENSITY of water	Table 10
RHOsolid	$\rho_{sd,sl}$	[$kg.m^{-3}$]	Mineral DENSITY sediment and soil	
SED.w1C.sd1C	$u_{sed,fw→fwsd[C]}$	[$m.s^{-1}$]	SEDIMENTATION to sediment	eq. (123)
SED.w1G.sd1G	$u_{sed,fw→fwsd[G]}$	[$m.s^{-1}$]		

USEtox variable	Symbol	Unit	Explanation	Equation
SED.w2C.sd2C	$u_{sed,sw\rightarrow swsd[C]}$	[m.s^{-1}]		
SED.w2G.sd2G	$u_{sed,sw\rightarrow swsd[G]}$	[m.s^{-1}]		
SETTLvelocity.C	$u_{sed,susp,w[C]}$	[m.s^{-1}]	SETTLING VELOCITY suspended particles	eq. (32)
SETTLvelocity.G	$u_{sed,susp,w[G]}$	[m.s^{-1}]		
Sol.25	$S_{w,25°C}$	[mg.L^{-1}]	Water SOLUBILITY of original species at 25 oC	Substance data
SOLIDadv.s1C	$u_{ad,solid,sl[C]}$	m.s^{-1}	SOLID-phase advection velocity soil	eq. (56)
SOLIDadv.s1G	$u_{ad,solid,sl[G]}$	[m.s^{-1}]		
SOLIDdiff.s1C	$D_{solid,sl[C]}$	m^2.s^{-1}	SOLID-phase turbation coefficient soil	eq. (60)
SOLIDdiff.s1G	$D_{solid,sl[G]}$	[m^2.s^{-1}]		
SUSP.w1C	$C_{susp,fw[C]}$	[mg.L^{-1}]	CONCENTRATION suspended matter in water	Table 10
SUSP.w1G	$C_{susp,fw[G]}$	[mg.L-1]		
SUSP.w2C	$C_{susp,sw[C]}$	[mg.L^{-1}]		
SUSP.w2G	$C_{susp,sw[G]}$	[mg.L-1]		
SYSTEMAREA.C	$A_{[C]}$	[km^2]	System area	Table 4
SYSTEMAREA.G	$A_{[G]}$	[km^2]		Table 5
SYSTEMAREA.U	$A_{[U]}$	[km^2]		Table 6
TAU.aC	$\tau_{air[C]}$	[d]	RESIDENCE TIME of air	eq. (16)
TAU.aU	$\tau_{air[U]}$	[d]		
TAU.w2C	$\tau_{sw[C]}$	[d]	RESIDENCE TIME of seawater on continental shelf	Table 10
tdry.C	$t_{dry[C]}$	[d]	Average duration of dry episodes	eq. (99)
tdry.G	$t_{dry[G]}$	[d]		
tdry.U	$t_{dry[U]}$	[d]		
TEMP.C	$T_{[C]}$	[°C]	Temperature	Table 4
TEMP.G	$T_{[G]}$	[°C]		Table 5
TEMP.U	$T_{[U]}$	[°C]		Table 10
twet.C	$t_{wet[C]}$	[d]	Average duration of wet episodes	eq. (100)
twet.G	$t_{wet[G]}$	[d]		
twet.U	$t_{wet[U]}$	[d]		
Veff.s1C	$u_{eff,adv,sl[C]}$	m.s^{-1}	Effective ADVECTIVE TRANSPORT in soil	eq. (55)
Veff.s1G	$u_{eff,adv,sl[G]}$	[m.s^{-1}]		
VOLAT.s1C.aC	$u_{volat,nsl\rightarrow air[C]}$	[m.s^{-1}]	VOLATILIZATION from soil	eq. (113)
VOLAT.s1G.aG	$u_{volat,nsl\rightarrow air[G]}$	[m.s^{-1}]		
VOLAT.s2C.aC	$u_{volat,asl\rightarrow air[C]}$	[m.s^{-1}]		

USEtox variable	Symbol	Unit	Explanation	Equation
VOLAT.s2G.aG	$\upsilon_{volat,asl\rightarrow air[G]}$	[m.s^{-1}]		
VOLAT.w1C.aC	$\upsilon_{volat,fw\rightarrow air[C]}$	[m.s^{-1}]	VOLATILIZATION from water	eq. (115)
VOLAT.w1G.aG	$\upsilon_{volat,fw\rightarrow air[G]}$	[m.s^{-1}]		
VOLAT.w2C.aC	$\upsilon_{volat,sw\rightarrow air[C]}$	[m.s^{-1}]		
VOLAT.w2G.aG	$\upsilon_{volat,sw\rightarrow air[G]}$	[m.s^{-1}]		
VOLUME.aC	$V_{air[C]}$	[m^3]	VOLUME air compartment	eq. (7)
VOLUME.aG	$V_{air[G]}$	[m^3]		
VOLUME.aU	$V_{air[U]}$	[m^3]		
VOLUME.s1C	$V_{nsl[C]}$	[m^3]	VOLUME soil compartment	eq. (43)
VOLUME.s1G	$V_{nsl[G]}$	[m^3]		
VOLUME.s2C	$V_{asl[C]}$	[m^3]		
VOLUME.s2G	$V_{asl[G]}$	[m^3]		
VOLUME.sd1C	$V_{fwsd[C]}$	[m^3]	VOLUME sediment compartment	eq. (37)
VOLUME.sd1G	$V_{fwsd[G]}$	[m^3]		
VOLUME.sd2C	$V_{swsd[C]}$	[m^3]		
VOLUME.sd2G	$V_{swsd[G]}$	[m^3]		
VOLUME.w1C	$V_{fw[C]}$	[m^3]	VOLUME water compartment	eq. (17)
VOLUME.w1G	$V_{fw[G]}$	[m^3]		
VOLUME.w2C	$V_{sw[C]}$	[m^3]		
VOLUME.w2G	$V_{sw[G]}$	[m^3]		
WATERflow.w1C.w2C	$Q_{des,fw\rightarrow sw[C]}$	[m^3.s^{-1}]	FLOW of continental fresh water to continental sea water	eq. (24)
WATERflow.w1G.w2G	$Q_{des,fw\rightarrow sw[G]}$	[m^3.s^{-1}]	FLOW of global fresh water to global sea water	eq. (29)
WATERflow.w2C.w2G	$Q_{adv,sw[C\rightarrow G]}$	[m^3.s^{-1}]	FLOW of continental sea water to the global ocean	eq. (28)
WATERflow.w2G.w2C	$Q_{adv,sw[G\rightarrow C]}$	[m^3.s^{-1}]	FLOW of global sea water to continental see water	eq. (31)
WATERrun.s1C	$Q_{runoff,water,nsl[C]}$	[m^3.s^{-1}]	Water run off from soil	eq. (26)
WATERrun.s1G	$Q_{runoff,water,nsl[G]}$	[m^3.s^{-1}]		
WATERrun.s2C	$Q_{runoff,water,asl[C]}$	[m^3.s^{-1}]		
WATERrun.s2G	$Q_{runoff,water,asl[G]}$	[m^3.s^{-1}]		
WINDspeed.C	$u_{[C]}$	[m.s^{-1}]	Wind speed	Table 4
WINDspeed.G	$u_{[G]}$	[m.s^{-1}]		Table 5

USEtox variable	Symbol	Unit	Explanation	Equation
WINDspeed.U	$u_{[U]}$	[m.s^{-1}]		Table 10

C. Human exposure

USEtox variable	Symbol	Unit	Explanation	Source
PestClassValues	α	[-]	Pesticide chemical class regression coefficient for pesticide dissipation in plant	Table 16
PestReg_wheat PestReg_rice PestReg_tomato PestReg_apple PestReg_lettuce PestReg_potato	β	[-]	Plant species regression coefficient for pesticide dissipation in plant	Table 17
Qtrans	Q_{transp}	[$m^3_{transpiration}$/ $m^2_{land\ area}$]	Area equivalent transpiration flow from soil through stems	Table 11
Vplant	V_{plant}	[$m^3_{tissues}$/$m^2_{land\ area}$]	Area equivalent volume of above ground plant tissues	Table 11
FAI.H_apple	$FAI_{H,apple}$	[$m^2_{leaf\ area}$/$m^2_{soil\ area}$]	Average fruit area index of apple at herbicide application time	Table 11
FAI.nH_apple	$FAI_{NH,apple}$	[$m^2_{leaf\ area}$/$m^2_{soil\ area}$]	Average fruit area index of apple at non-herbicide (insecticide, fungicide, etc.) application time	
FAI.H_rice	$FAI_{H,paddy}$	[$m^2_{leaf\ area}$/$m^2_{soil\ area}$]	Average fruit area index of paddy rice at herbicide application time	
FAI.nH_rice	$FAI_{NH,paddy}$	[$m^2_{leaf\ area}$/$m^2_{soil\ area}$]	Average fruit area index of paddy rice at non-herbicide (insecticide, fungicide, etc.) application time	
FAI.H_tomato	$FAI_{H,tomato}$	[$m^2_{leaf\ area}$/$m^2_{soil\ area}$]	Average fruit area index of tomato at herbicide application time	
FAI.nH_tomato	$FAI_{NH,tomato}$	[$m^2_{leaf\ area}$/$m^2_{soil\ area}$]	Average fruit area index of tomato at non-herbicide (insecticide, fungicide, etc.) application time	
FAI.H_wheat	$FAI_{H,wheat}$	[$m^2_{leaf\ area}$/$m^2_{soil\ area}$]	Average fruit area index of wheat at herbicide application time	
FAI.nH_wheat	$FAI_{NH,wheat}$	[$m^2_{leaf\ area}$/$m^2_{soil\ area}$]	Average fruit area index of wheat at non-herbicide (insecticide, fungicide, etc.) application time	
BAF.airgas_exp	$C^{air}_{plant-agpp}$	[kg_{airg}/kg_{veg}]	Bioaccumulation factor from air gas phase to above ground produce (BAFair_gas-above ground produce)	eq. (136)
BAF.air_exp	$C^{ap}_{plant-agpp}$	[kg_{airp}/kg_{veg}]	Bioaccumulation factor from air particulate matter to above ground produce (BAFair_particles-above ground produce)	eq. (135)
BAF.soil_exp	$BAF_{agp,sl}$	[kg_{soil}/kg_{veg}]	Bioaccumulation factor from soil to above ground produce (BAFsoil-above ground produce)	eq. (141)

USEtox variable	Symbol	Unit	Explanation	Source
BAF.soil_unexp	$BAF_{bgp,sl}$	[kg_{soil}/kg_{veg}]	Bioaccumulation factor from soil to below ground produce (BAFsoil-below ground produce)	eq. (142)
BAF.water_fish	$BAF_{dissolved.fish}$	[$L.kg^{-1}$]	BIOACCUMULATION FACTOR fish	eq. (163)
BAF.sea_fish	$BAF_{dissolved.fish}$	[$L.kg^{-1}$]		
diet.pork diet.beef diet.poultry diet.other1 diet.other2	$Pork_{diet}$ $Beef_{diet}$ $Poultry_{diet}$ $GoatSheep_{diet}$ $Other_{diet}$	[%] [%] [%] [%] [%]	Average composition of human meat consumption from different meat types	Table 11
Pork.air Beef.air Poultry.air Other.air	$Pork_{air}$ $Beef_{air}$ $Poultry_{air}$ $GoatSheep_{air}$	[m^3/d] [m^3/d] [m^3/d] [m^3/d]	Individual farm animal intake rate of air	Table 11
Pork.soil Beef.soil Poultry.soil Other.soil	$Pork_{soil}$ $Beef_{soil}$ $Poultry_{soil}$ $GoatSheep_{soil}$	[kg/d] [kg/d] [kg/d] [kg/d]	Individual farm animal intake rate of soil	Table 11
Pork.veg Beef.veg Poultry.veg Other.veg	$Pork_{veg}$ $Beef_{veg}$ $Poultry_{veg}$ $GoatSheep_{veg}$	[kg_{FM}/d] [kg_{FM}/d] [kg_{FM}/d] [kg_{FM}/d]	Individual farm animal intake rate of vegetation	Table 11
Pork.water Beef.water Poultry.water Other.water	$Pork_{water}$ $Beef_{water}$ $Poultry_{water}$ $GoatSheep_{water}$	[kg/d] [kg/d] [kg/d] [kg/d]	Individual farm animal intake rate of water	Table 11
fat.pork fat.beef fat.poultry fat.other	$Pork_{fat}$ $Beef_{fat}$ $Poultry_{fat}$ $GoatSheep_{fat}$	[%] [%] [%] [%]	Meat fat content	Table 11
BTF.beef	BTF_{meat}	[d/kg]	Biotransfer factor from chemical intake to beef meat (BTFmeat)	eqs. (144)-(146)
BTF.milk	BTF_{milk}	[d/kg]	Biotransfer factor from chemical intake to milk (BTFmilk)	eqs. (149)-(151)
fat.meat	Fat_{meat}	-	Weighted average meat fat content	eq. (147)
Dairy.air Dairy.veg Dairy.water	DC_{air} DC_{veg} DC_{water}	[m^3/d] [kg/d] [kg_{FM}/d]	Individual dairy cattle intake rates of air, vegetation (roughage), water, and soil	eq. (156) eq. (162) eq. (158)

USEtox variable	Symbol	Unit	Explanation	Source
Dairy.soil	DC_{soil}	[kg/d]		eq. (160)
vd	v_d	[m/d]	Deposition ratio accounting for both wet and dry particle deposition of particles from air to plant surfaces	Table 11
fp.wheat fp.rice fp.tomato fp.apple fp.lettuce fp.potato	$fp_{wheat,bread}$ $fp_{paddy,parb}$ $fp_{tomato,wash}$ $fp_{apple,wash}$ $fp_{lettuce,wash}$ $fp_{potato,cook}$	[$kg_{intake}/kg_{in\ harvest}$]	Food processing factor for wheat (bread making) Food processing factor for paddy rice (parboiling) Food processing factor for tomato (washing) Food processing factor for apple (washing) Food processing factor for lettuce (washing) Food processing factor for potato (cooking)	Table 11
fr.air_wheat fr.air_rice fr.air_tomato fr.air_apple fr.air_lettuce fr.air_potato	$fr_{rem,wheat}$ $fr_{rem,paddy}$ $fr_{rem,tomato}$ $fr_{rem,apple}$ $fr_{rem,lettuce}$ $fr_{rem,potato}$	[$kg_{in\ air}/kg_{applied}$]	Fraction of pesticide applied mass transferred to air	Table 11
fr.soil_wheat fr.soil_rice fr.soil_tomato fr.soil_apple fr.soil_lettuce fr.soil_potato	$fr_{soil,wheat}$ $fr_{soil,paddy}$ $fr_{soil,tomato}$ $fr_{soil,apple}$ $fr_{soil,lettuce}$ $fr_{soil,potato}$	[$kg_{in\ soil}/kg_{applied}$]	Fraction of pesticide applied mass transferred to soil for different crops	eqs. (168)-(169)
lambdag	λ_g	[1/d]	Growth dilution rate constant	Table 11
hF.wheat hF.rice hF.tomato hF.apple hF.lettuce hF.potato	$fr_{harv[wheat]}$ $fr_{harv[paddy]}$ $fr_{harv[tomato]}$ $fr_{harv[apple]}$ $fr_{harv[lettuce]}$ $fr_{harv[potato]}$	[$kg_{in\ harvest}/kg_{applied}$]	Harvest fraction	eq. (164)
LAI.H_wheat LAI.H_rice LAI.H_tomato LAI.H_apple LAI.H_lettuce LAI.H_potato	$LAI_{H,wheat}$ $LAI_{H,paddy}$ $LAI_{H,tomato}$ $LAI_{H,apple}$ $LAI_{H,lettuce}$ $LAI_{H,potato}$	[$m^2_{leaf\ area}/m^2_{soil\ area}$]	Leaf area index of crop at herbicide application time	Table 11
LAI.nH_wheat LAI.nH_rice LAI.nH_tomato LAI.nH_apple LAI.nH_lettuce LAI.nH_potato	$LAI_{NH,wheat}$ $LAI_{NH,paddy}$ $LAI_{NH,tomato}$ $LAI_{NH,apple}$ $LAI_{NH,lettuce}$ $LAI_{NH,potato}$	[$m^2_{leaf\ area}/m^2_{soil\ area}$]	Leaf area index of crop at non-herbicide (insecticide, fungicide, etc.) application time	

USEtox variable	Symbol	Unit	Explanation	Source
LAI	LAI	[$m^2_{leaf\ surfaces}/m^2_{land\ area}$]	Vegetation leaf area index, the one-sided area of plant leaf surfaces per unit land area	Table 11
MTC	MTC	[m/d]	Mass transfer coefficient at the air-leaf interface	Table 11
cattle.air cattle.veg cattle.water cattle.soil	MC_{air} MC_{veg} MC_{water} MC_{soil}	[m^3/d] [kg/d] [kg_{FM}/d] [kg/d]	Weighted average meat cattle (meat producing farm animals) intake rates for air, vegetation (roughage), water, and soil	eq. (152) eq. (148) eq. (153) eq. (154)
kdiss.wheat kdiss.rice kdiss.tomato kdiss.apple kdiss.lettuce kdiss.potato	$Diss_{[wheat]}$ $Diss_{[paddy]}$ $Diss_{[tomato]}$ $Diss_{[apple]}$ $Diss_{[lettuce]}$ $Diss_{[potato]}$	[1/d]	Overall rate constant for dissipation (proxy for degradation) from different crops (see also the half-lives calculator at http://half-lives.dynamicrop.org)	eq. (165)-(167)
RHO.plant	ρ_{plant}	[kg/m^3]	Plant density	Table 11
lambdat	λ_t	[1/d]	Rate constant for elimination by chemical transformation (dissipation as proxy) within above-ground plant tissues	eqs. (138)-(139)
RCF	RCF	[kg_{FM}/l]	Root concentration factor (RCF)	eq. (133)
ccs.wheat ccs.rice ccs.tomato ccs.apple ccs.lettuce ccs.potato	CSS_{wheat} CSS_{paddy} CSS_{tomato} CSS_{apple} $CSS_{lettuce}$ CSS_{potato}	[$(kg/m^2_{leaf})/(kg/m^2_{soil})$]	Substance capture coefficient for different crops	Table 11
tapp.H_wheat tapp.H_rice tapp.H_tomato tapp.H_apple tapp.H_lettuce tapp.H_potato	$\tau_{H,wheat}$ $\tau_{H,paddy}$ $\tau_{H,tomato}$ $\tau_{H,apple}$ $\tau_{H,lettuce}$ $\tau_{H,potato}$	[d]	Time of herbicide application before harvest for different crops	Table 11
tapp.nH_wheat tapp.nH_rice tapp.nH_tomato tapp.nH_apple tapp.nH_lettuce tapp.nH_potato	$\tau_{NH,wheat}$ $\tau_{NH,paddy}$ $\tau_{NH,tomato}$ $\tau_{NH,apple}$ $\tau_{NH,lettuce}$ $\tau_{NH,potato}$	[d]	Time of non-herbicide (insecticide, fungicide, etc.) application before harvest for different crops	Table 11

D. Indoor fate and exposure

USEtox variable	Symbol	Unit	Explanation	Source
fkex.a1I.U	$f_{ex[H]}$	-	Air exchange fraction to urban air at home	Table 12
fkex.a2I.U	$f_{ex[O]}$	-	Air exchange fraction to urban air at work	
kex.a1I	$K_{ex[H]}$	h^{-1}	Air exchange rate in the building at home	Table 8

USEtox variable	Symbol	Unit	Explanation	Source
kex.a2l	$K_{ex[O]}$	h^{-1}	Air exchange rate in the building at work	Table 9
-	$A_{carpet[H]}$	m^2m^{-3}	Area per volume (carpet) at home	Table 12
-	$A_{carpet[O]}$	m^2m^{-3}	Area per volume (carpet) at work	
-	$A_{total[H]}$	m^2m^{-3}	Area per volume (total) at home	
-	$A_{total[O]}$	m^2m^{-3}	Area per volume (total) at work	eq. (176)
VOLUME.a1l	$V_{[H]}$	m^3	Building volume at home	Table 8
VOLUME.a2l	$V_{[O]}$	m^3	Building volume at work	Table 9
-	t_{home}	$h{\cdot}d^{-1}$	Daily time at home	Table 8
-	t_{work}	$h.d^{-1}$	Daily time at work	Table 9
$k_{deg\ wall}/k_{a\ indoor}$	$k_{deg,wall,indoor}$	-	Degradation rate on room surfaces	Table 12
IR.a2l	$IR_{a[O]}$	$m^3.d^{-1}$	Individual daily inhalation of air at work	eq. (183)
IR.a1l	$IR_{a[H]}$	$m^3{\cdot}d^{-1}{\cdot}pers^{-1}$	Individual daily inhalation rate at home	eq. (181)
-	$k_{IR[H]}$	$m^3{\cdot}h^{-1}{\cdot}pers^{-1}$	Individual hourly inhalation rate at home	Table 8
-	$k_{IR[O]}$	$m^3.h^{-1}$	Individual hourly inhalation rate at work	Table 9
h_m.a1l h_m.a2l	h_m	$m^3m^{-2}h^{-1}$	Mass transfer coefficient at wall surface	Table 12
m.a1l	$Mix_{[H]}$	-	Mixing factor at home	Table 12
m.a2l	$Mix_{[O]}$	-	Mixing factor at work	
$[NO_3]$.a1l $[NO_3]$.a2l	NO_3	ppbv	Nitrate concentration indoors	Table 12
N.a1l	$N_{[H]}$	-	Number of people in the building at home	Table 8
N.a2l	$N_{[O]}$	-	Number of people in the building at work	Table 9
[OH].a1l [OH].a2l	OH	ppbv	OH radical concentration indoors	Table 12
outOH	Out_{OH}	ppbv	Outdoor OH	Table 12
$[O_3]$.a1l $[O_3]$.a2l	O_3	ppbv	Ozone concentration indoors	Table 12
$K_{eq\ carpet}$	$K_{eq,carpet}$	-	Partitioning coefficient indoor air - carpet	eq. (177)
$K_{eq\ wall}$	$K_{eq,wall}$	-	Partitioning coefficient indoor air - wall surface	eq. (178)
-	$f_{intake[H]}$	-	Population household indoor exposure intake fraction	eq. (180)
-	$f_{intake[O]}$	-	Population occupational indoor exposure intake fraction	eq. (182)

USEtox variable	Symbol	Unit	Explanation	Source
kdeg.a1I	$k_{g,deg[H]}$	h^{-1}	Removal rate due to indoor air degradation at home	eq. (173)
kdeg.a2I	$k_{g,deg[O]}$	h^{-1}	Removal rate due to indoor air degradation at work	
ks.a1I	$k_{s[H]}$	h^{-1}	Removal rate due to surface net adsorption & degradation at home	eq. (175)
ks.a2I	$k_{s[O]}$	h^{-1}	Removal rate due to surface net adsorption & degradation at work	
K_{NO3}	k_{NO3}	$h^{-1}ppbv^{-1}$	Second order constant rate for NO3	Table 12
k_{O3}	k_{O3}	$h^{-1}ppbv^{-1}$	Second order constant rate for O3	Table 12
kOH	k_{OH}	$h^{-1}(ppbv)^{-1}$	Second order constant rate for OH	eq. (174)
ktot.a1I	$k_{total[H]}$	h^{-1}	Total removal rate at home	eq. (171)
ktot.a2I	$k_{total[O]}$	h^{-1}	Total removal rate at work	
V_p	$P_{vap,25°C}$	Pa	Vapour pressure	Substance data

E. Human and ecosystem toxicological effects

USEtox variable	Symbol	Unit	Explanation	Source
-	HC_{50}	$kg.m^{-3}$	Geometric mean of chronic aquatic EC50's	eq. (193)
-	f_{eco}	-	Multiplier	Table 13
$EF_{eco}(frw)$	EF_{eco}	$PAF.m^3/kg$	Ecotox effect factor freshwater aquatic ecosystems	eq. (192)
$ED50_{inh,noncanc}$	$ED_{50,inh,nc}$	kg_{intake}/lifetime	Lifetime inhalation dose inducing non-cancer desease in 50% of population	Substance data
$ED50_{ing,noncanc}$	$ED_{50,inh,c}$	kg_{intake}/lifetime	Lifetime ingestion dose inducing non-cancer desease in 50% of population	
$ED50_{inh,canc}$	$ED_{50,ing,nc}$	kg_{intake}/lifetime	Lifetime inhalation dose inducing cancer in 50% of population	
$ED50_{ing,canc}$	$ED_{50,ing,c}$	kg_{intake}/lifetime	Lifetime ingestion dose inducing cancer in 50% of population	
-	f_{nc}	-	Multiplier non cancer	Table 13
-	f_c	-	Multiplier cancer	
$EFhum_{inh,noncanc}$	$EF_{inh,nc}$	$cases.kg_{intake}^{-1}$	Effect factor non-cancer via inhalation	eq. (185)
$EFhum_{ing,noncanc}$	$EF_{ing,nc}$	$cases.kg_{intake}^{-1}$	Effect factor non-cancer via ingestion	eq. (186)
$EFhum_{inh,canc}$	$EF_{inh,c}$	$cases.kg_{intake}^{-1}$	Effect factor cancer via inhalation	eq. (187)
$EFhum_{ing,canc}$	$EF_{ing,c}$	$cases.kg_{intake}^{-1}$	Effect factor cancer via ingestion	eq. (188)