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SimpleBox 2.0: a nested multimedia fate model for evaluating the environmental fate of chemicals

L.J. Brandes; H. den Hollander; D. van de Meent

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National Institute of Public Health and the Environment (RIVM), P.O. Box 1, 3720 BA Bilthoven, the Netherlands
Tel: +31 - 30 - 274 30 15, Fax: +31 - 30 - 274 44 13

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PREFACE

This document gives the technical description of SimpleBox 2.0 and is a part of the project 719101 Exposure Assessment. The research has been carried out at the National Institute of Public Health and the Environment (RIVM), Laboratory of Ecotoxicology by order and for the account of the Ministry of Housing, Spatial Planning and the Environment (VROM) on commission of the Directorate-General for Environmental Protection (DGM), Directorate of Chemicals, Radiation and Safety.

A former version of the SimpleBox model has become part of the European Union System for the Evaluation of Substances (EC, 1996b). The SimpleBox version described here, contains several new items which are not described in the Technical Guidance Document of EUSES (EC, 1996a). The SimpleBox version used for EUSES has no global scales, temperature dependent chemical properties, temperature dependent degradation rates and chemical dependent penetration depth. In a footnote below the specific formulas is described how SimpleBox version 2.0 can be set to match the EUSES version of SimpleBox.

The model is developed in Excel for Windows. A copy of the spreadsheet code of the model can be obtained from the RIVM by contacting D. van de Meent (ECO).

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SUMMARY

This document describes the technical details of the revised multi-media fate model SimpleBox 2.0 (96-09-01). The former version, SimpleBox 1.0, has been used for prediction of intermedia concentration ratios for the purpose of harmonisation of environmental quality objectives and prediction of concentrations in the regional environment for the purpose of evaluation of chemicals. Model validation was recommended by a SETAC Taskforce on Application of Multi-Media Fate Models to Regulatory Decision Making and by the Health Council of the Netherlands. Also, the Health Council of the Netherlands advised a review of the model. SimpleBox 2.0 is developed in response to these recommendations. SimpleBox is meant to support regulatory decision making in the Netherlands.

SimpleBox 2.0 is a nested multi-media fate model of the "Mackay type". The environment is modeled as consisting of a set of well-mixed, homogeneous compartments (air, two water compartments, sediments, three soil compartments and two vegetation compartments) in regional, continental and global scales. The model takes emission rates and rate constants for transport and transformation of micropollutants as input and computes steady-state concentrations as output. SimpleBox is a generic model in the sense that it can be customised to represent specific environmental situations. The default settings of the regional and continental scales of the model are set to match the EU procedures for evaluation of substances.

With respect to SimpleBox 1.0, several changes have been made. The main modifications are the addition of more compartments and nesting of the regional scale into continental and global spatial scales.

A former version of the SimpleBox model has become part of the European Union System for the Evaluation of Substances (EUSES). The SimpleBox version described here, contains several new items which are not described in the Technical Guidance Document of EUSES (EU, 1996a).

This report is meant to provide the technical documentation of the new SimpleBox model. The spreadsheet code of the model can be obtained from the RIVM.

SAMENVATTING

Dit document beschrijft de technische details van het herziene multi-media model SimpleBox 2.0 (96-09-01). De vorige versie, SimpleBox 1.0, is gebruikt voor het berekenen van steady-state concentratieverhoudingen voor de harmonisatie van milieu-kwaliteitsdoelstellingen en voor de evaluatie van stoffen. Validatie van het model was aanbevolen door de SETAC Workshop on Application of Multi-Media Fate Models to Regulatory Decision Making en door de Gezondsheidsraad. De Gezondheidsraad stelde tevens voor om een aantal model-aannamen te herzien. SimpleBox 2.0 is ontwikkeld als antwoord op de aanbevelingen van de SETAC Workshop en de Gezondheidsraad.

SimpleBox 2.0 is een "genest" multi-media lotgevallen model van het "Mackay type". Het milieu is gemodelleerd als een verzameling van goed gemengde, homogene compartimenten (lucht, twee watercompartimenten, sediment, drie bodemcompartimenten en twee vegetatiecompartimenten op natuurlijke bodem en landbouw bodem) in een regionale, continentale en globale ruimtelijke schaal. Het model gebruikt emissies en transport en transformatie snelheidsconstanten als input en berekent hiermee de steady-state concentraties in de diverse compartimenten.
SimpleBox is een generiek model, het kan worden aangepast om specifieke milieu-situaties te simuleren. De standaard-instellingen van het model voor de regionale en continentale schaal zijn gezet volgens de EU-procedure voor de evaluatie van stoffen.

Vergeleken met de vorige versie is er een aantal wijzigingen. De belangrijkste hiervan zijn het toevoegen van meerdere compartimenten en het toevoegen van continentale en globale schalen.

Een eerdere versie is onderdeel van het "European Union System for the Evaluation of Substances (EUSES)". SimpleBox 2.0 bevat een aantal nieuwe toevoegingen/wijzigingen die niet zijn beschreven in het "Technical Guidance Document of EUSES" (EU, 1996a).

Dit rapport is bedoeld als technisch achtergronddocument voor het nieuwe SimpleBox model. De spreadsheetcode van het model kan worden verkregen bij het RIVM.

1. INTRODUCTION

SimpleBox is a nested multimedia environmental fate model in which the environmental compartments are represented by homogeneous boxes. In the last few years some major changes have been made, resulting in a new version; SimpleBox 2.0. SimpleBox is a generic model, it can be customised to represent specific environmental situations. In its default setting, the SimpleBox computation represents the behaviour of micropollutants in regional and continental scale; representing a densely populated Western European region, and the whole of the European Union, respectively.

The work on SimpleBox started in 1982, when the development of a systematic procedure to evaluate the environmental risk associated with the introduction of new chemicals was initiated at RIVM. The earliest versions “SimpleMac” in Basic and Fortran codes are developed for “Mackay level 1 and level 2” computations. The first spreadsheet version “SimpleSal” in Multiplan for the Apple IIe, was made in 1984. This was an exact replica of the "Mackay level 3 computation" as published earlier by Mackay (1979). The SimpleSal sheet was found useful as an instrument to aid systematic environmental chemical reasoning. The multimedia modeling approach found its application in the Integrated Criteria Documents for existing chemicals. SimpleSal was also found useful as a means to direct the research in the field of environmental chemistry at the RIVM.
In the course of time, many minor and major changes have been made to the SimpleSal sheet. A major change was the replacement, in 1986, of the original Apple/Multiplan version of SimpleSal by a more generic MS-DOS/Lotus123 version. In this generic form, the spreadsheet became a framework to design multimedia box models for various purposes, rather then a specific model. Another development was the coupling, also in 1986, of the spreadsheet-based "level 3 computation" of SimpleSal with a numeric integrator: the "level 4 computation. Other applications of the SimpleBox modeling framework have been produced under the names: “SimpleSingh”, a spatially inhomogeneous multimedia box model (Singh and Van de Meent, 1989), “SimpleTreat”, a model of a waste water treatment plant (Struijs and Van de Meent, 1988; OECD, 1989; Struijs *et al.* 1991), and “WaterBox”, a water version of SimpleSal for teaching purposes. In 1993, the first documented version was produced: SimpleBox 1.0.
The SimpleBox model version 1.0 was used for two specific purposes:

1. to predict intermedia concentration ratios for the purpose of harmonization environmental quality objectives for air, water, sediment and soil (Van de Meent and De Bruijn, 1993).
2. to predict concentrations in the regional environment for the purpose of evaluation of chemicals.

The Health Council of the Netherlands identified model validation as a prerequisite for application of the model in regulatory practice. The development of SimpleBox 2.0 is a part of the response to this call for validation. A project “Validation SimpleBox-Computed Steady-State Concentration Ratios” (Van de Meent, 1996) was started; it was decided to validate an updated version of the model. This document gives the technical description of the revised SimpleBox 2.0 model.

1.1 Update of SimpleBox

As a response to the recommendations of the Health Council on the project "Setting Integrated Environmental Quality Objectives" (Health Council of the Netherlands, 1995) and the recommendations by the users of the USES model, the previous version of SimpleBox (version 1.0) is updated. The new additions and changes in SimpleBox 2.0 are given in Table 1. The main modifications are nesting of the regional scale into continental and global spatial scales and the addition of more compartments. The original model had one (fresh) water compartment and the three soil compartments were not covered with vegetation. In the revised model, a second (sea) water compartment is added, and vegetation compartments are added to the soil compartments. Water is treated as a bulk compartment, assuming thermodynamic equilibrium between dissolved phases and sub-phases. Furthermore, estimation equations for partition coefficients and degradation rates are made temperature dependent and the soil depth is derived from the chemical-specific penetration depth.

Table 1: *New items in SimpleBox 2.0.*

Differences of SimpleBox 2.0 with original SimpleBox 1.0 (930801)	**References**
Nesting of the regional scale in continental and global scales	Van de Meent and Van der Burg, 1995a. Van de Meent, 1995b.
Partition coefficients and degradation rates temperature dependent	Mackay *et al.*, 1991. Verbruggen *et al.*, 1996.
Two separate water compartments at regional and continental scales	Severinsen *et al.*, 1996. Henderson-Sellers and McGuffie, 1987.
Terrestrial vegetation compartments added	EC, 1996a. Trapp and MacFarlane, 1995a. Trapp and MacFarlane, 1995b.
Depth soil derived from chemical-specific penetration depth	Cowan *et al.*, 1995. Mackay *et al.*, 1991.
Water as bulk compartment, assuming thermodynamic equilibrium between dissolved phases and subphases	
Default settings according to EU procedures for evaluation of substances	EC, 1996a. EC, 1995.
Output tables adjusted to changed use	
Risk quotients (output) replaced by "potentially affected fraction" (PAF)	Hamers *et al.*, 1996
Format changed from LOTUS 1-2-3 to Excel	
Computation routine for time-dependent solutions replaced	

1.2 Reader's guide

In Chapter 2 the model concept is described. The third chapter gives a detailed description of SimpleBox. Chapter 4 gives a description of the model output. In Chapter 5 the SimpleBox model code is described. Model data and parameter descriptions are given in Appendix 1.
This report is meant to provide the technical documentation that is necessary to use the model for the above mentioned purposes.

2. THE SIMPLEBOX MODEL

2.1 Model concept

SimpleBox is a multimedia environmental fate model in which the environmental compartments are represented by homogeneous boxes.

SimpleBox is a generic model, it can be customised to represent specific environmental situations. In its default setting, the SimpleBox computation represents the behaviour of micropollutants in an regional and continental scale, representing a densely populated Western European region, and the whole of the European Union, respectively. SimpleBox follows the Mackay concept of sequentially carrying out the modelling procedure at different stages of conceptual sophistication or "levels" (Mackay, 1991). In SimpleBox, the non-equilibrium, steady-state computation (level 3) and the quasi-dynamic non-equilibrium, non-steady-state computation (level 4) can be performed.

Unlike the fugacity approach as adopted by Mackay, computation of mass flows and concentration levels in SimpleBox is done with concentration-based "piston velocity" type mass transfer coefficients [$m.s^{-1}$]. The reason for this is that, in most of the scientific literature, mass transfer is expressed in these terms, rather than in terms of the fugacity-based "conductivity" type coefficients [$mol.hr^{-1}.Pa^{-1}$]. As is done in the Mackay models, transfer and transformation phenomena are treated as simple pseudo first-order processes.

Environmental compartments are represented by boxes. The concentration of a chemical in these boxes is affected by processes that cause mass flows of the chemical to and from the boxes. The chemical can be *INPUT* into a box from outside the system, *OUTPUT* from a box to outside the system, or transported by means of *ADVECTIVE* or *DIFFUSIVE* processes to and from other boxes. A mass balance equation can be written for each of the boxes. The mass balance equations have the following format:

$$V_i.\frac{dC_i}{dt} = EMIS_i + IMP_i - EXP_i - DEGRD_i - LCH_i - BRL_i + ADV_{ij} + DIFF_{ij} \qquad \mathbf{1}$$

with

V_i : volume of box i [m^3]
C_i : concentration of the chemical in box i [$mol.m^{-3}$]
t : time [s]
$EMIS_i$: mass flow of the chemical from outside the system into box i by emission [$mol.s^{-1}$]
IMP_i : mass flow of the chemical from outside the system into box i by import [$mol.s^{-1}$]
EXP_i: mass flow of the chemical from box i to outside the system by export [$mol.s^{-1}$]
$DEGRD_i$:apparent degradation mass flow of the chemical from box i [$mol.s^{-1}$]
LCH_i : mass flow of the chemical from box i to outside the system by leaching [$mol.s^{-1}$]
BRL_i : mass flow of the chemical from box i to outside the system by sediment burial [$mol.s^{-1}$]
ADV_{ij} : advective exchange mass flow of the chemical from one box to another [$mol.s^{-1}$]
$DIFF_{ij}$: diffusive exchange mass flow of the chemical from one box to another [$mol.s^{-1}$]

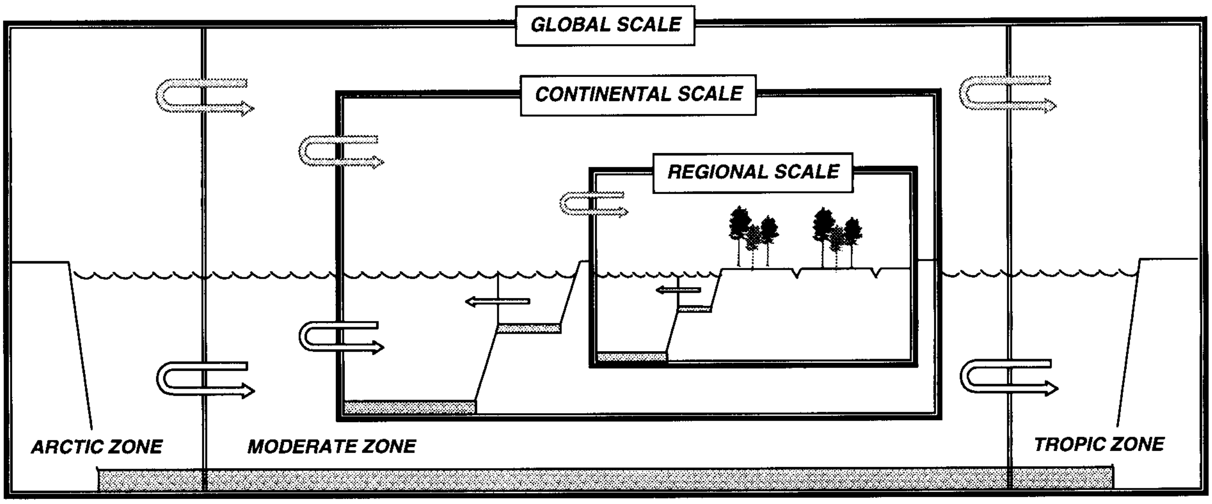

Figure 1: *SimpleBox 2.0 model*

The terms of the mass balance equations each represent a mass flow of the chemical [mol.s^{-1}]. Generally, the magnitudes of these mass flows depend on the concentration of the chemical in the boxes. If mathematical expressions that relate the mass flows to the concentrations are available, the set of mass balance equations (one for each box) can be solved: the concentrations in each of the boxes can be computed.

2.2 overview of the new SimpleBox multimedia model

2.2.1 scales

SimpleBox version 2.0 is a nested multimedia model, it consists of five spatial scales; a regional scale, a continental scale and a global scale consisting of three parts, reflecting arctic, moderate and tropic geographic zones (Figure 1). The global scale is not implemented in the distribution module of the European Union System for Evaluation of Substances (EUSES). The default settings of the regional and continental scale of the model are set to match the EU procedures for evaluating of substances. In this case, the regional scale is represented as a densely populated Western European region. The continental scale is a copy of the regional scale, with adjusted parameters to represent the whole European region. The global scales are added to serve as background for the continental and regional scales.
In SimpleBox is advective transport of air and water between the spatial scales and zones, see Figure 2; the global scale is modelled as a closed system, without transport across the system boundaries. The major characteristics of the different scales are given in Appendix 1.

2.2.2 compartments

The regional and continental environments modelled consist of ten homogeneous environmental compartments: air, two separate water compartments, sediments, three separate soil compartments, and vegetation on natural and agricultural soil. The global scales consist of 4 homogeneous compartments: air, water, sediment and soil. The atmospheric phases (gas, rain, aerosol) and the terrestrial phases (solids, water, air and roots) are considered to be in a state of thermodynamic equilibrium at all times.

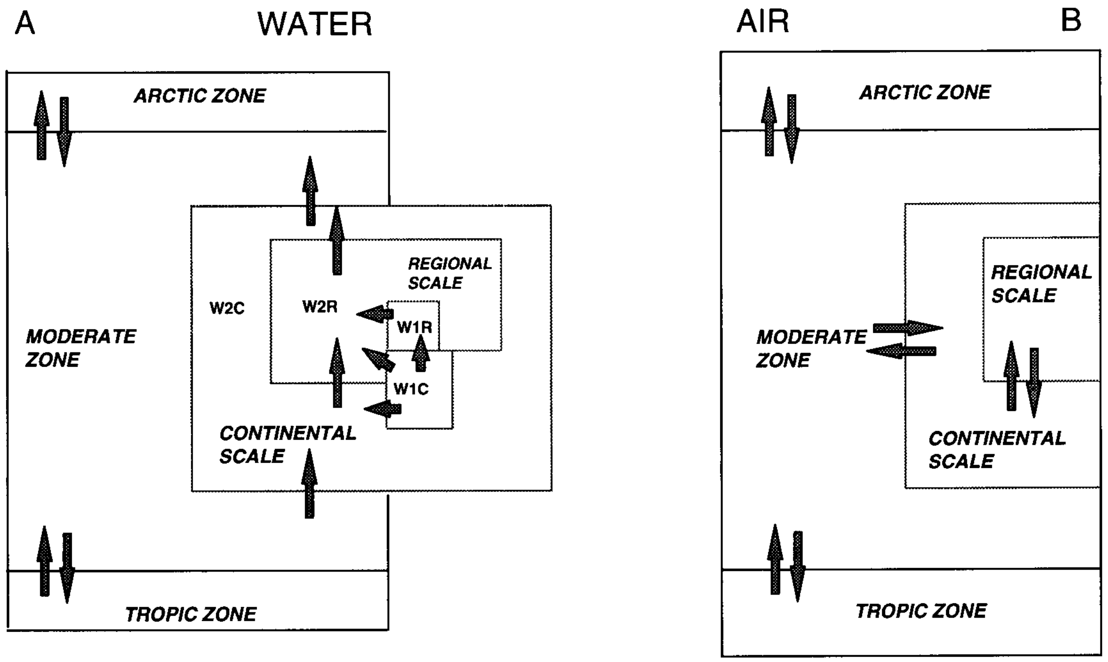

Figure 2: *Water and air flows in and between the spatial scales.*

In contrast with the former version of SimpleBox, the aquatic phases (water, suspended particles, biota) are treated as a bulk compartment and considered to be in thermodynamic equilibrium. The water compartments represents a fresh-water (lakes, rivers, etc.) and sea-water compartment.

The soil compartments can be used to define different geographic areas, different soil types or different soil use. In SimpleBox, the soil compartments stand for natural, agricultural and industrially/urban used soil. Vegetation is situated on natural soil and soil used for agriculture on the regional and continental scale, with different parameter settings for each vegetation compartment.

2.2.3 temperature dependent properties

Chemical properties as vapour pressure, solubility, Henry's Law constant and degradation rates are strongly temperature dependent. In the new SimpleBox version, this is taken into account (Mackay *et al.*,1991. Verbruggen *et al.*,1996).

2.2.4 chemical dependent soil depth

In the former version of SimpleBox the average total concentration of a chemical in the soil compartment was calculated with a fixed soil depth. In the new SimpleBox version it is assumed that the soil depth of natural, agricultural and industrially/urban used soil depends on the properties of the chemical. The chemical tends to migrate vertically down into the soil, whereby processes of leaching, diffusion, adsorption and degradation control the depth of migration. The penetration depth or "effective soil depth" of the chemical can be calculated with the modified Damköhler Number, D_a^* (Cowan *et al.*, 1995) The penetration depth of the chemical is the depth at which, at steady-state, the rate of chemical reaction disappearance is equal to its rate of movement into the soil by advective and diffusive processes. The depth at which these rates are equal is chosen as the penetration depth.

The soil depth depends not only on the chemical properties but also on the soil use. For readily degradable and/or hydrophobic chemicals the penetration depth is small. The top layer of the soil is usually broken up and reworked by biota, thus a minimum soil depth of 3 cm is suggested. For agricultural soil, which is frequently reworked by mechanical action (by plowing, etc.), the minimum soil depth is chosen as the actual mixing depth, 20 cm as a default value. In the Netherlands, the groundwater table is present at about 1 metre, below that level the soil characteristics changes to a lower organic carbon content and lower porosity. Therefore, a maximum soil depth of 1 metre is suggested for the three different soil compartments.

2.2.5 vegetation module

Another modification of SimpleBox is the addition of terrestrial vegetation compartments at the regional and continental scales. The detailed description of the vegetation module in SimpleBox is given in Severinsen and Jager (in prep.). In this vegetation model, the above parts of the vegetation are represented by one well-mixed box, whereas roots are treated as an integral part of the soil compartment. The root phase is assumed to be in equilibrium with the pore water phase of the soil. The vegetation compartments represent natural and agricultural vegetation, vegetation on industrial soil is neglected.

The processes taken into account are: diffusive exchange between air and leaves, atmospheric deposition, advective transport from soil to vegetation with the transpiration stream, advective transport from vegetation to soil by plant death, degradation in plant tissue and removal by harvesting. Harvesting of roots crops is treated as removal from the soil compartment.

The degradation rates of chemicals in plants, transpiration rates and residence times are uncertain, but important parameters. Conceptual problems such as which part of the vegetation must be included in the vegetation compartment (stems, foliage) and the assumption that water is taken up by trees from the top soil or deeper soil layers, lead to a higher uncertainly in the SimpleBox model.

Comparison of calculations with and without the vegetation module, inclusion of the vegetation module resulted in concentrations in air and soil within a factor 2 different. Considering this, in SimpleBox the vegetation module has default settings to have no impact on the fate of the chemical.

2.3 Processes in SimpleBox

EMISSION can go into the compartments air, water and soil compartments of all scales. Emissions may be direct or indirect. Direct emission rates may be derived as the product of a production volume and an emission factor. Indirect emissions result from rerouting of emissions to water upon sewage treatment. During sewage treatment, a fraction of the chemical is degraded; the remainder is rerouted to air (volatilization), water and suspended matter (effluent), soil (sludge application as fertilizer) or dump sites (not considered here). Indirect emissions may be derived from actual knowledge of concentrations of the chemical in effluent and sludge from a sewage treatment plant, or alternatively, as the product of the total load of the sewage treatment plant, the fraction of time that the sewage treatment plant is actually loaded with the chemical, and the fraction rerouted. SimpleBox anticipates the use of sewage treatment plant models like SimpleTreat (Struijs *et al.*, 1991,1996) to estimate these rerouting fractions.

IMPORT takes place in the air and water compartments of all scales. Import is the result of refreshment of the air and water in the system with air and water from a larger spatial scale. Import may be derived from the concentrations at the larger spatial scale, and the atmospheric and hydraulic residence times, which are system characteristics. The residence times may be derived from windspeed and stream flows. Import is considered to be constant in time.

EXPORT mass flows are computed as the product of refreshment flow rates and concentrations in the compartment. The refreshment flow rates are obtained from the atmospheric and hydraulic residence times and the compartment volumes. *DEGRADATION* makes the chemical disappear from the system and is considered as an output term. All degradation is assumed to obey (pseudo) first order kinetics. The degradation mass flows follow from the degradation rate constant, the volume of the compartment and the concentration in the compartment. Degradation rate constants must be entered as input, although SimpleBox does provide an indicative estimation possibility for biodegradation rates from the results of biodegradability tests. *LEACHING* transports the chemical from the top layer of the soil to the groundwater, which is not considered to be part of the system modeled. The leaching mass flow, therefore, is considered as an output term. Leaching is computed as the product of a mass transfer coefficient, the cross sectional area of the soil, and the concentration in the soil compartment. The leaching transfer coefficients may be estimated on the basis of percolation rates and equilibrium partition coefficients between the solid and water phases of the soil. Similarly, older sediment layers that are buried under the active, freshly deposited surface layer, are not considered as part of the system modeled. Therefore, the apparent mass flow due to *BURIAL* is also treated as an output process. Burial is determined by a mass transfer coefficient, which may be estimated from the net sedimentation rate, the cross sectional area of the sediment-water interface, and the concentration in the sediment compartment. Unlike the input mass flows, output mass flows are concentration dependent and become constant with time only at steady state.

Intermedia exchange by *ADVECTION* and *DIFFUSION* takes place between nearly all the compartments. Atmospheric deposition to soil and water in aerosol particles and rain droplets, sediment-water exchange by sedimentation and resuspension, run-off from soil to water, and soil-groundwater transport by percolation are examples of advective transport. Gas absorption and volatilization across the air-soil and air-water interfaces are examples of diffusive transport. Distinguishing between these types of transport is helpful because they imply differences in the direction of the resulting mass flows. Diffusive mass transfer between two compartments goes both ways. The net mass flow that results from it may be either way, depending on the actual concentrations of the chemical in the two media and the concentration ratio at equilibrium. Diffusive intermedia mass transfer is classically treated as a process that is driven by differences in chemical potentials in the two media (or, in terms of the Mackay approach, by fugacity differences). If the chemical potentials (or fugacities) in two media are the same, the media are at thermodynamic equilibrium. In that case the transport in both directions is equal and the net transport is zero. In the case of advective transport, a chemical is carried from one compartment into another by a carrier that physically flows from one compartment into the other. Advective mass transfer, therefore, is strictly one-way. The direction of the resulting mass flow is determined only by the direction of the carrier flow. Its magnitude is determined only by the rate of carrier flow and the concentration in the carrier; it is independent of the concentration in the receiving compartment. Advective mass transfer can carry the chemical against the chemical potential or fugacity gradients.

In SimpleBox, intermedia mass flows [mol.s^{-1}] are computed as the product of a transport coefficient [m^3.s^{-1}] and the concentration in the compartment from which the mass flow originates [mol.m^{-3}]. The transport coefficients (internal parameters) are found as the product of intermedia mass transfer coefficients and the interfacial areas (definition parameters). The mass transfer coefficients for forward and backward diffusive processes have different magnitudes; the coefficient for the "backward" advective process has the value zero. SimpleBox provides guidelines and in most cases estimation equations to derive the mass transfer coefficients from properties of the chemicals and characteristics of the environment (auxiliary parameters).

3. MODEL CALCULATIONS

In this section, the SimpleBox model is described in detail. In the following paragraphs the parameters and the equations for the chemical characteristics, partition coefficients, environmental characteristics, degradation and transformation rates, intermedia partitioning and transfer processes are specified. In paragraph 3.7-3.11 the mass balances for the compartments are presented. For each of these mass balances, the transfer processes (input and output of the compartment) are described.

3.1 Model parameters

The parameters that characterize the SimpleBox model definition can be categorized as follows:

1. Definition parameters *(D)* determine the mass balance equations. With these values, the SimpleBox computation can be carried out, without them it can not. The definition parameters are a "necessary and sufficient" requirement for the SimpleBox computation. Definition parameters are expressed in MKS-units. To derive values for the definition parameters, the user may chose to use either the suggested estimation equations or default values that are based on auxiliary parameters. Alternatively, values may be entered directly, overruling the suggested estimations and defaults.
2. Auxiliary parameters *(A)* are used to derive default values for the definition parameters. Values for the auxiliary parameters may be entered in the format that is available, which is often non-MKS units. Values for the auxiliary parameters must be entered if the user chooses to use the suggested estimation equations in setting one or more definition parameters.
3. Internal parameters *(I)* are used in SimpleBox to carry out the computation in an orderly manner. MKS-units are used. Values for these parameters cannot be entered by the user. Their existence is mentioned in this document only to explicitly describe what is being calculated in SimpleBox.
4. Constants *(C)*.
5. System variables *(S)*.
6. Output variables *(O)*.

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

- Parameters are mainly denoted in capitals, which indicate the type of the parameter (and its units).
- Specification of the parameter is in lower case.
- Specification of the compartment for which the parameter is specified is shown as a subscript, the index i specifies which compartment is considered in case of more compartments with the same name.
- Specification of the scale is shown as a subscript in capital.

As an example, the symbol $FRdisslvd_{water\ i[S]}$ means the fraction (*FR*) dissolved (*disslvd*) of the chemical in water i ($_{water\ i}$); where i can be 1 or 2, specifying the fresh water compartment or the sea water of at a certain scale [S], denoted in the subscript ($_{[S]}$); [S] may be the regional [R], continental [C], moderate [M], arctic [A] and tropic [T] scale.

3.2 Parameters that describe the properties of the chemical

3.2.1 Molecular weight

The molecular weight of the chemical, *MOL WEIGHT*, is one of the most often used parameters in the SimpleBox spreadsheet. In all but two cases, this is to convert the amount of chemical from mole-based units to mass-based units. If only mass-based units are used, the value of *MOL WEIGHT* is irrelevant to this purpose. The only instance where the molecular weight is used as a characteristic of the chemical is in the formulas for estimating partial mass transfer coefficients, where the parameter *MOL WEIGHT* is used as indicator of the size of the molecule. The following default value

$$MOL\ WEIGHT = 250\ g.mol^{-1} \qquad \mathbf{2}$$

with

MOL WEIGHT: molecular weight of the chemical [$kg.mol^{-1}$] *(A)*

may be taken as a starting point; it is a value for a medium-large molecule.

3.2.2 Octanol-water partition coefficient

The octanol-water partition coefficient, K_{ow}, is the basis for estimating intermedia partition coefficients (sed-water, soil-water) for organic chemicals. If the user chooses to use any of these formulas, a value for the K_{ow} of the chemical needs to be entered. SimpleBox does not provide an estimation routine to derive K_{ow} from knowledge of the chemical structure. The default value

$$\text{Octanol-water partition } K_{ow} = 10^5 \qquad \mathbf{3}$$

with

K_{ow} : octanol-water partition coefficient of the chemical [$mol.m_{octanol}^{-3}/mol.m_{water}^{-3}$] *(A)*

may be taken as a starting point; it is a value for a rather hydrophobic chemical.

3.2.3 Vapor pressure

The vapor pressure of the chemical, *VAPOR PRESSURE*, is also used in the formulas for estimating the fraction of the chemical that is associated with aerosol particles in air and the air-water partition coefficient. As for K_{ow}, a value for *VAPOR PRESSURE* needs to be entered if it has been decided that either one of these estimation formulas is to be used. *The VAPOR PRESSURE* of a chemical is temperature dependent[a]. When applying simple temperature corrections for the vapour pressure, care must be taken when the melting point is within the

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[a] EUSES: Setting the enthalpy of vaporization (H_{0vapor}) and the enthalpy of solution (H_{0solut}) to zero results in a temperature independent *VAPORPRESSURE* and *SOLUBILITY.*

extrapolated temperature range. The vapour pressure of the solid phase is always lower than the extrapolated vapour pressure of the liquid phase. A correction will therefore tend to overestimate the vapour pressure.

$$VAPORPRESSURE(T) = VAPORPRESSURE(25).e^{\frac{H_{0vapor}}{R}.(\frac{1}{298} - \frac{1}{TEMPERATURE_{[S]}})} \qquad \mathbf{4}$$

with

VAPOR PRESSURE (T) :	vapor pressure of the chemical at temperature T (^oC) [Pa] *(A)*
VAPOR PRESSURE (25):	vapor pressure of the chemical at temperature 25°C [Pa] *(A)*
H_{0vapor}:	enthalpy of vaporization [$J.mol^{-1}$] *(A)*
R :	gas constant, = 8.314 $Pa.m^3.mol^{-1}.K^{-1}$ *(C)*
$TEMPERATURE_{[S]}$:	temperature at the air-water interface at scale S [K] *(A)*

A suggested default enthalpy of vaporization is:

$$H_{0vapor} = 50kJ.mol^{-1} \qquad \mathbf{5}$$

with

H_{0vapor}:	enthalpy of vaporization [$J.mol^{-1}$] *(A)*

A suggested default *VAPOR PRESSURE(25)* is:

$$VAPORPRESSURE(25) = 10^{-3} Pa \qquad \mathbf{6}$$

with

VAPOR PRESSURE (25):	vapor pressure of the chemical at temperature 25°C [Pa] *(A)*

as a starting point, a typical value of a semi-volatile chemical.

3.2.4 Solubility

The solubility of the chemical in water, *SOLUBILITY*, is also used in the formula for estimating the air-water partition coefficient. If a value for the octanol-water partition coefficient has been entered already, *SOLUBILITY* may be estimated from K_{ow} by means of one of the many available regression formulas. SimpleBox uses the formula of Hansch *et al.* (1968), as mentioned by Lyman *et al.* (1982) for general purposes, corrected for temperature dependency[a]:

$$SOLUBILITY(T) = SOLUBILITY(25).e^{\frac{H_{0solut}}{R}.(\frac{1}{298} - \frac{1}{TEMPERATURE_{[S]}})} \qquad \mathbf{7}$$

with

SOLUBILITY (T) :	solubility of the chemical at temperature *T* (^oC) at scale S [$mol.m_{water}^{-3}$] *(A)*
SOLUBILITY (25):	solubility of the chemical at temperature 25°C [$mol.m_{water}^{-3}$] *(A)*
H_{0solut}:	enthalpy of solution [$J.mol^{-1}$] *(A)*
R :	gas constant, = 8.314 $Pa.m^3.mol^{-1}.K^{-1}$ *(C)*

TEMPERATURE : temperature at the air-water interface at scale [K] *(A)*

A suggested default enthalpy of solution is:

$$H_{0solut} = 10 kJ.mol^{-1} \qquad \mathbf{8}$$

with

H_{0solut}: enthalpy of solution [J.mol^{-1}] *(A)*

A suggested default *SOLUBILITY(25)* is:

$$SOLUBILITY(25) = 10^{-1.214.log\,Kow+0.85}.1000 \qquad \mathbf{9}$$

with

SOLUBILITY (25): vapor pressure of the chemical at temperature 25°C [mol.m$_{water}^{-3}$] *(A)*
Kow: octanol-water partitioning coefficient of the chemical [-] *(A)*
1000: conversion factor [l.m^{-3}] *(A)*

3.2.5 Melting Point

The melting point of the chemical, *MELTING POINT*, is used in the formula for estimating the fraction of the chemical that is associated with aerosol particles in air. As for K_{ow}, a value for *MELTING POINT* needs to be entered. As for K_{ow}, no estimation formula for *MELTING POINT* is provided in SimpleBox. The default value

$$MELTINGPOINT = 0\ ^{\circ}C \qquad \mathbf{10}$$

with

MELTINGPOINT : melting point of the chemical [°C] *(A)*

may be taken as a starting point (the chemical is liquid at environmental temperatures).

3.2.6 Biodegradability

The results of standard screening tests for aerobic degradability in water may be used as a starting point for estimating the rate constants for transformation of the chemical in water, sediment and soil (Struijs and Van den Berg, 1993). A positive result ("readily degradable") may be interpreted in this context as a property of the chemical. No estimation routine to derive estimates for the biodegradability are provided by SimpleBox. By default, the chemical is suggested to be treated as "not readily degradable":

$$PASSreadytest = n \qquad \mathbf{11}$$

with

PASSreadytest : the result of a standard screening test, expressed in the generally used "yes/no" format *(A)*

3.2.7 Potentially Affected Fraction

SimpleBox can calculate the Potentially Affected Fraction[b] (PAF) as an indicator for "environmental risk" for water, sediment and soil (Hamers *et al.*, 1995). This equation determines the percentile of species for which the NOEC is exceeded at the steady-state concentration:

$$PAF_{water\,i[S]} = \frac{1}{\left(1+e^{\frac{-(\log(CSS_{water i}\cdot MOLWEIGHT)-\alpha_{water[S]})}{\beta_{water[S]}}}\right)} \qquad \mathbf{12}$$

with

$PAF_{water\,i[S]}$:	predicted affected fraction for water [-] *(A)*
$CSS_{water\,i[S]}$:	steady-state concentration in water i [mol.m^{-3}] *(O)*
MOL WEIGHT:	molecular weight of the chemical [kg.mol^{-1}] *(A)*
$\alpha_{water[S]}$:	mean of log NOEC's for water at scale S [g.l^{-1}]
$\beta_{water[S]}$:	beta for water at scale S [-]

$$\beta_{water[S]} = stdev_{water[S]} \cdot \frac{\sqrt{3}}{\pi} \qquad \mathbf{13}$$

with

$\beta_{water[S]}$:	beta for water at scale S [-] *(D)*
$stdev_{water[S]}$:	standard deviation of log NOEC's for water [-] *(D)*

$$PAF_{sed\,i[S]} = \frac{1}{\left(1+e^{\frac{-(\log(CSS_{sed\,i}\cdot MOLWEIGHT)-\alpha_{sed[S]})}{\beta_{water[S]}}}\right)} \qquad \mathbf{14}$$

with

$PAF_{sed\,i[S]}$:	predicted affected fraction for sediment i [-] *(A)*
$CSS_{sed\,i[S]}$:	steady-state concentration in sediment i [mol.m^{-3}] *(O)*
MOL WEIGHT:	molecular weight of the chemical [kg.mol^{-1}] *(A)*
$\alpha_{sed\,[S]}$:	mean of log NOEC's for sediment at scale S [g.l^{-1}]
$\beta_{water\,[S]}$:	beta for water at scale S [-] *(D)*

$$PAF_{soil\,i[S]} = \frac{1}{\left(1+e^{\frac{-(\log(CSS_{soil\,i}\cdot MOLWEIGHT)-\alpha_{soil[S]})}{\beta_{soil[S]}}}\right)} \qquad \mathbf{15}$$

with

$PAF_{soil\,i[S]}$:	predicted affected fraction for soil i at scale S [-] *(A)*
$CSS_{soil\,i[S]}$:	steady-state concentration in soil i [mol.m^{-3}] *(O)*
$MOL\ WEIGHT$:	molecular weight of the chemical [kg.mol^{-1}] *(A)*
$\alpha_{soil[S]}$:	mean of log NOEC's for soil at scale S [g.l^{-1}]
$\beta_{soil[S]}$:	beta for soil at scale S [-]

$$\beta_{soil[S]} = stdev_{soil[S]} \cdot \frac{\sqrt{3}}{\pi} \qquad \textbf{16}$$

with

$\beta_{soil\,[S]}$:	beta for soil at scale S [-] *(D)*
$stdev_{soil\,[S]}$:	standard deviation of log NOEC's for soil [-] *(D)*

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[b] EUSES: the calculation of Potentially Affected Fraction is not implemented in EUSES.

3.3 Parameters that describe intermedia partitioning of the chemical

Intermedia equilibrium constants (air/water; air/aerosol, air/soil, air/vegetation; sediment/ water; soil/water; soil/vegetation) or partition coefficients are required for various purposes, but principally for estimating intermedia mass transfer coefficients. The coefficients represent concentration ratios. The concentrations can be expressed on a volume basis [mol.m^{-3}] or on a weight basis [mol.kg^{-1}].

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.

3.3.1 Air-water

The air-water equilibrium distribution constant, $K_{\text{air-water}}$, also known as the "dimensionless" Henry's law constant, can be estimated from the ratio of the vapor pressure and the water solubility. The air-water equilibrium distribution constant is temperature dependent. The estimation in SimpleBox is:

$$K_{air\text{-}water[S]} = \frac{H}{R.TEMPERATURE} = \frac{VAPORPRESSURE(T)/SOLUBILITY(T)}{R.TEMPERATURE_{[S]}} \qquad \mathbf{17}$$

with

$K_{air\text{-}water\,[S]}$:	air-water equilibrium distribution constant at scale S [mol.m$_{\text{air}}^{-3}$/mol.m$_{\text{water}}^{-3}$] *(A)*
H :	Henry's law constant [Pa.m^3.mol^{-1}]
VAPOR PRESSURE(T) :	vapor pressure of the chemical at temperature T (^{o}C) at scale S [Pa] *(A)*
SOLUBILITY(T) :	solubility of the chemical in water at temperature T (^{o}C) at scale S[mol.m^{-3}] *(A)*
R :	gas constant, = 8.314 Pa.m^3.mol^{-1}.K^{-1} *(C)*
$TEMPERATURE_{[S]}$:	temperature at the air-water interface at scale S [K] *(A)*

3.3.2 Air-aerosol

Air-aerosol partition coefficients are usually not known. However, some information is frequently available on the fraction of the chemical that occurs in association with the aerosol phase. SimpleBox uses this information for the computations. A value for the fraction of the chemical that is associated with the aerosol phase, $FRass_{aerosol}$, can be entered directly, or estimated on the basis of the chemical's vapor pressure, according to Junge (1977). In this equation, the sub-cooled liquid vapour pressure should be used. For solids, a correction is applied according to Mackay (1991):

If $MELTINGPOINT < TEMPERATURE_{[S]}$ (substance is liquid):

$$FRass_{aerosol[S]} = \frac{CONST.\theta}{VAPORPRESSURE(T) + CONST.\theta} \tag{18}$$

If $MELTINGPOINT > TEMPERATURE_{[S]}$ (substance is solid):

$$FRass_{aerosol[S]} = \frac{CONST.\theta}{VAPORPRESSURE(T).e^{6.79.(1-\frac{MELTINGPOINT}{TEMPERATURE_{[S]}})} + CONST.\theta} \tag{19}$$

with

$FRass_{aerosol[S]}$:	fraction of the chemical in air that is associated with aerosol particles at scale S [-] *(A)*
$VAPOR\ PRESSURE(T)$:	vapor pressure of the chemical at temperature T at scale S [Pa] *(A)*
$MELTINGPOINT$:	melting point of the chemical [K] *(A)*
$CONST$:	constant [Pa.m] *(C)*
θ :	surface area of aerosol phase [$m_{aerosol}^2/m_{air}^3$] *(C)*
$TEMPERATURE_{[S]}$:	temperature at the air-water interface at scale S [K] *(A)*

with the product $CONST \cdot \theta$ set equal to 10^{-4} Pa.

3.3.3 Air-rain

The scavenging ratio may be known from measurements or estimated:

$$SCAVratio_{[S]} = \frac{1 - FRass_{aerosol[S]}}{K_{air\text{-}water[S]}} + FRass_{aerosol[S]} COLLECTeff_{[S]} \tag{20}$$

with

$SCAVratio_{[S]}$:	scavenging ratio (quotient of the total concentration in rainwater and the total concentration in air) of the chemical at scale S [-] *(A)*
$FRass_{aerosol[S]}$:	fraction of the chemical in air that is associated with aerosol particles at scale S [-] *(A)*
$K_{air\text{-}water[S]}$:	air-water equilibrium distribution constant at scale S [$mol.m_{air}^{-3}/mol.m_{water}^{-3}$] *(A)*
$COLLECTeff_{[S]}$:	aerosol collection efficiency at scale S [-] *(A)*

The first term represents an estimate of the (equilibrium) distribution between rain water in air and the gas phase of air. The second term represents the scavenging of aerosol particles by rain droplets. The proportionality constant of $2 \cdot 10^5$ is taken from Mackay (1991).

3.3.4 Solid-Water partition coefficients

Commonly used estimation methods for the partition coefficients for sediment-(pore)water and soil-(pore)water are based on the assumption of the "hydrophobic sorption" mechanism. This mechanism is classically modeled using the organic carbon content of the soil or sediment and the octanol-water partition coefficient of the chemical. A common equation is:

$$\log Kp = \log(Koc.CORG) = a \log Kow + b + \log CORG \qquad \mathbf{21}$$

with

Kp :	solid(sediment/susp/soil)-water partition coefficient [$l_{water}.kg_{solid}^{-1}$] *(A)*
Koc :	organic carbon referenced solid-water partition coefficient [$l_{water}.kg_{oc}^{-1}$]*(A)*
$CORG$:	organic carbon content of the solid [$kg_{org.\ carbon}.kg_{solid}^{-1}$] *(A)*
Kow :	octanol-water partition coefficient of the chemical [-] *(A)*

Of the many regression formulas that have been reported for different classes of organic compounds, the most simple one appears to be the equation proposed by DiToro *et al.* (1991), in which the coefficients a and b are set to the values 1 and 0, respectively. Their equation is used here:

$$\log Kp = \log Kow + \log CORG \quad or \quad Kp = CORG.Kow \qquad \mathbf{22}$$

It should be stressed that this estimation method is valid only for non-ionic organic chemicals. This partition model is not to be applied to:

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

3.3.5 Sediment-water

Solid-water partition coefficients are commonly expressed as [$mol.kg_{solid}^{-1}/mol.l_{water}^{-1}$] or [$l_{water}.kg_{solid}^{-1}$]. The "dimensionless" form [$mol.m_{sorbent}^{-3}/mol.m_{water}^{-3}$] or [$m_{water}^{3}.m_{sorbent}^{-3}$] is often required in calculations. Values for these equililibrium distribution constants may be derived from:

$$K_{sed\text{-}water\ i[S]} = FRwater_{sed\ i[S]} + (1 - FRwater_{sed\ i[S]}).Kp_{sed\ i[S]}.RHOsolid_{[S]}/1000 \qquad \mathbf{23}$$

with

$K_{sed\text{-}water\ i[S]}$:	sediment-water equilibrium distribution constant at scale S [$mol.m_{sed}^{-3}/mol.m_{water}^{-3}$] *(A)*
$Frwater_{sed\ i[S]}$:	volume fraction of the water phase of sediment of scale S [-] *(A)*
$Kp_{sed\ i[S]}$:	sediment-water partition coefficient at scale S [$l_{water}.kg_{solid}^{-1}$] *(I)*
$RHOsolid_{[S]}$:	density of the solid phase at scale S [$kg_{solid}.m_{solid}^{-3}$] *(A)*
1000 :	conversion factor [$l.m^{-3}$] *(C)*

3.3.6 Soil-water

$$K_{soil\ i\text{-}water[S]} = FRwater_{soil\ i[S]} + FRsolid_{soil\ i[S]} \cdot Kp_{soil\ i[S]} \cdot RHOsolid_{[S]} / 1000 \qquad 24$$

with

$K_{soil\ i\text{-}water[S]}$: soil-water equilibrium distribution constant at scale S $[\mathrm{mol.m_{soil}^{-3}/mol.m_{water}^{-3}}]$ *(A)*

$FRwater_{soil\ i[S]}$: volume fraction of the water phase of soil at scale S[-] *(A)*

$FRsolid_{soil\ i[S]}$: volume fraction of the solid phase of soil at scale S[-] *(A)*

$Kp_{soil\ i[S]}$: soil-water partition coefficient at scale S$[\mathrm{l_{water}.kg_{solid}^{-1}}]$ *(I)*

$RHOsolid_{[S]}$: density of the solid phase at scale S $[\mathrm{kg_{solid}.m_{solid}^{-3}}]$ *(A)*

1000 : conversion factor $[\mathrm{l.m^{-3}}]$ *(C)*

3.3.7 Dissolved fraction of the chemical in water, sediment and soil

The fraction of a chemical, present in the total water column (suspended matter, biota and water) can be estimated on the basis of the partition coefficient and bioconcentration factor:

$$FRdisslvd_{water\ i[S]} = 100/(1 + \frac{Kp_{susp\text{-}water\ i[S]} \cdot SUSP_{water\ i[S]} + BCF_{fish\ i[S]} \cdot BIO_{water\ i[S]}}{1000}) \qquad 25$$

with

$FRdisslvd_{water\ i[S]}$: dissolved fraction of water column i at scale S [-] *(A)*

$Kp_{susp\text{-}water\ i[S]}$: suspended matter-water partition coefficient at scale S $[\mathrm{l_{water}.kg_{solid}^{-1}}]$ *(I)*

$SUSP_{water\ i\ [S]}$: concentration suspended matter in water column i at scale S $[\mathrm{kg_{solid}.m_{water}^{-3}}]$ *(D)*

$BCF_{fish\ i[S]}$: bioconcentration factor for fish in water column i at scale S $[\mathrm{l_{water}.kg_{fish}^{-1}}]$ *(A)*

$BIO_{water\ [S]}$: concentration of biota in the water column $[\mathrm{kg_{solid}.m_{water}^{-3}}]$ *(D)*

1000 : conversion factor $[\mathrm{l.m^{-3}}]$ *(C)*

For non-ionic organic chemicals, the bioconcentration factor can be estimated from the hydrophobicity of the chemical in the same way as the solids-water partition coefficients. Most of the available measurements and regression equations refer to fish.

$$BCF_{fish\ i[S]} = FAT_{fish\ i[S]} \cdot K_{ow} \qquad 26$$

with

$BCF_{fish\ i[S]}$: bioconcentration factor for fish in water column i at scale S $[\mathrm{l_{water}.kg_{fish}^{-1}}]$ *(A)*

$FAT_{fish\ i[S]}$: volume fraction of fat in fish in water column i at scale S [-] *(A)*

K_{ow} : octanol-water partition coefficient of the chemical [-] *(A)*

in which, by default, the following value may be considered:

$$FAT_{fish\ i[S]} = 0.05 \qquad 27$$

with

$FAT_{fish\ i[S]}$: volume fraction of fat in fish in water column i at scale S [-] *(A)*

$$FRdisslvd_{sed\ i[S]} = \frac{FRwater_{sed\ i[S]}}{K_{sed\text{-}water\ i[S]}} \cdot 100 \qquad \mathbf{28}$$

with

$FRdisslvd_{sed\ i[S]}$: fraction of the chemical present in the water phase of the sediment [-] *(A)*

$FRwater_{sed\ i[S]}$: volume fraction of the water phase of the sediment [-] *(A)*

$K_{sed\text{-}water\ i[S]}$: sediment-water equilibrium distribution constant at scale S [mol.m_{sed}^{-3}/mol.m_{water}^{-3}] *(A)*

$$FRdisslvd_{soil\ i[S]} = \frac{FRwater_{soil\ i[S]}}{K_{soil\ i\text{-}water[S]}} \cdot 100 \qquad \mathbf{29}$$

with

$FRdisslvd_{soil\ i[S]}$: fraction of the chemical present in the water phase of soil i at scale S [-] *(A)*

$FRwater_{soil\ i[S]}$: volume fraction of the water phase of the soil at scale S[-] *(A)*

$K_{soil\ i\text{-}water[S]}$: soil-water equilibrium distribution constant for soil i at scale S [mol.m_{sed}^{-3}/mol.m_{water}^{-3}] *(A)*

3.4 Parameters that characterize the environment

3.4.1 General parameter settings for the regional, continental and global scales

The default settings of SimpleBox are set to reflect a densely populated Western European region (regional scale), and the whole of the European Union (continental scale).

3.4.1.1 Area of the system

$$SYSTEMAREA_{[R]} = 80000\ km^2 \qquad \mathbf{30}$$

with

$SYSTEMAREA_{[R]}$:	total area of the regional scale (air/water + air/soil interfaces) [m^2] *(D)*
80000 :	area of the regional scale (soil + water 1 + water 2)

the area of the region (typical 200 x 200km^2 area, without sea water). The area of sea water is set equal to the typical area. The total systemarea is the typical area plus the area of sea water.

$$SYSTEMAREA_{[C]} = 7120000 - SYSTEMAREA_{[R]}\ km^2 \qquad \mathbf{31}$$

with

$SYSTEMAREA_{[C]}$:	total area of the continental scale (air/water + air/soil interfaces) [m^2] *(D)*
7120000:	area of the continental scale (soil + water 1 + water 2)
$SYSTEMAREA_{[R]}$:	total area of the regional scale (air/water + air/soil interfaces) [m^2] *(D)*

the area of the European Union, including sea water. The area of the continental scale is corrected by subtracting the area of the regional scale.

Table 2: *Systemarea of the global scales* (Henderson-Sellers and McCuffie, 1987)

Scale	*SYSTEMAREA* [km^2]
Moderate	$3.89.10^7$-$SYSTEMAREA_{[C]}$[a]
Arctic	$2.55.10^7$
Tropic	$8.93.10^7$

[a] The area of the moderate scale is corrected by subtracting the area of the continental scale.

3.4.1.2 Population

Population is needed for the calculation of indirect emmision by the waste water treatment population is corrected for the area fraction of sea water in the systems:

$$POPULATION_{[R]} = 500.\frac{SYSTEMAREA_{[R]}}{2}/10^{6} \qquad \textbf{32}$$

with

$POPULATION_{[R]}$:	total population of the regional scale [inh] *(A)*
500 :	average population density in the region [inh.km^{-2}] *(C)*
$SYSTEMAREA_{[R]}$:	total area of the regional scale (air/water + air/soil interfaces) [m^{2}] *(D)*
10^{6} :	conversion factor [m^{2}.km^{-2}] *(C)*
2 :	correction factor for soil+water1 *(C)*

$$POPULATION_{[C]} = 104.\frac{SYSTEMAREA_{[C]}}{2}/10^{6} \qquad \textbf{33}$$

with

$POPULATION_{[C]}$:	total population of the continental scale [inh] *(A)*
104 :	average population density of the continental scale [inh.km^{-2}] *(C)*
$SYSTEMAREA_{[C]}$:	total area of the continental scale (air/water + air/soil interfaces) [m^{2}]*(D)*
2 :	correction factor for soil+water1 *(C)*
10^{6} :	conversion factor [m^{2}.km^{-2}] *(C)*

3.4.1.3 Production

$$PRODUCTION_{[R]} = (1\cdot 10^{-6}/MOLWEIGHT)\cdot POPULATION_{[R]}\cdot(24\cdot 3600) \qquad \textbf{34}$$

with

$PRODUCTION_{[R]}$:	total amount produced or imported in the system [mol.s^{-1}] *(A)*
1.10^{-6} :	production per inhabitant [kg.inh^{-1}.d^{-1}]
$24\cdot 3600$:	conversion factor [s.d^{-1}]
$MOL\ WEIGHT$:	molecular weight of the chemical [kg.mol^{-1}] *(A)*
$POPULATION_{[R]}$:	total population of the regional scale [inh] *(A)*

$$PRODUCTION_{[C]} = 9\cdot PRODUCTION_{[R]} \qquad \textbf{35}$$

with

$PRODUCTION_{[C]}$:	total amount produced or imported in the continental scale [mol.s^{-1}] *(A)*
$PRODUCTION_{[R]}$:	total amount produced or imported in the regional scale [mol.s^{-1}] *(A)*

as a starting point;

3.4.1.4 Temperature

Table 3: *Temperature of the scales*

Scale	*TEMPERATURE* [°C]
Regional	12[a]
Continental	12
Moderate	12
Arctic	-10[b]
Tropic	25[b]

[a] the average temperature at ground level in the Netherlands
[b] Peixoto and Oort, 1992.

3.4.2 Air

Air is treated in SimpleBox as a bulk 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 3A. The air compartment is considered to be well-mixed. The refreshment rate is characterized by the atmospheric residence time.

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

$$VOLUME_{air[S]} = SYSTEMAREA_{[S]}.HEIGHT_{air[S]} \qquad \textbf{36}$$

with

$VOLUME_{air[S]}$:	volume of the air compartment of scale S [m^3] *(D)*
$SYSTEMAREA_{[S]}$:	total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$HEIGHT_{air[S]}$:	atmospheric mixing height of scale S [m] *(A)*

for which, by default, the following values may be considered:

$$HEIGHT_{air[S]} = 1000\ m \qquad \textbf{37}$$

with

$HEIGHT_{air[S]}$:	atmospheric mixing height of scale S [m] *(A)*

the average thickness of the atmospheric mixing layer.

To estimate the atmospheric residence time, it is assumed that wind blows at constant speed in one direction through a well-mixed cylindrical box:

$$TAU_{air[S]} = \frac{\sqrt{SYSTEMAREA_{[S]}.\pi/4}}{WINDSPEED_{[S]}} \qquad \textbf{38}$$

with

$TAU_{air\,[S]}$: residence time of air in scale S [s] *(D)*
$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$WINDSPEED_{[S]}$: average windspeed at 10 m above the surface of scale S [$m.s^{-1}$] *(A)*

in which the following may be considered as a default:

$$WINDSPEED_{[S]} = 3\; m.\,s^{-1} \tag{39}$$

with

$WINDSPEED_{[S]}$: average windspeed above the surface of scale S [$m.s^{-1}$] *(A)*

This is a typical windspeed for the regional scale (EC, 1996a).

3.4.2.1 Air flows between the scales

The $FLOW_{air}$ between the different scales may be estimated as:

$$FLOW_{air[R]-air[C]} = FLOW_{air[C]-air[R]} = \frac{VOLUME_{air[R]}}{TAU_{air[R]}} \tag{40}$$

with

$FLOW_{air[R]-air[C]}$: rate of air flow from the regional scale to the continental scale [$m_{air}^3.s^{-1}$] *(A)*
$FLOW_{air[C]-air[R]}$: rate of air flow from the continental scale to the regional scale [$m_{air}^3.s^{-1}$] *(A)*
$VOLUME_{air[R]}$: volume of the air compartment of the regional scale [m^3] *(D)*
$TAU_{air[R]}$: residence time of air in the regional scale [s] *(D)*

$$FLOW_{air[C]-air[M]} = FLOW_{air[M]-air[C]} = \frac{VOLUME_{air[C]}}{TAU_{air[C]}} \tag{41}$$

with

$FLOW_{air[C]-air[M]}$: rate of air flow from the continental scale to the moderate scale [$m_{air}^3.s^{-1}$] *(A)*
$FLOW_{air[M]-air[C]}$: rate of air flow from the moderate scale to the continental scale [$m_{air}^3.s^{-1}$] *(A)*
$VOLUME_{air[C]}$: volume of the air compartment of the continental scale [m^3] *(D)*
$TAU_{air[C]}$: residence time of air in the continental scale [s] *(D)*

$$FLOW_{air[M]-air[A]} = FLOW_{air[A]-air[M]} = \frac{VOLUME_{air[A]}}{TAU_{air[A]}} \tag{42}$$

with

$FLOW_{air[M]-air[A]}$: rate of air flow from the moderate scale to the arctic scale [$m_{air}^3.s^{-1}$] *(A)*
$FLOW_{air[A]-air[M]}$: rate of air flow from the arctic scale to the moderate scale [$m_{air}^3.s^{-1}$] *(A)*
$VOLUME_{air[A]}$: volume of the air compartment of the arctic scale [m^3] *(D)*
$TAU_{air[A]}$: residence time of air in the arctic scale [s] *(D)*

$$FLOW_{air[M]-air[T]} = FLOW_{air[T]-air[M]} = \frac{VOLUME_{air[T]}}{TAU_{air[T]}} \quad \mathbf{43}$$

with

$FLOW_{air[M]-air[T]}$:	rate of air flow from the moderate scale to the tropic scale $[m_{air}^3.s^{-1}]$ *(A)*
$FLOW_{air[T]-air[M]}$:	rate of air flow from the tropic scale to the moderate scale $[m_{air}^3.s^{-1}]$ *(A)*
$VOLUME_{air[T]}$:	volume of the air compartment of the tropic scale $[m^3]$ *(D)*
$TAU_{air[T]}$:	residence time of air in the tropic scale [s] *(D)*

Deposition mass flows of the chemical depend on the rate of wet precipitation and the rate of dry aerosol deposition. Deposition velocities and collection efficiencies of aerosols vary greatly with the size of the particles. As chemicals may be associated with particles of a specific size, the deposition velocities and collection efficiencies depend also on the chemical. The values given are typical values, to be used as a starting point:

$$AEROSOLDEPRATE_{[S]} = 0.1\ cm.s^{-1} \quad \mathbf{44}$$

with

$AEROSOLDEPRATE_{[S]}$:	deposition velocity of the aerosol particles with which the chemical is associated at scale S $[m.s^{-1}]$ *(A)*

$$COLLECTeff_{[S]} = 2.10^5 \quad \mathbf{45}$$

with

$COLLECTeff_{[S]}$:	aerosol collection efficiency at scale S [-] *(A)*

Table 4: *Rainrate of the scales*

Scale	*RAINRATE* $[mm.yr^{-1}]$
Regional	700
Continental	700
Moderate	700
Arctic	250[a]
Tropic	1300[a]

[a] from Wania and Mackay (1995)

3.4.3 Water

Two separate water compartments are defined in both the regional and continental scale; a fresh water and a sea water compartment. At the global scales, one water compartment is defined (seawater). In SimpleBox, "water" is treated as a homogeneous bulk compartment, consisting of a suspended matter phase, and a biota phase. The presence of suspended matter and biota influences the fate of chemicals in a very similar way to that of aerosols and rainwater 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. Concentration ratios among suspended matter, biota and water are often close to equilibrium. For the purpose of 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 and biota.

The water compartments at the regional and continental scales are continuously flushed with water (and biota, suspended matter) from outside that scale. The chemical in the fresh water compartment of the continental scale can be transported to the fresh water compartment of the regional scale (rivers). The chemical in the sea water compartment at the regional scale can be "exported" and "imported" to and from the continental scale. The chemical at the continental scale can be "exported" and “imported" from and to the sea water compartment of the regional scale and the water compartment of the moderate scale. The chemical at the moderate scale can be "exported" and "imported" from and to the sea water compartment of the continental scale and the water compartments of the arctic and tropic scales. The water flows between the scales are shown in Figure 3A.

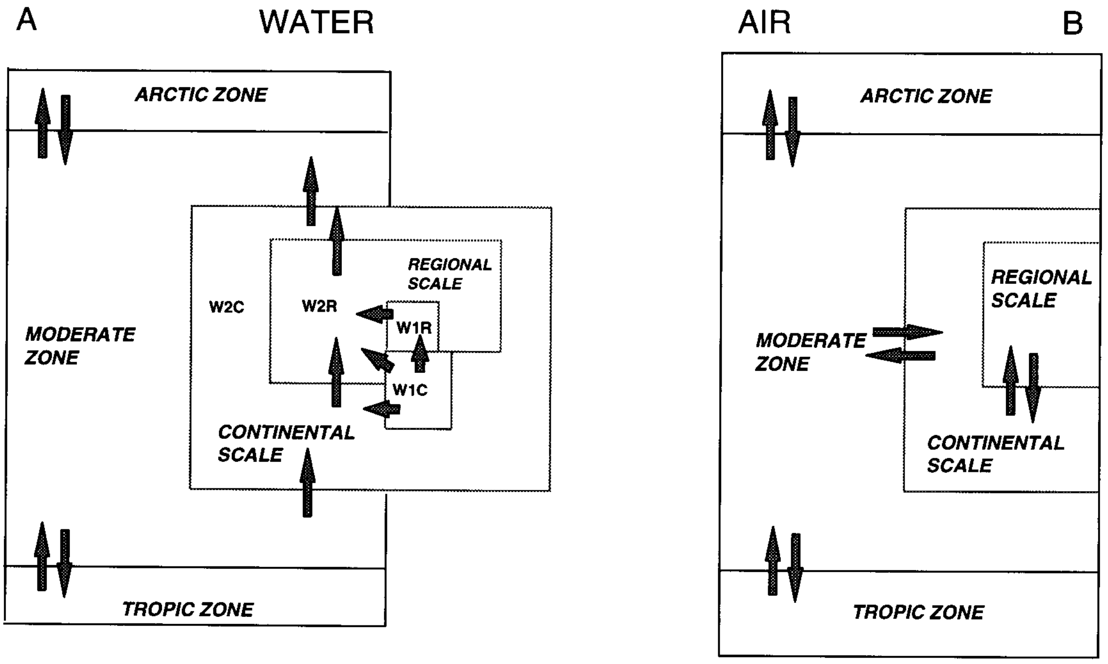

Figure 3: *Water and air flows in and between the spatial scales.* W1R is water compartment 1 of the regional scale, W2R is water compartment 2 of the regional scale. W1C is water compartment 1 of the continental scale, W2C is water compartment 2 of the continental scale.

The water flows between the global scales are equal, e.g. $FLOW_{water[M]\text{-}water[A]} = FLOW_{water[A]\text{-}water[M]}$ and $FLOW_{water[M]\text{-}water[T]} = FLOW_{water[T]\text{-}water[M]}$ in order to calculate a reasonable water balance for the total system modeled.
The rate of refreshment is characterized by means of a single hydraulic residence time. This assumption strongly caricaturizes reality since typically multimedia environmental contain many different water bodies with different characteristics. Naturally, the two separate water compartments of the regional and continental scale and the water compartments of the global scales cannot represent all of these. Instead, the water compartments that are modeled here are chosen to be "typical" --an exemplification of any real water body in the system.

The volume of the water compartments at the regional, continental and global scales may be obtained from:

$$VOLUME_{water\,i[S]} = SYSTEMAREA_{[S]} \cdot AREAFRAC_{water\,i[S]} \cdot DEPTH_{water\,i[S]} \qquad \textbf{46}$$

with

$VOLUME_{water\,i[S]}$: volume of water compartment i at scale S [m^3] *(D)*
$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{water\,i[S]}$: fraction of the system area that is water i at scale S [-] *(D)*
$DEPTH_{water\,i[S]}$: depth of water column i at scale S [m] *(A)*

for which, by default, the following may be considered:

$$AREAFRAC_{water\,1[R]} = 1.5\% \qquad \textbf{47}$$

with

$AREAFRAC_{water\,1[R]}$: fraction of the regional scale that is water 1 [-] *(D)*

the area percentage of fresh water (rivers, lakes, canals, ditches) in the region;

$$AREAFRAC_{water2[R]} = 50\% \qquad \textbf{48}$$

with

$AREAFRAC_{water\,2[R]}$: fraction of the regional scale that is water 2 [-] *(D)*

the area percentage of sea water in the region;

$$AREAFRAC_{water1[C]} = 1.5\% \qquad \textbf{49}$$

with

$AREAFRAC_{water\,1[C]}$: fraction of the continental scale that is water 1 [-] *(D)*

the area percentage of fresh water (rivers, lakes, canals, ditches) in Europe;

$$AREAFRAC_{water2[C]} = 50\% \qquad \textbf{50}$$

with

$AREAFRAC_{water\,2[C]}$: fraction of the continental scale that is water 2 [-] *(D)*

the area percentage of sea water in Europe;

Table 5: *Area fraction of water for the global scales*

Scale	*compartment*	$AREAFRAC_{water}$ [%]
Moderate	water	50
Arctic	water	60
Tropic	water	70

Table 6: *Water depth of the global scales*

Scale	*compartment*	$DEPTH_{water}$ [m]
Regional	water 1	3
Regional	water 2	25
Continental	water 1	3
Continental	water 2	200
Moderate	water	1000
Arctic	water	1000
Tropic	water	1000

A typical hydraulic residence[c] time may be obtained by calculating a water balance. The water compartments at the all scales receive water from four sources: water flows to the compartment, surface run-off, urban run-off and precipitation. Precipitation is considered to be equal to evaporation and has no influence on the residence time of water. The urban run-off, *EFFLUENTstp*, is very small compared with the incoming flows and can therefore be ignored. The same amount of the incoming flows flows out of the fresh water compartment of system into the sea water compartment of the system:

$$TAU_{water\,i[S]} = \frac{VOLUME_{water\,i[S]}}{FLOWS_{i[S]} + RUNOFF_{[S]}} \qquad \mathbf{51}$$

with

$TAU_{water\,i[S]}$: hydraulic residence time of water compartment i at scale S [s] *(D)*

$VOLUME_{water\,i[S]}$: volume of water compartment i at scale S [m^3] *(D)*

---

[c] In EUSES, the residence time is based on the incoming water flows, surface run-off, urban run-off (effluent of the sewage treatment plant) and precipitation: the effluent of the sewage treatment plant in $m^3.d^{-1}$ is calculated by: *WASTEW* = *POPULATION* * 0.2 *(24*3600); where 0.2 is the water use per inhabitant in $m^3.inh^{-1}.d^{-1}$ and (24*3600) is the conversion factor ($s.d^{-1}$). The water flow through the system due to rainfall directly into surface water is calculated by: *RAINDIRECT* = *RAINRATE* * *SYSTEMAREA* * *AREAFRACwater* i * (24*3600); where *RAINRATE* is the average daily precipitation ($m.d^{-1}$). The EUSES settings can be simulated in SimpleBox by setting TAU to the value computed in EUSES.

$FLOWS_{i[S]}$: sum of the discharges of all streams crossing the scale boundaries to water compartment i [$m^3.s^{-1}$] *(D)*

$RUNOFF_{[S]}$: total run off from soil 1, (soil 2 and soil 3) of scale S into the water compartment of scale S [$m^3.s^{-1}$] *(A)*

$$FLOWS_{1[R]} = FLOW_{water1[C]-water1[R]} \tag{52}$$

with

$FLOWS_{1[R]}$: sum of the discharges of all streams crossing the regional scale boundaries to water 1 [$m^3.s^{-1}$] *(A)*

$FLOW_{water1[C]-water1[R]}$: flow from water 1 of the continental scale to water 1 of the regional scale [$m^3.s^{-1}$] *(A)*

the total discharge of the major rivers, entering the fresh waters of the region;

$$FLOWS_{2[R]} = FLOW_{water1[C]-water2[R]} + FLOW_{water1[R]-water2[R]} + FLOW_{water2[C]-water2[R]} \tag{53}$$

with

$FLOWS_{2[R]}$: sum of the discharges of all streams crossing the regional scale boundaries to water 1 [$m^3.s^{-1}$] *(A)*

$FLOW_{water1[C]-water2[R]}$: flow from water 1 of the continental scale to water 2 of the regional scale [$m^3.s^{-1}$] *(A)*

$FLOW_{water1[R]-water2[R]}$: flow from water 1 of the regional scale to water 2 of the regional scale [$m^3.s^{-1}$] *(A)*

$FLOW_{water2[C]-water2[R]}$: flow from water 2 of the continental scale to water 2 of the regional scale [$m^3.s^{-1}$] *(A)*

the total discharge of the major rivers and flow of sea water, entering sea water of the region;

$$FLOWS_{1[C]} = 0 \tag{54}$$

with

$FLOWS_{1[C]}$: sum of the discharges of all streams crossing the continental scale boundaries to water 1 [$m^3.s^{-1}$] *(A)*

there are no water flows from other water compartments to water compartment 1 of the continental scale;

$$FLOWS_{2[C]} = FLOW_{water1[C]-water2[C]} + FLOW_{water[M]-water2[C]} + FLOW_{water2[R]-water2[C]} \tag{55}$$

with

$FLOWS_{2[C]}$: sum of the discharges of all streams crossing the continental scale boundaries to water 2 [$m^3.s^{-1}$] *(A)*

$FLOW_{water1[C]-water2[C]}$: flow from water 1 of the continental scale to water 2 of the continental scale [$m^3.s^{-1}$] *(A)*

$FLOW_{water[M]\text{-}water2[C]}$: flow from water of the moderate scale to water 2 of the continental scale $[m^3.s^{-1}]$ *(A)*

$FLOW_{water2[R]\text{-}water2[C]}$: flow from water 2 of the regional scale to water 2 of the continental scale $[m^3.s^{-1}]$ *(A)*

the total flow of water entering the sea water compartment of the continental scale;

$$FLOWS_{[M]} = FLOW_{water2[C]-water[M]} + FLOW_{water[A]-water[M]} + FLOW_{water[T]-water[M]} \qquad 56$$

with

$FLOWS_{[M]}$: sum of the discharges of all streams crossing the moderate scale boundaries to the water compartment $[m^3.s^{-1}]$ *(A)*

$FLOW_{water2[C]\text{-}water[M]}$: flow from water 2 of the continental scale to water of the moderate scale $[m^3.s^{-1}]$ *(A)*

$FLOW_{water[A]\text{-}water\ [M]}$: flow from water of the arctic scale to water of the moderate scale $[m^3.s^{-1}]$ *(A)*

$FLOW_{water[T]\text{-}water[M]}$: flow from water of the tropic scale to water of the moderate scale $[m^3.s^{-1}]$ *(A)*

the total flow of sea water, entering the water compartment of the moderate scale;

$$FLOWS_{[A]} = FLOW_{water[M]-water[A]} \qquad 57$$

with

$FLOWS_{[A]}$: sum of the discharges of all flows crossing the arctic scale boundaries to the water compartment $[m^3.s^{-1}]$ *(A)*

$FLOW_{water[M]\text{-}water[A]}$: flow from water of the moderate scale to water of the arctic scale $[m^3.s^{-1}]$ *(A)*

the total flow of water entering the water compartment of the arctic scale;

$$FLOWS_{[T]} = FLOW_{water[M]-water[T]} \qquad 58$$

with

$FLOWS_{[T]}$: sum of the discharges of all flows crossing the tropic scale boundaries to the water compartment $[m^3.s^{-1}]$ *(A)*

$FLOW_{water[M]\text{-}water[T]}$: flow from water of the moderate scale to water of the tropic scale $[m^3.s^{-1}]$ *(A)*

the total flow of water entering the water compartment of the arctic scale;

$$\begin{aligned} RUNOFF_{to\ water\ i[S]} = {} & \Sigma(FRACrun_{soil\ i-water\ i[S]} \cdot AREAFRAC_{soil\ i[S]}) \cdot \\ & RAINRATE_{[S]} . SYSTEMAREA_{[S]} \end{aligned} \qquad 59$$

with

$RUNOFF_{to\ water\ i[S]}$: total run off from soil 1, (soil 2 and soil 3) into water compartment i at scale S $[m^3.s^{-1}]$ *(A)*

$FRACrun_{soil\ i\ \text{-}water\ i[S]}$: fraction of the wet precipitation that runs off soil i to water i at scale S [-] *(A)*

$AREAFRAC_{soil\ i[S]}$: fraction of the systemarea of scale S that is soil i [-] *(D)*

$RAINRATE_{[S]}$: rate of wet precipitation at scale S $[m_{rain}.s^{-1}]$ *(A)*

$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*

3.4.3.1 Water flows between the scales

The water flows between the water compartments of the different scales are defined by:

$$FLOW_{water\ 1[R]-water\ 2[R]} = VOLUME_{water\ 1[R]}/TAU_{water\ 1[R]} \qquad 60$$

with

$FLOW_{water\ 1[R]-water\ 2[R]}$: rate of water flow from water 1 to water 2 of the regional scale [$m_{water}^3.s^{-1}$] *(A)*

$VOLUME_{water}$: volume of the water compartment [m^3] *(D)*

TAU_{water} : residence time of water in the system [s] *(D)*

$$\begin{aligned} FLOW_{water\ 2[R]-water\ 2[C]} = {} & RUNOFF_{soil\ 1[R]-water\ 2[R]} + RUNOFF_{soil\ 2[R]-water\ 2[R]} \\ & + RUNOFF_{soil\ 3[R]-water\ 2[R]} + FLOW_{water\ 1[R]-water\ 2[R]} \\ & + FLOW_{water\ 1[C]-water\ 2[R]} + FLOW_{water\ 2[C]-water\ 2[R]} \end{aligned} \qquad 61$$

with

$FLOW_{water\ 2[R]-water\ 2[C]}$: rate of water flow from water 2 of the regional scale to water 2 of the continental scale [$m_{water}^3.s^{-1}$] *(A)*

$RUNOFF_{soil\ 1-water\ 2[R]}$: transport coefficient for run-off from soil 1 to water 2 at the regional scale [$m_{soil}^3 s^{-1}$] *(D)*

$RUNOFF_{soil\ 2-water\ 2[R]}$: transport coefficient for run-off from soil 2 to water 2 at the regional scale [$m_{soil}^3 s^{-1}$] *(D)*

$RUNOFF_{soil\ 3-water\ 2[R]}$: transport coefficient for run-off from soil 2 to water 2 at the regional scale [$m_{soil}^3 s^{-1}$] *(D)*

$FLOW_{water\ 1[R]-water\ 2[R]}$: rate of water flow from water 1 to water 2 of the regional scale [$m_{water}^3.s^{-1}$] *(A)*

$FLOW_{water\ 1[C]-water\ 2[R]}$: rate of water flow from water 1 of the continental scale to water 2 of the regional scale [$m_{water}^3.s^{-1}$] *(A)*

$FLOW_{water\ 2[C]-water\ 2[R]}$: rate of water flow from water 2 of the continental scale to water 2 of the regional scale [$m_{water}^3.s^{-1}$] *(A)*

$$FLOW_{water\ 1[C]-water\ 2[C]} = \frac{VOLUME_{water\ 1[C]}}{TAU_{water\ 1[C]}} . FRACout_{water\ 2[C]} \qquad 62$$

with

$FLOW_{water\ 1[C]-water\ 2[C]}$: rate of water flow from water 1 to water 2 of the continental scale [$m_{water}^3.s^{-1}$] *(A)*

$VOLUME_{water\ 1[C]}$: volume of water compartment 1 of the continental scale [m^3] *(D)*

$TAU_{water\ 1[C]}$: residence time of water 1 in the continental scale [s] *(D)*

$FRACout_{water\ 2[C]}$: fraction of water 1 of the continental scale that flows to water 2 of the continental scale [-] *(D)*

$$FLOW_{water\ 1[C]-water\ 1[R]} = \frac{VOLUME_{water\ 1[C]}}{TAU_{water\ 1[C]}}.FRACout_{water\ 1[R]} \qquad \textbf{63}$$

with

$FLOW_{water\ 1[C]-water\ 1[R]}$: rate of water flow from water 1 of the continental scale to water 1 of the regional scale [$m_{water}^3.s^{-1}$] *(A)*

$VOLUME_{water\ 1[C]}$: volume of water compartment 1 of the continental scale [m^3] *(D)*

$TAU_{water\ 1[C]}$: residence time of water 1 in the continental scale [s] *(D)*

$FRACout_{water\ 1[R]}$: fraction of water 1 of the continental scale that flows to water 1 of the regional scale [-] *(D)*

$$FLOW_{water\ 1[C]-water\ 2[R]} = \frac{VOLUME_{water\ 1[C]}}{TAU_{water\ 1[C]}}.FRACout_{water\ 2[R]} \qquad \textbf{64}$$

with

$FLOW_{water\ 1[C]-water\ 2[R]}$: rate of water flow from water 1 of the continental scale to water 2 of the regional scale [$m_{water}^3.s^{-1}$] *(A)*

$VOLUME_{water\ 1[C]}$: volume of water compartment 1 of the continental scale m^3] *(D)*

$TAU_{water\ 1[C]}$: residence time of water 1 in the continental scale [s] *(D)*

$FRACout_{water\ 2[R]}$: fraction of water 1 of the continental scale that flows to water 2 of the regional scale [-] *(D)*

$$FLOW_{water\ 2[C]-water\ 2[R]} = \frac{VOLUME_{water\ 2[R]}}{\left(\dfrac{\sqrt{SYSTEMAREA_{[R]} \cdot AREAFRAC_{water\ 2[R]}}}{0.03}\right)} \qquad \textbf{65}$$

with

$FLOW_{water\ 2[C]-water\ 2[R]}$: rate of water flow from water 2 of the continental scale to water 2 of the regional scale [$m_{water}^3.s^{-1}$] *(A)*

$VOLUME_{water\ 2[R]}$: volume of water compartment 2 of the regional scale [m^3] *(D)*

$SYSTEMAREA_{[R]}$: area of the regional scale [m^2] *(D)*

$AREAFRAC_{water\ 2[R]}$: fraction of the regional scale that is water 2 [-] *(D)*

0.03 : sea current at the continental scale [$m.s^{-1}$] *(D)*

$$FLOW_{water\ 2[C]-water[M]} = \frac{VOLUME_{water\ 2[C]}}{TAU_{water\ 2[C]}} \qquad \textbf{66}$$

with

$FLOW_{water\ 2[C]-water[M]}$: rate of water flow from water 2 of the continental scale to water of the moderate scale [$m_{water}^3.s^{-1}$] *(A)*

$VOLUME_{water\ 2[C]}$: volume of water compartment 2 of the continental scale [m^3] *(D)*

$TAU_{water\ 2[C]}$: residence time of water 2 in the continental scale [s] *(D)*

$$FLOW_{water[M]-water\,2[C]} = \frac{VOLUME_{water\,2[C]}}{\left(\frac{\sqrt{SYSTEMAREA_{[C]} * AREAFRAC_{water\,2[C]}}}{0.01}\right)} \qquad \textbf{67}$$

with

$FLOW_{water[M]-water\,2[C]}$: rate of water flow from water of the moderate scale to water 2 of the continental scale $[m_{water}^{3}.s^{-1}]$ *(A)*

$VOLUME_{water\,2[C]}$: volume of water compartment 2 of the continental scale $[m^{3}]$ *(D)*

TAU_{water} : residence time of water in the system [s] *(D)*

$SYSTEMAREA_{[C]}$: area of the continental scale $[m^{2}]$ *(D)*

$AREAFRAC_{water\,2[C]}$: fraction of the continental scale that is water 2 [-] *(D)*

0.01: sea current at the moderate scale [-] *(D)*

$$FLOW_{water[M]-water[A]} = \frac{VOLUME_{water[A]}}{\left(\frac{\sqrt{SYSTEMAREA_{[A]}}}{0.01}\right)} \qquad \textbf{68}$$

with

$FLOW_{water[M]-water[A]}$: rate of water flow from water of the moderate scale to water of the arctic scale $[m_{water}^{3}.s^{-1}]$ *(A)*

$VOLUME_{water[A]}$: volume of the water compartment of the arctic scale $[m^{3}]$ *(D)*

$SYSTEMAREA_{[A]}$: area of the arctic scale $[m^{2}]$ *(D)*

0.01: sea current at the arctic scale [-] *(D)*

$$FLOW_{water[M]-water[T]} = \frac{VOLUME_{water[T]}}{\left(\frac{\sqrt{SYSTEMAREA_{[T]}}}{0.01}\right)} \qquad \textbf{69}$$

with

$FLOW_{water[M]-water[T]}$: rate of water flow from water of the moderate scale to water of the tropic scale $[m_{water}^{3}.s^{-1}]$ *(A)*

$VOLUME_{water[T]}$: volume of the water compartment of the tropic scale $[m^{3}]$ *(D)*

$SYSTEMAREA_{[T]}$: area of the arctic scale $[m^{2}]$ *(D)*

0.01: sea current at the moderate scale [-] *(D)*

$$FLOW_{water[A]-water[M]} = \frac{VOLUME_{water[A]}}{TAU_{water[A]}} \qquad \textbf{70}$$

with

$FLOW_{water[A]-water[M]}$: rate of water flow from water of the arctic scale to water of the moderate scale $[m_{water}^{3}.s^{-1}]$ *(A)*

$VOLUME_{water[A]}$: volume of the water compartment of the arctic scale $[m^{3}]$ *(D)*

$TAU_{water[A]}$: residence time of water in the arctic scale [s] *(D)*

$$FLOW_{water[T]-water[M]} = \frac{VOLUME_{water[T]}}{TAU_{water[T]}} \qquad \mathbf{71}$$

with

$FLOW_{water[T]-water[M]}$: rate of water flow from water of the tropic scale to water of the moderate scale [$m_{water}^3.s^{-1}$] *(A)*

$VOLUME_{water[T]}$: volume of the water compartment of the tropic scale [m^3] *(D)*

$TAU_{water[T]}$: residence time of water in the tropic scale [s] *(D)*

Table 7: *Fraction of water flow out of water 1 of the continental scale to other water compartments*

Scale	*compartment*	$FRACout_{water\ i[S]}$ [-]
Regional	water 1	0.0391[a]
Regional	water 2	0.01
Continental	water	0.951

a The fraction water out of water compartment 1 of the continental scale is set to calculate the flow $FLOW_{water\ 1[C]-water\ 1[R]} = 750\ m^2.s^{-1}$.

3.4.4 Water, suspended matter

In this context, "suspended matter" refers to all abiotic colloidal or macromolecular materials (debris of organisms, "humic" material, "dissolved" organic matter, "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 fresh water compartment of the continental scale can be transported to the fresh water compartment of the regional scale (rivers). The suspended matter in the sea water compartment at the regional scale can be “imported" and "exported" to and from the continental scale. The suspended matter at the continental scale can be “imported" and "exported" to and from the sea water compartment of the regional scale and the water compartment of the moderate scale. The suspended matter at the moderate scale can be “imported" and "exported" to and from the sea water compartment of the continental scale and the water compartments of the arctic and tropic scales. This transport is characterized by the flow of water and the concentrations of suspended matter in the incoming and outgoing water. Suspended matter may also be produced in the system itself, by growth of small aquatic organisms (bacteria, algae). Sewage treatment plant effluents are another source of suspended matter. 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.

Suspended matter is transported into the system with the inflowing water from a larger scale. The inflow of suspended matter is given by the concentration of suspended matter in the larger spatial scale. The outflow of suspended matter is given by the concentration of suspended matter in the water in the system, $SUSP_{water\ i[S]}$:

Table 8: *Suspended matter concentration*

Scale	*compartment*	$SUSP_{water}$ [mg.l^{-1}]
Regional	water 1	15
Regional	water 2	5
Continental	water 1	25
Continental	water 2	5
Moderate	water	5
Arctic	water	5
Tropic	water	5

Particle exchange between sediment and water is characterized by:

$$\text{If } \frac{SETTLEvelocity_{[S]} \cdot SUSP_{water\ i[S]}}{(1\ -\ FRwater_{sed\ i[S]}) \cdot RHOsolid_{[S]}} > NETsedrate_{i[s]}, \text{ then:}$$

72

$$GROSSsedrate_{i[S]} = \frac{SETTLEvelocity_{[S]} \cdot SUSP_{water\ i[S]}}{(1\ -\ FRwater_{sed\ i[S]}) \cdot RHOsolid_{[S]}}, \text{ else:}$$

$$GROSSsedrate_{i[S]} = NETsedrate_{i[S]}$$

with

$GROSSsedrate_{i[S]}$	gross sedimentation rate for sediment i at scale S [m$_{sed}$.s^{-1}] *(A)*
$SETTLEvelocity_{[S]}$:	settling velocity of suspended particles at scale S [m$_{water}$.s^{-1}] *(A)*
$SUSP_{water\ i[S]}$:	concentration of suspended matter in water column i at scale S [kg$_{solid}$.m$_{water}^{-3}$] *(D)*
$FRwater_{sed\ i[S]}$:	volume fraction water of the sediment i at scale S [-] *(A)*
$RHOsolid_{[s]}$:	density of the solid phase of sediment i at scale S [kg.m^{-3}] *(A)*
$NETsedrate_{i[S]}$:	net sedimentation rate for sediment i at scale S[m$_{sed}$.s^{-1}] *(A)*

for which, by default, the following values may be considered:

$$SETTLvelocity_{[S]} = 2.5\ m.d^{-1}$$ **73**

with

$SETTLvelocity_{[S]}$:	settling velocity of suspended particles at scale S [m$_{water}$.s^{-1}] *(A)*

a value typical for the fine muddy sediments that are common in the region;

$$RESUSPrate_{i[S]} = GROSSsedrate_{i[S]} - NETsedrate_{i[S]} \qquad \mathbf{74}$$

with

$RESUPrate_{i\,[S]}$:	resuspension rate for sediment i at scale S $[m_{sed}.s^{-1}]$ *(A)*
$GROSSsedrate_{i\,[S]}$:	gross sedimentation rate for sediment i at scale S $[m_{sed}.s^{-1}]$ *(A)*
$NETsedrate_{i\,[S]}$:	net sedimentation rate for sediment i at scale S $[m_{sed}.s^{-1}]$ *(A)*

$$\mathbf{75}$$

$$\begin{aligned} NETsedrate_{1[R]} = {} & (PROD_{susp\,1[R]} + SUSP_{water\,1[C]} . FLOW_{water\,1[C]-water\,1[R]} + \\ & SUSPeff_{stp[R]} . FRstpwater_{1[R]} . EFFLUENT_{stp[R]} + \\ & \Sigma\; EROSION_{soil\,i[R]} . AREAFRAC_{soil\,i[R]} . SYSTEMAREA_{[R]} . FRsolid_{soili[R]} \\ & . RHOsolid_{[R]} - SUSP_{water\,1[R]} . FLOW_{water\,1[R]-water\,2[R]}) . \\ & \frac{1}{(1\ -\ FRwater_{sed[R]}) . RHOsolid_{[R]}} . \frac{1}{(SYSTEMAREA_{[R]} . AREAFRAC_{water\,1[R]})} \end{aligned}$$

with

$NETsedrate_{1[R]}$:	net sedimentation rate for sediment 1 at the regional scale $[m_{sed}.s^{-1}]$ *(A)*
$PROD_{susp\,1[R]}$:	rate of production of suspended matter in water column 1 at the regional scale $[kg_{solid}.s^{-1}]$ *(A)*
$FLOW_{water\,1[C]-water1[R]}$:	the stream of water that flows to water compartment 1 at the regional scale $[m_{water}^{3}.s^{-1}]$ *(A)*
$SUSP_{water\,i[S]}$:	concentration of suspended matter in water column i at scale S $[kg_{solid}.m_{water}^{-3}]$ *(D)*
$SUSPeff_{stp[R]}$:	concentration of suspended matter in STP-effluents at the regional scale $[kg_{solid}.m_{eff}^{-3}]$ *(A)*
$EFFLUENT_{stp[R]}$:	total of all STP-effluent discharges to the water compartment at the regional scale $[m_{eff}^{3}.s^{-1}]$ *(A)*
$EROSION_{soil\,i[R]}$:	rate of erosion of soil i at the regional scale $[m_{soil}.s^{-1}]$ *(A)*
$AREAFRAC_{soil\,i[R]}$:	fraction of the systemarea that is soil i at the regional scale [-] *(D)*
$FRsolid_{soil\,i[R]}$:	volume fraction solid of soil i at the regional scale [-] *(A)*
$RHOsolid_{[R]}$:	density of the solid phase of the sediment at the regional scale $[kg.m^{-3}]$ *(A)*
$SYSTEMAREA_{[R]}$:	total area of the regional scale(air/water + air/soil interfaces) $[m^{2}]$ *(D)*
$FRwater_{sed\,[R]}$:	volume fraction water of sediment at the regional scale [-] *(A)*
$AREAFRAC_{water\,1[R]}$:	fraction of the systemarea of the regional scale that is water 1 [-] *(D)*

$$\begin{aligned}NETsedrate_{2[R]} = {} & (PROD_{susp\,2[R]} + SUSP_{water\,1[R]} . FLOW_{water\,1[R]-water\,2[R]} \\ & + SUSP_{water\,1[C]} . FLOW_{water\,1[C]-water\,2[R]} + SUSP_{water\,2[C]} . FLOW_{water\,2[C]-water\,2[R]} \\ & + SUSPeff_{stp[R]} . FRstpwater_{2[R]} . EFFLUENT_{stp[R]} + \\ & \Sigma\ EROSION_{soil\,i[R]} . AREAFRAC_{soil\,i[R]} . SYSTEMAREA_{[R]} . FRsolid_{soili[R]} \\ & . RHOsolid_{[R]} - SUSP_{water\,2[R]} . FLOW_{water\,2[R]-water\,2[C]}) . \\ & \frac{1}{(1\ -\ FRwater_{sed[R]}) . RHOsolid_{[R]}} . \frac{1}{(SYSTEMAREA_{[R]} . AREAFRAC_{water\,2[R]})}\end{aligned} \qquad \mathbf{76}$$

with

$NETsedrate_{2[R]}$:	net sedimentation rate for sediment 2 at the regional scale $[m_{sed}.s^{-1}]$ *(A)*
$PROD_{susp\,2[R]}$:	rate of production of suspended matter in water column 2 at the regional scale $[kg_{solid}.s^{-1}]$ *(A)*
$FLOW_{water\,i[S]-water\,2[R]}$:	the stream of water that flows to water compartment 2 at the regional scale $[m_{water}^{3}.s^{-1}]$ *(A)*
$SUSP_{water\,i[S]}$:	concentration of suspended matter in water column i at scale S $[kg_{solid}.m_{water}^{-3}]$ *(D)*
$SUSPeff_{stp[R]}$:	concentration of suspended matter in STP-effluents at the regional scale $[kg_{solid}.m_{eff}^{-3}]$ *(A)*
$EFFLUENT_{stp[R]}$:	total of all STP-effluent discharges to the water compartment at the regional scale $[m_{eff}^{3}.s^{-1}]$ *(A)*
$EROSION_{soil\,i[R]}$:	rate of erosion of soil i at the regional scale $[m_{soil}.s^{-1}]$ *(A)*
$AREAFRAC_{soil\,i[R]}$:	fraction of the systemarea that is soil i at the regional scale [-] *(D)*
$FRsolid_{soil\,i[R]}$:	volume fraction solid of soil i at the regional scale [-] *(A)*
$RHOsolid_{[R]}$:	density of the solid phase of the sediment at the regional scale $[kg.m^{-3}]$ *(A)*
$SYSTEMAREA_{[R]}$:	total area of the regional scale(air/water + air/soil interfaces) $[m^{2}]$ *(D)*
$FRwater_{sed\,[R]}$:	volume fraction water of sediment at the regional scale [-] *(A)*
$AREAFRAC_{water\,2[R]}$:	fraction of the systemarea of the regional scale that is water 2 [-] *(D)*

$$\begin{aligned}NETsedrate_{1[C]} = {} & (PROD_{susp\,1[C]} + SUSPeff_{stp[C]} . FRstpwater_{1[C]} . EFFLUENT_{stp[C]} + \\ & \Sigma\ EROSION_{soil\,i[C]} . AREAFRAC_{soil\,i[C]} . SYSTEMAREA_{[C]} . FRsolid_{soili[C]} \\ & . RHOsolid_{[C]} - SUSP_{water\,1[C]} . FLOW_{water\,1[C]-water\,1[R]} \\ & - SUSP_{water\,1[C]} . FLOW_{water\,1[C]-water\,2[R]} - SUSP_{water\,1[C]} . FLOW_{water\,1[C]-water\,2[C]}) . \\ & \frac{1}{(1\ -\ FRwater_{sed[C]}) . RHOsolid_{[C]}} . \frac{1}{(SYSTEMAREA_{[C]} . AREAFRAC_{water\,1[C]})}\end{aligned} \qquad \mathbf{77}$$

with

$NETsedrate_{1[C]}$:	net sedimentation rate for sediment 1 at the continental scale $[m_{sed}.s^{-1}]$ *(A)*
$PROD_{susp\,1[C]}$:	rate of production of suspended matter in water column 1 at the continental scale $[kg_{solid}.s^{-1}]$ *(A)*

$FLOW_{water\,i[S]-water1[C]}$: the stream of water that flows to water compartment 1 at the continental scale $[m_{water}^{3}.s^{-1}]$ *(A)*
$SUSP_{water\,i[S]}$: concentration of suspended matter in water column i at scale S $[kg_{solid}.m_{water}^{-3}]$ *(D)*
$SUSPeff_{stp[C]}$: concentration of suspended matter in STP-effluents at the continental scale $[kg_{solid}.m_{eff}^{-3}]$ *(A)*
$EFFLUENT_{stp[C]}$: total of all STP-effluent discharges to the water compartment at the continental scale $[m_{eff}^{3}.s^{-1}]$ *(A)*
$EROSION_{soil\,i[C]}$: rate of erosion of soil i at the continental scale $[m_{soil}.s^{-1}]$ *(A)*
$AREAFRAC_{soil\,i[C]}$: fraction of the systemarea that is soil i at the continental scale [-] *(D)*
$FRsolid_{soil\,i[C]}$: volume fraction solid of soil i at the continental scale [-] *(A)*
$RHOsolid_{[C]}$: density of the solid phase of the sediment at the continental scale $[kg.m^{-3}]$ *(A)*
$SYSTEMAREA_{[C}$: total area of the continental scale(air/water + air/soil interfaces) $[m^{2}]$ *(D)*
$FRwater_{sed\,[C}$: volume fraction water of sediment at the continental scale [-] *(A)*
$AREAFRAC_{water\,1[C]}$: fraction of the systemarea of the continental scale that is water 1 [-] *(D)*

$$
\begin{aligned}
NETsedrate_{2[C]} = {} & (PROD_{susp\,2[C]} + SUSP_{water[M]}.FLOW_{water[M]-water\,2[C]} \\
& + SUSP_{water\,1[C]}.FLOW_{water\,1[C]-water\,2[C]} + SUSP_{water\,2[R]}.FLOW_{water\,2[R]-water\,2[C]} \\
& + SUSPeff_{stp[C]}.FRstpwater_{2[C]}.EFFLUENT_{stp[C]} + \\
& \Sigma\ EROSION_{soil\,i[C]}.AREAFRAC_{soil\,i[C]}.SYSTEMAREA_{[C]}.FRsolid_{soili[C]} \\
& .RHOsolid_{[C]} - SUSP_{water\,2[C]}.FLOW_{water\,2[C]-water\,2[R]} \\
& - SUSP_{water\,2[C]}.FLOW_{water\,2[C]-water[M]}). \\
& \frac{1}{(1\ -\ FRwater_{sed[C]}).RHOsolid_{[C]}}.\frac{1}{(SYSTEMAREA_{[C]}.AREAFRAC_{water\,1[C]})}
\end{aligned}
\tag{78}
$$

with

$NETsedrate_{2[C]}$: net sedimentation rate for sediment 2 at the continental scale $[m_{sed}.s^{-1}]$ *(A)*
$PROD_{susp\,2[C]}$: rate of production of suspended matter in water column 2 at the continental scale $[kg_{solid}.s^{-1}]$ *(A)*
$FLOW_{water\,i[S]-water2[C]}$: the stream of water that flows to water compartment 2 at the continental scale $[m_{water}^{3}.s^{-1}]$ *(A)*
$SUSP_{water\,i[S]}$: concentration of suspended matter in water column i at scale S $[kg_{solid}.m_{water}^{-3}]$ *(D)*
$SUSPeff_{stp[C]}$: concentration of suspended matter in STP-effluents at the continental scale $[kg_{solid}.m_{eff}^{-3}]$ *(A)*
$EFFLUENT_{stp[C]}$: total of all STP-effluent discharges to the water compartment at the continental scale $[m_{eff}^{3}.s^{-1}]$ *(A)*
$EROSION_{soil\,i[C]}$: rate of erosion of soil i at the continental scale $[m_{soil}.s^{-1}]$ *(A)*
$AREAFRAC_{soil\,i[C]}$: fraction of the systemarea that is soil i at the continental scale [-] *(D)*
$FRsolid_{soil\,i[C]}$: volume fraction solid of soil i at the continental scale [-] *(A)*
$RHOsolid_{[C]}$: density of the solid phase of the sediment at the continental scale $[kg.m^{-3}]$ *(A)*
$SYSTEMAREA_{[C}$: total area of the continental scale(air/water + air/soil interfaces) $[m^{2}]$ *(D)*
$FRwater_{sed\,[C}$: volume fraction water of sediment at the continental scale [-] *(A)*
$AREAFRAC_{water\,2[C]}$: fraction of the systemarea of the continental scale that is water 2 [-] *(D)*

$$\begin{aligned} NETsedrate_{[M]} = {} & (PROD_{susp\,[M]} + SUSP_{water\,2[C]} \cdot FLOW_{water\,2[C]-water[M]} \\ & + SUSP_{water[A]} \cdot FLOW_{water[A]-water[M]} + SUSP_{water[T]} \cdot FLOW_{water[T]-water[M]} \\ & + \Sigma \;\; EROSION_{soil[M]} \cdot AREAFRAC_{soil[M]} \cdot SYSTEMAREA_{[M]} \cdot FRsolid_{soil[M]} \\ & .\, RHOsolid_{[M]} - SUSP_{water\,1[C]} \cdot FLOW_{water\,1[C]-water\,1[R]} \\ & - SUSP_{water[M]} \cdot FLOW_{water[M]-water\,2[C]} - SUSP_{water[M]} \cdot FLOW_{water[M]-water[A]} \\ & - SUSP_{water[M]} \cdot FLOW_{water[M]-water[T]} \;). \\ & \frac{1}{(1 \; - \; FRwater_{sed[M]}) .\, RHOsolid_{[M]}} \cdot \frac{1}{(SYSTEMAREA_{[M]} \cdot AREAFRAC_{water[M]})} \end{aligned} \tag{79}$$

with

$NETsedrate_{[M]}$:	net sedimentation rate for sediment at the moderate scale [$m_{sed}.s^{-1}$] *(A)*
$PROD_{susp[M]}$:	rate of production of suspended matter in the water column at the moderate scale [$kg_{solid}.s^{-1}$] *(A)*
$FLOW_{water\,i[S]-water[M]}$:	the stream of water that flows to the water compartment at the moderate scale [$m_{water}^{3}.s^{-1}$] *(A)*
$SUSP_{water\,i[S]}$:	concentration of suspended matter in water column i at scale S [$kg_{solid}.m_{water}^{-3}$] *(D)*
$EROSION_{soil\,[M]}$:	rate of erosion of soil at the moderate scale [$m_{soil}.s^{-1}$] *(A)*
$AREAFRAC_{soil\,[M]}$:	fraction of the systemarea that is soil at the moderate scale [-] *(D)*
$Frsolid_{soil\,[M]}$:	volume fraction solid of soil at the moderate scale [-] *(A)*
$RHOsolid_{[M]}$:	density of the solid phase of the sediment at the moderate scale [$kg.m^{-3}$] *(A)*
$SYSTEMAREA_{[M]}$:	total area of the moderate scale(air/water + air/soil interfaces) [m^{2}] *(D)*
$FRwater_{sed\,[M]}$:	volume fraction water of sediment at the moderate scale [-] *(A)*
$AREAFRAC_{water[M]}$:	fraction of the systemarea of the moderate scale that is water [-] *(D)*

$$\begin{aligned} NETsedrate_{[A]} = {} & (PROD_{susp\,[A]} + SUSP_{water[M]} \cdot FLOW_{water[M]-water[A]} \\ & + \Sigma \;\; EROSION_{soil[A]} \cdot AREAFRAC_{soil[A]} \cdot SYSTEMAREA_{[A]} \cdot FRsolid_{soil[A]} \\ & .\, RHOsolid_{[A]} - SUSP_{water[A]} \cdot FLOW_{water[A]-water[M]} \;). \\ & \frac{1}{(1 \; - \; FRwater_{sed[A]}) .\, RHOsolid_{[A]}} \cdot \frac{1}{(SYSTEMAREA_{[A]} \cdot AREAFRAC_{water[A]})} \end{aligned} \tag{80}$$

with

$NETsedrate_{[A]}$:	net sedimentation rate for sediment at the arctic scale [$m_{sed}.s^{-1}$] *(A)*
$PROD_{susp[A]}$:	rate of production of suspended matter in the water column at the arctic scale [$kg_{solid}.s^{-1}$] *(A)*
$FLOW_{water\,[S]-water[A]}$:	the stream of water that flows to the water compartment at the arctic scale [$m_{water}^{3}.s^{-1}$] *(A)*
$SUSP_{water\,i[S]}$:	concentration of suspended matter in water column i at scale S [$kg_{solid}.m_{water}^{-3}$] *(D)*
$EROSION_{soil\,[A]}$:	rate of erosion of soil at the arctic scale [$m_{soil}.s^{-1}$] *(A)*
$AREAFRAC_{soil\,[A]}$:	fraction of the systemarea that is soil at the arctic scale [-] *(D)*
$Frsolid_{soil\,[A]}$:	volume fraction solid of soil at the arctic scale [-] *(A)*

$RHOsolid_{[A]}$:	density of the solid phase of the sediment at the arctic scale [kg.m^{-3}] *(A)*
$SYSTEMAREA_{[A]}$:	total area of the arctic scale(air/water + air/soil interfaces) [m^2] *(D)*
$FRwater_{sed\,[A]}$:	volume fraction water of sediment at the arctic scale [-] *(A)*
$AREAFRAC_{water[A]}$:	fraction of the systemarea of the arctic scale that is water [-] *(D)*

$$\begin{aligned} NETsedrate_{[T]} = {} & (PROD_{susp\,[T]} + SUSP_{water[M]} . FLOW_{water[M]-water[T]} \\ & + \sum EROSION_{soil[T]} . AREAFRAC_{soil[T]} . SYSTEMAREA_{[T]} . FRsolid_{soil[T]} \\ & . RHOsolid_{[T]} - SUSP_{water[T]} . FLOW_{water[T]-water[M]}) . \\ & \frac{1}{(1 - FRwater_{sed[T]}) . RHOsolid_{[T]}} . \frac{1}{(SYSTEMAREA_{[T]} . AREAFRAC_{water[T]})} \end{aligned} \tag{81}$$

with

$NETsedrate_{[T]}$:	net sedimentation rate for sediment at the tropic scale [m$_{sed}$.s^{-1}] *(A)*
$PROD_{susp[T]}$:	rate of production of suspended matter in the water column at the tropic scale [kg$_{solid}$.s^{-1}] *(A)*
$FLOW_{water\,[S]-water[T]}$:	the stream of water that flows to the water compartment at the tropic scale [m$_{water}^3$.s^{-1}] *(A)*
$SUSP_{water\,i[S]}$:	concentration of suspended matter in water column i at scale S [kg$_{solid}$.m$_{water}^{-3}$] *(D)*
$EROSION_{soil\,[T]}$:	rate of erosion of soil at the tropic scale [m$_{soil}$.s^{-1}] *(A)*
$AREAFRAC_{soil\,[T]}$:	fraction of the systemarea that is soil at the tropic scale [-] *(D)*
$Frsolid_{soil\,[T]}$:	volume fraction solid of soil at the tropic scale [-] *(A)*
$RHOsolid_{[T]}$:	density of the solid phase of the sediment at the tropic scale [kg.m^{-3}] *(A)*
$SYSTEMAREA_{[T]}$:	total area of the tropic scale(air/water + air/soil interfaces) [m^2] *(D)*
$FRwater_{sed\,[T]}$:	volume fraction water of sediment at the tropic scale [-] *(A)*
$AREAFRAC_{water[T]}$:	fraction of the systemarea of the tropic scale that is water [-] *(D)*

for which, by default, the following values may be considered:

Table 9: *Production of suspended matter*

Scale	*compartment*	$PROD_{SUSPwater}$ [g$_{solid}$.m^{-2}.y^{-1}]
Regional	water 1	10
Regional	water 2	1
Continental	water 1	10
Continental	water 2	1
Moderate	water	1
Arctic	water	1
Tropic	water	1

$$SUSPeff_{stp[R]} = 30\ mg(dry).l^{-1}$$ **82**

with

$SUSPeff_{stp[R]}$: concentration of suspended matter in STP-effluents at the regional scale[$kg_{solid}.m_{eff}^{-3}$] *(A)*

a typical value for communal water treatment facilities in the Netherlands.

$$SUSPeff_{stp[C]} = 40\ mg(dry).l^{-1}$$ **83**

with

$SUSPeff_{stp[C]}$: concentration of suspended matter in STP-effluents at the continental scale[$kg_{solid}.m_{eff}^{-3}$] *(A)*

a typical value for communal water treatment facilities in Europe.

Estimation of the susp-water partition coefficient takes the organic carbon content of the suspended matter as input. By default, the following value may be considered:

$$CORG_{susp[S]} = 0.1$$ **84**

with

$CORG_{susp[S]}$: organic carbon content of suspended matter at scale S [$kg_{org.\ carbon}.kg_{solid}^{-1}$] *(A)*

a typical value for suspended particulate matter in surface waters.

3.4.5 Water, biota

"Biota" refers to all living organisms in water, from bacteria to mammals. The fraction biota in the water compartment is usually small, compared to even the fraction of suspended matter in the water compartment. As a result, biota usually plays an insignificant role with regard to the overall fate of the chemicals. Concentration ratios among biota and water are often close to equilibrium. Therefore, in SimpleBox equilibrium is assumed at all times among water and biota.

$$BIO_{water[S]} = 1\ mg(dry).l^{-1}$$ **85**

with

$BIO_{water[S]}$: concentration of biota in the water column [$kg_{solid}.m_{water}^{-3}$] *(D)*

as a starting point.

3.4.6 Sediment

Sediment is treated as a bulk compartment, consisting of a water phase and a solid phase; the concentration in sediment is a total concentration. Equilibrium is assumed between the pore water and solid phases of the sediment.
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 volume of the sediment compartment may be obtained from:

$$V_{sed\,i[S]} = VOLUME_{sed\,i[S]} = SYSTEMAREA_{[S]} \cdot AREAFRAC_{water\,i[S]} \cdot DEPTH_{sed\,i[S]} \tag{86}$$

with

$V_{sed\ i[S]}$:	volume of sediment compartment i at scale S [m^3] *(I)*
$VOLUME_{sed\ i[S]}$:	volume of sediment compartment i at scale S [m^3] *(D)*
$SYSTEMAREA_{[S]}$:	total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{water\ i[S]}$:	fraction of the area of scale S that is water i [-] *(D)*
$DEPTH_{sed\ i[S]}$:	mixing depth of sediment i at scale S [m] *(A)*

for which, by default, the following values may be considered:

$$DEPTH_{sed\,i[S]} = 3\ cm \tag{87}$$

with

$DEPTH_{sed\,i[S]}$:	mixing depth of the sediment at all scales [m] *(A)*

a value that may be considered typical for the muddy sediments in the shallow waters of the region.

The apparent mass flow of the chemical from the top layer to the deeper sediment is characterized by:

$$BURIAL_{sed\,i[S]} = NETsedrate_{i[S]} \tag{88}$$

with

$BURIAL_{sed\ i[S]}$:	burial rate of old sediment i under fresh deposits at scale S [$m_{sed}.s^{-1}$] *(A)*
$NETsedrate_{i[S]}$:	net sedimentation rate for sediment i at scale S [$m_{sed}.s^{-1}$] *(A)*

$$FRwater_{sed[S]} = 0.8 \tag{89}$$

with

$FRwater_{sed[S]}$:	volume fraction water of the sediment at scale S [-] *(A)*

Estimation of the sediment-water partition coefficient takes the organic carbon content of the sediment as input. By default, the following value may be considered:

$$CORG_{sed\,i[S]} = 0.05 \tag{90}$$

with

$CORG_{sed\,i[S]}$: organic carbon content of sediment i at scale S $[kg_{org.\,carbon} \cdot kg_{solid}^{-1}]$ *(A)*

a typical value for the sediments in surface waters.

3.4.7 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. SimpleBox, therefore, comes with three separate soil compartments. The first soil compartment may be thought of as "natural soil". The second soil compartment may be thought of as "agricultural soil". The third soil compartment may be used to reflect the existence of "urban" or "industrially used" soil.

Only the top layer of the soil is considered in this modeling concept. The effective soil depth is chemical dependent, see paragraph 3.4.8 .

Soil is treated as a bulk 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:

$$V_{soil\,i[S]} = VOLUME_{soil\,i[S]} = SYSTEMAREA_{[S]} \cdot AREAFRAC_{soil\,i[S]} \cdot DEPTH_{soil\,i[S]} \tag{91}$$

with

$V_{soil\,i[S]}$: volume of the soil compartment i at scale S $[m^3]$ *(I)*

$VOLUME_{soil\,i[S]}$: volume of the soil compartment i at scale S $[m^3]$ *(D)*

$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) $[m^2]$ *(D)*

$AREAFRAC_{soil\,i[S]}$: fraction of the area of scale S that is soil i [-] *(D)*

$DEPTH_{soil\,i[S]}$: mixing depth of soil i at scale S [m] *(A)*

for which, by default, the following values may be considered:

$$AREAFRAC_{soil\,1[R,C]} = 30\% \tag{92}$$

with

$AREAFRAC_{soil\,1[R,C]}$: fraction of the regional or continental scale that is soil 1 [-] *(D)* the approximate area percentage of soil that is not in agricultural use,

$$AREAFRAC_{soil(2)[R,C]} = 13.5\%$$ **93**

with

$AREAFRAC_{soil\,2[R,C]}$: fraction of the regional scale or continental that is soil 2 [-] *(D)*

the approximate area percentage of agricultural land,

$$AREAFRAC_{soil(3)[R,C]} = 5\%$$ **94**

with

$AREAFRAC_{soil\,3[R,C]}$: fraction of the regional or continental scale that is soil 3 [-] *(D)*

$$AREAFRAC_{soil[M,A,T]} = 1 - AREAFRAC_{water[M,A,T]} \cdot 100\%$$ **95**

with

$AREAFRAC_{soil\,[M,A,T]}$: fraction of the moderate, arctic or tropic scale that is soil [-] *(D)*

$AREAFRAC_{water\,[M,A,T]}$: fraction of the moderate, arctic or tropic scale that is water [-]*(D)*

The soil depth of the different compartments in given in paragraph 3.4.8.
It is assumed that the sludge produced in the area considered is applied onto soil 2 of that area.

$$RHO_{solid} = 2500\ kg.m^{-3}$$ **96**

with

RHO_{solid} : density of the solid phase [kg.m^{-3}] *(A)*

a typical value for minerals.

Surface run-off and infiltration of rain water play an important role in transport of chemicals out of the soil compartment. By default, values for the fraction of rain water that runs off to the water compartments and the fraction that infiltrates may be taken as:

$$FRACrun_{soil\,i-water\,1[S]} = 0.25$$ **97**

with

$FRACrun_{soil\,i\text{-}water\,1[S]}$: fraction of rain water that runs of from soil i to water 1 at scale S [-] *(A)*

$$FRACrun_{soil\,i-water\,2[S]} = 0$$ **98**

with

$FRACrun_{soil\ i\text{-}water\ 2[S]}$: fraction of rain water that runs of from soil i to water 2 at scale S [-] *(A)*

the sum of these fractions is the total fraction that runs off from the soil compartment, and is set to 0.25.

$$FRACinf_{soil\ i[S]} = 0.25 \qquad \mathbf{99}$$

with

$FRACinf_{soil\ i[S]}$: fraction of rain water that infiltrates into soil i of scale S [-] *(A)*

These values may be regarded as typical for the region.

The rain water that runs off the soil transports soil particles to the water compartment, eroding the soil and carrying the chemical that is associated with the soil particles with it. The rate of erosion varies with the topography. By default, values for this *EROSION* may be taken as:

$$EROSION_{soil\ i[S]} = 0.03\ mm.yr^{-1} \qquad \mathbf{100}$$

with

$EROSION_{soil\ i[S]}$: rate at which soil that is washed from soil i into surface water of scale S [m.s^{-1}] *(A)*

typical for flat terrain.

$$FRair_{soil\ i[S]} = 0.2 \qquad \mathbf{101}$$

with

$Frair_{soil\ i[S]}$: volume fraction air of soil i at scale S [-] *(A)*

$$FRwater_{soil\ i[S]} = 0.2 \qquad \mathbf{102}$$

with

$Frwater_{soil\ i[S]}$: volume fraction water of soil i at scale S [-] *(A)*

$$FRsolid_{soil\ i[S]} = 0.6 \qquad \mathbf{103}$$

with

$Frsolid_{soil\ i[S]}$: volume fraction solid of soil i at scale S [-] *(A)*

typical values for soil in the Netherlands (van Grinsven, RIVM, personal communication).

Estimation of the soil-water partition coefficient takes the organic carbon content of the soil as input. By default, the following values may be considered:

$$CORG_{soil\ 1[S]} = 0.05 \qquad \mathbf{104}$$

with

$CORG_{soil\ 1[S]}$: organic carbon content of soil 1 at scale S [$kg_{org.\ carbon}.kg_{solid}^{-1}$] *(A)*

$$CORG_{soil\ 2[S]} = 0.05$$ **105**

with

$CORG_{soil\ 2[S]}$: organic carbon content of soil 2 at the regional and continental scale $[kg_{org.\ carbon}.kg_{solid}^{-1}]$ *(A)*

$$CORG_{soil\ 3[S]} = 0.05$$ **106**

with

$CORG_{soil\ 3[S]}$: organic carbon content of soil 3 at the regional and continental scale $[kg_{org.\ carbon}.kg_{solid}^{-1}]$ *(A)*

3.4.8 Chemical dependent soil depth

In contrast with the former version of SimpleBox, it is assumed that the soil depth is dependent on the properties of the chemical[d]. For agricultural soil, which is frequently reworked by mechanical action (by plowing, etc.), the soil depth is chosen as the actual mixing depth, 20 cm as a minimum value. For natural and industrially soil a chemical-specific soil depth is defined, depending on the actual penetration depth of the chemical. The chemical tends to migrate vertically down into the soil, whereby processes of leaching, diffusion, absorption and degradation control the depth of migration. The penetration depth or "effective soil depth" of the chemical can be calculated with the modified Damköhler Number, D_a^*, (Cowan *et al.*, 1995). The penetration depth of the chemical is the depth at which, at steady-state, the rate of chemical reaction disappearance is equal to its rate of movement into the soil by diffusive processes. When these rates are equal, the penetration depth is calculated from $(D_E/k)^{1/2}$, where k is the first order degradation rate and D_E is the dispersion coefficient (diffusion + advection) (Cowan *et al.*, 1995). Although the SETAC approach was cast in terms of the Damköhler Number, in reality it is the result of a species mass balance of a section of soil near the air/soil interface, (Genuchten and Alves, 1982 and Thibodeaux, 1996) :

$$\frac{dC}{dt} = D_E.\frac{d^2C}{dx^2} - v_E\frac{dC}{dx} - kC = 0 \qquad \mathbf{107}$$

with

C : total concentration in soil [kg.m^{-3}]
D_E: effective diffusion coefficient in an unsaturated soil [m^2.s^{-1}]
k: first order degradation rate [s^{-1}]
v_E: effective solute convection velocity [m.s^{-1}]
x: soil depth [m]

The penetration depth d_p is calculated from the equivalent macroscopic mass balance, with an advection term, diffusion term and a first-order degradation term:

with

$$v_E.A.C/K_{sw} = -D_E.A.\frac{C}{d_p} - k.\frac{C}{2}.A.d_p \qquad \mathbf{108}$$

d_p: penetration depth of the chemical [m]
D_E: effective diffusion coefficient in an unsaturated soil [m^2.s^{-1}]
k: first order degradation rate [s^{-1}]

---

[d] EUSES: setting the soil depth of "natural soil" and "industially used soil" to 5 cm and the "agricultural used soil" to 20 cm simulates the default settings of EUSES. Chemical dependent penetration depth is not implemented in the EUSES-system.

v_E: effective solute convection velocity [m.s^{-1}]
C : total concentration in soil [kg.m^{-3}]
A : area of the soil compartment [kg.m^{-3}]
K_{sw}: soil-water partition coefficient [-]

Equation 108 can be rewritten as:

$$\tfrac{1}{2}kd_p^2 + \frac{v_E}{K_{sw}}d_p + D_E = 0 \qquad \mathbf{109}$$

with

d_p: penetration depth of the chemical [m]
D_E: effective diffusion coefficient in an unsaturated soil [m^2.s^{-1}]
k: first order degradation rate [s^{-1}]
v_E: effective solute convection velocity [m.s^{-1}]
C : total concentration in soil [kg.m^{-3}]
A : area of the soil compartment [kg.m^{-3}]
K_{sw}: soil-water partition coefficient [-]

The solution of equation 109 is:

$$d_p = \frac{\frac{v_E}{K_{sw}} + \sqrt{(\frac{v_E}{K_{sw}})^2 + 4D_E.k}}{2k} \qquad \mathbf{110}$$

with

d_p : chemical dependent penetration depth [m]
v_E: effective solute convection velocity [m.s^{-1}]
D_E: effective diffusion coefficient in an unsaturated soil [m^2.s^{-1}]
k: first order degradation rate [s^{-1}]
K_{sw}: soil-water partition coefficient [-]

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.

$$D_E = D_W\phi_W^{1.5} + D_A\phi_A^{1.5}.K_{aw} \qquad \mathbf{111}$$

with:

D_e: effective diffusion coefficient in an unsaturated soil [m^2.s^{-1}]
D_w: diffusion coefficient in water [m^2.s^{-1}]
ϕ_W: volume fraction of water in soil [-]
D_A: diffusion coefficient in air [m^2.s^{-1}]

ϕ_A: volume fraction of air in soil [-]
K_{aw}: soil-water partition coefficient [-]
K_{sa}: soil-air partition coefficient [-]

in which, by default, the following may be considered:

$$\begin{aligned} \phi_W &= 0.3 \\ \phi_A &= 0.2 \end{aligned} \tag{112}$$

with:

ϕ_W: volume fraction of water in soil [-]
ϕ_A: volume fraction of air in soil [-]

$$v_E = \frac{RAINrate.\, FRACinf(soil)}{\varepsilon} \tag{113}$$

with

$RAINrate$: rainrate [$m^3 m^{-2} s^{-1}$]
ε: air content of soil [$m^3.m^{-3}$]
$FRACinf(soil)$: fraction of rainwater that infiltrates into the soil [-]

in which, by default, the following may be considered:

$$\varepsilon = 0.5 \tag{114}$$

with

ε: air content of soil [$m^3.m^{-3}$]

The soil depth of the soil compartment 1 and 3 is (natural and industrial/urban soil):

If $0.01\ m < d_p < 1\ m$:

$$DEPTH_{soil\,1,3[S]} = d_p \tag{115}$$

with:

$DEPTH_{soil1[S]}$: mixing depth of soil 1 at scale S [m]
$DEPTH_{soil3[S]}$: mixing depth of soil 3 at scale S [m]
d_p : chemical dependent penetration depth [m]

The minimum soil depth of the soil compartment 2 (agricultural soil) is:

$$DEPTH_{soil2[S]} = 0.20m \qquad \mathbf{116}$$

$DEPTH_{soil2[S]}$: mixing depth of soil 2 at scale S [m] *(A)*

a typical mechanical reworking depth for agricultural soil. If the penetration depth is larger than 20 centimeter an smaller than 1 meter, the penetration depth is used to set the depth of the soil compartment.

3.4.9 Sewage treatment plant

On the regional and continental scale, it is assumed that 70% of the wastewater is treated in a biological sewage treatment plant (STP). The chemical loading of the STP can be estimated by the production of the chemical in the system and the emission factor to fresh water (rivers, lakes, etc.). The total effluent of the STP is calculated from the capacity of the sewage treatment plant. From these parameters the STP emissions to air, the water compartments (water 1 and water 2) and agricultural soil (soil 2) are calculated.

Emission to air

$$Estp_{air[S]} = STPload_{[S]}.ACTIVEtime_{[S]}.FR_{volatstp[S]} \qquad \textbf{117}$$

with

$Estp_{air[S]}$:	indirect emission to air of scale S, resulting from volatilization during sewage treatment at scale S [mol.s^{-1}] *(D)*
$STPload_{[S]}$:	load of the sewage treatment plant at scale S during release episodes at scale S [mol.s^{-1}] *(A)*
$ACTIVEtime_{[S]}$:	fraction of the time that the sewage treatment plant is loaded with the chemical at scale S [-] *(A)*
$FR_{volatstp[S]}$:	fraction of the load that is rerouted to the air compartment as a result of volatilization during sewage treatment at scale S [-] *(A)*

emission to water compartment i:

$$Estp_{water\,i[S]} = ACTIVEtime_{[S]}..FRstp_{water\,i[S]}EFFLUENT_{stp[S]}.CONCstp_{water[S]} \qquad \textbf{118}$$

with

$Estp_{water\,i[S]}$:	indirect emission to water with effluent from sewage treatment [mol.s^{-1}] *(D)*
$ACTIVEtime_{[S]}$:	fraction of the time that the sewage treatment plant of scale S is loaded with the chemical [-] *(A)*
$FRstp_{water\,i[S]}$:	fraction of the STP-effluent discharged into the water compartment i of scale S [m_{water}^{3}.s^{-1}] *(A)*
$EFFLUENT_{stp[S]}$:	amount of STP-effluent discharged into the water compartment i of scale S [m_{water}^{3}.s^{-1}] *(A)*
$CONCstp_{water[S]}$:	concentration of the chemical, dissolved in STP-effluent of scale S [mol.m_{water}^{-3}] *(A)*

emission to soil compartment 2, agricultural soil:

$$Estp_{soil\,2[S]} = ACTIVEtime_{[S]}.SOLIDS_{stp[S]}.CONCstp_{sludge[S]} \qquad \textbf{119}$$

with

$Estp_{soil\,2[S]}$	indirect emission to soil 2, resulting from application of sewage sludge at scale S [l.s^{-1}] *(D)*

$ACTIVEtime_{[S]}$: fraction of the time that the sewage treatment plant is loaded with the chemical at scale S [-] *(A)*

$SOLIDS_{stp[S]}$: rate of sewage sludge production at scale S [$kg_{solid}.s^{-1}$] *(A)*

$CONCstp_{sludge[S]}$: concentration of the chemical in sewage sludge at scale S [$mol.kg_{solid}^{-1}$] *(A)*

$$CONCstp_{water[S]} = \frac{STPload_{[S]} \cdot FR_{effstp[S]}}{EFFLUENT_{stp[S]} \cdot (1 + Kp_{susp[S]} \cdot SUSPeff_{stp[S]} / 1000)} \qquad \textbf{120}$$

with

$CONCstp_{water[S]}$: concentration of the chemical, dissolved in STP-effluent at scale S [$mol.m_{water}^{-3}$] *(A)*

$STPload[S]$: load of the sewage treatment plant during release episodes at scale S [$mol.s^{-1}$] *(A)*

$FR_{effstp[S]}$: fraction of the load that is rerouted to the water compartment with effluent (water + particles) upon sewage treatment at scale S [-] *(A)*

$EFFLUENT_{stp[S]}$: amount of STP-effluent discharged into the water compartment of scale S [$m_{water}^{3}.s^{-1}$] *(A)*

$Kp_{susp[S]}$: suspended matter-water partition coefficient at scale S [$l_{water}.kg_{solid}^{-1}$] *(A)*

$SUSPeff_{stp[S]}$: concentration of suspended matter in STP-effluents at scale S [$kg_{solid}.m_{eff}^{-3}$] *(A)*

1000 : conversion factor [$l.m^{-3}$] *(C)*

$$CONC_{sludge[s]} = \frac{STPload_{[S]} \cdot FR_{sludgestp[S]}}{SOLIDS_{stp[S]}} \qquad \textbf{121}$$

with

$CONCstp_{sludge[S]}$: concentration of the chemical in the solid phase of STP-sludge at scale S [$mol.kg_{solid}^{-1}$] *(A)*

$STPload_{[S]}$: load of the sewage treatment plant during release episodes at scale S [$mol.s^{-1}$] *(A)*

$FR_{sludgestp[S]}$: fraction of the load that is rerouted to the soil compartment with sludge upon sewage treatment at scale S [-] *(A)*

$SOLIDS_{stp[S]}$: rate of sewage sludge production at scale S [$kg_{solid}.s^{-1}$] *(A)*

$$FRstp_{water\,1[R]} = 0.9 \qquad \textbf{122}$$

with

$FRstp_{water\,1[R]}$: fraction of the STP-effluent discharged into the water compartment 1 of the regional scale [$m_{water}^{3}.s^{-1}$] *(A)*

$$FRstp_{water\,2[R]} = 1 - FRstp_{water1[R]} \qquad \textbf{123}$$

with

$Frstp_{water\,2[R]}$: fraction of the STP-effluent discharged into the water compartment 2 of the regional scale [$m_{water}^3.s^{-1}$] *(A)*

$$FRstp_{water\,1[C]} = 0.9 \tag{124}$$

with

$Frstp_{water\,1[C]}$: fraction of the STP-effluent discharged into the water compartment 1 of the continental scale [$m_{water}^3.s^{-1}$] *(A)*

$$FRstp_{water2[C]} = 1 - FRstp_{water1[C]} \tag{125}$$

with

$Frstp_{water\,2[C]}$: fraction of the STP-effluent discharged into the water compartment 2 of the continental scale [$m_{water}^3.s^{-1}$] *(A)*

$$EFFLUENT_{stp[S]} = STPcapacity_{[S]}.0.2 \tag{126}$$

with

$EFFLUENT_{stp[S]}$: amount of STP-effluent discharged into the water compartment of scale S [$m_{water}^3.s^{-1}$] *(A)*

$STPcapacity_{[S]}$: total capacity of all sewage treatment plants in scale S [eq] *(A)*

0.2 : sewage production [$m_{water}^3.eq^{-1}$] *(C)*

$$STPcapacity_{[S]} = POPULATION_{[S]}.PRCNTconnect_{[S]} \tag{127}$$

with

$STPcapacity_{[S]}$: total capacity of the sewage treatment plant of scale S [eq] *(A)*

$POPULATION_{[S]}$: number of inhabitants of scale S [eq] *(A)*

$PRCNTconnect_{[S]}$: the fraction of householdings connected to the sewage treatment plant of scale S [-] *(A)*

$$PRCNTconnect_{[S]} = 70\% \tag{128}$$

with

$PRCNTconnect_{[S]}$: the percentage of householdings connected to the sewage treatment plant of scale S [%] *(A)*

The rate of production of sludge may be obtained from Struijs *et al.* (1991):

$$SOLIDS_{stp[S]} = STPcapacity_{[S]}.(0.15.0.40 + 0.0355) \tag{129}$$

with

$SOLIDS_{stp[S]}$: rate of sewage sludge production at scale S $[kg_{solid}.s^{-1}]$ *(A)*
$STPcapacity_{[S]}$: total capacity of all sewage treatment plants in the system [eq] *(A)*
0.15 : sewage production $[m_{water}{}^{3}.eq^{-1}]$ *(C)*
0.4 : primary settling solids $[kg_{solid}.m_{water}{}^{-3}]$ *(C)*
0.0355 : amount of sludge produced in sewage treatment plant $[kg_{solid}.eq^{-1}]$ *(C)*

$$STPload_{[S]} = PRODUCTION_{[S]}.EMISfact_{water1[S]} \tag*{\textbf{130}}$$

with

$STPload$: load of the sewage treatment plant at scale S during release episodes $[mol.s^{-1}]$ *(A)*
$PRODUCTION_{[S]}$: total amount produced or imported in scale S $[mol.s^{-1}]$ *(A)*
$EMISfact_{water[S]}$: emission factor for water: the fraction of the production volume that is released to water compartment 1 of scale S [-] *(A)*

as a starting point;

$$ACTIVEtime_{[S]} = 365d.yr^{-1} = 1 \tag*{\textbf{131}}$$

with

$ACTIVEtime_{[S]}$: fraction of the time that the sewage treatment plant is loaded with the chemical at scale S [-] *(A)*

assuming continuous activity;

$$FR_{volatstp[S]} = 0.1 \tag*{\textbf{132}}$$

with

$FR_{volatstp[S]}$: fraction of the load that is rerouted to the air compartment of scale S as a result of volatilization during sewage treatment [-] *(A)*

as a starting point.

$$FR_{effstp[S]} = 0.2 \tag*{\textbf{133}}$$

with

$FR_{effstp[S]}$: fraction of the load that is rerouted to the water compartment with effluent (water + particles) upon sewage treatment at scale S [-] *(A)*

$$FR_{sludgestp[S]} = 0.6 \tag*{\textbf{134}}$$

with

$FR_{sludgestp[S]}$: fraction of the STPload that is rerouted to (agricultural) soil through application of sewage sludge at scale S*(A)*

$$SUSPeff_{stp[R]} = 30\ mg(dry).l^{-1} \tag{135}$$

with

$SUSPeff_{stp[R]}$: concentration of suspended matter in STP-effluents at the regional scale[$kg_{solid}.m_{eff}^{-3}$] (A)

a typical value for communal water treatment facilities in the Netherlands.

$$SUSPeff_{stp[C]} = 40\ mg(dry).l^{-1} \tag{136}$$

with

$SUSPeff_{stp[C]}$: concentration of suspended matter in STP-effluents at the continental scale[$kg_{solid}.m_{eff}^{-3}$] (A)

a typical value for communal water treatment facilities in Europe.

3.5 Parameters that describe the transformation processes

3.5.1 Degradation in air

$$kdeg_{air[S]} = (1 - FRass_{aerosol[S]}) \cdot krad_{OH[S]} \tag{137}$$

with

$kdeg_{air[S]}$: pseudo first order transformation rate constant in air at scale S [s^{-1}] *(D)*
$FRass_{aerosol[S]}$: fraction of the chemical in air that is associated with aerosol particles at scale S [-] *(A)*
$krad_{OH[S]}$: pseudo first order rate constant for reaction with OH-radicals at scale S [s^{-1}] *(A)*

As a default for $krad_{OH}$, it may be considered that nearly all organic chemicals show some reactivity with OH-radicals. According to Peijnenburg (personal communication), a half life of 160 days, equivalent to

$$krad_{OH[S]} = \frac{\ln 2}{160}\ d^{-1} \tag{138}$$

with

$krad_{OH[S]}$: pseudo first order rate constant for reaction with OH-radicals at scale S [d^{-1}] *(A)*
160 : maximum half-life for organic chemicals in air [d]

may be taken as a minimum reactivity.

3.5.2 Degradation in water

A value for $kdeg_{water}$ may be obtained by means of the scaling procedure proposed by Struijs and Van den Berg (1993). This procedure assumes that the pseudo first order rate constant for degradation in water is proportional to the concentration of bacteria in the water. The degradation rate is corrected by an empirical relationship which changes the degradation rate 50% per 10 degrees[e]. The rate constant for surface water may be deduced from the rate constant observed in laboratory tests at 20 °C by scaling:

---

[e] : the degradation rates in the EUSES-system are not temperature dependent. For a simulation of EUSES with SimpleBox 2.0 the kdeg-values of EUSES must be entered.

$$kdeg_{water\,i[S]} = kdeg_{test}.(1.072^{TEMPERATURE_{[S]}-293}).\frac{BACT_{water}}{BACT_{test}}.FRdisslvd_{water\,i[S]} \qquad \textbf{139}$$

with

$kdeg_{water\,i[S]}$:	pseudo first order degradation rate constant in water i at scale S[s^{-1}] *(D)*
$FRdisslvd_{water(i)\,[S]}$:	dissolved fraction of water column i at scale S [-] *(A)*
$kdeg_{test}$:	pseudo first order degradation rate constant in laboratory test [s^{-1}] *(A)*
$BACT_{water}$:	concentration of bacteria in the water compartment [$cfu.ml_{water}^{-1}$] *(A)*
$BACT_{test}$:	concentration of bacteria in the laboratory test water [$cfu.ml_{test\ water}^{-1}$]*(A)*
$TEMPERATURE_{[S]}$:	temperature at scale S [K] *(A)*

It is further assumed in this procedure that a pseudo first order degradation rate constant may be obtained by extrapolation from the results of standard screening tests for ready biodegradability in water:

$$kdeg_{test} = \frac{ln\,2}{5}\ d^{-1}\ \ if\ \ PASSreadytest = y$$

$$kdeg_{test} = \frac{ln\,2}{1000}\ d^{-1}\ \ if\ \ PASSreadytest = n \qquad \textbf{140}$$

with

$kdeg_{test}$:	pseudo first order degradation rate constant in laboratory test [d^{-1}] *(A)*
$PASSreadytest$:	the result of a standard screening test; expressed as "y" if the chemical is "readily biodegradable" and "n" if the chemical is not "readily biodegradable"

For derivation of the degradation rate in water, the following default-values may be considered:

$$BACT_{test} = 4.10^{4}\,cfu.ml^{-1} \qquad \textbf{141}$$

with

$BACT_{test}$:	concentration of bacteria in the laboratory test water [$cfu.ml_{test\ water}^{-1}$] *(A)*

$$BACT_{water} = 4.10^{4}\,cfu.ml^{-1} \qquad \textbf{142}$$

with

$BACT_{water}$:	concentration of bacteria in the water compartment [$cfu.ml_{water}^{-1}$] *(A)*

3.5.3 Degradation in sediment

A value for $kdeg_{sed}$ may be obtained by means of the scaling procedure proposed by Struijs and Van den Berg (1993). The degradation rate is corrected by an empirical relationship which changes the degradation rate 50% per 10 degrees. As with degradation in water, it is assumed that the degradation rate is related to the degradation rate constant observed in standard tests for (aerobic) ready degradability in water. Degradation in sediment is treated as disappearance from the water phase of the sediment. The concentration of bacteria, present in the pore water or at the surface of the solid phase (or both), in the sediment compartment is expressed on a pore water volume basis:

$$kdeg_{sed\,i[S]} = kdeg_{test}.(1.072^{TEMPERATURE_{[S]}-293}).\frac{BACT_{sed\,i[S]}}{BACT_{test}}.FRdisslvd_{sed\,i[S]} \qquad \mathbf{143}$$

with

$kdeg_{sed\,i[S]}$:	pseudo first order degradation rate constant in sediment [s^{-1}] *(D)*
$kdeg_{test}$:	pseudo first order degradation rate constant in laboratory test [s^{-1}] *(A)*
$BACT_{sed\,i[S]}$:	concentration of bacteria in sediment, expressed on a pore water basis [$cfu.ml_{pore\ water}^{-1}$] *(A)*
$BACT_{test}$:	concentration of bacteria in the laboratory test water [$cfu.ml_{test\ water}^{-1}$]*(A)*
$Frdisslvd_{sed\,i[S]}$:	fraction of the chemical in sediment, present in the pore water phase of the sediment [-]
$TEMPERATURE_{[S]}$:	temperature at scale S [K] *(A)*

For derivation of the degradation rate in sediment, a value for $BACT_{sed}$ may be derived from:

$$BACT_{sed\ i[S]} = \frac{1.8.10^{9}}{FRwater_{sed\ i[S]}} \qquad \mathbf{144}$$

with

$BACT_{sed\,i[S]}$:	concentration of bacteria in sediment i, expressed on a pore water basis at scale S [$cfu.ml_{pore\ water}^{-1}$] *(A)*
$1.8 \cdot 10^{9}$:	concentration of bacteria reported in aerobic sediment [$cfu.cm_{sed}^{-3}$]
$Frwater_{sed\,i[S]}$:	volume fraction of the water phase of the sediment i at scale S [-] *(A)*

It should be noted that this procedure to derive a degradation rate constant in sediment applies only to aerobic sediments and that generally only the top few millimeters of the sediment are aerobic.

3.5.4 Degradation in soil

A value for $kdeg_{soil}$ may be obtained by means of the scaling procedure proposed by Struijs and Van den Berg (1993), in analogy with the derivation of $kdeg_{sed}$. The degradation rate is corrected by an empirical relationship which changes the degradation rate 50% per 10 degrees.

$$kdeg_{soil\,i[S]} = \frac{kdeg_{water\,1[S]}.(1.072^{TEMPERATURE_{[S]}-293})}{FRdisslvd_{water\,1[S]}}.\frac{BACT_{soilwater}}{BACT_{water}}.FRdisslvd_{soil\,i[S]} \qquad \mathbf{145}$$

with

$kdeg_{soil\,i[S]}$: pseudo first order degradation rate constant in soil i at scale S [s^{-1}] *(D)*
$kdeg_{water\,i[S]}$: pseudo first order degradation rate constant in water i at scale S [s^{-1}] *(D)*
$BACT_{soil}$: concentration of bacteria in soil, expressed on a pore water basis [$cfu.ml_{pore\,water}^{-1}$] *(A)*
$FRdisslvd_{soil\,i[S]}$: fraction of the chemical in soil i at scale S, present in the pore water phase [-]
$FRdisslvd_{water\,i[S]}$: dissolved fraction of water column i at scale S [-] *(A)*
$BACT_{water}$: concentration of bacteria in the water compartment [$cfu.ml_{water}^{-1}$] *(A)*
$TEMPERATURE_{[S]}$: temperature at scale S [K] *(A)*

For derivation of the degradation rate in soil, a value for $BACT_{soil}$ may be derived from Struijs and Van den Berg (1993):

$$BACT_{soil} = \frac{10^6/1.4}{FRwater_{soil\,i[S]}} \qquad \mathbf{146}$$

with

$BACT_{soil}$: concentration of bacteria in soil, expressed on a pore water basis [$cfu.ml_{pore\,water}^{-1}$] *(A)*
10^6 : concentration of bacteria reported in aerobic soil [$cfu.g_{soil}$]
1.4 : bulk density of soil [$kg_{soil}.m_{soil}^{-3}$] *(A)*
$FRwater_{soil\,i[S]}$: volume fraction water of soil i at scale S [-] *(A)*

It should be noted that this procedure for deriving a degradation rate constant in soil applies only to aerobic systems.

3.6 Parameters that describe the intermedia transfer processes

3.6.1 Deposition

Values for the deposition mass transfer coefficients $DRYDEP_{aerosol}$ and $WASHOUT$ may be obtained by means of:

$$DRYDEP_{aerosol[S]} = AEROSOLDEPRATE_{[S]}.FRass_{aerosol[S]} \qquad \mathbf{147}$$

with

$DRYDEP_{aerosol[S]}$:	mass transfer coefficient for dry deposition of aerosol-associated chemical at scale S [$m_{air}.s^{-1}$] *(D)*
$AEROSOLDEPRATE_{[S]}$:	deposition velocity of the aerosol particles at scale S with which the chemical is associated [$m.s^{-1}$] *(A)*
$FRass_{aerosol[S]}$:	fraction of the chemical in air that is associated with aerosol particles at scale S [-] *(A)*

$$WASHOUT_{[S]} = RAINRATE_{[S]}.SCAVratio_{[S]} \qquad \mathbf{148}$$

with

$WASHOUT_{[S]}$:	mass transfer coefficient for wet atmospheric deposition at scale S [$m_{air}.s^{-1}$] *(D)*
$RAINRATE_{[S]}$:	rate of wet precipitation at scale S [$m_{rain}.s^{-1}$] *(A)*
$SCAVratio_{[S]}$:	scavenging ratio (quotient of the total concentration in rainwater and the total concentration in air) of the chemical at scale S [-] *(A)*

3.6.2 Gas absorption and volatization

Values for the overall mass transfer coefficients for gas absorption and 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 following equations may be used:

$$GASABS_{water\,i[S]} = \frac{kaw_{air[S]}.kaw_{water[S]}}{kaw_{air[S]}.K_{air\text{-}water[S]} + kaw_{water[S]}}.(1 - FRass_{aerosol[S]}) \qquad \mathbf{149}$$

with

$GASABS_{water\,i[S]}$:	overall mass transfer coefficient for gas absorption across the air-water interface, referenced to air at scale S [$m_{air}.s^{-1}$] *(D)*
$kaw_{air[S]}$:	partial mass transfer coefficient at the air-side of the air-water interface at scale S [$m_{air}.s^{-1}$] *(A)*
$kaw_{water[S]}$:	partial mass transfer coefficient at the water-side of the air-water interface at scale S [$m_{water}.s^{-1}$] *(A)*

$K_{air\text{-}water[S]}$: air-water equilibrium distribution constant at scale S [$m_{water}^{3}.m_{air}^{-3}$] *(A)*
$FRass_{aerosol[S]}$: fraction of the chemical in air that is associated with aerosol particles at scale S [-] *(A)*

$$GASABS_{soil\,i[S]} = \frac{kasl_{air[S]}\cdot kasl_{soilair[S]} + kasl_{air[S]}\cdot kasl_{soilwater[S]}/K_{air\text{-}water[S]}}{kasl_{air[S]} + kasl_{soilair[S]} + kasl_{soilwater[S]}/K_{air\text{-}water[S]}} \cdot (1 - FRass_{aerosol[S]}) \qquad \mathbf{150}$$

with

$GASABS_{soil\,i[S]}$: overall mass transfer coefficient for gas absorption across the air-soil interface, referenced to air at scale S [$m_{air}.s^{-1}$] *(D)*
$kasl_{air[S]}$: partial mass transfer coefficient at the air-side of the air-soil interface at scale S [$m_{air}.s^{-1}$] *(A)*
$kasl_{spoilair[S]}$: partial mass transfer coefficient at the soilair-side of the air-soil interface at scale S [$m_{air}.s^{-1}$] *(A)*
$kasl_{spoilwater[S]}$: partial mass transfer coefficient at the soilwater-side of the air-soil interface at scale S [$m_{water}.s^{-1}$] *(A)*
$K_{air\text{-}water[S]}$: air-water equilibrium distribution constant at scale S [$m_{water}^{3}.m_{air}^{-3}$] *(A)*
$FRass_{aerosol[S]}$: fraction of the chemical in air that is associated with aerosol particles at scale S [-] *(A)*

And, since the quotient of the mass transfer coefficients for gas absorption and volatilization is equal to the volume-based intermedia partition coefficient:

$$VOLAT_{water\,i[S]} = \frac{GASABS_{water\,i[S]}}{1 - FRass_{aerosol[S]}} \cdot K_{air\text{-}water[S]} \cdot FRdisslvd_{water\,i[S]} \qquad \mathbf{151}$$

with

$VOLAT_{water\,i[S]}$: overall mass transfer coefficient for volatilization across the air-water interface, referenced to water at scale S *(D)*
$GASABS_{water\,i[S]}$: overall mass transfer coefficient for gas absorption across the air-water interface, referenced to air at scale S [$m_{air}.s^{-1}$] *(D)*
$FRass_{aerosol[S]}$: fraction of the chemical in air that is associated with aerosol particles at scale S [-] *(A)*
$K_{air\text{-}water[S]}$: air-water equilibrium distribution constant at scale S [$m_{water}^{3}.m_{air}^{-3}$] *(A)*
$FRdisslvd_{water(i)\,[S]}$: dissolved fraction of water column i at scale S [-] *(A)*

$$VOLAT_{soil\,i[S]} = \frac{GASABS_{soil\,i[S]}}{1 - FRass_{aerosol[S]}} \cdot \frac{K_{air\text{-}water[S]}}{K_{soil\,i\text{-}water[S]}} \qquad \mathbf{152}$$

with

$VOLAT_{soil\,i[S]}$: overall mass transfer coefficient for volatilization across the air-soil interface, referenced to soil at scale S [$m_{soil}.s^{-1}$] *(D)*

$GASABS_{soil\,i[S]}$:	overall mass transfer coefficient for gas absorption across the air-soil interface, referenced to air at scale S [$m_{air}.s^{-1}$] *(D)*
$FRass_{aerosol[S]}$:	fraction of the chemical in air that is associated with aerosol particles at scale S [-] *(A)*
$K_{air\text{-}water[S]}$:	air-water equilibrium distribution constant at scale S [$m_{water}^{3}.m_{air}^{-3}$] *(A)*
$K_{soil\,i\text{-}water[S]}$:	soil i-water equilibrium distribution constant at scale S [$m_{water}^{3}.m_{soil}^{-3}$] *(A)*

A value for the partial mass transfer coefficient at the air-side of the air-water interface may be derived from the equation (Schwarzenbach *et al.,* 1993):

$$kaw_{air} = 0.01 \cdot (0.3 + 0.2 \cdot WINDSPEED_{[S]}) \cdot (\frac{0.018}{MOL\ WEIGHT})^{0.4355} \qquad \mathbf{153}$$

with

kaw_{air} :	partial mass transfer coefficient at the air side of the air-water interface [$m_{air}.s^{-1}$] *(A)*
$WINDSPEED_{[S]}$:	average windspeed at 10 m above the surface at scale S [$m.s^{-1}$] *(A)*
$MOL\ WEIGHT$:	molecular weight of the chemical [$kg.mol^{-1}$] *(A)*
0.018 :	molecular weight of water *(C)*

For the partial mass transfer coefficient at the water side of the air-water interface, the equation of (Schwarzenbach *et al.,* 1993) may be used:

$$kaw_{water} = 0.01 \cdot (0.004 + 0.00004 \cdot WINDSPEED_{[S]}) \cdot (\frac{0.032}{MOLWEIGHT})^{0.4047} \qquad \mathbf{154}$$

with

kaw_{water} :	partial mass transfer coefficient at the water-side of the air-water interface [$m_{water}.s^{-1}$] *(A)*
$WINDSPEED_{[S]}$:	average windspeed at 10 m above the surface at scale S [$m.s^{-1}$] *(A)*
$MOL\ WEIGHT$:	molecular weight of the chemical [$kg.mol^{-1}$] *(A)*

The partial mass transfer coefficients at the air-soil interface may be derived using the reasoning suggested by Mackay *et al.* (1992).
According to this reasoning, the value for the air side may be taken equal to the value at the air-water interface:

$$kasl_{air} = kaw_{air} \qquad \mathbf{155}$$

with

$kasl_{air}$:	partial mass transfer coefficient at the air-side of the air-soil interface [$m_{air}.s^{-1}$] *(A)*
kaw_{air} :	partial mass transfer coefficient at the air-side of the air-water interface [$m_{air}.s^{-1}$] *(A)*

Mass transfer in the soil air phase is treated as molecular diffusion in the gas phase of a porous solid medium, characterized by an effective diffusivity of 10^{-3} $m^2.hr^{-1}$ and a diffusion path length of 5 cm. This leads to:

$$kasl_{soilair} = 5.56.10^{-6}\, m.s^{-1} \qquad \mathbf{156}$$

with

$kasl_{soilair}$: partial mass transfer coefficient at the soilair-side of the air-soil interface $[m_{air}.s^{-1}]$ *(A)*

Mass transfer in the soil water phase is similarly treated as molecular diffusion in the water phase of a porous solid medium, characterized by an effective diffusivity of 10^{-7} $m^2.hr^{-1}$ and a diffusion path length of 2 cm, leading to:

$$kasl_{soilwater} = 5.56.10^{-10}\, m.s^{-1} \qquad \mathbf{157}$$

with

$kasl_{soilwater}$: partial mass transfer coefficient at the soilwater-side of the air-soil interface $[m_{water}.s^{-1}]$ *(A)*

3.6.3 Water/sediment exchange

Values for the overall mass transfer coefficients for direct adsorption and desorption across the sediment-water interface may be obtained using the two-film resistance model, in analogy to the description of mass transfer across the air-water and air-soil interfaces.

$$ADSORB_{sed\, i[S]} = \frac{kws_{water} \cdot kws_{sed}}{kws_{water} + kws_{sed}} . FRdisslvd_{water\, i[S]} \qquad \mathbf{158}$$

with

$ADSORB_{sed\, i[S]}$: overall mass transfer coefficient for adsorption across the sedi ment-water interface, referenced to water at scale S $[m_{water}.s^{-1}]$ *(D)*

kws_{water} : partial mass transfer coefficient at the water side of the sediment-water interface $[m_{water}.s^{-1}]$ *(A)*

kws_{sed} : partial mass transfer coefficient at the pore water side of the sediment-water interface $[m_{pore\ water}.s^{-1}]$ *(A)*

$FRdisslvd_{water(i)\, [S]}$: dissolved fraction of water column i at scale S [-] *(A)*

And, since the quotient of the mass transfer coefficients for adsorption and desorption is equal to the volume-based sediment-water partition coefficient:

$$DESORB_{sed\, i[S]} = \frac{ADSORB_{sed\, i[S]}}{K_{sed\text{-}water\, i[S]}} . FRdisslvd_{water\, i[S]} \qquad \mathbf{159}$$

with

$DESORB_{sed\ i[s]}$:	overall mass transfer coefficient for desorption across the sediment-water interface, referenced to sediment i at scale S [$m_{sed}.s^{-1}$] *(D)*
$ADSORB_{sed\ i[S]}$:	overall mass transfer coefficient for adsorption across the sediment-water interface, referenced to water i at scale S [$m_{water}.s^{-1}$] *(D)*
$K_{sed\text{-}water\ i[S]}$	sediment-water equilibrium distribution constant at scale S [$mol.m_{sed}^{-3}/mol.m_{water}^{-3}$] *(A)*
$FRdisslvd_{water(i)\ [S]}$:	dissolved fraction of water column i at scale S [-] *(A)*

As a value for the mass transfer coefficient at the water-side of the sediment-water interface, the following fixed value (Mackay *et al.*, 1985) may serve:

$$kws_{water} = 2.778.10^{-6} m.s^{-1} \qquad \mathbf{160}$$

with

kws_{water} :	partial mass transfer coefficient at the water-side of the sediment-water interface [$m_{water}.s^{-1}$] *(A)*

Mass transfer at the pore water side of the sediment-water interface is treated, according to Mackay's reasoning (Mackay *et al.*, 1992), as molecular diffusion in the aqueous phase of a porous solid material, characterized by an effective diffusivity of $2\cdot10^{-6}$ $m^2.hr^{-1}$ and a diffusion path length of 2 cm. This leads to:

$$kws_{sed} = 2.778.10^{-8} m.s^{-1} \qquad \mathbf{161}$$

with

kws_{sed} :	partial mass transfer coefficient at the pore water side of the sediment-water interface [$m_{porewater}.s^{-1}$] *(A)*

3.6.4 Soil to water transfer

The apparent mass flow of the chemical from the top layer to the water compartiment is characterized by:

$$RUNOFF_{soil\ i[S]} = \frac{FRACrun_{soil\ i[S]}.RAINrate_{[S]}}{K_{soil\ i\text{-}water[S]}} + EROSION_{soil\ i[S]}\cdot\left(\frac{FRACrun_{soil\ i-water\ i[S]}}{FRACrun_{soil\ i-water\ 1[S]} + FRACrun_{soil\ i-water\ 1[S]}}\right) \qquad \mathbf{162}$$

with

$RUNOFF_{soil\ i[s]}$:	mass transfer coefficient for run-off from soil i at scale S [$m_{soil}.s^{-1}$] *(D)*
$FRACrun_{soil\ i\text{-}water\ i[s]}$:	fraction of rain water that runs off from soil i to water i at scale S [-] *(A)*
$RAINRATE_{[S]}$:	rate of wet precipitation at scale S [$m_{rain}.s^{-1}$] *(A)*
$K_{soil\ i\text{-}water[s]}$:	soil i-water equilibrium distribution constant at scale S [$m_{water}^3.m_{solid}^{-3}$] *(A)*

$EROSION_{soil\,i[S]}$:	rate at which soil is washed from soil i into surface water at scale S [$m_{soil}.s^{-1}$] *(A)*

3.6.5 Removal from the system

The apparent mass flow of the chemical from the top layer to the deeper sediment is characterized by:

$$BURIAL_{sed\,i[S]} = NETsedrate_{i[S]} \tag{163}$$

with

$BURIAL_{sed\,i[S]}$:	sediment burial rate for water column i at scale S [$m_{sed}.s^{-1}$] *(D)*
$NETsedrate_{i[S]}$:	net sedimentation rate for sediment/water i at scale S [$m_{sed}.s^{-1}$] *(D)*

$$LEACH_{soil\,i[S]} = \frac{FRACinf_{soil\,i[S]} . RAINrate_{[S]}}{K_{soil\,i\text{-}water[S]}} \tag{164}$$

with

$LEACH_{soil\,i[S]}$:	mass transfer coefficient for leaching from soil i at scale S [$m_{soil}.s^{-1}$] *(D)*
$FRACinf_{soil\,i[S]}$:	fraction of rain water that infiltrates into soil i at scale S [-] *(A)*
$RAINRATE_{[S]}$:	rate of wet precipitation at scale S [$m_{rain}.s^{-1}$] *(A)*
$K_{soil\,i\text{-}water[S]}$:	soil i-water equilibrium distribution constant at scale S [$m_{water}^{3}.m_{solid}^{-3}$] *(A)*

3.7 The air compartment

3.7.1 Mass balance

The mass balance equation for the air compartment is:

$$\begin{aligned} V_{air[S]} . \frac{dC_{air[S]}}{dt} = {} & + EMIS_{air[S]} + IMP_{air[S]} - EXP_{air[S]} \\ & - V_{air[S]} . DEG_{air[S]} . C_{air[S]} - \sum DEP_{water\,i[S]} . C_{air[S]} \\ & - \sum DEP_{soil\,i[S]} . C_{air[S]} - \sum DEP_{veg\,i[S]} . C_{air[S]} - \sum XCH_{air\text{-}water\,i[S]} . C_{air[S]} \\ & - \sum XCH_{air\text{-}soil\,i} . C_{air} - \sum XCH_{air\text{-}veg\,i[S]} . C_{air[S]} + \sum XCH_{water\,i\text{-}air[S]} . C_{water\,i[S]} \\ & + \sum XCH_{soil\,i\text{-}air[S]} . C_{soil\,i[S]} + \sum XCH_{veg\,i\text{-}air[S]} . C_{veg\,i[S]} \end{aligned} \tag{165}$$

with

$V_{air[S]}$:	volume of the air compartment of scale S [m_{air}^{3}] *(I)*

$C_{air[S]}$:	total concentration in air at scale S (gas phase + aerosol phase + rain water phase) [mol.m$_{air}^{-3}$] *(S)*
t :	time [s] *(S)*
$EMIS_{air[S]}$:	emission mass flow into the air compartment at scale S [mol.s^{-1}] *(I)*
$IMP_{air[S]}$:	import mass flow into air at scale S [mol.s^{-1}] *(I)*
$FLOW_{air[S]}$:	refreshment flow through the air compartment at scale S [m$_{air}^{3}$.s^{-1}] *(I)*
$DEG_{air[S]}$:	pseudo first order transformation rate constant in air at scale S [s^{-1}] *(I)*
$DEP_{water\ i[S]}$:	transport coefficient for atmospheric deposition (wet and dry) to water i at scale S [m$_{air}^{3}$.s^{-1}] *(I)*
$DEP_{soil\ i[S]}$:	transport coefficient for atmospheric deposition (wet and dry) to soil i at scale S [m$_{air}^{3}$.s^{-1}] *(I)*
$DEP_{veg\ i[S]}$:	transport coefficient for atmospheric deposition (wet and dry) to vegetation i at scale S [m$_{air}^{3}$.s^{-1}] *(I)*
$XCH_{air\text{-}water\ i\ [S]}$:	transport coefficient gas absorption to water i at scale S [m$_{air}^{3}$.s^{-1}] *(I)*
$XCH_{air\text{-}soil\ i[S]}$:	transport coefficient gas absorption to soil i at scale S [m$_{air}^{3}$.s^{-1}] *(I)*
$XCH_{air\text{-}veg\ i[S]}$:	transport coefficient gas absorption to vegetation i at scale S [m$_{air}^{3}$.s^{-1}]*(I)*
$XCH_{water\ i\ \text{-}air[S]}$:	transport coefficient volatilization from water i at scale S [m$_{water}^{3}$.s^{-1}]*(I)*
$XCH_{veg\ i\ \text{-}air[S]}$:	transport coefficient volatilization from vegetation i at scale S [m$_{water}^{3}$.s^{-1}] *(I)*
$XCH_{soil\ i\text{-}air[S]}$:	transport coefficient volatilization from soil i at scale S [m$_{soil}^{3}$.s^{-1}] *(I)*
$C_{water\ i[S]}$:	concentration in water i (dissolved) at scale S [mol.m$_{water}^{-3}$] *(S)*
$C_{soil\ i[S]}$:	concentration in soil i at scale S [mol.m$_{soil}^{-3}$] *(S)*
$C_{veg\ i[S]}$:	concentration in vegetation i at scale S [mol.m$_{water}^{-3}$] *(S)*

3.7.2 Emissions

The emission mass flow to air is obtained from:

$$EMIS_{air[S]} = Edirect_{air[S]} + Estp_{air[S]} \qquad \textbf{166}$$

with

$EMIS_{air[S]}$:	total emission mass flow into the air compartment of scale S [mol.s^{-1}] *(I)*
$Edirect_{air[S]}$:	sum of all direct emissions to the air compartment of scale S [mol.s^{-1}] *(D)*
$Estp_{air[S]}$:	indirect emission to air of scale S, resulting from volatilization during sewage treatment [mol.s^{-1}] *(D)*

$Edirect_{air}$ may be derived by means of:

$$Edirect_{air[S]} = PRODUCTION_{[S]}.EMISfact_{air[S]} \qquad \textbf{167}$$

with

$Edirect_{air[S]}$:	sum of all direct emissions to the air compartment of scale S [mol.s^{-1}]*(D)*
$PRODUCTION_{[S]}$:	total amount produced or imported in scale S [mol.s^{-1}] *(A)*
$EMISfact_{air[S]}$:	emission factor for air: the fraction of the production volume that is released to the air compartment of scale S [-] *(A)*

The following defaults may be considered:

$$EMISfact_{air[S]} \;=\; 0.1\% \qquad \textbf{168}$$

with

$EMISfact_{air[S]}$: emission factor for air: the fraction of the production volume that is released to the air compartment of scale S [-] *(A)*

as a starting point.

3.7.3 *Import*

The import mass flow into air is obtained from:

$$IMP_{air} \;=\; IMPORT_{air} \qquad \textbf{169}$$

with

IMP_{air} : import mass flow into the air compartment [mol.s^{-1}] *(I)*
$IMPORT_{air}$: transport of the chemical with air (wind) across the system boundaries [mol.s^{-1}] *(D)*

A value for $IMPORT_{air}$ for the different scales may be derived as follows:

$$IMPORT_{air[R]} \;=\; FLOW_{air[C]-air[R]} \cdot C_{air[C]} \qquad \textbf{170}$$

with

$IMPORT_{air[R]}$: transport of the chemical with air (wind) across the regional system boundaries [mol.s^{-1}] *(D)*
$FLOW_{air[C]-air[R]}$: rate of air flow from the continental scale to the regional scale [m$_{air}^{3}$.s^{-1}] *(A)*
$C_{air[C]}$: concentration of the chemical in the air compartment of the continental scale [mol.m$_{air}^{-3}$] *(A)*

$$IMPORT_{air[C]} \;=\; FLOW_{air[R]-air[C]} \cdot C_{air[R]} + FLOW_{air[M]-air[C]} \cdot C_{air[M]} \qquad \textbf{171}$$

with

$IMPORT_{air[C]}$: transport of the chemical with air (wind) across the continental system boundaries [mol.s^{-1}] *(D)*
$FLOW_{air[R]-air[C]}$: rate of air flow from the regional scale to the continental scale [m$_{air}^{3}$.s^{-1}] *(A)*

$C_{air[R]}$: concentration of the chemical in the air compartment of the regional scale $[\mathrm{mol.m_{air}^{-3}}]$ *(A)*

$FLOW_{air[M]-air[C]}$: rate of air flow from the moderate scale to the continental scale $[\mathrm{m_{air}^{3}.s^{-1}}]$ *(A)*

$C_{air[M]}$: concentration of the chemical in the air compartment of the moderate scale $[\mathrm{mol.m_{air}^{-3}}]$ *(A)*

$$IMPORT_{air[M]} = FLOW_{air[C]-air[M]} \cdot C_{air[C]} + FLOW_{air[A]-air[M]} \cdot C_{air[A]} + FLOW_{air[T]-air[M]} \cdot C_{air[T]} \qquad \mathbf{172}$$

with

$IMPORT_{air[M]}$: transport of the chemical with air (wind) across the moderate system boundaries $[\mathrm{mol.s^{-1}}]$ *(D)*

$FLOW_{air[C]-air[M]}$: rate of air flow from the continental scale to the moderate scale $[\mathrm{m_{air}^{3}.s^{-1}}]$ *(A)*

$C_{air[C]}$: concentration of the chemical in the air compartment of the continental scale $[\mathrm{mol.m_{air}^{-3}}]$ *(A)*

$FLOW_{air[A]-air[M]}$: rate of air flow from the arctic scale to the moderate scale $[\mathrm{m_{air}^{3}.s^{-1}}]$ *(A)*

$C_{air[A]}$: concentration of the chemical in the air compartment of the arctic scale $[\mathrm{mol.m_{air}^{-3}}]$ *(A)*

$FLOW_{air[T]-air[M]}$: rate of air flow from the tropic scale to the moderate scale $[\mathrm{m_{air}^{3}.s^{-1}}]$ *(A)*

$C_{air[T]}$: concentration of the chemical in the air compartment of the tropic scale $[\mathrm{mol.m_{air}^{-3}}]$ *(A)*

$$IMPORT_{air[A]} = FLOW_{air[M]-air[A]} \cdot C_{air[M]} \qquad \mathbf{173}$$

with

$IMPORT_{air[A]}$: transport of the chemical with air (wind) across the arctic system boundaries $[\mathrm{mol.s^{-1}}]$ *(D)*

$FLOW_{air[M]-air[A]}$: rate of air flow from the moderate scale to the arctic scale $[\mathrm{m_{air}^{3}.s^{-1}}]$ *(A)*

$C_{air[M]}$: concentration of the chemical in the air compartment of the moderate scale $[\mathrm{mol.m_{air}^{-3}}]$ *(A)*

$$IMPORT_{air[T]} = FLOW_{air[M]-air[T]} \cdot C_{air[M]} \qquad \mathbf{174}$$

with

$IMPORT_{air[T]}$: transport of the chemical with air (wind) across the tropic system boundaries $[\mathrm{mol.s^{-1}}]$ *(D)*

$FLOW_{air[M]-air[T]}$: rate of air flow from the moderate scale to the tropic scale $[\mathrm{m_{air}^{3}.s^{-1}}]$ *(A)*

$C_{air[M]}$: concentration of the chemical in the air compartment of the moderate scale $[\mathrm{mol.m_{air}^{-3}}]$ *(A)*

3.7.4 Export

The export mass flow into air is obtained from:

$$EXP_{air} = EXPORT_{air} \tag{175}$$

with

EXP_{air} :	export mass flow into the air compartment [mol.s^{-1}] *(I)*
$EXPORT_{air}$:	transport of the chemical with air (wind) across the system boundaries [mol.s^{-1}] *(D)*

A value for $EXPORT_{air}$ for the different scales may be derived as follows:

$$EXPORT_{air[R]} = FLOW_{air[R]-air[C]} \cdot C_{air[R]} \tag{176}$$

with

$EXPORT_{air[R]}$:	transport of the chemical with air (wind) across the regional system boundaries [mol.s^{-1}] *(D)*
$FLOW_{air[R]-air[C]}$:	rate of air flow from the regional scale to the continental scale [m$_{air}^{3}$.s^{-1}] *(A)*
$C_{air[R]}$:	concentration of the chemical in the air compartment of the regional scale [mol.m$_{air}^{-3}$] *(A)*

$$EXPORT_{air[C]} = FLOW_{air[C]-air[R]} \cdot C_{air[C]} + FLOW_{air[C]-air[M]} \cdot C_{air[C]} \tag{177}$$

with

$EXPORT_{air[C]}$:	transport of the chemical with air (wind) across the continental system boundaries [mol.s^{-1}] *(D)*
$FLOW_{air[C]-air[R]}$:	rate of air flow from the continental scale to the regional scale [m$_{air}^{3}$.s^{-1}] *(A)*
$FLOW_{air[C]-air[M]}$:	rate of air flow from the continental scale to the moderate scale [m$_{air}^{3}$.s^{-1}] *(A)*
$C_{air[C]}$:	concentration of the chemical in the air compartment of the continental scale [mol.m$_{air}^{-3}$] *(A)*

$$\begin{aligned} EXPORT_{air[M]} = {} & FLOW_{air[M]-air[C]} \cdot C_{air[M]} + FLOW_{air[M]-air[A]} \cdot C_{air[M]} \\ & + FLOW_{air[M]-air[T]} \cdot C_{air[M]} \end{aligned} \tag{178}$$

with

$EXPORT_{air[M]}$:	transport of the chemical with air (wind) across the moderate system boundaries [mol.s^{-1}] *(D)*
$FLOW_{air[M]-air[C]}$:	rate of air flow from the moderate scale to the continental scale [m$_{air}^{3}$.s^{-1}] *(A)*
$FLOW_{air[M]-air[A]}$:	rate of air flow from the moderate scale to the arctic scale [m$_{air}^{3}$.s^{-1}] *(A)*
$FLOW_{air[M]-air[T]}$:	rate of air flow from the moderate scale to the tropic scale [m$_{air}^{3}$.s^{-1}] *(A)*
$C_{air[M]}$:	concentration of the chemical in the air compartment of the moderate scale [mol.m$_{air}^{-3}$] *(A)*

$$EXPORT_{air[A]} = FLOW_{air[A]-air[M]} \cdot C_{air[A]} \tag{179}$$

with

$EXPORT_{air[A]}$: transport of the chemical with air (wind) across the arctic system boundaries [mol.s^{-1}] *(D)*

$FLOW_{air[A]-air[M]}$: rate of air flow from the arctic scale to the moderate scale [m$_{air}^{3}$.s^{-1}] *(A)*

$C_{air[A]}$: concentration of the chemical in the air compartment of the arctic scale [mol.m$_{air}^{-3}$] *(A)*

$$EXPORT_{air[T]} = FLOW_{air[T]-air[M]} \cdot C_{air[T]} \tag{180}$$

with

$EXPORT_{air[T]}$: transport of the chemical with air (wind) across the tropic system boundaries [mol.s^{-1}] *(D)*

$FLOW_{air[T]-air[M]}$: rate of air flow from the tropic scale to the moderate scale [m$_{air}^{3}$.s^{-1}]*(A)*

$C_{air[T]}$: concentration of the chemical in the air compartment of the tropic scale [mol.m$_{air}^{-3}$] *(A)*

3.7.5 Degradation

The apparent degradation mass flow from air of the different scales is obtained from:

$$DEGRD_{air[S]} = V_{air[S]} \cdot DEG_{air[S]} \cdot C_{air[S]} \tag{181}$$

with

$DEGRD_{air[S]}$: degradation mass flow from the air compartment of scale S [mol.s^{-1}]*(I)*

$V_{air[S]}$: volume of the air compartment of scale S [m^{3}] *(I)*

$DEG_{air[S]}$: pseudo first order transformation rate constant in air at scale S [s^{-1}] *(I)*

$C_{air[S]}$: total concentration in air (gas phase + aerosol phase + rain water phase) at scale [mol.m$_{air}^{-3}$] *(S)*

$$DEG_{air[S]} = kdeg_{air[S]} \tag{182}$$

with

$DEG_{air[S]}$: pseudo first order transformation rate constant in air at scale S [s^{-1}] *(I)*

$kdeg_{air[S]}$: pseudo first order transformation rate constant in air at scale S [s^{-1}] *(D)*

A value for $kdeg_{air}$ is obtained from the equation 137 paragraph 3.5.1.

3.7.6 Advective transport

Advective transport from air to water and soil takes place by wet and dry atmospheric deposition. The deposition mass flows are obtained from:

$$ADV_{air\text{-}water\,i[S]} = DEP_{water\,i[S]} \cdot C_{air[S]} \qquad \mathbf{183}$$

with

$ADV_{air\text{-}water\,i[S]}$: advective mass flow from air to water i at scale S by atmospheric deposition [$mol.s^{-1}$] *(I)*

$DEP_{water\,i[S]}$: transport coefficient for atmospheric deposition (wet and dry) to water i at scale S [$m_{air}^{3}.s^{-1}$] *(I)*

$C_{air[S]}$: total concentration in air (gas phase + aerosol phase + rain water phase) at scale S [$mol.m_{air}^{-3}$] *(S)*

$$ADV_{air\text{-}soil\,i[S]} = DEP_{soil\,i[S]} \cdot C_{air[S]} \qquad \mathbf{184}$$

with

$ADV_{soil\,i[S]}$: advective mass flow from air to soil i at scale S by atmospheric deposition [$mol.s^{-1}$] *(I)*

$DEP_{soil\,i[S]}$: transport coefficient for atmospheric deposition (wet and dry) to soil i at scale S [$m_{air}^{3}.s^{-1}$] *(I)*

$C_{air[S]}$: total concentration in air (gas phase + aerosol phase + rain water phase) at scale S [$mol.m_{air}^{-3}$] *(S)*

$$DEP_{water\,i[S]} = (DRYDEP_{aerosol[S]} + WASHOUT_{[S]}).SYSTEMAREA_{[S]} \cdot AREAFRAC_{water\,i[S]} \qquad \mathbf{185}$$

with

$DEP_{water\,i[S]}$: transport coefficient for atmospheric deposition (wet and dry) to water i at scale S [$m_{air}^{3}.s^{-1}$] *(I)*

$DRYDEP_{aerosol[S]}$: mass transfer coefficient for dry deposition of aerosol-associated chemical at scale S [$m_{air}.s^{-1}$] *(D)*

$WASHOUT_{[S]}$: mass transfer coefficient for wet atmospheric deposition at scale S [$m_{air}.s^{-1}$] *(D)*

$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*

$AREAFRAC_{water\,i[S]}$: fraction of scale S that is water [-] *(D)*

$$DEP_{soil\,i[S]} = (DRYDEP_{aerosol[S]} + WASHOUT_{[S]}).SYSTEMAREA_{[S]} \cdot AREAFRAC_{soil\,i[S]} \qquad \mathbf{186}$$

with

$DEP_{soil\,i[S]}$: transport coefficient for atmospheric deposition (wet and dry) to soil i at scale S [$m_{air}^{3}.s^{-1}$] *(I)*

$DRYDEP_{aerosol[S]}$: mass transfer coefficient for dry deposition of aerosol-associated chemical at scale S [$m_{air}.s^{-1}$] *(D)*

$WASHOUT_{[S]}$: mass transfer coefficient for wet atmospheric deposition at scale S [$m_{air}.s^{-1}$] *(D)*

$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*

$AREAFRAC_{soil\,i[S]}$: fraction of scale S that is soil i [-] *(D)*

Values for the deposition mass transfer coefficients $DRYDEP_{aerosol}$ and $WASHOUT$ can be found in paragraph 3.6.1.

3.7.7 Diffusive transport

Diffusive transport to and from air takes place by gas absorption and volatilization. The absorption mass flows are obtained from:

$$DIFF_{air\text{-}water\,i[S]} = XCH_{air\text{-}water\,i[S]} \cdot C_{air[S]} \tag{187}$$

with

$DIFF_{air\text{-}water\,i[S]}$: diffusive mass flow from air to water i at scale S by gas absorption [mol.s^{-1}] *(I)*
$XCH_{air\text{-}water\,i[S]}$: transport coefficient for gas absorption to water i at scale S [$m_{air}^3.s^{-1}$]*(I)*
$C_{air[S]}$: total concentration in air (gas phase + aerosol phase + rain water phase) at scale S [mol. m_{air}^{-3}] *(S)*

$$DIFF_{air\text{-}soil\,i[S]} = XCH_{air\text{-}soil\,i[S]} \cdot C_{air[S]} \tag{188}$$

with

$DIFF_{air\text{-}soil\,i[S]}$: diffusive mass flow from air to soil i at scale S by gas absorption [mol.s^{-1}] *(I)*
$XCH_{air\text{-}soil\,i[S]}$: transport coefficient for gas absorption by soil i at scale S [$m_{air}^3.s^{-1}$] *(I)*
$C_{air[S]}$: total concentration in air (gas phase + aerosol phase + rain water phase) at scale S [mol. m_{air}^{-3}] *(S)*

$$DIFF_{air\text{-}veg\,i[S]} = XCH_{air\text{-}veg\,i[S]} \cdot C_{air[S]} \tag{189}$$

with

$DIFF_{air\text{-}veg\,i[S]}$: diffusive mass flow from air to vegetation i at scale S by gas absorption [mol.s^{-1}] *(I)*
$XCH_{air\text{-}veg\,i[S]}$: transport coefficient for gas absorption by vegetation i at scale S [$m_{air}^3.s^{-1}$] *(I)*
$C_{air[S]}$: total concentration in air (gas phase + aerosol phase + rain water phase) at scale S [mol. m_{air}^{-3}] *(S)*

$$XCH_{air\text{-}water\,i[S]} = GASABS_{water\,i[S]} \cdot SYSTEMAREA_{[S]} \cdot AREAFRAC_{water\,i[S]} \tag{190}$$

with

$XCH_{air\text{-}water\,i[S]}$: transport coefficient for gas absorption to water i at scale S [$m_{air}^3.s^{-1}$] *(I)*
$GASABS_{water\,i[S]}$: overall mass transfer coefficient for gas absorption across the air-water interface, referenced to air at scale S [$m_{air}.s^{-1}$] *(D)*
$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{water\,i[S]}$: fraction of the system area that is water i at scale S [-] *(D)*

$$XCH_{air\text{-}soil\ i[S]} = GASABS_{soil\ i[S]} . SYSTEMAREA_{[S]} . AREAFRAC_{soi\ li[S]} \qquad \mathbf{191}$$

with

$XCH_{air\text{-}soil\ i[S]}$: transport coefficient for gas absorption to soil i at scale S [$m_{air}^3.s^{-1}$] *(I)*
$GASABS_{soil\ i[S]}$: overall mass transfer coefficient for gas absorption across the air-soil interface, referenced to air at scale S [$m_{air}.s^{-1}$] *(D)*
$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{soil\ i[S]}$: fraction of scale S that is soil i [-] *(D)*

The volatilization mass flows are obtained from:

$$DIFF_{water\ i\text{-}air[S]} = XCH_{water\ i\text{-}air[S]} . C_{water\ i[S]} \qquad \mathbf{192}$$

with

$DIFF_{water\ i\text{-}air[S]}$: diffusive mass flow from water i to air at scale S by volatilization [$mol.s^{-1}$] *(I)*
$XCH_{water\ i\ air[S]}$: transport coefficient for volatilization from water i at scale S [$m_{water}^3.s^{-1}$] *(I)*
$C_{water\ i[S]}$: dissolved concentration in water i at scale S [$mol.m_{water}^{-3}$] *(S)*

$$DIFF_{soil\ i\text{-}air[S]} = XCH_{soil\ i\text{-}air[S]} . C_{soil\ i[S]} \qquad \mathbf{193}$$

with

$DIFF_{soil\ i\text{-}air[S]}$: diffusive mass flow from soil i to air at scale S by volatilization [$mol.s^{-1}$] *(I)*
$XCH_{soil\ i\text{-}air[S]}$: transport coefficient for volatilization from soil i at scale S [$m_{soil}^3.s^{-1}$]*(I)*
$C_{soil\ i[S]}$: total concentration in soil i at scael S (gas phase + water phase + solid phase) [$mol.m_{soil}^{-3}$] *(S)*

$$XCH_{water\ i\text{-}air[S]} = VOLAT_{water\ i[S]} . SYSTEMAREA_{[S]} . AREAFRAC_{water\ i[S]} \qquad \mathbf{194}$$

with

$XCH_{wateri\ \text{-}air}$: transport coefficient for volatilization from water i at scale S[$m_{water}^3.s^{-1}$] *(I)*
$VOLAT_{water\ i[S]}$: overall mass transfer coefficient for volatilization across the water-air interface, referenced to water i at scale S [$m_{water}.s^{-1}$] *(D)*
$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{water\ i[S]}$: fraction of scale S that is water i [-] *(D)*

$$XCH_{soil\ i\text{-}air[S]} = VOLAT_{soil\ i[S]} . SYSTEMAREA_{[S]} . AREAFRAC_{soil\ i[S]} \qquad \mathbf{195}$$

with

$XCH_{soil\ i\text{-}air[S]}$: transport coefficient for volatilization from soil i at scale S [$m_{soil}^3.s^{-1}$] *(I)*
$VOLAT_{soil\ i[S]}$: overall mass transfer coefficient for volatilization across the soil-air interface, referenced to soil i at scale S [$m_{soil}.s^{-1}$] *(D)*
$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{soil\ i[S]}$: fraction of scale S that is soil i [-] *(D)*

Values for the overall mass transfer coefficients for gas absorption and volatilization can be found in paragraph 3.6.2.

3.8 The water compartments

3.8.1 Mass balance

The mass balance equation for the water compartment is:

$$\begin{aligned} V_{water\,i[S]} \cdot \frac{dC_{water\,i[S]}}{dt} = & + EMIS_{water\,i[S]} + IMP_{water\,i[S]} - EXP_{water\,i[S]} \\ & - V_{water\,i[S]} \cdot DEG_{water\,i[S]} \cdot C_{water\,i[S]} + DEP_{water\,i[S]} \cdot C_{air[S]} \\ & + \Sigma RUN\text{-}OFF_{soil\,i[S]} \cdot C_{soil\,i[S]} - XCH_{water\,i\text{-}air[S]} \cdot C_{water\,i[S]} \\ & - XCH_{water\,i\text{-}sed\,i[S]} \cdot C_{water\,i[S]} + XCH_{air\text{-}water\,i[S]} \cdot C_{air[S]} \\ & + XCH_{sed\,i\text{-}water\,i[S]} \cdot C_{sed\,i[S]} \end{aligned} \qquad \mathbf{196}$$

with

$V_{water\,i[S]}$:	volume of water compartment i at scale S [m_{water}^3] *(I)*
$C_{water\,i[S]}$:	concentration in water compartment i (dissolved) at scale S [$mol.m_{water}^{-3}$] *(S)*
t :	time [s] *(S)*
$EMIS_{water\,i[S]}$:	emission to water compartment i at scale S [$mol.s^{-1}$] *(I)*
$IMP_{water\,i[S]}$:	import mass flow into water compartment i at scale S [$mol.s^{-1}$] *(I)*
$EXP_{water\,i[S]}$:	export mass flow from water compartment i at scale S [$mol.s^{-1}$] *(I)*
$DEG_{water\,i[S]}$:	pseudo first order transformation rate constant in water i at scale S [s^{-1}] *(I)*
$DEP_{water\,i[S]}$:	transport coefficient for atmospheric deposition (wet and dry) to water i at scale S [$m_{air}^3.s^{-1}$] *(I)*
$RUN\text{-}OFF_{soil\,i[S]}$:	transport coefficient for run off from soil i to water i at scale S [$m_{soil}^3.s^{-1}$] *(I)*
$C_{soil\,i[S]}$:	concentration in soil i at scale S [$mol.m_{soil}^{-3}$] *(S)*
$XCH_{water\,i\text{-}air[S]}$:	transport coefficient for volatilization from water i at scale S [$m_{water}^3.s^{-1}$] *(I)*
$XCH_{water\,i\text{-}sed\,i[S]}$:	transport coefficient for uptake by sediment i at scale S [$m_{water}^3.s^{-1}$] *(I)*
$XCH_{air\text{-}water\,i[S]}$:	transport coefficient for gas absorption from air at scale S [$m_{air}^3.s^{-1}$] *(I)*
$C_{air[S]}$:	concentration in air at scale S [$mol.m_{air}^{-3}$] *(S)*
$XCH_{sed\,i\text{-}water\,i[S]}$:	transport coefficient for release from sediment i at scale S [$m_{sed}^3.s^{-1}$] *(I)*
$C_{sed\,i[S]}$:	concentration in sediment i at scale S [$mol.m_{sed}^{-3}$] *(S)*

3.8.2 Emissions

$$EMIS_{water\,i[S]} = Edirect_{water\,i[S]} + Estp_{water\,i[S]} \qquad \mathbf{197}$$

The emission mass flow to the water compartment is obtained from:

with

$EMIS_{water\,i[S]}$:	total emission mass flow into water compartment i at scale S [$mol.s^{-1}$] *(I)*

$Edirect_{water\ i[S]}$:	sum of all direct emissions to water compartment i at scale S [mol.s^{-1}] *(D)*
$Estp_{water\ i[S]}$:	indirect emission to water i with effluent from sewage treatment at scale S [mol.s^{-1}] *(D)*

$Edirect_{water}$ may be derived by means of:

$$Edirect_{water\ i[S]} = PRODUCTION_{[S]}.EMISfact_{water\ i[S]} \qquad \textbf{198}$$

with

$Edirect_{water\ i[S]}$:	sum of all direct emissions to water compartment i at scale S [mol.s^{-1}] *(D)*
$PRODUCTION_{[S]}$:	total amount produced or imported in the system [mol.s^{-1}] *(A)*
$EMISfact_{water\ i[S]}$:	mission factor for water: the fraction of the production volume that is released to water compartment i at scale S [-] *(A)*

$$EMISfact_{water\ i[S]} = 0.1\% \qquad \textbf{199}$$

with

$EMISfact_{water\ i[S]}$:	emission factor for water i: the fraction of the production volume that is released to water compartment i of scale S [-] *(A)*

as a starting point.

3.8.3 Import

The import mass flow into water is obtained from:

$$IMP_{water} = IMPORT_{water} \qquad \textbf{200}$$

with

IMP_{water}:	import mass flow into the water compartment [mol.s^{-1}] *(I)*
$IMPORT_{water}$:	transport of the chemical with water across the system boundaries [mol.s^{-1}]*(D)*

A value for $IMPORT_{water}$ may be derived as follows:

$$IMPORT_{water\ 1[R]} = FLOW_{water\ 1[C]-water\ 1[R]}.C_{water\ 1[C]} \qquad \textbf{201}$$

with

$IMPORT_{water\ 1[R]}$:	transport of the chemical with water across the regional scale boundaries [mol.s^{-1}] *(D)*
$FLOW_{water\ 1[C]-water\ 1[R]}$:	rate of water flow from water 1 of the continental scale to water 1 of the regional scale [m_{water}^3.s^{-1}] *(A)*
$C_{water\ 1[C]}$:	concentration of the chemical in water 1 of the continental scale [mol.m_{water}^{-3}] *(A)*

$$IMPORT_{water\,2[R]} = +FLOW_{water\,1[R]-water\,2[R]} \cdot C_{water\,1[R]} + FLOW_{water\,1[C]-water\,2[R]} \cdot C_{water\,1[C]} + FLOW_{water\,2[C]-water\,2[R]} \cdot C_{water\,2[C]} \quad \mathbf{202}$$

with

$IMPORT_{water\,2[R]}$:	transport of the chemical with water across the regional scale boundaries to water 2 [mol.s^{-1}] *(D)*
$FLOW_{water\,1[R]-water\,2[R]}$:	rate of water flow from water 1 to water 2 of the regional scale [m$_{water}^{3}$.s^{-1}] (A)
$C_{water\,1[R]}$:	concentration of the chemical in water 1 of the regional scale [mol.m$_{water}^{-3}$]*(A)*
$FLOW_{water\,1[C]-water\,2[R]}$:	rate of water flow from water 1of the continental scale to water 2 of the regional scale [m$_{water}^{3}$.s^{-1}] *(A)*
$C_{water\,1[C]}$:	concentration of the chemical in water 1 of the continental scale [mol.m$_{water}^{-3}$] *(A)*
$FLOW_{water\,2[C]-water\,2[R]}$:	rate of water flow from water 2 of the continental scale to water 2 of the regional scale [m$_{water}^{3}$.s^{-1}] *(A)*
$C_{water\,2[C]}$:	concentration of the chemical in water 2 of the continental scale [mol.m$_{water}^{-3}$] *(A)*

$$IMPORT_{water\,1[C]} = 0 \quad \mathbf{203}$$

with

$IMPORT_{water\,1[C]}$:	transport of the chemical with water across the continental scale boundaries to water 1[mol.s^{-1}] *(D)*

$$IMPORT_{water\,2[C]} = +FLOW_{water\,1[C]-water\,2[C]} \cdot C_{water\,1[C]} + FLOW_{water\,2[R]-water\,2[C]} \cdot C_{water\,2[R]} + FLOW_{water[M]-water\,2[C]} \cdot C_{water[M]} \quad \mathbf{204}$$

with

$IMPORT_{water\,2[C]}$:	transport of the chemical with water across the continental scale boundaries to water 2 [mol.s^{-1}] *(D)*
$FLOW_{water\,1[C]-water\,2[C]}$:	rate of water flow from water 1 to water 2 of the continental scale [m$_{water}^{3}$.s^{-1}]*(A)*
$C_{water\,1[C]}$:	concentration of the chemical in water 1 of the continental scale [mol.m$_{water}^{-3}$]*(A)*
$FLOW_{water\,2[R]-water\,2[C]}$:	rate of water flow from water 2 of the regional scale to water 2 of the continental scale [m$_{water}^{3}$.s^{-1}] *(A)*
$C_{water\,2[R]}$:	concentration of the chemical in water 2 of the regional scale [mol.m$_{water}^{-3}$] *(A)*
$FLOW_{water[M]-water\,2[C]}$:	rate of water flow from water of the moderate scale to water 2 of the continental scale [m$_{water}^{3}$.s^{-1}] *(A)*
$C_{water[M]}$:	concentration of the chemical in water of the moderate scale [mol.m$_{water}^{-3}$] *(A)*

$$IMPORT_{water[M]} = +FLOW_{water\,2[C]-water[M]} \cdot C_{water\,2[C]} + FLOW_{water[A]-water[M]} \cdot C_{water[A]} + FLOW_{water[T]-water[M]} \cdot C_{water[T]} \quad \mathbf{205}$$

with

$IMPORT_{water[M]}$: transport of the chemical with water across the moderate scale [mol.s^{-1}]*(D)*

$FLOW_{water2[C]-water[M]}$: rate of water flow from water 2 of the continental scale to water of the moderate scale [m$_{water}^{3}$.s^{-1}] *(A)*

$C_{water2[C]}$: concentration of the chemical in water 2 of the continental scale [mol.m$_{water}^{-3}$]*(A)*

$FLOW_{water[A]-water[M]}$: rate of water flow from water of the arctic scale to water of the moderate scale [m$_{water}^{3}$.s^{-1}] *(A)*

$C_{water[A]}$: concentration of the chemical in water of the arctic scale [mol.m$_{water}^{-3}$]*(A)*

$FLOW_{water[T]-water[M]}$: rate of water flow from water of the arctic scale to water of the moderate scale [m$_{water}^{3}$.s^{-1}] *(A)*

$C_{water[T]}$: concentration of the chemical in water of the tropic scale [mol.m$_{water}^{-3}$] *(A)*

$$IMPORT_{water[A]} = +FLOW_{water[M]-water[A]} \cdot C_{water[M]} \qquad \mathbf{206}$$

with

$IMPORT_{water[A]}$: transport of the chemical with water across the arctic scale [mol.s^{-1}] *(D)*

$FLOW_{water[M]-water[A]}$: rate of water flow from water of the moderate scale to water of the arctic scale [m$_{water}^{3}$.s^{-1}] *(A)*

$C_{water[M]}$: concentration of the chemical in water of the moderate scale [mol.m$_{water}^{-3}$]*(A)*

$$IMPORT_{water[T]} = +FLOW_{water[M]-water[T]} \cdot C_{water[M]} \qquad \mathbf{207}$$

with

$IMPORT_{water[T]}$: transport of the chemical with water across the tropic scale [mol.s^{-1}] *(D)*

$FLOW_{water[M]-water[T]}$: rate of water flow from water of the moderate scale to water of the tropic scale [m$_{water}^{3}$.s^{-1}] *(A)*

$C_{water[M]}$: concentration of the chemical in water of the moderate scale [mol.m$_{water}^{-3}$]*(A)*

3.8.4 Export

The export mass flow from water is obtained from:

$$EXP_{water} = FLOW_{water} \cdot C_{water} \qquad \mathbf{208}$$

with

EXP_{water}: export mass flow from the water compartment [mol.s^{-1}] *(I)*

$FLOW_{water}$: refreshment flow through the water compartment [m$_{water}^{3}$.s^{-1}] *(I)*

C_{water}: dissolved concentration in water [mol.m$_{water}^{-3}$] *(S)*

A value for $EXPORT_{water}$ for the different scales may be derived as follows:

$$EXPORT_{water1[R]} = FLOW_{water1[R]-water2[R]} \cdot C_{water1[R]} \qquad \mathbf{209}$$

with

$EXPORT_{water\,1[R]}$: transport of the chemical with water across the regional scale boundaries $[mol.s^{-1}]$ *(D)*

$FLOW_{water\,1[R]-water\,2[R]}$: rate of water flow from water 1 to water 2 of the regional scale $[m_{water}^{3}.s^{-1}]$ *(A)*

$C_{water\,1[R]}$: concentration of the chemical in water 1 of the regional scale $[mol.m_{water}^{-3}]$ *(A)*

$$EXPORT_{water\,2[R]} = FLOW_{water\,2[R]-water\,2[C]} \cdot C_{water\,2[R]} \tag{210}$$

with

$EXPORT_{water\,2[R]}$: transport of the chemical with water across the regional scale boundaries to water 2 of the continental scale $[mol.s^{-1}]$ *(D)*

$FLOW_{water\,2[R]-water\,2[C]}$: rate of water flow from water 2 of the regional scale to water 2 of the continental scale $[m_{water}^{3}.s^{-1}]$ *(A)*

$C_{water\,2[R]}$: concentration of the chemical in water 2 of the regional scale $[mol.m_{water}^{-3}]$ *(A)*

$$\begin{aligned} EXPORT_{water\,1[C]} = {} & FLOW_{water\,1[C]-water\,2[C]} \cdot C_{water\,1[C]} + FLOW_{water\,1[C]-water\,1[R]} \cdot C_{water\,1[C]} \\ & + FLOW_{water\,1[C]-water\,2[R]} \cdot C_{water\,1[C]} \end{aligned} \tag{211}$$

with

$EXPORT_{water\,1[C]}$: transport of the chemical with water 1 across the continental scale boundaries $[mol.s^{-1}]$ *(D)*

$FLOW_{water\,1[C]-water\,2[C]}$: rate of water flow from water 1 to water 2 of the continental scale $[m_{water}^{3}.s^{-1}]$*(A)*

$FLOW_{water\,1[C]-water\,1[R]}$: rate of water flow from water 1 of the continental scale to water 1 of the regional scale $[m_{water}^{3}.s^{-1}]$ *(A)*

$FLOW_{water\,1[C]-water\,2[R]}$: rate of water flow from water 1 of the continental scale to water 2 of the regional scale $[m_{water}^{3}.s^{-1}]$ *(A)*

$C_{water\,1[C]}$: concentration of the chemical in water 1 of the continental scale $[mol.m_{water}^{-3}]$ *(A)*

$$EXPORT_{water\,2[C]} = +FLOW_{water\,2[C]-water\,2[R]} \cdot C_{water\,2[C]} + FLOW_{water\,2[C]-water[M]} \cdot C_{water\,2[C]} \tag{212}$$

with

$EXPORT_{water\,2[C]}$: transport of the chemical with water 2 across the continental scale boundaries $[mol.s^{-1}]$ *(D)*

$FLOW_{water\,2[C]-water\,2[R]}$: rate of water flow from water 1 of the continental scale to water 2 of the regional scale $[m_{water}^{3}.s^{-1}]$ *(A)*

$FLOW_{water\,2[C]-water[M]}$: rate of water flow from water 2 of the continental scale to water of the moderate scale $[m_{water}^{3}.s^{-1}]$ *(A)*

$C_{water\,2[C]}$: concentration of the chemical in water 2 of the continental scale $[mol.m_{water}^{-3}]$*(A)*

$$\begin{aligned} EXPORT_{water[M]} = {} & FLOW_{water[M]-water\,2[C]} \cdot C_{water[M]} + FLOW_{water[M]-water[A]} \cdot C_{water[M]} \\ & + FLOW_{water[M]-water[T]} \cdot C_{water[M]} \end{aligned} \tag{213}$$

with

$EXPORT_{water[M]}$: transport of the chemical with water across the moderate scale $[mol.s^{-1}]$ *(D)*

$FLOW_{water[M]\text{-}water2[C]}$: rate of water flow from water of the moderate scale to water of the continental scale [$m_{water}^3.s^{-1}$] *(A)*
$FLOW_{water[M]\text{-}water[A]}$: rate of water flow from water of the moderate scale to water of the arctic scale [$m_{water}^3.s^{-1}$] *(A)*
$FLOW_{water[M]\text{-}water[T]}$: rate of water flow from water of the moderate scale to water of the tropic scale [$m_{water}^3.s^{-1}$] *(A)*
$C_{water[M]}$: concentration of the chemical in water of the moderate scale [$mol.m_{water}^{-3}$] *(A)*

$$EXPORT_{water[A]} = FLOW_{water[A]-water[M]} \cdot C_{water[A]} \qquad \mathbf{214}$$

with

$EXPORT_{water[A]}$: transport of the chemical with water across the arctic scale [$mol.s^{-1}$] *(D)*
$FLOW_{water[A]\text{-}water[M]}$: rate of water flow from water of the arctic scale to water of the moderate scale [$m_{water}^3.s^{-1}$] *(A)*
$C_{water[A]}$: concentration of the chemical in water of the arctic scale [$mol.m_{water}^{-3}$] *(A)*

$$EXPORT_{water[T]} = FLOW_{water[T]-water[M]} \cdot C_{water[T]} \qquad \mathbf{215}$$

with

$EXPORT_{water[T]}$: transport of the chemical with water across the tropic scale [$mol.s^{-1}$] *(D)*
$FLOW_{water[T]\text{-}water[M]}$: rate of water flow from water of the tropic scale to water of the moderate scale [$m_{water}^3.s^{-1}$] *(A)*
$C_{water[T]}$: concentration of the chemical in water of the tropic scale [$mol.m_{water}^{-3}$] *(A)*

3.8.5 Degradation

The apparent degradation mass flow from water is obtained from:

$$DEGRD_{water\,i[S]} = V_{water\,i[S]} \cdot DEG_{water\,i[S]} \cdot C_{water\,i[S]} \qquad \mathbf{216}$$

with

$DEGRD_{water\,i[S]}$: degradation mass flow from water compartment i of scale S [$mol.s^{-1}$] *(I)*
$V_{water\,i[S]}$: volume of water compartment i at scale S [m_{water}^3] *(I)*
$DEG_{wateri[S]}$: pseudo first order transformation rate constant in water i at scale S [s^{-1}] *(I)*
$C_{water\,i[S]}$: bulk concentration in water i at scale S [$mol.m_{water}^{-3}$] *(S)*

$$DEG_{water\,i[S]} = kdeg_{water\,i[S]} \qquad \mathbf{217}$$

with

$DEG_{water\,i[S]}$: pseudo first order transformation rate constant in water i at scale S [s^{-1}] *(I)*
$kdeg_{water\,i[S]}$: pseudo first order transformation rate constant in water i at scale S [s^{-1}] *(D)*

A value for $kdeg_{water}$ may be obtained by the equations in paragraph 3.5.2

3.8.6 Advective transport

Advective transport from air to water takes place by wet and dry atmospheric deposition, as described in paragraph 3.6.1 and 3.7.6 See equations 183, 185, 147 and 148.

Advective transport from soil to water by run-off is described in paragraph 3.6.4.

3.8.7 Diffusive transport

Diffusive transport between air and water takes place by gas absorption and volatilization. The formulas for this have been given in paragraph 3.6.2, equations 149, 151, 187, 190, 192, 194.

Diffusive transport across the sediment-water interface by means of adsorption and desorption is described in paragraph 3.9.7 and 3.6.3, equations 226, 227, 228, 158, 159.

3.9 The sediment compartments

3.9.1 Mass balance

The mass balance equation for the sediment compartment is:

$$V_{sed\ i[S]} \cdot \frac{dC_{sed\ i[S]}}{dt} = -\ V_{sed\ i[S]} \cdot DEG_{sed\ i[S]} \cdot C_{sed\ i[S]}\ -\ SEDBURIAL_{i[S]} \cdot C_{sed\ i[S]}$$
$$-\ RESUSPENSION_{i[S]} \cdot C_{sed\ i[S]} +\ SEDIMENTATION_{i[S]} \cdot C_{water\ i[S]}$$
$$-\ XCH_{sed\ i\text{-}water\ i[S]} \cdot C_{sed\ i[S]} +\ XCH_{water\ i\text{-}sed\ i[S]} \cdot C_{water\ i[S]} \qquad \textbf{218}$$

with

$V_{sed\ i[S]}$:	volume of sediment compartment i at scale S [m_{sed}^3] *(I)*
$C_{sed\ i[S]}$:	total concentration in sediment i (water phase + solid phase) at scale S [$mol.m_{sed}^{-3}$] *(S)*
t :	time [s] *(S)*
$DEG_{sed\ i[S]}$:	pseudo first order transformation rate constant in sediment i at scale S [s^{-1}] *(I)*
$SEDBURIAL_{i[S]}$:	transport coefficient for sediment burial for water column i at scale S [$m_{sed}^3.s^{-1}$] *(I)*
$RESUSPENSION_{i[S]}$:	transport coefficient for resuspension for water column i at scale S [$m_{sed}^3.s^{-1}$] *(I)*
$SEDIMENTATION_{i[S]}$:	transport coefficient for sedimentation for water column i at scale S [$m_{susp}^3.s^{-1}$] *(I)*
$XCH_{sed\ i\text{-}water\ i[S]}$:	transport coefficient for release from sediment i to water i at scale S [$m_{sed}^3.s^{-1}$] *(I)*
$XCH_{water\ i\text{-}sed\ i[S]}$:	transport coefficient for uptake by sediment i at scale S [$m_{water}^3.s^{-1}$] *(I)*
$C_{water\ i[S]}$:	concentration in water i at scale S [$mol.m_{water}^{-3}$] *(S)*

3.9.2 Degradation

The apparent degradation mass flow from sediment is obtained from:

$$DEGRD_{sed\ i[S]} = V_{sed\ i[S]} \cdot DEG_{sed\ i[S]} \cdot C_{sed\ i[S]} \qquad \textbf{219}$$

with

$DEGRD_{sed\ i[S]}$:	degradation mass flow from sediment compartment i at scale S [$mol.s^{-1}$] *(I)*
$V_{sed\ i[S]}$:	volume of sediment compartment i at scale S [m_{sed}^3] *(I)*
$DEG_{sed\ i[S]}$:	pseudo first order transformation rate constant in sediment i at scale S [s^{-1}] *(I)*

$C_{sed\,i[S]}$: bulk concentration in sediment i at scale S [mol.m_{sed}^{-3}] *(S)*

$$DEG_{sed\,i[S]} = kdeg_{sed\,i[S]} \qquad \textbf{220}$$

with

$DEG_{sed\,i[S]}$: pseudo first order transformation rate constant in sediment i at scale S [s^{-1}] *(I)*
$kdeg_{sed\,i[S]}$: pseudo first order transformation rate constant in sediment i at scale S [s^{-1}] *(D)*

A value for $kdeg_{sed}$ is given by the equations in paragraph3.5.3.

3.9.3 Sedimentation

Advective mass flows between suspended matter of the water compartment and the sediment compartment by means of sedimentation and resuspension are obtained from:

$$SEDIMENTATION_{i[S]} = \frac{GROSSsedrate_{i[S]}.(1 - FRwater_{sed\,i[S]}).RHOsolid_{[S]}}{SUSP_{water\,i[S]}}. \\ (\frac{Kp_{susp\,i[S]}.SUSP_{water\,i[S]}}{1000}.FRdisslvd_{water\,i[S]}). \\ SYSTEMAREA_{[S]}.AREAFRAC_{water\,i[S]} \qquad \textbf{221}$$

with

$SEDIMENTATION_{i[S]}$: transport coefficient for sedimentation of suspended matter in water column i at scale S [$m_{susp}^{3}.s^{-1}$] *(I)*
$GROSSsedrate_{i[S]}$: gross sedimentation rate of suspended matter in water column i at scale S [$m_{sed}.s^{-1}$] *(A)*
$Frwater_{sed\,i[S]}$: volume fraction of the water phase of sediment i at scale S [-] *(A)*
$RHOsolid_{[S]}$: density of the solid phase [kg.m^{-3}] *(D)*
$Kp_{susp\,i[S]}$: suspended matter-water partition coefficient at scale S[$l_{water}.kg_{solid}^{-1}$] *(I)*
$SUSP_{water\,i\,[S]}$: concentration of suspended matter in water column i at scale S [$kg_{solid}.m_{water}^{-3}$] *(D)*
$Frdisslvd_{water\,i[S]}$: dissolved fraction of water column i at scale S [%] *(A)*
$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{water\,i[S]}$: fraction of scale S that is water i [-] *(D)*

3.9.4 Resuspention

The apparent mass flow from the sediment as a result of resuspention is obtained from:

$$RESUSPENSION_{i[S]} = RESUSPrate_{i[S]}.SYSTEMAREA_{[S]}.AREAFRAC_{water\,i[S]} \qquad \textbf{222}$$

with

$RESUSPENSION_{i[S]}$:	transport coefficient for resuspension for sediment compartment i at scale S $[m_{sed}^3.s^{-1}]$ *(I)*
$RESUSPrate_{i[S]}$:	resuspension rate for sediment compartment i at scale S$[m_{sed}.s^{-1}]$ *(A)*
$SYSTEMAREA_{[S]}$:	total area of scale S (air/water + air/soil interfaces) $[m^2]$ *(D)*
$AREAFRAC_{water\ i[S]}$:	fraction of scale S that is water i [-] *(D)*

3.9.5 Burial

The apparent mass flow from the sediment as a result of burial is obtained from:

$$BRL_{sed\ i[S]} = SEDBURIAL_{i[S]} . C_{sed\ i[S]} \qquad \mathbf{223}$$

with

$BRL_{sed\ i[S]}$:	apparent burial mass flow from sediment compartment i at scale S $[mol.s^{-1}]$ *(I)*
$SEDBURIAL_{i[S]}$:	transport coefficient for sediment burial for water compartment i at scale S $[m_{sed}^3.s^{-1}]$ *(I)*
$C_{sed\ i[S]}$:	bulk concentration in sediment i at scale S $[mol.m_{sed}^{-3}]$ *(S)*

$$SEDBURIAL_{i[S]} = BURIAL_{sed\ i[S]} . SYSTEMAREA_{[S]} . AREAFRAC_{water\ i[S]} \qquad \mathbf{224}$$

with

$SEDBURIAL_{i[S]}$:	transport coefficient for sediment burial for water column i at scale S $[m_{sed}^3.s^{-1}]$ *(I)*
$BURIAL_{sed\ i[S]}$:	sediment burial rate for water column i at scale S $[m_{sed}.s^{-1}]$ *(D)*
$SYSTEMAREA[S]$:	total area of the system (air/water + air/soil interfaces) $[m^2]$ *(D)*
$AREAFRAC_{water\ i[S]}$:	fraction of the system area that is water i at scale S [-] *(D)*

3.9.6 Advective transport

Advective transport between sediment and suspended matter by sedimentation and resuspension is described in paragraph 3.4.6 and 3.4.4, equations 88, 72-81.

3.9.7 Diffusive transport

Diffusive mass flows between sediment and water, by direct adsorption and desorption across the sediment-water interface, are obtained from:

$$DIFF_{sed\ i\text{-}water\ i[S]} = XCH_{sed\ i\text{-}water\ i[S]} . C_{sed\ i[S]} \qquad \mathbf{225}$$

with

$DIFF_{sed\ i\text{-}water\ i[S]}$:	diffusive desorption mass flow from sediment i to water i at scale S $[mol.s^{-1}]$ *(I)*
$XCH_{sed\ i\text{-}water\ i[S]}$:	transport coefficient for desorption from sediment i at scale S $[m_{sed}^3.s^{-1}]$ *(I)*
$C_{sed\ i[S]}$:	concentration in sediment i at scale S $[mol.m_{sed}^{-3}]$ *(S)*

$$XCH_{sed\,i\text{-}water\,i[S]} = DESORB_{sed\,i[S]} \cdot SYSTEMAREA_{[S]} \cdot AREAFRAC_{water\,i[S]} \tag{226}$$

with

$XCH_{sed\,i\text{-}water\,i[S]}$: transport coefficient for desorption from sediment i at scale S $[m_{sed}^3.s^{-1}]$ *(I)*
$DESORB_{sed\,i[S]}$: overall mass transfer coefficient for desorption across the sediment-water interface, referenced to sediment i at scale S $[m_{sed}.s^{-1}]$ *(D)*
$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) $[m^2]$ *(D)*
$AREAFRAC_{water\,i[S]}$: fraction of the system area that is water [-] *(D)*

$$DIFF_{water\,i\text{-}sed\,i[S]} = XCH_{water\,i\text{-}sed\,i[S]} \cdot C_{water\,i[S]} \tag{227}$$

with

$DIFF_{water\,i\text{-}sed\,i[S]}$: diffusive adsorption mass flow to sediment i to water i at scale S $[mol.s^{-1}]$ *(I)*
$XCH_{water\,i\text{-}sed\,i[S]}$: transport coefficient for adsorption to sediment i at scale S $[m_{water}^3.s^{-1}]$ *(I)*
$C_{water\,i[S]}$: concentration in water i at scale S $[mol.m_{water}^{-3}]$ *(S)*

$$XCH_{water\,i\text{-}sed\,i[S]} = ADSORB_{sed\,i[S]} \cdot SYSTEMAREA_{[S]} \cdot AREAFRAC_{water\,i[S]} \tag{228}$$

with

$XCH_{water\,i\text{-}sed\,i[S]}$: transport coefficient for adsorption to sediment $[m_{water}^3.s^{-1}]$ *(I)*
$ADSORB_{sed\,i[S]}$: overall mass transfer coefficient for adsorption across the sediment-water interface, referenced to water i at scale S $[m_{water}.s^{-1}]$ *(D)*
$SYSTEMAREA[S]$: total area of scale S (air/water + air/soil interfaces) $[m^2]$ *(D)*
$AREAFRAC_{water\,i[S]}$: fraction of scale S that is water i [-] *(D)*

Values for the overall mass transfer coefficients for direct adsorption and desorption across the sediment-water interface are given in paragraph 3.6.3.

3.10 The soil compartments

3.10.1 Mass balance

The mass balance equations for the soil compartments are:

$$\begin{aligned} V_{soil\,i[S]} \cdot \frac{dC_{soil\,i[S]}}{dt} = &+ EMIS_{soil\,i[S]} \\ &- V_{soil\,i[S]} \cdot DEG_{soil\,i[S]} \cdot C_{soil\,i[S]} - LEACHING_{soil\,i[S]} \cdot C_{soil\,i[S]} \\ &- \Sigma RUN-OFF_{soil\,i\text{-}water\,i[S]} \cdot C_{soil\,i[S]} + DEP_{soil\,i[S]} \cdot C_{air[S]} \\ &- XCH_{soil\,i\text{-}air[S]} \cdot C_{soil\,i[S]} + XCH_{air\text{-}soil\,i[S]} \cdot C_{air[S]} \end{aligned} \tag{229}$$

with

$V_{soil\,i[S]}$:	volume of the compartment soil i at scale S [m_{soil}^3] *(I)*
$C_{soil\,i[S]}$:	total concentration in soil i (gas phase + water phase + solid phase) at scale S mol.m_{soil}^{-3}] *(S)*
t :	time [s] *(S)*
$EMIS_{soil\,i[S]}$:	emission to soil i at scale S [mol.s^{-1}] *(I)*
$DEG_{soil\,i[S]}$:	pseudo first order transformation rate constant in soil i at scale S [s^{-1}] *(I)*
$LEACHING_{soil\,i[S]}$:	transport coefficient for leaching from soil i at scale S [m_{soil}^3.s^{-1}] *(I)*
$RUN\text{-}OFF_{soil\,i[S]}$:	transport coefficient for run off from soil i to water i at scale S [m_{soil}^3.s^{-1}] *(I)*
$DEP_{soil\,i[S]}$:	transport coefficient for atmospheric deposition (wet and dry) to soil i at scale S [m_{air}^3.s^{-1}] *(I)*
$C_{air[S]}$:	total concentration in air at scale S [mol.m_{air}^{-3}] *(S)*
$XCH_{soil\,i\text{-}air[S]}$:	transport coefficient volatilization from soil i at scale S [m_{soil}^3.s^{-1}] *(I)*
$XCH_{air\text{-}soil\,i[S]}$:	transport coefficient gas absorption to soil i at scale S [m_{air}^3.s^{-1}] *(I)*

3.10.2 Emission

Soil 1 and soil 3 only receive direct emissions. In addition to this, soil 2 may receive indirect emission through application of the sludge that is produced upon sewage treatment. Emission mass flows to soil are obtained from:

$$EMIS_{soil\,1[S]} = Edirect_{soil\,1[S]} \tag{230}$$

$$EMIS_{soil\,2[S]} = Edirect_{soil\,2[S]} + Estp_{soil\,2[S]} \tag{231}$$

$$EMIS_{soil\,3[S]} = Edirect_{soil3[S]} \tag{232}$$

with

$EMIS_{soil\,1[S]}$:	total emission mass flow to soil i at scale S [mol.s^{-1}] *(I)*
$Edirect_{soil\,2[S]}$:	sum of all direct emissions to soil i at scale S [mol.s^{-1}] *(D)*

$Estp_{soil\,2[S]}$: indirect emission to soil 2, resulting from application of sewage sludge at scale S [mol.s^{-1}] *(D)*

$Edirect_{\mathrm{soil\,i}}$ may be derived by means of:

$$Edirect_{soil\,i[S]} = PRODUCTION_{[S]}\, EMISfact_{soil\,i[S]} \qquad \textbf{233}$$

with

$Edirect_{soil\,i[S]}$: sum of all direct emissions to soil i at scale S [mol.s^{-1}] *(D)*
$PRODUCTION_{[S]}$: total amount produced or imported in scale S [mol.s^{-1}] *(A)*
$EMISfact_{soil\,i[S]}$: emission factor for soil i: the fraction of the production volume that is released to soil i at scale S [-] *(A)*

The following default values may serve as a starting point:

$$EMISfact_{soil\,1[S]} = 0 \qquad \textbf{234}$$

$$EMISfact_{soil\,2[S]} = 0.1\% \qquad \textbf{235}$$

$$EMISfact_{soil\,3[S]} = 0.1\% \qquad \textbf{236}$$

with

$EMISfact_{soil\,i[S]}$: emission factor for soil i: the fraction of the production volume that is released soil i at scale S [-] *(A)*

3.10.3 Degradation

The apparent degradation mass flows from soil are obtained from:

$$DEGRD_{soil\,i[S]} = V_{soil\,i[S]} \cdot DEG_{soil\,i[S]} \cdot C_{soil\,i[S]} \qquad \textbf{237}$$

with

$DEGRD_{soil\,i[S]}$: degradation mass flow from the soil i at scale S [mol.s^{-1}] *(I)*
$V_{soil\,i[S]}$: volume of soil i at scale S [m$_{\mathrm{soil}}^{3}$] *(I)*
$DEG_{soil\,i[s]}$: pseudo first order transformation rate constant in soil i at scale S [s^{-1}] *(I)*
$C_{soil\,i[S]}$: bulk concentration in soil i at scale S [mol.m$_{\mathrm{soil}}^{-3}$] *(S)*

$$DEG_{soil\,i[S]} = kdeg_{soil\,i[S]} \qquad \textbf{238}$$

with

$DEG_{soil\,i[S]}$: pseudo first order transformation rate constant in soil i at scale S [s^{-1}] *(I)*
$kdeg_{soil\,i[S]}$: pseudo first order transformation rate constant in soil i at scale S [s^{-1}] *(D)*

A value for $kdeg_{soil}$ may be obtained by the equations given in paragraph 3.5.4.

3.10.4 Leaching

The mass flows for removal from soil by leaching are obtained from:

$$LCH_{soil\,i[S]} = LEACHING_{soil\,i[S]} \cdot C_{soil\,i[S]} \tag{239}$$

with

$LCH_{soil\,i[S]}$: leaching mass flow from soil i at scale S [$mol.s^{-1}$] *(I)*
$LEACHING_{soil\,i[S]}$: transport coefficient for leaching from soil i at scale S [$m_{soil}^{3}.s^{-1}$] *(I)*
$C_{soil\,i[S]}$: bulk concentration in soil i at scale S [$mol.m_{soil}^{-3}$] *(S)*

$$LEACHING_{soil\,i[S]} = LEACH_{soil\,i[S]} \cdot SYSTEMAREA_{[S]} \cdot AREAFRAC_{soil\,i[S]} \tag{240}$$

with

$LEACHING_{soil\,i[S]}$: transport coefficient for leaching from soil i at scale S [$m_{soil}^{3}.s^{-1}$] *(I)*
$LEACH_{soil\,i[S]}$: mass transfer coefficient for leaching from soil i at scale S [$m_{soil}.s^{-1}$] *(D)*
$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^{2}] *(D)*
$AREAFRAC_{soil\,i[S]}$: fraction of the scale S that is soil i at scale S [-] *(D)*

The mass transfer coefficient for leaching can be found in paragraph 3.6.5.

3.10.5 Advection

The mass flows for advective transport from soil to water by run-off are obtained from:

$$ADV_{soil\,i\text{-}water[S]} = RUN\text{-}OFF_{soil\,i[S]} \cdot C_{soil\,i[S]} \tag{241}$$

with

$ADV_{soil\,i\text{-}water[S]}$: run-off mass flow from the soil i to water at scale S [$mol.s^{-1}$] *(I)*
$RUN\text{-}OFF_{soil\,i[S]}$: transport coefficient for run-off from soil i at scale S [$m_{soil}^{3}.s^{-1}$] *(I)*
$C_{soil\,i[S]}$: bulk concentration in soil i at scale S [$mol.m_{soil}^{-3}$] *(S)*

$$RUN\text{-}OFF_{soil\,i[S]} = RUNOFF_{soil\,i[S]} \cdot SYSTEMAREA_{[S]} \cdot AREAFRAC_{soil\,i[S]} \tag{242}$$

with

$RUN\text{-}OFF_{soil\,i[S]}$: transport coefficient for run-off from soil i at scale S [$m_{soil}^{3}.s^{-1}$] *(I)*
$RUNOFF_{soil\,i[S]}$: mass transfer coefficient for run-off from soil i at scale S [$m_{soil}.s^{-1}$] *(D)*
$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^{2}] *(D)*
$AREAFRAC_{soil\,i[S]}$: fraction of scale S that is soil i [-] *(D)*

The equation for the mass transfer coefficient for *RUNOFF* can be found in paragraph 3.6.4.

Advective transport from air to soil by atmospheric deposition has been described in paragraph 3.6.1 and 3.7.6, equations 147, 148, 184, 186.

3.10.6 Diffusion

Diffusive transport between air and soil by means of gas absorption and volatilization has been described in paragraph 3.6.2 and 3.7.7, equations 150, 152, 188, 191, 193, 195.

3.11 The vegetation compartment

In SimpleBox 2.0 a vegetation compartment[f] is defined on the natural and agricultural soil compartments at the regional and continental scales. A more detailed discription of the vegetation module can be found in Severinsen et al. (in prep.). The vegetation sub-model treats the above-ground parts of the vegetation as one well-mixed box. The roots of the vegetation are treated as an integral part of the soil compartment. The used equations presented here are only valid for for nonionized organic micropollutants. The fate processes included for this compartment are: diffusive exhange with air, advective transport from air to vegetation by deposition, degradation in plant tissue, uptake from soil with the transpiration stream, advective transport to soil by plant death and harvest.

3.11.1 Mass balance

The mass balance equations for the vegetation compartments are:

$$\begin{aligned} V_{veg\,i[S]}\cdot\frac{dC_{veg\,i[S]}}{dt} &= + DEP_{veg\,i[S]}\cdot C_{air[S]} - V_{veg\,i[S]}\cdot DEG_{veg\,i[S]}\cdot C_{veg\,i[S]} \\ &\quad + XCH_{air\text{-}veg\,i[S]}\cdot C_{air[S]} - XCH_{veg\,i\text{-}air[S]}\cdot C_{veg\,i[S]} \\ &\quad + \sum ADV_{soil\,i-veg\,i[S]}\cdot C_{soil\,i[S]} - \sum ADV_{veg\,i-soil\,i[S]}\cdot C_{veg\,i[S]} \\ &\quad - REMOVAL_{veg\,i[S]}\cdot C_{veg\,i[S]} \end{aligned} \tag{243}$$

with

$V_{veg\,i[S]}$: volume of the vegetation compartment i at scale S [m_{soil}^3] *(I)*

$C_{veg\,i[S]}$: total concentration in vegetation compartment i at scale S [$mol.m_{veg}^{-3}$] *(S)*

$C_{soil\,i[S]}$: total concentration in soil i (gas phase + water phase + solid phase) at scale S [$mol.m_{soil}^{-3}$] *(S)*

$C_{air[S]}$: total concentration in air at scale S [$mol.m_{air}^{-3}$] *(S)*

t : time [s] *(S)*

$DEP_{veg\,i[S]}$: transport coefficient for atmospheric deposition to vegetation i at scale S [$m_{air}^3.s^{-1}$] *(I)*

$DEG_{veg\,i[S]}$: pseudo first order transformation rate constant in vegetation i at scale S [s^{-1}] *(I)*

$XCH_{veg\,i\text{-}air[S]}$: transport coefficient volatilization from vegetation i at scale S [$m_{soil}^3.s^{-1}$] *(I)*

$XCH_{air\text{-}veg\,i[S]}$: transport coefficient gas absorption to vegetation i at scale S [$m_{air}^3.s^{-1}$] *(I)*

$ADV_{soil\,i\text{-}veg\,i[S]}$: transport coefficient of the transpiration stream from soil i to vegetation I at scale S [$m_{soil}^3.s^{-1}$] *(I)*

$ADV_{veg\,i\text{-}soil\,i[S]}$: transport coefficient for plant death at scale S [$m_{soil}^3.s^{-1}$] *(I)*

$REMOVAL_{veg\,i[S]}$: transport coefficient for harvesting of vegetation i at scale S [$m_{soil}^3.s^{-1}$] *(I)*

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[f] The vegetation module for calculating the environmental fate of chemicals as described here, is not a part of EUSES.

3.11.2 Vegetation compartment characteristics

The volume of the vegetation compartment can be obtained from:

$$VOLUME_{veg\ i[S]} = SYSTEMAREA_{[S]} \cdot AREAFRAC_{soil\ i[S]} \cdot \frac{D_{veg\ i[S]}}{RHO_{veg\ i[S]}} \qquad \mathbf{244}$$

with

$VOLUME_{veg\ i[S]}$: volume of the above-ground plant parts [m^3] *(D)*
$D_{veg\ i[S]}$: area specific above-ground biomass [$\mathrm{kg_{plant}.m^{-2}}$] *(D)*
$RHO_{veg\ i[S]}$: density of plant tissue [$\mathrm{kg_{plant}.m^{-3}}$] *(D)*
$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{soil\ i[S]}$: fraction of scale S that is soil i [-] *(D)*

The area specific above-ground biomass and density are taken from Severinsen and Jager (in prep.):

$$D_{veg\ 1[S]} = 1.2\ kg.m^{-2} \qquad \mathbf{245}$$

with

$D_{veg\ 1[S]}$: area specific above-ground biomass of vegetation 1 [$\mathrm{kg_{plant}.m^{-2}}$] *(D)*

$$D_{veg\ 2[S]} = 1.8\ kg.m^{-2} \qquad \mathbf{246}$$

with

$D_{veg\ 2[S]}$: area specific above-ground biomass of vegetation 2 [$\mathrm{kg_{plant}.m^{-2}}$] *(D)*

$$RHO_{veg\ i[S]} = 900\ kg.m^{-3} \qquad \mathbf{247}$$

with

$RHO_{veg\ i[S]}$: density of plant tissue at scale S [$\mathrm{kg_{plant}.m^{-3}}$] *(D)*

The leaf surface area is obtained from the leaf area index and the area of the soil:

$$AREA_{leaves\ i[S]} = K_{leaf-soilarea\ i[S]} \cdot SYSTEMAREA_{[S]} \cdot AREAFRAC_{soil\ i[S]} \qquad \mathbf{248}$$

with

$AREA_{leaves\ i[S]}$: leaf surface area of vegetation i at scale S [m^2] *(D)*
$K_{leaf\text{-}soilarea\ i[S]}$: leaf area index of vegetation i at scale S [$\mathrm{m_{leaf\ surface}^{2}.m_{soil}^{-2}}$] *(D)*
$SYSTEMAREA_{[S]}$: total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{soil\ i[S]}$: fraction of scale S that is soil i [-] *(D)*

$$K_{leaf-soilarea\ 1[S]} = 3.9 \qquad \mathbf{249}$$

with

$K_{leaf\text{-}soilarea\ i[S]}$: leaf area index of vegetation 1 at scale S [$\mathrm{m_{leaf\ surface}}^{2}.\mathrm{m_{soil}}^{-2}$] *(D)*

$$K_{leaf-soilarea\ 1[S]} = 2.7 \tag{250}$$

with

$K_{leaf\text{-}soilarea\ i[S]}$: leaf area index of vegetation 1 at scale S [$\mathrm{m_{leaf\ surface}}^{2}.\mathrm{m_{soil}}^{-2}$] *(D)*

3.11.3 Transformation processes

The apparent degradation mass flow from air of the different scales is obtained from:

$$DEGRD_{veg\ i[S]} = VOLUME_{veg\ i[S]} \cdot DEG_{veg\ i[S]} \cdot C_{veg\ i[S]} \tag{251}$$

with

$DEGRD_{veg\ i[S]}$: degradation mass flow from the vegetation compartment i of scale S [$\mathrm{mol.s^{-1}}$] *(I)*
$VOLUME_{veg\ i[S]}$: volume of the vegetation compartment i of scale S [$\mathrm{m^3}$] *(I)*
$DEG_{veg\ i[S]}$: pseudo first order transformation rate constant of vegetation i at scale S [$\mathrm{s^{-1}}$] *(I)*
$C_{veg\ i[S]}$: total concentration in the vegetation compartment i at scale S [$\mathrm{mol.m_{vegetation}}^{-3}$] *(S)*

$$DEG_{veg\ i[S]} = kdeg_{veg\ i[S]} \tag{252}$$

with

$DEG_{veg\ i[S]}$: pseudo first order transformation rate constant of vegetation i at scale S [$\mathrm{s^{-1}}$] *(I)*
$kdeg_{veg\ i[S]}$: pseudo first order transformation rate constant of vegetation i at scale S [$\mathrm{s^{-1}}$] *(D)*

The removal process metabolism in the vegetation is based on the degradation rate in soil, photodegradation in plants is excluded:

$$kdeg_{veg\ i[S]} = kdeg_{meta[S]} \tag{253}$$

with

$kdeg_{veg\ i[S]}$: pseudo first order transformation rate constant of vegetation i at scale S [$\mathrm{s^{-1}}$] *(D)*
$kdeg_{meta[S]}$ pseudo first order metabolism rate constant of vegetation i at scale S [$\mathrm{s^{-1}}$] *(D)*

$$kdeg_{meta[S]} = kdeg_{soil\ 1[S]} \cdot 10 \tag{254}$$

with

$kdeg_{meta[S]}$ pseudo first order metabolism rate constant of vegetation i at scale S [$\mathrm{s^{-1}}$] *(D)*
$kdeg_{soil\ 1[S]}$: pseudo first order transformation rate constant in soil 1 at scale S [$\mathrm{s^{-1}}$] *(D)*

as a starting point.

3.11.4 Partition coefficients for plant tissue

For non-ionized xenobiotics, the concentration ratio between plant tissue and water in thermodynamic equilibrium is estimated from the water and lipid contents of plant tissue (Severinsen and Jager, in prep.):

$$K_{leaf\,i-water[S]} = FRwater_{veg\,i[S]} + FRlipid_{veg\,i[S]} * Kow^{0.95} \tag{255}$$

with

$K_{leaf\,i\text{-}water[S]}$: plant tissue-water partition coefficient at scale S $[m^3.m^{-3}]$ *(A)*

$FRwater_{veg\,i[S]}$: volume fraction water in plant tissue at scale S $[m^3.m^{-3}]$ *(A)*

$FRlipid_{veg\,i[S]}$: volume fraction water in plant tissue at scale S $[m^3.m^{-3}]$ *(A)*

Kow : octanol-water partitioning coeffient of the chemical $[mol.m_{octanol}^{3}.mol.m_{water}^{-3}]$ *A)*

b : correction exponent for difference fat and octanol [-] *(A)*

The concentration ratio between plant tissue and air in thermodynamic equilibrium is estimated from the concentation ratio between plant tissue and water and the dimensionless Henry's law constant: (Severinsen and Jager, in prep.):

$$K_{leaf\,i-air[S]} = K_{leaf\,i-water[S]} \cdot K_{air-water[S]} \tag{256}$$

with

$K_{leaf\,i\text{-}water[S]}$: plant tissue-water partition coefficient at scale S $[m^3.m^{-3}]$ *(A)*

$K_{leaf\,i\text{-}air[S]}$: plant tissue-air partition coefficient at scale S $[m^3.m^{-3}]$ *(A)*

$K_{air\text{-}water\,[S]}$: air-water equilibrium distribution constant at scale S $[mol.m_{air}^{-3}.mol.m_{water}^{-3}]$ *(A)*

3.11.5 Diffusive transport

Diffusive transport between air and vegetation by means of gas absorption and volatilization is described by:

$$DIFF_{air\text{-}veg\,i[S]} = XCH_{air\text{-}veg\,i[S]} \cdot C_{air[S]} \tag{257}$$

with

$DIFF_{air\text{-}veg\,i[S]}$: diffusive mass flow from air to vegetation i at scale S by gas absorption $[mol.s^{-1}]$ *(I)*

$XCH_{air\text{-}veg\,i[S]}$: transport coefficient for gas absorption by vegetation i at scale S $[m_{air}^{3}.s^{-1}]$ *(I)*

$C_{air[S]}$: total concentration in air (gas phase + aerosol phase + rain water phase) at scale S $[mol.\ m_{air}^{-3}]$ *(S)*

$$XCH_{air\text{-}veg\,i[S]} = GASABS_{veg\,i[S]} \cdot AREA_{leaves\,i[S]} \tag{258}$$

with

$XCH_{air\text{-}veg\ i[S]}$:	transport coefficient for gas absorption to vegetation i at scale S [$m_{air}^3.s^{-1}$] *(I)*
$GASABS_{veg\ i[S]}$:	overall mass transfer coefficient for gas absorption across the air-vegetation interface, referenced to air at scale S [$m_{air}.s^{-1}$] *(D)*
$AREA_{leaves\ i[S]}$:	leaf surface area at scale S [-] *(D)*

$$GASABS_{veg\ i[S]} = (1 - FRass_{aerosol[S]}) \cdot g_{veg\ i[S]} \tag{259}$$

with

$GASABS_{veg\ i[S]}$:	overall mass transfer coefficient for gas absorption across the air-vegetation interface, referenced to air at scale S [$m_{air}.s^{-1}$] *(D)*
$FRass_{aerosol[S]}$:	fraction of the chemical in air that is associated with aerosol particles at scale S [-] *(A)*
$g_{veg\ i[S]}$:	conductance [$m.s^{-1}$] *(D)*

The conductance, g_{veg}, depends on the chemical properties, plant species and environmental conditions (Trapp and Matthies, 1995):

$$g_{veg\ i[S]} = 0.001\ m.s^{-1} \tag{260}$$

with

$g_{veg\ i[S]}$:	conductance [$m.s^{-1}$] *(D)*

may be taken as default value.

The volatilization mass flows are obtained from:

$$DIFF_{veg\ i\text{-}air[S]} = XCH_{veg\ i\text{-}air[S]} \cdot C_{veg\ i[S]} \tag{261}$$

with

$DIFF_{veg\ i\text{-}air[S]}$:	diffusive mass flow from vegetation i to air at scale S by volatilization [$mol.s^{-1}$] *(I)*
$XCH_{veg\ i\ air[S]}$:	transport coefficient for volatilization from vegetation i at scale S [$m_{veg}^3.s^{-1}$] *(I)*
$C_{veg\ i[S]}$:	dissolved concentration in vegetation i at scale S [$mol.m_{veg}^{-3}$] *(S)*

$$XCH_{veg\ i\text{-}air[S]} = VOLAT_{veg\ i[S]} \cdot AREA_{leaves\ i[S]} \tag{262}$$

with

$XCH_{veg\ i\ \text{-}air}$:	transport coefficient for volatilization from vegetation i at scale S [$m_{veg}^3.s^{-1}$] *(I)*
$VOLAT_{veg\ i[S]}$:	overall mass transfer coefficient for volatilization across the vegetation-air interface, referenced to vegetation i at scale S [$m_{water}.s^{-1}$] *(D)*
$AREA_{leaves\ i[S]}$:	leaf surface area at scale S [-] *(D)*

$$VOLAT_{veg\ i[S]} = \frac{g_{veg\ i[S]}}{K_{leafi\text{-}air[S]}} \tag{263}$$

with

$VOLAT_{veg\ i[S]}$:	overall mass transfer coefficient for volatization across the air-vegetation interface, referenced to vegetation at scale S [$m_{air}.s^{-1}$] *(D)*
$g_{veg\ i[S]}$:	conductance [$m.s^{-1}$] *(D)*
$K_{leaf\ i\text{-}air[S]}$:	plant tissue-air partition coefficient at scale S [$m^3.m^{-3}$] *(A)*

3.11.6 Advective transport

3.11.6.1 Deposition

Advective transport from air to vegetation takes place by atmospheric deposition of the chemical associated with small particles. The deposition mass flows are obtained from:

$$ADV_{air\text{-}veg\ i[S]} = DEP_{veg\ i[S]} \cdot C_{air[S]} \qquad \textbf{264}$$

with

$ADV_{veg\ i[S]}$:	advective mass flow from air to vegetation i at scale S by atmospheric deposition [$mol.s^{-1}$] *(I)*
$DEP_{veg\ i[S]}$:	transport coefficient for atmospheric depositionto vegetation i at scale S [$m_{air}^3.s^{-1}$] *(I)*
$C_{air[S]}$:	total concentration in air (gas phase + aerosol phase + rain water phase) at scale S [$mol.m_{air}^{-3}$] *(S)*

$$DEP_{veg\ i[S]} = DEP_{air-veg\ i[S]}.SYSTEMAREA_{[S]}.AREAFRAC_{soil\ i[S]} \qquad \textbf{265}$$

with

$DEP_{veg\ i\ [S]}$:	transport coefficient for atmospheric deposition (wet and dry) to water i at scale S [$m_{air}^3.s^{-1}$] *(I)*
$DEP_{air\text{-}veg\ i[S]}$:	mass transfer coefficient for dry deposition of aerosol-associated chemical at scale S [$m_{air}.s^{-1}$] *(D)*
$SYSTEMAREA_{[S]}$:	total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{soil\ i[S]}$:	fraction of scale S that is soil i [-] *(D)*

$$DEP_{air-veg\ i[S]} = vgrowth_{veg\ i[S]} \cdot \frac{FRcarbon_{veg\ i[S]}}{FRcarbon_{air[S]}} \cdot D_{veg\ i[S]} \cdot FRass_{aerosol[S]} \qquad \textbf{266}$$

with

$DEP_{air\text{-}veg\ i[S]}$:	mass transfer coefficient for dry deposition of aerosol-associated chemical at scale S [$m_{air}.s^{-1}$] *(D)*
$vgrowth_{veg\ i[S]}$:	above ground vegetation growth rate [s^{-1}] *(A)*
$FRcarbon_{veg\ i[S]}$:	weight fraction carbon of vegetation [$kgC.kg_{plant}^{-1}$] *(A)*
$FRcarbon_{air\ i[S]}$:	carbon concentration in air [$kgC.m^{-3}$] *(A)*
$D_{veg\ i[S]}$:	area specific above-ground biomass [$kg_{plant}.m^{-2}$] *(D)*

$$vgrowth_{veg\ i[S]} = \frac{1}{Residencetime_{veg\ i[S]}}$$ **267**

with

$vgrowth_{veg\ i[S]}$:	above ground vegetation growth rate [s^{-1}] *(A)*
$Residencetime_{veg\ i[S]}$:	residence time for above-ground plant tissue [s] *(S)*

The residence time for "natural" and "agricultural" vegetation is taken from Severinsen and Jager (in prep.):

$$Residencetime_{veg\ 1[S]} = 402\ days$$ **268**

with

$Residencetime_{veg\ 1[S]}$:	residence time for above-ground plant tissue of vegetation 1[d] *(S)*

$$Residencetime_{veg\ 2[S]} = 91\ days$$ **269**

with

$Residencetime_{veg\ i[S]}$:	residence time for above-ground plant tissue of vegetation 2[d] *(S)*

3.11.6.2 Transpiration

The uptake from soil via the roots with the transpiration stream of the xylem sap is calculated from the concentration in soil and the transpiration rate:

$$ADV_{soil\text{-}veg\ i[S]} = TRANS_{veg\ i[S]} \cdot C_{soil\ i[S]}$$ **270**

with

$ADV_{soil\text{-}veg\ i[S]}$:	advective mass flow from soil i to vegetation i at scale S by transpiration stream [$mol.s^{-1}$] *(I)*
$TRANS_{veg\ i[S]}$:	transport coefficient for evapotranspiration to vegetation i at scale S [$m^3.s^{-1}$] *(I)*
$C_{soil\ i[S]}$:	concentration in soil i at scale S [$mol.m^{-3}$] *(S)*

$$TRANS_{veg\ i[S]} = TRANS_{soili-veg\ i[S]} \cdot SYSTEMAREA_{[S]} \cdot AREAFRAC_{soil\ i[S]}$$ **271**

with

$TRANS_{veg\ i\ [S]}$:	transport coefficient for evapotranspiration to vegetation i at scale S [$m_{air}^3.s^{-1}$] *(I)*
$TRANS_{soil\ i\text{-}veg\ i[S]}$:	mass transfer coefficient for evapotranspiration stream at scale S [$m_{water}.s^{-1}$] *(D)*
$SYSTEMAREA_{[S]}$:	total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{soil\ i[S]}$:	fraction of scale S that is soil i [-] *(D)*

$$TRANS_{soil\,i-veg\,i[S]} = Q_{veg\,i[S]} \cdot TSCF_{vegi[S]} \,/\, K_{soili-water[S]} \qquad 272$$

with

$TRANS_{soil\,i\text{-}veg\,i[S]}$:	mass transfer coefficient for evapotranspiration stream at scale S [$m_{water}.s^{-1}$] *(D)*
$Q_{veg\,i[S]}$:	area specific transpiration rate [s^{-1}] *(A)*
$TSCF_{veg\,i[S]}$:	transpiration stream concentration factor [$m_{soilwater}^{3}.m_{xylem\ sap}^{-3}$] *(A)*
$K_{soil\,i\text{-}water[S]}$:	soil-water equilibrium distribution constant at scale S [$mol.m_{soil}^{-3}.molm_{water}^{-3}$] *(A)*

For organic xenobiotics, the transpiration stream concentration factor, *TSCF*, is related to *Kow*. The estimation method of Briggs et al. (1982) is adopted here:

$$TSCF_{veg\,i[S]} = 0.784 \cdot e^{\frac{-(log\,Kow-1.78)^2}{2.44}} \qquad 273$$

with

$TSCF_{veg\,i[S]}$:	transpiration stream concentration factor [$m_{soilwater}^{3}.m_{xylem\ sap}^{-3}$] *(A)*
Kow :	octanol-water partitioning coeffient of the chemical [$mol.m_{octanol}^{3}.mol.m_{water}^{-3}$] *A)*

$$Q_{veg\,1[S]} = 8.40 \cdot 10^{-9} \qquad 274$$

with

$Q_{veg\,1[S]}$:	area specific transpiration rate for “natural” vegetation [s^{-1}] *(A)*

may be taken as default value for transpiration (transpiration by trees excluded), (Severinsen and Jager, in prep.).

$$Q_{veg\,2[S]} = 2.50 \cdot 10^{-8} \qquad 275$$

with

$Q_{veg\,2[S]}$:	area specific transpiration rate for “agricultural” vegetation [s^{-1}] *(A)*

average transpiration based on a total production of 7800 $kgC.ha_{agricultural\ soil}.yr^{-1}$.

3.11.6.3 Plant death, harvest and growth

Death of above-ground plant parts will result in transport of the chemical from the vegetation compartment to the soil/roots compartment. Harvest will result in transport of the chemical from the vegetation compartment out of the system. Growth dilutes the mass of chemical in the vegetation, plant growth supplies unpolluted plant tissue to the vegetation compartment. In SimpleBox constant mass is assumed of the vegetation compartment. Therefore, the growth rate, *vgrowth,* must be equal to the sum of the harvest rate, *vharvest*, and the death rate, *vdeath.*

$$ADV_{veg\,i-soil\,i[S]} = DEATH_{veg\,i[S]} \cdot C_{veg\,i[S]} \qquad 276$$

with

$ADV_{veg\,i\text{-}soil\,i[S]}$:	advective mass flow from vegetation to soil i at scale S by plant death [$mol.s^{-1}$] *(I)*

$DEATH_{veg\,i[S]}$: transport coefficient for plant death at scale S [$m_{vegetation}^{3}.s^{-1}$] *(I)*
$C_{veg\,i[S]}$: total concentration in vegetation compartment i at scale S [$mol.m_{vegetation}^{-3}$] *(S)*

$$DEATH_{veg\,i[S]} = vdeath_{veg\,i-soil\,i[S]} \cdot VOLUME_{veg\,i[S]} \tag{277}$$

with

$DEATH_{veg\,i[S]}$: transport coefficient for plant death at scale S [$m_{air}^{3}.s^{-1}$] *(I)*
$vdeath_{veg\,i[S]}$: vegetation death rate [s^{-1}] *(A)*
$VOLUME_{veg\,i[S]}$: volume of the above-ground plant parts [m^{3}] *(D)*

$$vdeath_{veg\,i[S]} = \frac{1 - EFFharvest_{veg\,i[S]}}{Residencetime_{veg i[S]}} \tag{278}$$

with

$vdeath_{veg\,i[S]}$: vegetation death rate [s^{-1}] *(A)*
$EFFharvest_{veg\,i[S]}$: harvest efficiency of vegetation i at scale S [-] *(I)*
$Residencetime_{veg\,i[S]}$: residence time for above-ground plant tissue [$mol.m_{air}^{-3}$] *(S)*

$$REMOVAL_{veg\,i[S]} = (REMOVAL_{above-veg\,i[S]} + REMOVALroots_{veg\,i[S]}) \cdot C_{veg\,i[S]} \tag{279}$$

with

$HARVEST_{veg\,i[S]}$: advective mass flow from vegetationout of the system by harvest [$mol.s^{-1}$] *(I)*
$REMOVAL_{above-veg\,i[S]}$: transport coefficient for harvesting of above-plant parts at scale S [$m_{vegetation}^{3}.s^{-1}$] *(I)*
$REMOVALroots_{veg\,i[S]}$: transport coefficient for harvesting of roots of the vegetation at scale S [$m_{vegetation}^{3}.s^{-1}$] *(I)*
$C_{veg\,i[S]}$: total concentration in vegetation compartment i at scale S[$mol.m_{vegetation}^{-3}$] *(S)*

$$REMOVAL_{above-veg\,i[S]} = vharvest_{veg\,i[S]} \cdot VOLUME_{veg\,i[S]} \tag{280}$$

with

$REMOVAL_{above-veg\,i[S]}$: transport coefficient for harvesting of above-plant parts at scale S [$m_{vegetation}^{3}.s^{-1}$] *(I)*
$vharvest_{veg\,i[S]}$: vegetation harvest rate [s^{-1}] *(A)*
$VOLUME_{veg\,i[S]}$: volume of the above-ground plant parts [m^{3}] *(D)*

$$vharvest_{veg\,i[S]} = \frac{EFFharvest_{veg\,i[S]}}{Residencetime_{veg\,i[S]}} \tag{281}$$

with

$vharvest_{veg\,i[S]}$: vegetation harvest rate [s^{-1}] *(A)*
$EFFharvest_{veg\,i[S]}$: harvest efficiency of vegetation i at scale S [-] *(A)*
$Residencetime_{veg\,i[S]}$: residence time for above-ground plant tissue [s] *(S)*

$$EFFharvest_{veg\,2[S]} = 0.59 \qquad \mathbf{282}$$

with

$EFFharvest_{veg\,2[S]}$:	harvest efficiency of vegetation 2 at scale S [-] *(A)*

$$REMOVALroots_{veg\,2[S]} = 0.0021 \cdot SYSTEMAREA_{[S]} \cdot AREAFRAC_{soil\,i[S]} \qquad \mathbf{283}$$

with

$REMOVALroots_{-veg\,2[S]}$:	transport coefficient for harvesting of root crops at scale S [$m_{vegetation} \cdot s^{-1}$] *(I)*
$SYSTEMAREA_{[S]}$:	total area of scale S (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{soil\,i[S]}$:	fraction of scale S that is soil i [-] *(D)*
0.0021	root crops harvest rate [-] *(D)*

4. MODEL OUTPUT

SimpleBox produces two sorts of output:

1. Steady-state or "level 3" output. If the conditions (loadings and environmental conditions) remain constant in time for a sufficiently long period of time, eventually a steady state, in which all mass flows and concentrations are constant in time, will develop. At steady state, the sum of the mass balance equation terms is equal to zero for all boxes, and the n steady-state concentrations can be solved from the n linear mass balance equations. This steady-state solution is obtained in SimpleBox by means of a matrix inversion routine. The mass flows and concentrations that characterize this steady state are written by SimpleBox in output tables.
2. Quasi-dynamic or "level 4" output. After a change in conditions (loadings or environmental conditions), mass flows and concentrations develop toward a new steady state, according to the mass balance equations. The "level 4" computation is done by numerical integration of the set of mass balance equations from time zero, with all concentrations at zero, to infinite time with all concentrations constant at steady state.

The standard procedure in SimpleBox is to compute the steady-state solution first and carry out the dynamic response computation afterwards, as an option.

4.1 Steady-state Computation

The model description in SimpleBox consists of the eight mass balance equations described in the previous paragraphs. In SimpleBox 10 boxes are defined for the regional and the continental system, the global scales consists of 4 boxes. InTable 10, the box numbers are given for the compartments of the different scales:

Table 10: The boxes of SimpleBox

Box	Scale	Compartment	Box	Scale	Compartment
1	regional	air	17	moderate	air
2	regional	water 1	18	moderate	water
3	regional	water 2	19	moderate	sediment
4	regional	sediment 1	20	arctic	air
5	regional	sediment 2	21	arctic	water
6	regional	soil 1	22	arctic	sediment
7	regional	soil 2	23	tropic	air
8	regional	soil 3	24	tropic	water
9	continental	air	25	tropic	sediment
10	continental	water 1	26	moderate	soil
11	continental	water 2	27	arctic	soil
12	continental	sediment 1	28	tropic	soil
13	continental	sediment 2	29	regional	vegetation
14	continental	soil 1	30	regional	vegetation
15	continental	soil 2	31	continental	vegetation
16	continental	soil 3	32	continental	vegetation

At steady state, all balances become equal to zero:

$$V_i \cdot \frac{dC_i}{dt} = EMIS_i + IMP_i - EXP_i - LCH_i - BRL_i - DEGRD_i + \sum ADV_{i\text{-}j} + \sum DIFF_{i\text{-}j} = 0 \qquad \mathbf{284}$$

with

$V_{i,S}$:	volume of box i [m^3] *(I)*
$C_{i,S}$:	concentration in box i [mol.m^{-3}] *(S)*
$EMIS_{i,S}$:	emission mass flow into box i [mol.s^{-1}] *(I)*
t :	time [s] *(S)*
$IMP_{i,S}$:	import mass flow into box i [mol.s^{-1}] *(I)*
$EXP_{i,S}$:	export mass flow from box i [mol.s^{-1}] *(I)*
$LCH_{i,S}$:	leaching mass flow from box i [mol.s^{-1}] *(I)*
$BRL_{i,S}$:	apparent burial mass flow from box i [mol.s^{-1}] *(I)*
$DEGRD_{i,S}$:	apparent degradation mass flow from box i [mol.s^{-1}] *(I)*
$ADV_{(i\text{-}j),S}$:	advective mass flows to and from box i [mol.s^{-1}] *(I)*
$DIFF_{(i\text{-}j),S}$:	diffusive mass flows to and from box i [mol.s^{-1}] *(I)*

The mass balances are rewritten as:

$$CNST_i = CF_{ii} \cdot Css_i + \sum (CF_{ij} \cdot Css_j) \qquad \mathbf{285}$$

with

$CNST_i$:	constant term in mass balance of box i [mol.s^{-1}] *(I)*
CF_{ii} :	sum of coefficients for (apparent) transport from box i to elsewhere [m$^3_{\text{medium i}}$.s^{-1}] *(I)*
CF_{ij} :	sum of coefficients for transport from compartment j to box I [m$^3_{\text{medium i}}$.s^{-1}] *(I)*
Css_i :	steady-state concentration in box i [mol.m$_{\text{medium i}}^{-3}$] *(I)*
Css_j :	steady-state concentration in compartment j [mol.m$_{\text{medium j}}^{-3}$] *(I)*

where

$$CNST_i = -EMIS_i - IMP_i \qquad \mathbf{286}$$

with

$CNST_i$:	constant term in mass balance of box i [mol.s^{-1}] *(I)*
$EMIS_i$:	emission mass flow into box i [mol.s^{-1}] *(I)*
IMP_i :	import mass flow into box i [mol.s^{-1}] *(I)*

In matrix-format, the set of eight mass balances reads:

$$\overline{CNST} = CF.\overline{Css} \qquad \textbf{287}$$

with

CNST :	vector of constant terms of mass balance equations *(I)*
CF :	matrix of coefficients *(I)*
Css :	vector of steady-state concentrations *(I)*

As the product of a matrix and its inverse is equals to 1, the solution of the set of mass balances can be obtained by multiplying the left and right parts of287 by the inverse of the matrix of coefficients:

$$CF^{-1}.CF.\overline{Css} = \overline{Css} = CF^{-1}.\overline{CNST} \qquad \textbf{288}$$

SimpleBox uses this matrix-inversion method to produce the steady-state output. The steady-state computation procedure produces the following output:

Steady-state concentrations in "standard units"

The elements Css_1-Css_{32} of the vector *Css*, computed as described above, are expressed in the internal SimpleBox-dimensions of $mol.m_{medium}^{-3}$. These variables are only used internally; they are not shown in the SimpleBox output tables.

Steady-state hold-up

The amount of the chemical present in each of the compartments at steady state is computed by:

$$HOLD\text{-}UP_i = Css_i.V_i \qquad \textbf{289}$$

with

$HOLD\text{-}UP_i$:	amount of the chemical in box i at steady state [mol] *(I)*
Css_i :	steady-state concentration in box i [$mol.m^{-3}$] *(I)*
V_i :	volume of box i [m^3] *(I)*

The total hold-up in the system is obtained by summation:

$$SYSTEMHOLD\text{-}UP = \Sigma HOLD\text{-}UP_i \qquad \textbf{290}$$

with

SYSTEM HOLD-UP :	total amount of the chemical in the system at steady state [mol] *(I)*

$HOLD\text{-}UP_i$:	hold-up at steady state in box i [mol] *(I)*

These variables are not shown in the SimpleBox output tables.

Steady-state distribution

The steady-state distribution of the chemical is obtained by expressing the steady-state hold-ups as a percentage of the *SYSTEM HOLD-UP*:

$$DISTRIBUTION_i = \frac{HOLD\text{-}UP_i}{SYSTEMHOLD\text{-}UP}.100 \qquad \mathbf{291}$$

with

$DISTRIBUTION_i$:	percentage of the chemical in box i at steady state [%] *(O)*
$HOLD\text{-}UP_i$:	amount of the chemical in box i at steady state [mol] *(I)*
SYSTEM HOLD-UP :	total amount of the chemical in the system at steady state [mol] *(I)*

The distribution percentages are shown in the SimpleBox output table 3.

Steady-state mass flows

The steady-state mass flows of the chemical, i.e. the terms of equation 284, are computed by means of the equations described in the previous paragraphs. As a check for the integrity of the steady-state computation, the mass flows are summed for each of the boxes:

$$INPUT_i = EMIS_i + IMP_i + \Sigma ADV_{j\text{-}i} + \Sigma DIFF_{j\text{-}i} \qquad \mathbf{292}$$

$$OUTPUT_i = EXP_i + LCH_i + BRL_i + DEGRD_i + \Sigma ADV_{i\text{-}j} + \Sigma DIFF_{i\text{-}j} \qquad \mathbf{293}$$

with

$INPUT_i$:	sum of the mass flows into box i [mol.s^{-1}] *(I)*
$EMIS_i$:	emission mass flow into box i [mol.s^{-1}] *(I)*
IMP_i :	import mass flow into box i [mol.s^{-1}] *(I)*
$ADV_{j\text{-}i}$:	advective mass flows to box i [mol.s^{-1}] *(I)*
$DIFF_{j\text{-}i}$:	diffusive mass flows to box i [mol.s^{-1}] *(I)*
$OUTPUT_i$:	sum of the mass flows out of box i [mol.s^{-1}] *(I)*
EXP_i :	export mass flow from box i [mol.s^{-1}] *(I)*
LCH_i :	leaching mass flow from box i [mol.s^{-1}] *(I)*
BRL_i :	apparent burial mass flow from box i [mol.s^{-1}] *(I)*
$DEGRD_i$:	apparent degradation mass flow from box i [mol.s^{-1}] *(I)*
$ADV_{i\text{-}j}$:	advective mass flows from box i [mol.s^{-1}] *(I)*
$DIFF_{i\text{-}j}$:	diffusive mass flows from box i [mol.s^{-1}] *(I)*

At steady state, *INPUT* and *OUTPUT* for each of the boxes as well as in total, should be equal:

$$THROUGHPUT = \Sigma INPUT_i = \Sigma OUTPUT_i \qquad \textbf{294}$$

with

THROUGHPUT:	sum of all mass flows into or out of the system [mol.s^{-1}] *(I)*
$INPUT_i$:	sum of the mass flows into box i [mol.s^{-1}] *(I)*
$OUTPUT_i$:	sum of the mass flows out of box i [mol.s^{-1}] *(I)*

A full mass balance checking table is produced; this is not shown as part of the SimpleBox output. Instead, a separate table of mass flows is produced as SimpleBox output table 2. This table can be displayed in different units to suit the demands of the specific analysis. To do so, the mass flows are expressed as the product of the mass flow in standard units (mol.s^{-1}) and a conversion factor:

$$FLOW_{shown} = FLOW_{standard} \cdot CONVFACTOR_i \qquad \textbf{295}$$

with

$FLOW_{shown}$:	mass flow in chosen units *(I)*
$FLOW_{standard}$:	mass flow in standard units [mol.s^{-1}] *(I)*
$CONVFACTOR_i$:	conversion factor of choice *(I)*

There are four options:

$$CONVFACTOR_1 = 1 \qquad \textbf{296}$$

To express the mass flows in table 2 as mol.s^{-1}.

$$CONVFACTOR_2 = \frac{100}{THROUGHPUT} \qquad \textbf{297}$$

To express the mass flows in table 2 as percentages of the total mass flow through the system at steady state. The most characteristic mass flows ($EMIS_i$, IMP_i, LCH_i, BRL_i, $DEGRD_i$) are shown in this unit in SimpleBox output table 1.

$$CONVFACTOR_3 = (MOLWEIGHT / 1000).(3600.24.365) \qquad \textbf{298}$$

To express the mass flows in table 2 as t.y^{-1}.

$$CONVFACTOR_4 = MOLWEIGHT.(3600.24) \qquad \textbf{299}$$

To express the mass flows in table 2 as kg.d^{-1}.

Steady-state concentrations in "common units"

Steady-state concentrations expressed in "common" units are shown in SimpleBox output table 1. The values are obtained by conversion of the elements of vector *Css*:

$$Css_{air[S]} = Css_i . MOLWEIGHT . 1000 \tag{300}$$

with

$Css_{air[R]}$: steady-state concentration in air at scale S [g.m^{-3}] *(O)*
Css_I : steady-state concentration in box i (1,9,17,20,23) [mol.m^{-3}] *(I)*
MOL WEIGHT : molecular weight of the chemical [kg.mol^{-1}] *(D)*
1000 : conversion factor [g.kg^{-1}]

$$Css_{water\, i[S]} = Css_i . MOLWEIGHT \tag{301}$$

with

$Css_{water\, i[S]}$: steady-state concentration in water i of scale S [g.l^{-1}] *(O)*
Css_i : steady-state concentration in box i (2,3,10,11,18,21,24) [mol.m^{-3}] *(I)*
MOL WEIGHT : molecular weight of the chemical [kg.mol^{-1}] *(D)*

$$Css_{sed\, i[S]} = Css_i . \frac{MOLWEIGHT . Kp_{sed\, i[S]}}{K_{sed\, i\text{-}water[S]}} \tag{302}$$

with

$Css_{sed\, i[S]}$: steady-state concentration in sediment i of scale S [g.kg$_{solid}^{-1}$] *(O)*
Css_i : steady-state concentration in box i (4,5,12,13,19,22,25) [mol.m^{-3}] *(I)*
MOL WEIGHT : molecular weight of the chemical [kg.mol^{-1}] *(D)*
$Kp_{sed\, i[S]}$: sediment-water partition coefficient at scale S [l$_{water}$.kg$_{solid}^{-1}$] *(I)*
$K_{sed\, i\text{-}water[S]}$: sediment-water equilibrium distribution coefficient at scale S [m$_{water}^{3}$.m$_{sed}^{-3}$] *(A)*

$$Css_{pwsed\, i[S]} = Css_i . \frac{MOLWEIGHT}{K_{sed\, i\text{-}water[S]}} \tag{303}$$

with

$Css_{pw\, sed\, i[S]}$: steady-state concentration in pore water of sediment i of scale S [g.l^{-1}] *(O)*
Css_i : steady-state concentration in box i (4,5,12,13,19,22,25) [mol.m^{-3}] *(I)*
MOL WEIGHT : molecular weight of the chemical [kg.mol^{-1}] *(D)*
$K_{sed\, i\text{-}water[S]}$: sediment-water equilibrium distribution coefficient at scale S [m$_{water}^{3}$.m$_{sed}^{-3}$] *(A)*

$$Css_{soil\, i[S]} = Css_i . \frac{MOLWEIGHT . Kp_{soil\, i[S]}}{K_{soil\, i\text{-}water[S]}} \tag{304}$$

with

$Css_{soil\,i}$: steady-state concentration in soil i of scale S $[g.kg_{solid}^{-1}]$ *(O)*
Css_i : steady-state concentration in box i (6,7,8,14,15,16,26,27,28) $[mol.m^{-3}]$ *(I)*
MOL WEIGHT : molecular weight of the chemical $[kg.mol^{-1}]$ *(D)*
$Kp_{soil\,i[S]}$: soil i-water partition coefficient at scale S $[l_{water}.kg_{solid}^{-1}]$ *(I)*
$K_{soil\,i\text{-}water[S]}$: soil i-water equilibrium distribution coefficient at scale S $[m_{water}^{3}.m_{soil}^{-3}]$ *(A)*

$$Css_{pwsoil\,i[S]} = Css_i \cdot \frac{MOLWEIGHT}{K_{soil\ i\text{-}water[S]}} \tag{305}$$

with

$Css_{pw\,soil\,i[S]}$: steady-state concentration in pore water of soil i at scale S $[g.l^{-1}]$ *(O)*
Css_i : steady-state concentration in box i (6,7,8,14,15,16,26,27,28) $[mol.m^{-3}]$ *(S)*
MOL WEIGHT : molecular weight of the chemical $[kg.mol^{-1}]$ *(D)*
$K_{soil\,i\text{-}water[S]}$: soil i-water equilibrium distribution constant at scale S $[m_{water}^{3}.m_{soil}^{-3}]$*(A)*

4.2 Quasi-dynamic Computation

As an option, the response of the system to changes in loadings (emissions or imports), i.e., the development toward an eventual steady state, may be computed. This computation is called "quasi-dynamic" since, besides the loadings, all the model parameters are assumed to be constant in time. The computation is done by a separate integration routine that numerically integrates the mass balance equations described in the previous paragraphs. To this end, the mass balances are rewritten in the following format:

$$\underline{\frac{dc(i)}{dt}} = \frac{\underline{emis(i) + imp(i) + cf(i1).c(1) + cf(i2).c(2) + \ldots\ldots\ldots\ldots + cf(i8).c(8)}}{v(i)} \tag{306}$$

with

$c(i)$: concentration in box i $[mol.m^{-3}]$ *(S)*
t : time [s] *(S)*
$emis(i)$: emission mass flow into box i $[mol.s^{-1}]$ *(I)*
$imp(i)$: import mass flow into box i $[mol.s^{-1}]$ *(I)*
$cf(ij)$: sum of coefficients for (apparent) transport to and from box i $[m^{3}_{medium\,i}.s^{-1}]$ *(I)*
$v(i)$: volume of box i $[m^{3}]$ *(I)*

In these mass balance equations, the parameters *v(i)* and *cf(ij)* have the same values as their equivalents V_i and CF_{ij} in equations 284 and 285, used for computation of the steady-state solution. These parameter values are written into a settings table, which is read by the integration routine. The parameters *emis(i)* and *imp(i)* are read by the integration routine from a scenario table. The most commonly used loadings scenario is a "block scenario", in which the loadings have the value used in the steady-state computation for a period of time, long enough to approach the steady state, followed by the value zero for an equally long period of time. Using this scenario, both the development toward the steady state that has been computed and the recovery upon elimination of sources are computed. This computation is known in "Mackay-nomenclature" as "level 4 computation". The quasi-dynamic computation routine is described by the following:

The format of equation 1 can be seen as:

$$\begin{cases} \frac{dc}{dt} = A.c + b \\ c(0) = c_0 \end{cases} \qquad \textbf{307}$$

with

c, b, c_0 :	vectors with dimension N
A :	matrix with dimension N*N

$$A = p\Lambda p^{-1} \qquad \textbf{308}$$

with

Λ:	diagonal matrix with eigenvalues $\lambda_1, \ldots, \lambda_N$ at the diagonal, dimension N*N
A :	matrix with dimension N*N
p :	matrix with eigenvectors as columns, dimension N*N
p^{-1} :	inverse matrix from p, dimension N*N

If *a* is written as:

$$a = p^{-1}c \qquad \textbf{309}$$

with

a:	vector, dimension N
p^{-1} :	inverse matrix from p, dimension N*N
c :	vector, dimension N

Then:

$$\begin{cases} p\frac{dp^{-1}c}{dt} = p\Lambda p^{-1}c + b \\ p^{-1}c(0) = p^{-1}c_0 \end{cases} \qquad \textbf{310}$$

or:

$$\begin{cases} p\dfrac{da}{dt} = \Lambda a + p^{-1}b \\ a(0) = p^{-1}c_0 \end{cases} \tag{311}$$

This can be solved as:

$$a = a_H + a_p \tag{312}$$

with:

$$a_H = (\Lambda^{-1}p^{-1}b + p^{-1}c_0)e^{\Lambda t} \tag{313}$$

$$a_p = -\Lambda p^{-1}b \tag{314}$$

equation 6,7,8 into equation 5 gives:

$$\begin{gathered} \frac{da_i}{dt} = \lambda_i a_i + (p^{-1}b)_i \\ \Rightarrow a_i(t) = -\lambda_i^{-1}(p^{-1}b)_i + [\lambda_i^{-1}(p^{-1}b)_i + (p^{-1}c_0)_i] * e^{\lambda_i t} \\ c = p.a \end{gathered} \tag{315}$$

Thus:

$$c = (p\Lambda^{-1}p^{-1}b + c_0)e^{\Lambda t} + (-p\Lambda p^{-1}b) \tag{316}$$

5. THE SIMPLEBOX MODEL CODE

5.1 SimpleBox modules

The SimpleBox 2.0 model was developed as a MS Excel spreadsheet. The various versions that have been produced in the past all had the same basic structure, consisting of three main parts: an "input block", a "computation block" and an "output block". The present SimpleBox model still has the same basic modular structure. The spreadsheet consists of the following modules in each definition sheet: a definition block , output blocks and a picture of the SimpleBox model with mass flows. The steady-state computation block and quasi-dynamic computation blocks can be found in the engine sheet. SimpleBox also comes with a charts and macro sheet. The individual modules are further described in the following paragraphs.
The SimpleBox variables as described in the previous chapter appear in the spreadsheet as cells. As a general rule, these cells are placed directly to the right of a cell containing a text string that corresponds as closely as possible to the variable names used in this document. The cells are usually named with this text string ("name" in Excel).

5.1.1 Definition

The definition module consists of 2 blocks, *DEFINITION1* (Figure 4): regional scale model definition, continental scale model definition, moderate scale model definition, arctic scale model definition, tropic scale model definition and *DEFINITION 2* (Figure 5): the model definition in the engine sheet. The block *DEFINITION1* is where the actual model definition is entered into the spreadsheet; this is the first of the few places in the spreadsheet where user input is required. A value needs to be assigned by the user to each of the SimpleBox "definition parameters". Values can be assigned in two ways:

1. By entering a value into the cell to the right of the parameter name in the column labeled "User", using the units that are given in square brackets to the right of the variable name.
2. By accepting the value that appears in either the column labeled "Formula" (indicating that an estimation formula is producing the number shown) or the column labeled "Value" (indicating that a fixed default value is producing the number). This default formula or value is accepted by entering nothing into the cell. Usually a number appears in one of the columns only. When both columns contain a number, the number in the column "Formula" is used, unless the user overrides this by entering a number into the column "User".

The numbers in the column labeled "Formula" depend on the values assigned to other cells in the spreadsheet. The estimation formulas that produce the numbers take the values of auxiliary parameters as input. As a rule, the auxiliary parameters used are placed in the rows immediately below, the text strings that label them indented. The result returned by the estimation formulas changes when the value of any of the used auxiliary parameters are changed, as the spreadsheet is recalculated automatically after each data entry.
This way a value is assigned to the cell in the column labeled "Used". This is done by a conditional statement in this cell that takes either the user input (column "User"), the estimation formula (column "Formula") or the default value (column "Value") as input and converts this into internal SimpleBox units (SI). The values in the column "Used" are used as the SimpleBox model definition. The cells in this column carry the names of the corresponding variable names. The second definition block in the engine sheet serves as an

interface between the input block and the actual computation. *DEFINITION2* uses the values of the definition parameters set in *DEFINITION1* to produce the internal variables that are to be used in the mass balance equations. The output of this block is the full model definition. The values are used in the SimpleBox computation block; the box numbers used are indicated in the last column of this block.

5.1.2 Steady-state computation

The computation of the steady-sate solution as described in paragraph 4.1, is done in the engine sheet by the block *SIMPLEBOX STEADY-STATE COMPUTATION* (Figure 6). The values of the internal model parameters from *DEFINITION2* are assigned to numbered boxes. The output of this block: *STANDARD STEADY-STATE OUTPUT* (Figure 7) consists of the steady-state concentrations in standard units, shown in the row labeled "CONCENTRATION (mol.m^{-3})"; the total amount of chemical present in the total system at steady state, shown in the row labeled "HOLD-UP (mol)"; the percentual distribution at steady state, shown in the row labeled "DISTRIBUTION (%)"; and the throughput at steady state, shown in the row labeled "THROUGHPUT". There are two rows labeled "THROUGHPUT"; the first is computed as the sum of all inputs, the second is the sum of all outputs. These numbers are used in the development stage of new model definitions only; the two numbers should be equal for correctly defined models. Differences greater than the rounding error of the spreadsheet program indicate errors in the model definition.

The steady-state computation requires inversion of the matrix in mass balance coefficients, *cf*, in the block *MASS BALANCE COEFFICIENTS*,multiplication of the inverse matrix, cf^{1} in the block *INTERMEDIATE RESULTS* , with the vector of constants, *constants*, and recalculation of the spreadsheet. In the Excel code of SimpleBox, this calculation is done automatically after each change in the model definition by the user.

5.1.3 Quasi-dynamic computation

This part of the model code is discussed only briefly here. The integration is done on the basis of a integration routine written by Veling (1993) called integrat.exe . This process is briefly discussed in section 5.1.3 of this document.

The quasi-dynamic computation consists of three spreadsheet blocks plus the external integration program. The first block of the dynamic computation module, *SIMPLEBOX QUASI-DYNAMIC COMPUTATION* gives the initially concentations in the boxes and the emissions to these boxes (Figure 13). The second block of the dynamic computation module, *INPUT FILE DYNAMIC COMPUTATION*, produce the texts that are read by the integrator as a settings file and a scenario file, respectively, any time the integration routine is carried out. The integration process can be controlled by editing the first block of the dynamic computation module. For standard operation, it suffices to accept the settings and standard loadings scenario. Calling the integration routine then results in computation of the development towards a steady state with the same model definition as was used for computation of the steady-sate solution. The computation starts from time zero concentrations. A block scenario is assumed for the loadings: at time zero the constant loadings as used for the steady-state computation are applied for a period of 50 years, followed by a period of 50 years with zero loadings. It is suggested that only experienced users attempt to set custom integration scenarios.

The quasi-dynamic computation is carried out by *Ctrl-I.* This macro first creates the DOS-file that is necessary to externally perform the integration: it prints the contents of the block

INPUT FILE DYNAMIC COMPUTATION (area named *scenario*) to a text file with the name *INTEGRAT.SCN.* The file is used as the input file for the integration routine INTEGRAT.EXE . This routine writes the results of the integration to the file INTEGRAT.OUT, which is returned to the spreadsheet macro. The macro then reads the integration results from the file *INTEGRAT.OUT* and produces several graphs of these data in the sheet called "charts" (Figure 14).

5.1.4 Output

The SimpleBox output consists of four blocks, on each scale definition sheet. The fist block *STEADY-STATE OUTPUT;* table 1: Analysis report, is a table listing the general information (model version), used data, fate of the chemical (emissions) and the distribution & risk. (Figure 8 and Figure 9) The second block, *STEADY-STATE OUTPUT;* table 2: half life, is a table listing the half life of each process (Figure 10).
The third output block, *STEADY-STATE OUTPUT;* table 3:Transfer- and transformation mass flows, is a extensive listing of all steady-state mass flows (Figure 11). The mass flows can be read out in four different units:

1: moles per second [mol.s^{-1}]
2: % of THROUGHPUT [%]
3: metric tons per year [t.yr^{-1}]
4: kilograms per day [kg.d^{-1}]

This is controlled by the number in the cell right of the label "Units:" in the top line of the table. This number can be changed by the user.
The fourth output block is a picture of the SimpleBox model, with transfer- and transformation mass flows and steady state distribution (Figure 12). This picture can be read out the same way as table 3 by changing the number in the cell right of the label "Units" of table 3.

5.1.5 Operation

For the operation of SimpleBox Windows 3.x and Excel 5.0 are necessary.
The file *SIMBOX2.XLS* is the SimpleBox spreadsheet and the file *INTEGRAT.EXE,* which is described in the previous paragraph, is used for the integration procedure.
The spreadsheet is recalculated automatically after every change.
The integration macro in the sheet labeled *MACRO* can be started with *ALT-I.*

5.2 Running the model

The SimpleBox spreadsheet that is distributed with this document is a Excel spreadsheet. The spreadsheet was created originally in MS Excel version 5.0c.

The distribution diskette contains the following files:

- *SIMBOX2.XLS (961101)*
- *INTEGRAT.EXE (940617)*

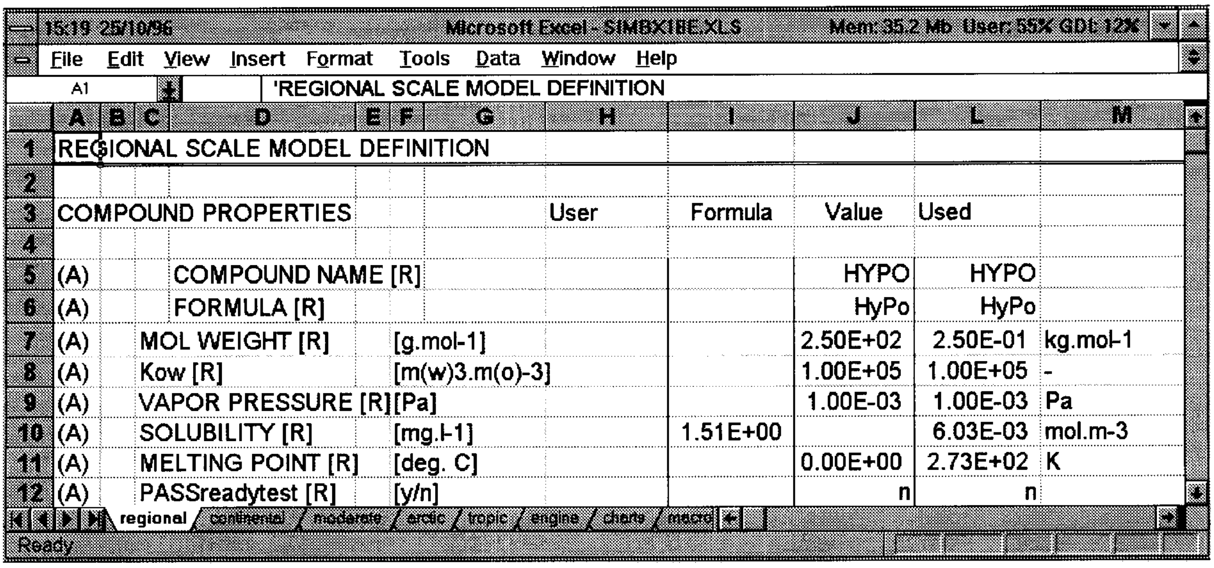
These files must be copied to the hard disk in the same directory.

To run SimpleBox, take the following steps:

1. In Windows, start Excel.
2. In Excel, open the file SIMBOX2.XLS.
3. Define a model by assigning values to the SimpleBox definition parameters. Some knowledge of the operation of Excel is required to do this.
   NOTE: leaving the cell blank leads to acceptance of the default estimation or default value.
   The computation of the steady state concentration and distribution takes place after every change/input. On slower machines this could take a while. In the Calculation Tab of the Options command of the Tools menu it is possible to change the automatic calculation to manual calculation. Then use F9 to calculate the SimpleBox spreadsheet after the changes in parameter values.
4. Complete the documentation of the analysis by typing the analyst's name and comments into the designated area of output table 1.
5. Optionally run the quasi-dynamic computation by pushing CTRL and I at the same time.
   NOTE 1: Depending on the model definition and the computing power available, this may take a long time; use of 80486 or better is advised.
6. Optionally save the model definition by using the 'save as' command in the File menu, followed by entering a file name.
7. End the SimpleBox session by exiting Microsoft Excel.

To change the SimpleBox model (e.g. turn off the global scales, second water compartment, vegetation compartment) take the following steps:

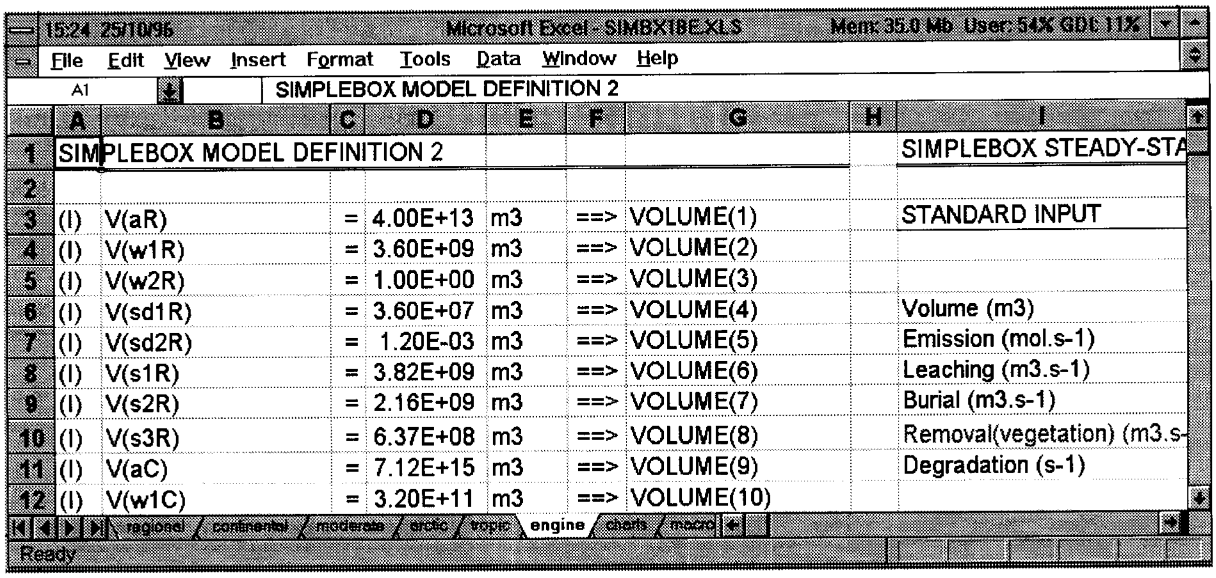
1. Turn off the sea water compartment : set AREAFRACwater2 to 1E-7 in the "User"-column and set the other fractions (soil, water) in such a way that the sum of the fractions is 100% (*Important: entering values smaller than 1E-7 for area fractions gives errors in the dynamic calculation*).
2. Turn off the vegetation compartment: type off in "User"-column in the row "Terrestrial vegetation module on/off".
3. Turn off the global scales: set degradation rates (kdeg) to 1E10 and emmision to zero.



'REGIONAL SCALE MODEL DEFINITION

	A	B	C	D	E	F	G	H	I	J	L	M
1	REGIONAL SCALE MODEL DEFINITION											
2												
3	COMPOUND PROPERTIES							User	Formula	Value	Used	
4												
5	(A)			COMPOUND NAME [R]						HYPO	HYPO	
6	(A)			FORMULA [R]						HyPo	HyPo	
7	(A)		MOL WEIGHT [R]			[g.mol-1]				2.50E+02	2.50E-01	kg.mol-1
8	(A)		Kow [R]			[m(w)3.m(o)-3]				1.00E+05	1.00E+05	-
9	(A)		VAPOR PRESSURE [R]			[Pa]				1.00E-03	1.00E-03	Pa
10	(A)		SOLUBILITY [R]			[mg.l-1]			1.51E+00		6.03E-03	mol.m-3
11	(A)		MELTING POINT [R]			[deg. C]				0.00E+00	2.73E+02	K
12	(A)		PASSreadytest [R]			[y/n]				n	n	

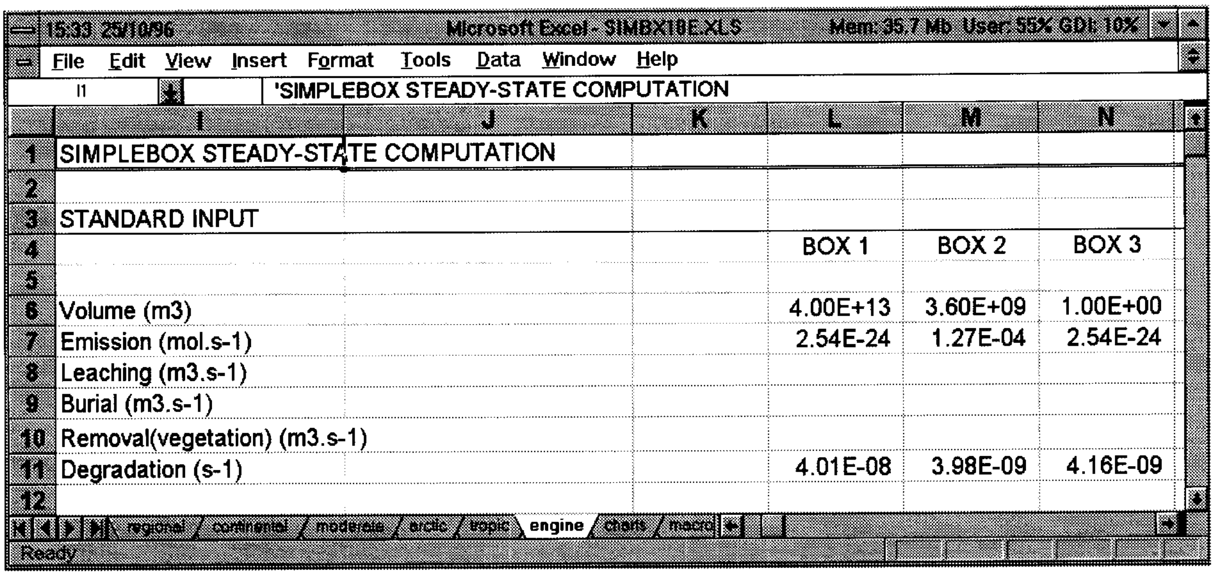
Figure 4: spreadsheet block *DEFINITION 1* for the regional scale.



A1 SIMPLEBOX MODEL DEFINITION 2

	A	B	C	D	E	F	G	H	I
1	SIMPLEBOX MODEL DEFINITION 2								SIMPLEBOX STEADY-STA
2									
3	(I)	V(aR)	=	4.00E+13	m3	==>	VOLUME(1)		STANDARD INPUT
4	(I)	V(w1R)	=	3.60E+09	m3	==>	VOLUME(2)		
5	(I)	V(w2R)	=	1.00E+00	m3	==>	VOLUME(3)		
6	(I)	V(sd1R)	=	3.60E+07	m3	==>	VOLUME(4)		Volume (m3)
7	(I)	V(sd2R)	=	1.20E-03	m3	==>	VOLUME(5)		Emission (mol.s-1)
8	(I)	V(s1R)	=	3.82E+09	m3	==>	VOLUME(6)		Leaching (m3.s-1)
9	(I)	V(s2R)	=	2.16E+09	m3	==>	VOLUME(7)		Burial (m3.s-1)
10	(I)	V(s3R)	=	6.37E+08	m3	==>	VOLUME(8)		Removal(vegetation) (m3.s-
11	(I)	V(aC)	=	7.12E+15	m3	==>	VOLUME(9)		Degradation (s-1)
12	(I)	V(w1C)	=	3.20E+11	m3	==>	VOLUME(10)		

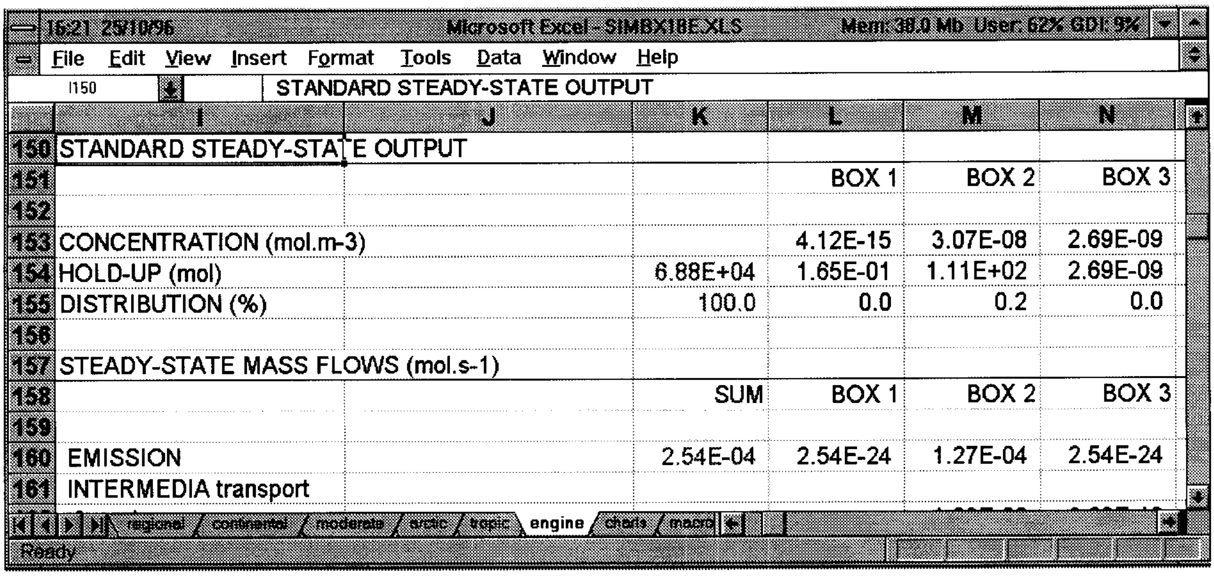
Figure 5: spreadsheet block *DEFINITION 2* on the engine sheet.



I1 'SIMPLEBOX STEADY-STATE COMPUTATION

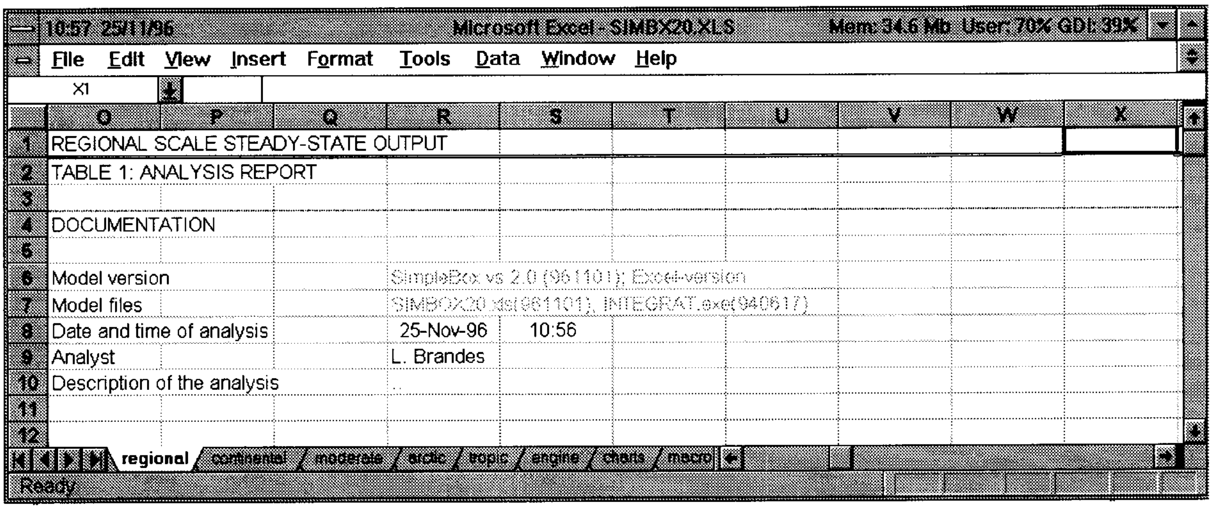
	I	J	K	L	M	N
1	SIMPLEBOX STEADY-STATE COMPUTATION					
2						
3	STANDARD INPUT					
4				BOX 1	BOX 2	BOX 3
5						
6	Volume (m3)			4.00E+13	3.60E+09	1.00E+00
7	Emission (mol.s-1)			2.54E-24	1.27E-04	2.54E-24
8	Leaching (m3.s-1)					
9	Burial (m3.s-1)					
10	Removal(vegetation) (m3.s-1)					
11	Degradation (s-1)			4.01E-08	3.98E-09	4.16E-09
12						

Figure 6: spreadsheet block *STEADY-STATE COMPUTATION* on the engine sheet.



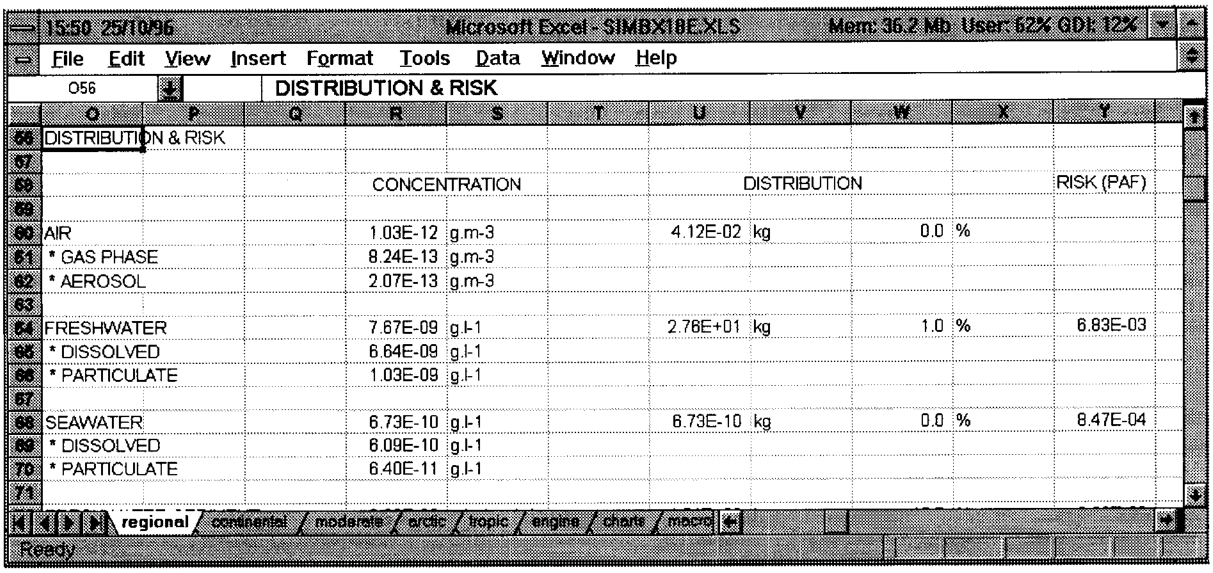
	I	J	K	L	M	N
150	STANDARD STEADY-STATE OUTPUT					
151				BOX 1	BOX 2	BOX 3
152						
153	CONCENTRATION (mol.m-3)			4.12E-15	3.07E-08	2.69E-09
154	HOLD-UP (mol)		6.88E+04	1.65E-01	1.11E+02	2.69E-09
155	DISTRIBUTION (%)		100.0	0.0	0.2	0.0
156						
157	STEADY-STATE MASS FLOWS (mol.s-1)					
158			SUM	BOX 1	BOX 2	BOX 3
159						
160	EMISSION		2.54E-04	2.54E-24	1.27E-04	2.54E-24
161	INTERMEDIA transport					

Figure 7: spreadsheet block *STEADY-STATE COMPUTATION: Output* on the engine sheet.



	O	P	Q	R	S	T	U	V	W	X
1	REGIONAL SCALE STEADY-STATE OUTPUT									
2	TABLE 1: ANALYSIS REPORT									
3										
4	DOCUMENTATION									
5										
6	Model version			SimpleBox vs 2.0 (961101); Excel-version						
7	Model files			SIMBOX20.xls(961101), INTEGRAT.exe(940617)						
8	Date and time of analysis			25-Nov-96	10:56					
9	Analyst			L. Brandes						
10	Description of the analysis			..						
11										
12										

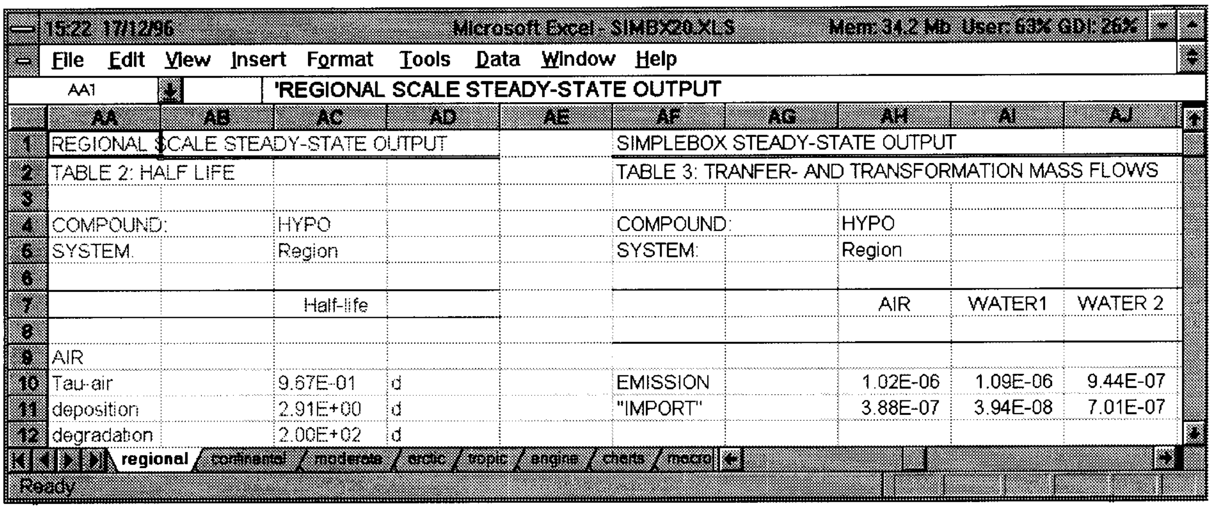
Figure 8: *STEADY-STATE OUTPUT TABLE 1: analysis report* on the regional sheet.



O56 DISTRIBUTION & RISK

	O	P	Q	R	S	T	U	V	W	X	Y
56	DISTRIBUTION & RISK										
57											
58				CONCENTRATION				DISTRIBUTION			RISK (PAF)
59											
60	AIR			1.03E-12	g.m-3		4.12E-02	kg	0.0	%	
61	* GAS PHASE			8.24E-13	g.m-3						
62	* AEROSOL			2.07E-13	g.m-3						
63											
64	FRESHWATER			7.67E-09	g.l-1		2.76E+01	kg	1.0	%	6.83E-03
65	* DISSOLVED			6.64E-09	g.l-1						
66	* PARTICULATE			1.03E-09	g.l-1						
67											
68	SEAWATER			6.73E-10	g.l-1		6.73E-10	kg	0.0	%	8.47E-04
69	* DISSOLVED			6.09E-10	g.l-1						
70	* PARTICULATE			6.40E-11	g.l-1						
71											

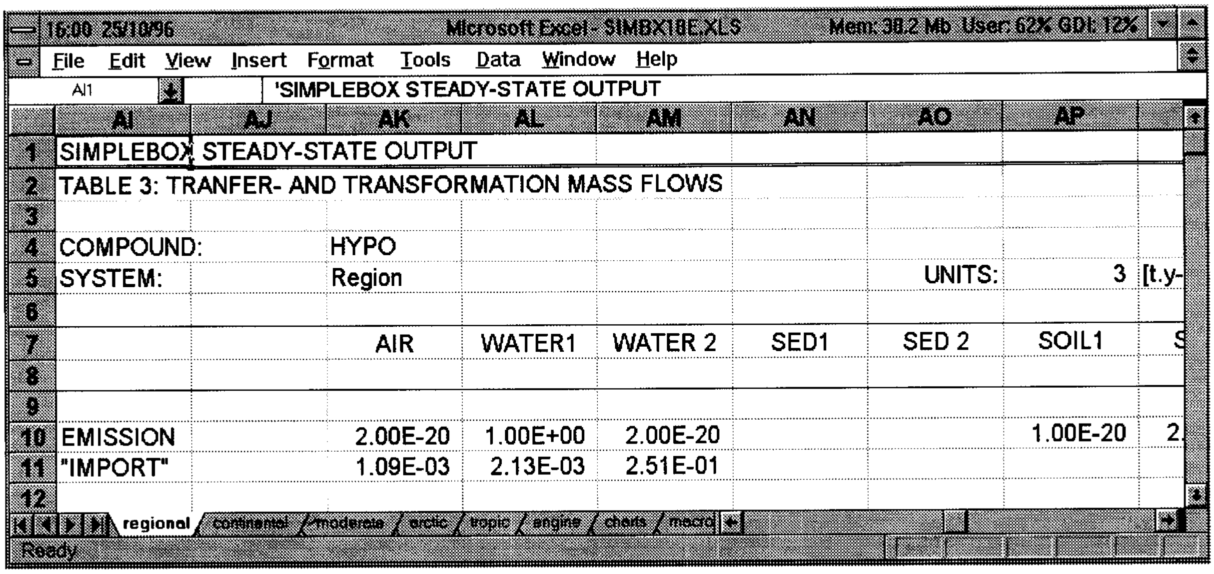
Figure 9: *STEADY-STATE OUTPUT TABLE 1: distribution and risk* on the regional sheet.



AA1 'REGIONAL SCALE STEADY-STATE OUTPUT

	AA	AB	AC	AD	AE	AF	AG	AH	AI	AJ
1	REGIONAL SCALE STEADY-STATE OUTPUT					SIMPLEBOX STEADY-STATE OUTPUT				
2	TABLE 2: HALF LIFE					TABLE 3: TRANFER- AND TRANSFORMATION MASS FLOWS				
3										
4	COMPOUND:		HYPO			COMPOUND:		HYPO		
5	SYSTEM.		Region			SYSTEM:		Region		
6										
7			Half-life					AIR	WATER1	WATER 2
8										
9	AIR									
10	Tau-air		9.67E-01	d		EMISSION		1.02E-06	1.09E-06	9.44E-07
11	deposition		2.91E+00	d		"IMPORT"		3.88E-07	3.94E-08	7.01E-07
12	degradation		2.00E+02	d						

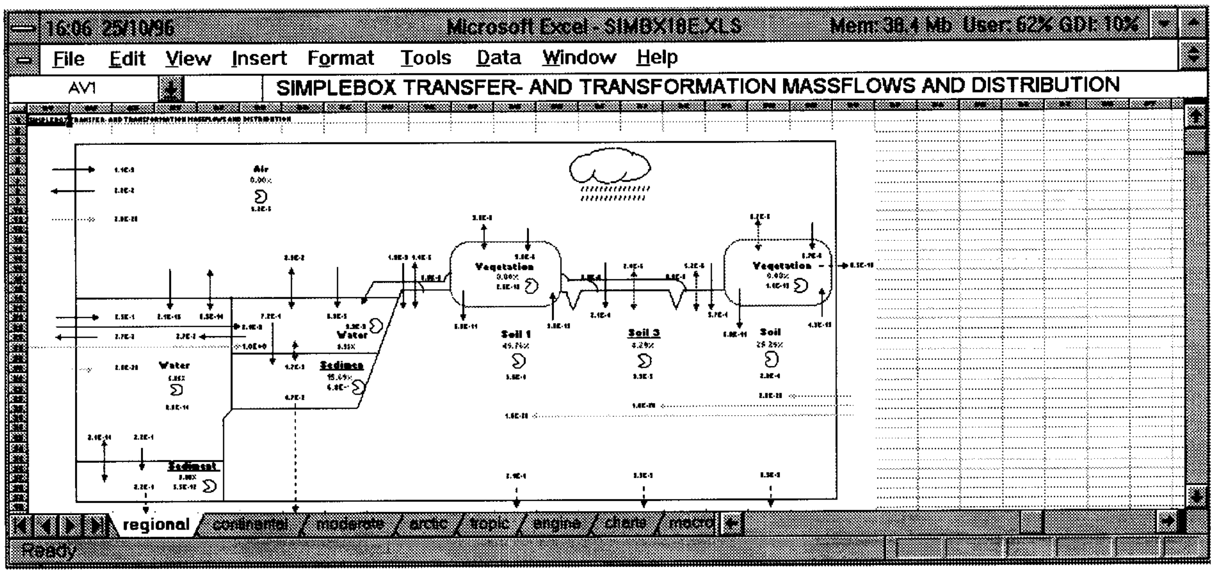
Figure 10: *STEADY-STATE OUTPUT TABLE 2:Steady-state concentrations* on the regional sheet.



'SIMPLEBOX STEADY-STATE OUTPUT

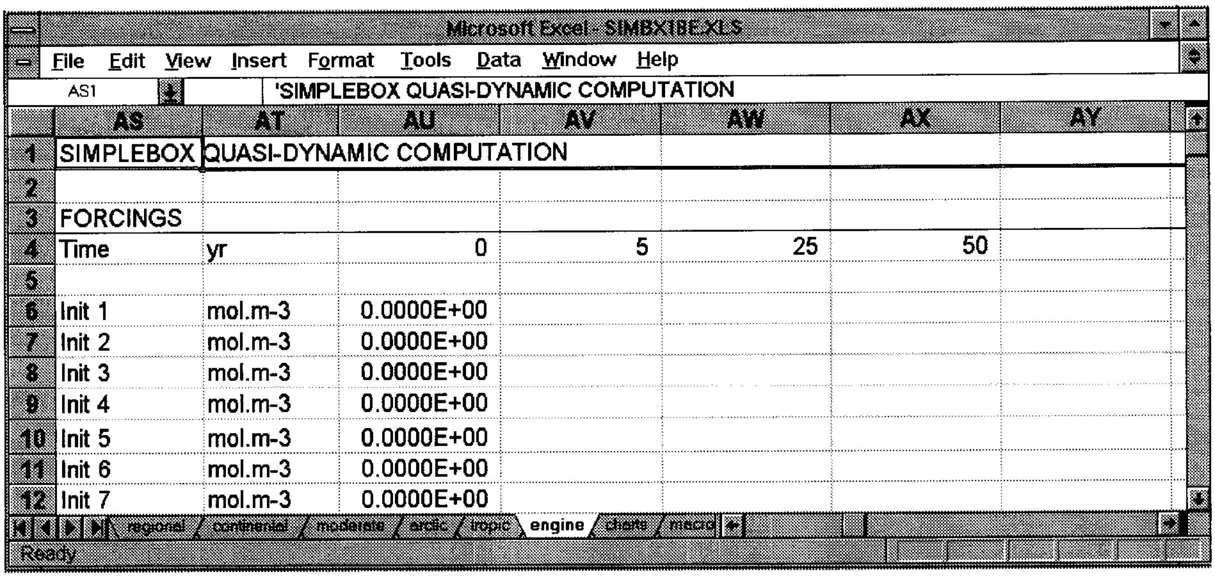
	AI	AJ	AK	AL	AM	AN	AO	AP	
1	SIMPLEBOX STEADY-STATE OUTPUT								
2	TABLE 3: TRANFER- AND TRANSFORMATION MASS FLOWS								
3									
4	COMPOUND:		HYPO						
5	SYSTEM:		Region				UNITS:	3	[t.y-
6									
7			AIR	WATER1	WATER 2	SED1	SED 2	SOIL1	S
8									
9									
10	EMISSION		2.00E-20	1.00E+00	2.00E-20			1.00E-20	2
11	"IMPORT"		1.09E-03	2.13E-03	2.51E-01				
12									

Figure 11: *STEADY-STATE OUTPUT TABLE 3: mass flows* on the regional sheet.



SIMPLEBOX TRANSFER- AND TRANSFORMATION MASSFLOWS AND DISTRIBUTION

Figure 12: SIMPLEBOX picture: *mass flows and distribution* on the regional sheet.



	AS	AT	AU	AV	AW	AX	AY
1	SIMPLEBOX	QUASI-DYNAMIC COMPUTATION					
2							
3	FORCINGS						
4	Time	yr	0	5	25	50	
5							
6	Init 1	mol.m-3	0.0000E+00				
7	Init 2	mol.m-3	0.0000E+00				
8	Init 3	mol.m-3	0.0000E+00				
9	Init 4	mol.m-3	0.0000E+00				
10	Init 5	mol.m-3	0.0000E+00				
11	Init 6	mol.m-3	0.0000E+00				
12	Init 7	mol.m-3	0.0000E+00				

Figure 13: *QUASI DYNAMIC COMPUTATION block* on the engine sheet.

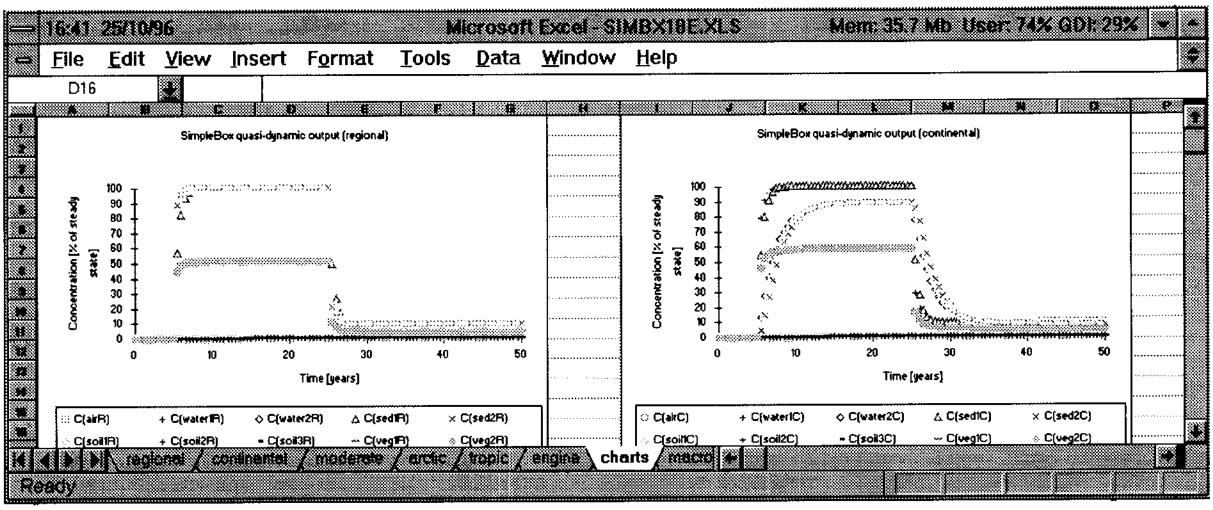


Figure 14: *QUASI DYNAMIC OUTPUT: charts* on the charts sheet.

REFERENCES

Cohen, Y. and Ryan, P.A. (1985). Multimedia modeling of environmental transport: trichloroethylene test case. Environ. Sci. Technol. 19, 412-417.

Cowan, C.E. et al. (1995) .The Multi-Media Fate Model: A vital tool for predicting the fate of chemicals. SETAC press, Pensacola, FL.

DiToro, D.M., Zarba, C.S., Hansen, D.J., Berry, W.J., Swartz, R.C., Cowan, C.E., Pavlou, S.P., Allen, H.E., Thomas, N.A. and Paquin, P.R. (1991). Technical basis for establishing sediment quality criteria for nonionic organic chemicals using equilibrium partitioning. Environ. Toxicol. Chem., 10, 1541-1583.

EC (1996a). Technical Guidance Documents in support of the Commission Directive 93/67/EEC on risk assessment for new notified substances and the Commission Regulation (EC) No. 1488/94 on risk assessment for existing substances. Brussels, Belgium, Commission of the European Communities.

EC (1996b). EUSES, the European Union System for the Evaluation of Substances. National Institute of Public Health and the Environment (RIVM), the Netherlands. Available from European Chemicals Bureau (EC/DGXI), Ispra, Italy.(1996a).

Frische, R., Klopffer, W., Rippen, G. and Gunther, K-L. (1984). The environmental model segment approach for estimating potential environmental concentrations. I. The model. Ecotoxicol. Environ. Safety, 8, 352-362.

Hamers, T., Aldenberg, T. and Van de Meent, D. (1995). Defenition report-Indicator Effects Toxic Substances (Itox). Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report nr. 607128001.

Hansch, C., Quinlan, J.E. and Lawrence, G.L. (1968). The linear free-energy relationships between partition coefficients and the aqueous solubility of organic liquids. J. Org. Chem., 33, 347-350.

Health Council of the Netherlands, (1995). Committee on Setting Integrated Environmental Quality Objectives. The project Setting Integrated Environmental Quality Objectives. The Hague, Health Council of the Netherlands, Publication no. 1995/07.

Henderson-Sellers, A. and McGuffie, K. (1987). A Climate Modelling Primer. Wiley, pp. 111.

Junge, C.E. (1977). In: Fate of pollutants in the air and water environment (I.H. Suffet, ed.), pp. 7-25, Wiley-Interscience.

Lyman, W.J., Rheel, W.F. and Rosenblatt, D.H. (1982). Handbook of environmental property estimation. McGraw-Hill.

Mackay, D. (1979). Finding fugacity feasible. Environ. Sci. Technol., 13, 1218.

Mackay, D. (1982). Correlation of bioconcentration factors. Environ. Sci. Technol., 16, 274-278.

Mackay, D. (1991). Multimedia environmental models. Lewis, Chelsea, MI.

Mackay, D. and Paterson, S. (1981). Calculating fugacity. Environ. Sci. Technol., 15, 1006-1014.

Mackay, D., Paterson, S., Cheung, B. and Neely, W.B. (1985). Evaluating the environmental behavior of chemicals with a level III model. Chemosphere, 14, 335-374.

Mackay, D., Paterson, S. and Shiu, W.Y. (1992). Generic models for evaluating the regional fate of chemicals. Chemosphere, 24, 695-717.

Mackay, D., Paterson, S. and Tam, D.D. (1991). Assessment of chemical fate in Canada: continued development of a fugacity model. Toronto. Institue of Environmental Studies, University of Toronto.

Meylan, W.M. and Howard, P.H. (1991). Bond contribution method for estimating Henry's law constants. Environ. Toxicol. Chem., 10, 1283-1293.

OECD (1989). Compedium of environmental exposure assessment methods for chemicals. Method 604: SIMPLEBOX (pp. 333-338); Method 506: SIMPLESAL (pp. 278-288); Method 109: SIM PLETREAT (pp. 51-58). OECD Environmental Monographs No. 27, Paris, July 1989, 350 pp.

Peixoto, J.P. and A.H. Oort (1992). Physics of Climate. American Institute of Physics, NY, 520 pp.

Rippen, G., Klopffer, W., Frische, R. and Gunther, K.O. (1984). The environmental model segment approach for estimating potential environmental concentrations. II. Application of the model to p-dichlorobenzene and trichlorobenzene. Ecotoxicol. Environ. Safety, 8, 363-377.

RPC (1991). Prototype model uniform substances evaluation system (UBS); a decision support system. Delft, Resources Planning Consultants, April 1991 [in Dutch].

Ryan, P.A. and Cohen, Y. (1986). Multimedia transport of particle-bound organics: benzo(a)pyrene test case. Chemosphere, 15, 21-47.

Schwarzenbach, R.P., Gschend, P.M., and Imboden, D.M. (1993). Environmental Organic Chemistry. New York: Wiley.

Severinsen, M., Andersen, M.B., Chen, F., and Nyholm, N. (1996). A regional chemical fate and exposure model suitable for Denmark and its coatal sea. Submitted for publication.

Singh, K.P. and Van de Meent, D. (1989). Mathematical modeling of transfer, transport and transformation of chemicals in the environment. SimpleSingh, a spacially inhomogeneous box modeling system. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report nr. 768803 002.

Struijs, J. and Van de Meent, D. (1988). The use of a multimedia box model to predict the emission patterns of xenobiotics in a waste water treatment plant. In: Proceedings of the CEC-COST 641 workshop on "Behaviour of organic micropollutants in biological waste water treatment", pp 181-184, Commission of the European Communities Report EUR 11356 (1987).

Struijs, J. and Van den Berg, R. (1993). Standardized biodegradability tests: extrapolation to aerobic environments. Water Res., submitted for publication.

Struijs, J., Stoltenkamp, J. and Van de Meent, D. (1991). SimpleTreat, a box model of the behavior of micropollutants during waste water treatment. Water Research, 25, 891-900.

Trapp, S. and MacFarlane, J.C. (1995). Plant Contamination: modelling and simulation of organic chemical processes. Lewis.

Trapp, S. and Matthies, M. (1995). Generic one-compartment model of organic chemicals by foliar vegetation. Environ. Sci. Technol., 29, 2333-2338.

Travis, C.C., Dennison, J.W. and Arms, A.D. (1987). The extend of multimedia partitioning of organic chemicals. Chemosphere, 16, 117-125.

Van de Meent, D. (1987). Intercompartment transfer of pollutants: The case of lead. Discussion paper presented at the ECE-Workshop "Transfer of pollutants from one compartment to another", Como, Italy, March 1987.

Van de Meent, D. (1988). Exposure modeling I: Principles, and Exposure modeling II: The use of simple box models. In: Manual on Aquatic Ecotoxicology (H.A.M. de Kruijf, D. de Zwart, P.K. Ray and P.N. Viswanathan, eds.), pp. 77-81, and pp. 82-87, Allied Publishers Pvt. Ltd., New Delhi.

Van de Meent, D. (1989). Evaluation System New Chemicals. SIMPLERISK, a model to estimate local concentrations in water and soil. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report nr. 718706 001 [in Dutch].

Van de Meent, D. (1990). Modelling intercompartment transfer of pollutants: the case of lead. Sci. Total Environ., 90, 41-54.

Van de Meent, D. and Toet, C. (1992) Dutch Priority Setting System for Existing Chemicals, a systematic procedure for ranking chemicals according to increasing environmental hazard. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report no. 679120 001.

Van de Meent, D. and De Bruijn, J.H.M. (1995). A modeling procedure to evaluate the coherence of independently derived environmental quality objectives for air, water and soil. Environ. Toxicol. Chem. 14, 177-186.

Van de Meent, D. and Van der Burg, P.A. (1995). Sensitivity of model-computed persistence for degradation rates. SETAC Brussels.

Van de Meent, D. (1995). Global Toxification: a manageble problem? SETAC Vancouver.

Van de Meent, D. (1996). Validating SimpleBox-computed steady-state concentration ratios. Project defenition report. ECO report no. 96-04. Bilthoven, National Institute of Public Health and the Environment.

Van Leeuwen, C.J., P.T.J. van der Zandt, T. Aldenberg, H.J.M. Verhaar and J.L.M. Hermens (1992). The application of QSARs, extrapolation and equilibrium partitioning in aquatic effects assessment for narcotic pollutants. Environ. Toxicol. Chem., 11, 267-282.

Verbruggen, E.J., Beusen, A., De Greef, J. and Van de Meent, D. (1996). GlobeTox: a global scale multi-media fate model. Bilthoven, National Institute for Public Health and the Environment, RIVM report no. 461501014 in press.

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APPENDIX 1. MODEL PARAMETERS

Symbol	***Explanation***	***Default value***	***Unit***
Parameters that describe the properties of the chemical			
MOL WEIGHT	molecular weight of the chemical	0.250	$kg.mol^{-1}$ *(A)*
K_{ow}	octanol-water partition coefficient of the chemical	10^5	$mol.m_{octanol}^{-3}/mol.m_{water}^{-3}$ *(A)*
VAPOR PRESSURE (25)	vapor pressure of the chemical at temperature 25°C	10^{-3}	Pa *(A)*
SOLUBILITY (25)	solubility of the chemical at temperature 25°C		$mol.m^{-3}$ *(A)*
H0vapor	enthalpy of vaporization	50	$J.mol^{-1}$ *(A)*
H0solut	enthalpy of solution	10	$J.mol^{-1}$ *(A)*
MELTINGPOINT	melting point of the chemical	273	K *(A)*
PASSreadytest	the result of a standard screening test, expressed in the generally used "yes/no" format	n	y/n *(A)*
alfa water	mean log NOEC water	-5.6	$g.l^{-1}$ *(A)*
alfa sediment	mean log NOEC sediment		$g.l^{-1}$ *(A)*
alfa soil	mean log NOEC soil	-2.4	$g.l^{-1}$ *(A)*
stdev log NOEC water	standard deviation of log NOEC's for water	0.916	- *(A)*
stdev log NOEC soil	standard deviation of log NOEC's for soil	0.5	- *(A)*
beta water	beta for water		- *(A)*
beta soil	beta for soil		- *(A)*
PAF_{water}	Potentially Affected Fraction water		- *(D)*

PAF_{sed}	Potentially Affected Fraction sediment		- *(D)*
PAF_{soil}	Potentially Affected Fraction soil		- *(D)*
Parameters that describe intermedia partitioning of the chemical			
$K_{air\text{-}water\,[S]}$	air-water equilibrium distribution constant at scale S		$mol.m_{air}^{-3}/mol.m_{water}^{-3}$ *(A)*
R	gas constant	8.314	$Pa.m^{3}.mol^{-1}.K^{-1}$ *(C)*
H	Henry's law constant		$Pa.m^{3}.mol^{-1}$
$FRass_{aerosol[S]}$	fraction of the chemical in air that is associated with aerosol particles at scale S		- *(A)*
$CONST$ θ	constant surface area of aerosol phase	10^{-4}	Pa.m *(C)* $m_{aerosol}^{2}/m_{air}^{3}$ *(C)*
$FRdisslvd_{water(i)\,[S]}$	dissolved fraction of the chemical in water column i at scale S		- *(A)*
$K_{susp\text{-}water\,i[S]}$	suspended matter-water equilibrium distribution constant at scale S		$l.kg(d)^{-1}$ *(A)*
$CORG_{suspi[S]}$	organic carbon content of suspended matter	10	% C *(A)*
$SUSP_{water\,1\,[R]}$	concentration of suspended matter in water column 1 at the regional scale	0.015	$kg_{solid}.m_{water}^{-3}$ *(D)*
$SUSP_{water\,2\,[R]}$	concentration of suspended matter in water column 2 at the regional scale	0.05	$kg_{solid}.m_{water}^{-3}$ *(D)*
$SUSP_{water\,1[C]}$	concentration of suspended matter in water column 1at the continental scale	0.025	$kg_{solid}.m_{water}^{-3}$ *(D)*
$SUSP_{water\,2\,[C]}$	concentration of suspended matter in water column 2 at the continental scale	0.005	$kg_{solid}.m_{water}^{-3}$ *(D)*
$SUSP_{water\,[M]}$	concentration of suspended matter in the water column of the moderate scale	0.005	$kg_{solid}.m_{water}^{-3}$ *(D)*
$SUSP_{water\,[A]}$	concentration of suspended matter in the water column of the arctic scale	0.005	$kg_{solid}.m_{water}^{-3}$ *(D)*
$SUSP_{water\,[T]}$	concentration of suspended matter in the water column of the tropic scale	0.005	$kg_{solid}.m_{water}^{-3}$ *(D)*
$BCF_{fish\,i[S]}$	bioconcentration factor for fish in water column i at scale S		$l_{water}.kg_{fish}^{-1}$ *(A)*
$FAT_{fish\,i\,[S]}$	volume fraction of fat in fish in water column i at scale S	0.05	- *(A)*
$BIO_{water\,[S]}$	concentration of biota in the water column	10^{-3}	$kg_{solid}.m_{water}^{-3}$ *(D)*

$K_{sed\text{-}water\ i[S]}$	sediment-water equilibrium distribution constant at scale S		$mol.m_{sed}^{-3}/mol.m_{water}^{-3}$ *(A)*
$FRdisslvd_{sed\ i[S]}$	fraction of the chemical present in the water phase of sediment i at scale S		- *(A)*
$Kp_{sed\ i\ [S]}$	sediment-water partition coefficient at scale S		$l_{water}.kg_{solid}^{-1}$ *(A)*
$CORG_{sed\ i[S]}$	organic carbon content of the sediment i at scale S	0.05	- *(A)*
$K_{soil\ i\text{-}water[S]}$	soil-water equilibrium distribution constant at scale S		$mol.m_{soil}^{-3}/mol.m_{water}^{-3}$ *(A)*
$FRdisslvd_{soil\ i\ [S]}$	fraction of the chemical present in the water phase of the soil at scale S		- *(A)*
$Kp_{soil\ i[S]}$	soil-water partition coefficient at scale S		$l_{water}.kg_{solid}^{-1}$ *(I)*
$CORG_{soil\ i[S]}$	organic carbon content of soil i at scale S	0.05	- *(A)*
Parameters that characterize the environment			
$TEMPERATURE_{[R]}$	temperature at the air-water interface at the regional scale	285	K *(A)*
$TEMPERATURE_{[C]}$	temperature at the air-water interface at the regional scale	285	K *(A)*
$TEMPERATURE_{[M]}$	temperature at the air-water interface at the moderate scale	285	K *(A)*
$TEMPERATURE_{[A]}$	temperature at the air-water interface at the arctic scale	298	K *(A)*
$TEMPERATURE_{[T]}$	temperature at the air-water interface at the tropic scale	263	K *(A)*
$RHOsolid_{[S]}$	density of the solid phase of scale S	2500	$kg_{solid}.m_{solid}^{-3}$ *(A)*
$VOLUME_{air[\ S]}$	volume of the air compartment of scale S		m^3 *(D)*
$VOLUME_{water\ i\ [S]}$	volume of water compartment i at scale S		m^3 *(D)*
$VOLUME_{sed\ i\ [S]}$	volume of sediment compartment i at scale S		m^3 *(D)*
$VOLUME_{soil\ i[S]}$	volume of the soil compartment i at scale S		m^3 *(D)*
$SYSTEMAREA_{\ [R]}$	total area of the regional scale air/water + air/soil interfaces)	$8.00.10^{10}$	m^2 *(D)*
$SYSTEMAREA_{\ [C]}$	total area of the continental scale air/water + air/soil interfaces)	$7.12.10^{12}$	m^2 *(D)*
$SYSTEMAREA_{\ [M]}$	total area of the moderate scale air/water + air/soil interfaces)	$3.89.10^{13}$	m^2 *(D)*

$SYSTEMAREA_{[A]}$	total area of the arctic scale air/water + air/soil interfaces)	$2.55.10^{13}$	m^2 *(D)*
$SYSTEMAREA_{[T]}$	total area of the tropic scale air/water + air/soil interfaces)	$8.93.10^{10}$	m^2 *(D)*
$AREAFRAC_{water\ i\ [S]}$	fraction of scale S that is water i		- *(D)*
$AREAFRAC_{soil\ i[S}$	fraction of the area of scale S that is soil i		- *(D)*
$HEIGHT_{air[\ S]}$	atmospheric mixing height of scale S	1000	m *(A)*
$DEPTH_{water\ 1\ [R]}$	depth of water column 1 at the regional scale	3	m *(A)*
$DEPTH_{water\ 2\ [R]}$	depth of water column 2 at the regional scale	25	m *(A)*
$DEPTH_{water\ 1\ [C]}$	depth of water column 1 at the continental scale	3	m *(A)*
$DEPTH_{water\ 2\ [C]}$	depth of water column 2 at the continental scale	200	m *(A)*
$DEPTH_{water\ [M]}$	depth of water column of the moderate scale	1000	m *(A)*
$DEPTH_{water\ [A]}$	depth of water column of the arctic scale	1000	m *(A)*
$DEPTH_{water\ [T]}$	depth of water column of the tropic scale	1000	m *(A)*
$DEPTH_{sed\ i\ [S]}$	mixing depth of sediment i at scale S	0.03	m *(A)*
$FRwater_{sed[S]}$	volume fraction of the water phase of sediment of scale S	0.08	- *(A)*
$DEPTH_{soil\ 1[S]}$	mixing depth of soil 1 at scale S		m *(A)*
$DEPTH_{soil\ 2[S]}$	mixing depth of soil 2 at scale S		m *(A)*
$DEPTH_{soil\ 3[S]}$	mixing depth of soil 3 at scale S		m *(A)*
$FRair_{soil[S]}$	volume fraction air of soil i at scale S	0.2	- *(A)*
$FRwater_{soil[S]}$	volume fraction of the water phase of soil at scale S	0.2	- *(A)*
$FRsolid_{soil[S]}$	volume fraction solid of soil i at scale S	0.6	- *(A)*
$TAU_{air\ [S]}$	residence time of air in scale S		s *(D)*
$WINDSPEED_{[S]}$	average windspeed at 10 m above the surface of scale S	3	$m.s^{-1}$ *(A)*

$TAU_{water\ i\ [S]}$	hydraulic residence time of water compartment i at scale S		s (*D*)
$RUNOFF_{[S]}$	total run off from soil 1, (soil 2 and soil 3) of scale S into the water compartment of scale S		$m^3.s^{-1}$ (*A*)
$FLOWS_{i[S]}$	sum of the discharges of all streams crossing compartment/scale boundaries to water i		$m^3.s^{-1}$ (*D*)
$FLOW_{water\ i[S]-water\ i[S]}$	flow from water i (of the larger spatial scale) to water i of scale S		$m^3.s^{-1}$ (*A*)
$FRACout_{water1[C]-water1[R]}$	fraction water out of water 1 of the continental scale to water 1 of the regional scale	0.0391389	-
$FRACout_{water1[C]-water2[R]}$	fraction water out of water 1 of the continental scale to water 2 of the regional scale	0.01	-
Direct emissions			
$Edirect_{air[S]}$	sum of all direct emissions to the air compartment of scale S		$mol.s^{-1}$ (*D*)
$Edirect_{water\ i[S]}$	sum of all direct emissions to water compartment i of scale S		$mol.s^{-1}$ (*D*)
$Edirect_{soil\ i[S]}$	sum of all direct emissions to soil compartment i of scale S		$mol.s^{-1}$ (*D*)
$POPULATION_{[S]}$	total population of the scale S		inh (*A*)
$PRODUCTION_{[S]}$	total amount produced or imported in the system		$mol.s^{-1}$ (*A*)
$EMISfact_{air[S]}$	emission factor for air: the fraction of the production volume that is released to the water compartment i at scale S	10^{-3}	- (*A*)
$EMISfact_{water\ i[S]}$	emission factor for water i: the fraction of the production volume that is released to the air compartment at scale S	10^{-3}	- (*A*)
$EMISfact_{soil\ i[S]}$	emission factor for soil i: the fraction of the production volume that is released to soil i at scale S	10^{-3}	- (*A*)
Emissions via sewage treatment plant [c]			
$Estp_{air[S]}$	indirect emission to air of scale S, resulting from volatilization during sewage treatment		$mol.s^{-1}$ (*D*)
$Estp_{water\ i[S]}$	indirect emission to water i with effluent from sewage treatment of scale S		$mol.s^{-1}$ (*D*)
$Estp_{soil\ 2[S]}$	indirect emission to soil 2, resulting from application of sewage sludge at scale S		$mol.s^{-1}$ (*D*)
$CONCstp_{water[S]}$	concentration of the chemical, dissolved in STP-effluent at scale S		$mol.m_{water}^{-3}$ (*A*)
$CONCstp_{sludge[S]}$	concentration of the chemical in sewage sludge at scale S		$mol.kg_{solid}^{-1}$ (*A*)

$Frstp_{water\ 2[R]}$	fraction of the STP-effluent discharged into the water compartment i of the scale S	0.9	$m_{water}^{3}.s^{-1}$ *(A)*
$EFFLUENT_{stp}$	amount of STP-effluent discharged into the water compartment of scale S		$m_{water}^{3}.s^{-1}$ *(A)*
$STPcapacity_{[S]}$	total capacity of the sewage treatment plant of scale S		eq *(A)*
$PRCNTconnect_{S]}$	the percentage of householdings connected to the sewage treatment plant of scale S	0.7	- *(A)*
$SOLIDS_{stp[S]}$	rate of sewage sludge production at scale S		$kg_{solid}.s^{-1}$ *(A)*
$STPload_{[S]}$	load of the sewage treatment plant during release episodes at scale S		$mol.s^{-1}$ *(A)*
$ACTIVEtime_{[S]}$	fraction of the time that the sewage treatment plant is loaded with the chemical at scale S	365	d.y-1
$FR_{volatstp[S]}$	fraction of the load that is rerouted to the air compartment of scale S as a result of volatilization during sewage treatment	0.1	- *(A)*
$FR_{effstp[S]}$	fraction of the load that is rerouted to the water compartment with effluent (water + particles) upon sewage treatment at scale S	0.2	- *(A)*
$FR_{sludgestp[S]}$:	fraction of the STPload that is rerouted to (agricultural) soil through application of sewage sludge at scale S	0.6	- *(A)*
Transformation processes			
$kdeg_{air[S]}$	pseudo first order transformation rate constant in air at scale S		s^{-1} *(D)*
$krad_{OH}$:	pseudo first order rate constant for reaction with OH-radicals	$5.01 \cdot 10^{-8}$	s^{-1} *(A)*
$kdeg_{water\ i[S]}$	pseudo first order degradation rate constant in water i at scale S		s^{-1} *(D)*
$kdeg_{test}$:	Peudo first order degradation rate constant in laboratory test		s^{-1} *(A)*
$BACT_{water}$	concentration of bacteria in the water compartment	$4.0 \cdot 10^{4}$	$cfu.ml_{water}^{-1}$ *(A)*
$BACT_{test}$	concentration of bacteria in the laboratory test water	$4.0 \cdot 10^{4}$	$cfu.ml_{test\ water}^{-1}$ *(A)*
$kdeg_{sed\ i[S]}$	pseudo first order degradation rate constant in sediment i at scale S		s^{-1} *(D)*
$BACT_{sed\ i[S]}$	concentration of bacteria in sediment, expressed on a pore water basis	$5.0 \cdot 10^{9}$	$cfu.ml_{water}^{-1}$ *(A)*
$kdeg_{soili[S]}$	pseudo first order degradation rate constant in soil i at scale S		s^{-1} *(D)*

$BACT_{soil}$	concentration of bacteria in soil, expressed on a pore water basis	$2.22\cdot10^{6}$	$cfu.ml_{water}^{-1}$ *(A)*
Intermedia transfer processes			
$DRYDEP_{aerosol[S]}$	mass transfer coefficient for dry deposition of aerosol-associated chemical at scale S		$m_{air}.s^{-1}$ *(D)*
$AEROSOLDEPRATE_{[S]}$	deposition velocity of the aerosol particles at scale S with which the chemical is associated)	10^{-3}	$m.s^{-1}$ *(A)*
$WASHOUT_{[S]}$	mass transfer coefficient for wet atmospheric deposition at scale S		$m_{air}.s^{-1}$ *(D)*
$RAINrate_{[R]}$	rate of wet precipitation at the regional scale 700 $mm.y^{-1}$	$2.22\cdot10^{-8}$	$m_{rain}.s^{-1}$ *(A)*
$RAINrate_{[C]}$	rate of wet precipitation at the continental scale 700 $mm.y^{-1}$	$2.22\cdot10^{-8}$	$m_{rain}.s^{-1}$ *(A)*
$RAINrate_{[M]}$	rate of wet precipitation at the moderate scale 700 $mm.y^{-1}$	$2.22\cdot10^{-8}$	$m_{rain}.s^{-1}$ *(A)*
$RAINrate_{[A]}$	rate of wet precipitation at the arctic scale 250 $mm.y^{-1}$	$7.93\cdot10^{-9}$	$m_{rain}.s^{-1}$ *(A)*
$RAINrate_{[T]}$	rate of wet precipitation at the tropic scale 1300 $mm.y^{-1}$	$4.12\cdot10^{-8}$	$m_{rain}.s^{-1}$ *(A)*
$SCAVratio_{[S]}$	scavenging ratio (quotient of the total concentration in rainwater and the total concentration in air) of the chemical at scale S		- *(A)*
$COLLECTeff_{[S]}$	aerosol collection efficiency at scale S	$2\cdot10^{5}$	- *(A)*
$GASABS_{water\,i[S]}$	overall mass transfer coefficient for gas absorption across the air-water interface, referenced to air at scale S		$m_{air}.s^{-1}$ *(D)*
$VOLAT_{water\,i[S]}$	overall mass transfer coefficient for volatilization across the air-water interface, referenced to water at scale S		$m_{air}.s^{-1}$ *(D)*
$kaw_{air[S]}$	partial mass transfer coefficient at the air-side of the air-water interface at scale S	$1.39\cdot10^{-3}$	$m_{air}.s^{-1}$ *(A)*
$kaw_{water[S]}$	partial mass transfer coefficient at the water-side of the air-water interface at scale S	$1.39\cdot10^{-5}$	$m_{water}.s^{-1}$ *(A)*
$GASABS_{soil\,i[S]}$	overall mass transfer coefficient for gas absorption across the air-soil interface, referenced to air at scale S		$m_{air}.s^{-1}$ *(D)*
$VOLAT_{soil\,i[S]}$:	overall mass transfer coefficient for volatilization across the air-soil interface, referenced to soil at scale S		$m_{soil}.s^{-1}$ *(D)*
$kasl_{air[S]}$	partial mass transfer coefficient at the air-side of the air-soil interface at scale S	$1.39\cdot10^{-3}$	$m_{air}.s^{-1}$ *(A)*

$kasl_{spoilair[S]}$	partial mass transfer coefficient at the soilair-side of the air-soil interface at scale S	$5.56\cdot10^{-6}$	$m_{air}.s^{-1}$ *(A)*
$kasl_{spoilwater[S]}$	partial mass transfer coefficient at the soilwater-side of the air-soil interface at scale S	$5.56\cdot10^{-10}$	$m_{water}.s^{-1}$ *(A)*
Water/sediment exchange			
$GROSSsedrate_{i\,[S]}$	gross sedimentation rate for sediment i at scale S		$m_{sed}.s^{-1}$ *(A)*
$RESUSPrate_{i[S]}$	resuspension rate for sediment compartment i at scale S		$m_{sed}.s^{-1}$ *(A)*
$SETTLEvelocity_{[S]}$	settling velocity of suspended particles at scale S	$2.89\cdot10^{-5}$	$m_{water}.s^{-1}$ *(A)*
$SUSP_{water\,i\,[S]}$	concentration of suspended matter in water column i at scale S	$2.50\cdot10^{-2}$	$kg_{solid}.m_{water}^{-3}$ *(D)*
$SUSPeff_{stp[R]}$	concentration of suspended matter in STP-effluents at the regional scale	$3.00\cdot10^{-2}$	$kg_{solid}.m_{eff}^{-3}$ *(A)*
$PROD_{susp\,1\,[R]}$	rate of production of suspended matter in water column 1 of the regional scale	10	$g(d).m^{-2}.yr^{-1}$ *(A)*
$PROD_{susp\,2\,[R]}$	rate of production of suspended matter in water column 1 of the regional scale	1	$g(d).m^{-2}.yr^{-1}$ *(A)*
$PROD_{susp\,1\,[C]}$	rate of production of suspended matter in water column 1 of the continental scale	10	$g(d).m^{-2}.yr^{-1}$ *(A)*
$PROD_{susp\,2\,[C]}$	rate of production of suspended matter in water column 1 of the continental scale	1	$g(d).m^{-2}.yr^{-1}$ *(A)*
$PROD_{susp\,[A]}$	rate of production of suspended matter in the water column of the arctic scale	1	$g(d).m^{-2}.yr^{-1}$ *(A)*
$PROD_{susp\,[T]}$	rate of production of suspended matter in the water column of the tropic scale	1	$g(d).m^{-2}.yr^{-1}$ *(A)*
$NETsedrate_{i\,[S]}$	net sedimentation rate for sediment i at scale S		$m_{sed}.s^{-1}$ *(A)*
$ADSORB_{sed\,i[S]}$	overall mass transfer coefficient for adsorption across the sediment-water interface, referenced to water at scale S		$m_{water}.s^{-1}$ *(D)*
$DESORB_{sed\,i[S]}$	overall mass transfer coefficient for desorption across the sediment-water interface, referenced to sediment i at scale S		$m_{sed}.s^{-1}$ *(D)*
kws_{water}	partial mass transfer coefficient at the water-side of the sediment-water interface	$2.78\cdot10^{-6}$	$m_{water}.s^{-1}$ *(A)*
kws_{sed}	partial mass transfer coefficient at the pore water side of the sediment-water interface	$2.78\cdot10^{-8}$	$m_{porewater}.s^{-1}$ *(A)*
Soil to water transfer			
$RUNOFF_{soil\,i\text{-}water\,i[S]}$	mass transfer coefficient for run-off from soil i to water i at scale S		$m_{soil}.s^{-1}$ *(D)*

$EROSION_{soil\ i[S]}$	rate at which soil is washed from soil i into surface water at scale S	0.03	$mm.y^{-1}$ *(A)*
$FRACrun_{soil\ i[S]}$	fraction of the wet precipitation that runs off soil i to water i at scale S	0.25	- *(A)*
Transport from system			
$BURIAL_{sed\ i[S]}$	sediment burial rate for water column i at scale S		$m_{sed}.s^{-1}$ *(D)*
$LEACH_{soil\ i[S]}$	mass transfer coefficient for leaching from soil i at scale S		$m_{soil}.s^{-1}$ *(D)*
$FRACinf_{soil\ i[S]}$	fraction of rain water that infiltrates into soil i at scale S	0.25	- *(A)*

[b] Only at the regional and continental scale

[c] Rerouting of the chemical due to sewage treatment is defined at the regional and continental scale only.