SimpleBox 4.0
A multimedia mass balance model for evaluating the fate of chemical substances

National Institute for Public Health
and the Environment
Ministry of Health, Welfare and Sport

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Publiekssamenvatting

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SimpleBox is een van de rekenmodellen die het RIVM ontwikkelt voor het milieubeleid. Met dit model kan worden geschat aan welke concentraties chemische stoffen mens en milieu blootstaan. SimpleBox wordt al twintig jaar gebruikt bij de ontwikkeling van Europese regelgeving voor chemische stoffen (tegenwoordig: REACH-procedures) om te berekenen welke concentraties als veilig mogen worden beschouwd. Het model is in 2014 geüpdatet op basis van de nieuwste wetenschappelijke inzichten en kan nu voor meer stoffen worden ingezet. Dit rapport bevat de gedetailleerde beschrijving voor technisch-wetenschappelijke onderzoekers en beleidsmakers.

Met SimpleBox kan de aanwezigheid van chemische stoffen in lucht, water en de bodem worden weergegeven. Het beschrijft ook hoe snel en in welke mate ze tussen deze compartimenten worden 'uitgewisseld'. Stoffen in de lucht kunnen bijvoorbeeld door regen in de bodem terechtkomen.

De eerste versie van SimpleBox stamt uit 1986; de huidige versie 3.0, die momenteel in REACH dienst doet, is uitgebracht in 2004. Het vernieuwde model kan ook worden gebruikt voor stoffen die in het milieu geheel of gedeeltelijk als elektrisch geladen deeltjes (ionen) aanwezig zijn, zoals zware metalen en organische zuren en basen. Toekomstige modelvernieuwingen van SimpleBox zullen bovendien bruikbaar zijn voor nanomaterialen. Het RIVM ontwikkelt momenteel zo'n SimpleBox4nano in samenwerking met de Radboud Universiteit Nijmegen.

Het model wordt voor gebruik door onderzoekers en beleidsmakers beschikbaar gesteld via de RIVM-website www.rivm.nl/SimpleBox.

Kernwoorden: milieumodellering, gifstoffen

Synopsis

SimpleBox 4.0

This document provides the technical description of the revised multi-media fate model SimpleBox 4.01 (20150331).

SimpleBox is a nested multi-media environmental fate model of the so-called Mackay level III/IV type. The environment is modelled as consisting of well-mixed environmental compartments (air, water, sediment, soil, etc.), at three spatial scales. Emissions to the compartments, transfer and partitioning between the compartments, and removal from the compartments are used to compute the steady-state and quasi-dynamic masses of chemical substance in the environment. The SimpleBox model simulates the environmental fates of different substances in different landscape settings, of which the characteristics are provided with the model database. In its default settings, SimpleBox returns results for a typical chemical, given a typical emission, to a typical environment.

SimpleBox vs. 4.01 (20150331) is an update of the SimpleBox vs 3.0 (20040614). Structural improvements made to the former version are the removal of the local scale and the vegetation compartments, and the addition of lake water and deep-sea water compartments. Further improvements are a number of updates which implement new scientific insights in transport and degradation processes. The model's application domain has been extended to cover a wider suite of chemical substances, notably ionizing compounds such as metals, organic acids, and bases.

This report has been written to provide technical documentation for the new SimpleBox model.

Keywords: environmental fate modeling, toxic substances

Contents

Samenvatting

Deze documentatie verstrekt de technische beschrijving van het herziene multimedia lotgevallenmodel SimpleBox 4.01 (31 maart 2015).

SimpleBox is een "genest" multimedia milieu lotgevallenmodel van het zogenaamde Mackay level III/IV-type. Het milieu wordt gemodelleerd als bestaande uit goed gemengde milieucompartimenten (lucht, water, sediment, bodem, et cetera) op drie ruimtelijke schalen. Emissies naar de compartimenten, transport en verdeling tussen de compartimenten, en verwijdering uit compartimenten worden gebruikt voor het berekenen van de steady-state en quasi-dynamische toestanden van milieuvervuiling, in termen van massa's van stoffen in het milieu. SimpleBox simuleert het gedrag van verschillende chemische stoffen in verschillende milieus, waarvan de parameters in de met het model meegeleverde database zijn terug te vinden. Met alleen standaardwaarden modelleert SimpleBox de massa's van een standaardstof in de compartimenten van een standaardmilieu.

SimpleBox vs 4.01 (20150331) is een aangepaste versie van SimpleBox vs 3.0 (20040614). Structurele verbeteringen zijn de verwijdering van de lokale schaal en de vegetatiecompartimenten, en het toevoegen van een zoetwatermeer- en diepzeewatercompartimenten. Verder zijn nieuwe wetenschappelijke inzichten in transport en omzetting van stoffen in het nieuwe model geïmplementeerd. Hierdoor is het toepassingsgebied van het model uitgebreid en kunnen er meer verschillende soorten stoffen worden gemodelleerd. Met name metalen en andere geheel of gedeeltelijk ionogene stoffen, zoals organische zuren en basen.

Dit rapport is bedoeld als technisch achtergronddocument voor het nieuwe SimpleBox model.

1   Introduction

A central issue in risk assessment of chemicals in the environment is the lack of information on the organisms' levels of exposure to these chemicals. In the late 1970s, the development of the first multimedia mass balance models (MMBM) provided an opportunity to predict the environmental fate of chemicals (Mackay, 1979). Thanks to these models, exposure levels of organisms to chemicals can now be predicted, resulting in more powerful risk assessment and management. While the first models focused on screening and evaluation of the behaviour of chemicals, currently MMBMs are used to identify the behaviour of chemicals and data gaps, as well as to provide input for environmental policy and legislation. MMBMs are made up of multiple homogeneous compartments in a box; these can be at a local, regional, continental, or global scale. The concentration of a chemical in each homogeneous compartment such as air, water, soil or sediment is predicted using a separate equation. By combining all the compartments' equations, the model predicts the steady states and/or non-steady states of the chemicals.

SimpleBox is a nested multimedia environmental fate model in which the environmental compartments are represented by boxes. In the past few years some major changes have been made, resulting in a new version; SimpleBox 4.0. 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 a typical substance in a typical environment.

In 1982, the first SimpleBox was introduced at the RIVM; its complete history has been published by Brandes et al. (1996).

1.1   Adjustments to the SimpleBox model

Both the transport processes between and the removal processes from all the compartments are described using equations. However, recent studies have shown that more accurate parameters or equations to describe certain processes are possible. An overview of all the improvements made to SimpleBox 4.0, are presented in Table 1.

For example, the enthalpy of vaporization is set to a constant value in SimpleBox 3.0, while a relationship between this vaporization enthalpy and the subcooled liquid vapour pressure of a compound has been described (MacLeod et al., 2007). In addition, precipitation patterns are assumed to be continuous over the year. This results in a possible overestimation of removal of hydrophilic compounds due to wet deposition (Jolliet & Hauschild, 2005). Franco & Trapp (2010) described new equations for more reliable predictions on ionized compounds. Therefore, the SimpleBox 3.0 model, which is only valid for neutral non-ionized compounds only, has been updated with routines for ionisable chemicals (Franco & Trapp, 2010), to obtain version 4.0. However, it is important to ensure that the partitioning of this class of chemicals depends on the pH of the compartment. As explained above, all

compartments are considered as being homogeneous, while an exponential concentration profile in soils is described by Hollander et al., (2004, 2007a). To obtain more reliable and up-to-date predictions, all of these findings have been implemented in the SimpleBox model.

Table 1. Adjustments made to SimpleBox 3.0 resulting in SimpleBox 4.0.

Differences in SimpleBox 4.0 compared to SimpleBox 3.0		References
Scales	Removal of the local scale; Inclusion of the moderate, arctic and trophic zones under global scale;	
Compart-ments	Removal of the vegetation compartments at the regional and continental scale; Addition of lake compartment to the regional and continental scale; Addition of deep sea water compartment to the global scales;	
Colloids	Addition of colloidal organic matter to the water compartments;	
Soil pene-tration	Implementation of corrections for exponential decrease of soil concentrations; Penetration depth in soil set to ten cm for all chemicals;	Hollander et al., 2004; Hollander et al., 2007a
Precipitation pattern	Implementation of intermittent rain algorithm; Distinction between water and solid phase of aerosols; Partitioning within the air compartment between gas, aerosol and cloud water made pKa dependent;	Jolliet & Hauschild, 2005 Franco & Trapp, 2010 Franco & Trapp, 2010
Enthalpy of vaporization	Implementation of algorithm for enthalpy of vaporization;	MacLeod et al., 2007
QSARs	Implementation of QSARs for calculating the K_{oc} from the K_{ow};	REACH 2012
Calculations and lay-out	Adjustments to lay-out of steady-state output; Improvements to the look-up from scenarios and cases	

1.2 Reader's guide

This report is complementary to the technical documentation as described by Brandes et al. (1996). Chapter 2 describes the model concept and all the processes in the SimpleBox model, chapter 3 describes the improvements made to the model, chapter 4 describes the output possibilities of the model, and chapter 5 describes the SimpleBox model code.

2 The SimpleBox model

2.1 Model concept

SimpleBox (version 4) is an example of a level III and level IV "Mackay type" model, where both non-equilibrium steady-state and non-equilibrium non-steady-state are computed. This model contains a local scale containing eight compartments, regional and continental scales each containing nine compartments, and global zones, each containing five compartments (Figure 1; Hollander et al., 2007b).

Environmental compartments are represented by boxes. The mass of a chemical in these boxes is the result of various mass flow processes to and from the boxes. Entry mechanisms of chemicals into a box are: (a) emission (EMIS), (b) import flows of air or water (IMP) from boxes outside the spatial scale to which the box belongs, and (c) intermedia transport (IMT) from another box inside the spatial scale. Loss mechanisms are: (d) degradation (DEG), (e) export (EXP) to outside the spatial scale, and (f) intermedia transport (IMT) to other boxes in the same spatial system. A mass balance equation can be written for each of the boxes. The mass balance equations have the following format:

$$\frac{\mathrm{d}\vec{m}_x(t)}{\mathrm{d}t} = EMIS_x + IMP_{y\to x} \cdot m_y - EXP_{x\to y} \cdot m_x + IMT_{z\to x} \cdot m_z - IMT_{x\to z} \cdot m_x \quad (1)$$
$$- DEG_x \cdot m_x$$

with
m_x :   mass of the chemical in box x [mol]
t :   time [s]
$EMIS_x$: emission rate of the chemical into box x [mol·s^{-1}]
$IMP_{y\to x}$: import rate of the chemical from box y into box x [s^{-1}]
$EXP_{x\to y}$: export rate of the chemical from box x into box y [s^{-1}]
$IMT_{z\to x}$: intermedia transfer rate of the chemical from box z into box x [s^{-1}]
$IMT_{x\to z}$: intermedia transfer rate of the chemical from box x into box z [s^{-1}]
DEG_x : loss rate of the chemical from box z [s^{-1}]

2.2 Scales and compartments

SimpleBox 4.0 is a nested multimedia model consisting of three scales: regional, continental, and global. The global scale includes three zones: the arctic, moderate, and tropic. The regional and continental scales include nine compartments: air, lake water, freshwater, fresh water sediment, sea water, sea water sediment, natural soil, agricultural soil, and urban/industrial soil (Figure 1). At the global scale, each scale includes five compartments: air, surface sea water, deep-sea water, sea water sediment, and soil (Figure 1).

2.3 Processes in SimpleBox

Emissions can enter the air, water and soil compartments of all scales. Emission rates are expressed as products of production volumes and
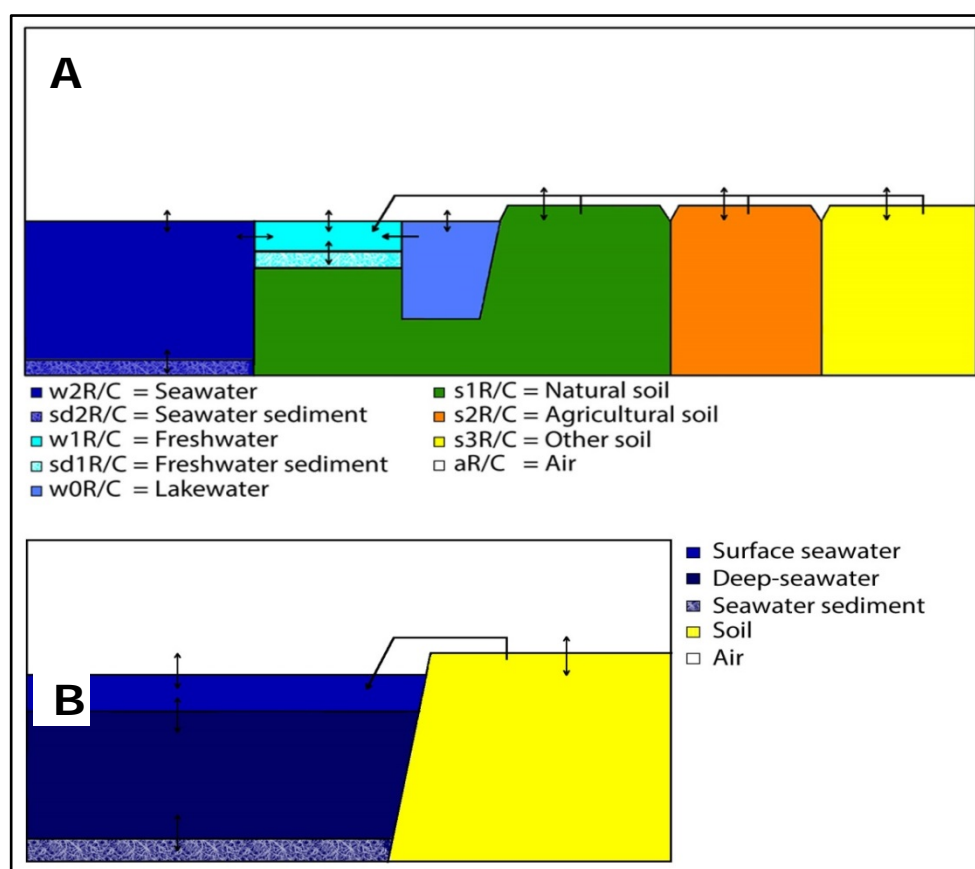
Figure 1. Schematic view of the system and its compartments. A: Regional and continental scale, B: global scale.

emission factors, each of which needs to be entered by the modeller as model input.

Imports and exports of a substance enter and leave the air and water compartments of all spatial scales. At the regional and continental scales, fresh water flows through the lake water compartments via the fresh water compartments into the coastal marine and the ocean water compartments At the global scale, the water flows from tropical surface water through the moderate zone to the arctic zone and back through deep-sea waters. At all scales and global zones, air masses carry chemicals between air compartments. Import and export flow rates of water and air are considered constant in time. In addition, export of a substance occurs from the air compartments of all spatial scales by diffusion to the stratosphere.

Degradation of the substance occurs in all compartments at all scales. As with export with flowing air and water, and escape by diffusive transfer, degradation is a loss mechanism, assumed to obey (pseudo) first order kinetics. The first-order degradation rate constants characterising the virtual degradation mass flows must be entered as input. Leaching of the substance occurs from the soil compartments into the groundwater, which is not considered to be part of the modelled system; leaching mass flows are considered as output terms. Unlike the

input mass flows, output mass flows are concentration dependent and become constant with time only when at steady state.

Intermedia transfer takes place between nearly all the compartments. Atmospheric deposition to soil and water in aerosol particles and rain droplets, run-off from soil to water, and leaching from soil 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 of the implications for the direction of the resulting (net) intermedia mass flows. Net transport between two compartments by diffusion can go both ways, depending on the concentrations of the chemical in the two adjacent media: diffusive transport from air to the earth's surface is called gas absorption, diffusive transport in the opposite direction is called volatilization. As described by Brandes *et al.* (1996), diffusive intermedia transfer was successfully addressed by Mackay (2001) in his 'fugacity approach'. In the case of advective transport, a chemical is carried physically from one compartment into another so that the chemical mass flow strictly takes the direction of the carrier flow, independent of the (direction of) concentration gradients. Advective mass transfer can carry the chemical against the chemical potential or fugacity gradients.

3 Model calculations

In this chapter, the SimpleBox model is described in detail. In the following sections, the parameters and the equations for the landscape characteristics, chemical characteristics, partition coefficients, degradation and transformation rates, intermedia partitioning and transfer processes are specified.

3.1 Model parameters

SimpleBox 4.0 contains multiple categories of parameters:
1. Default parameters: parameters that have a default value which is generally accepted or described in the literature (Table 2).
2. Input parameters: parameters that describe the substances or landscape.
3. Calculated parameters: parameters that are described by a formula which contains other default, input and/or calculated parameters.

The following conventions are applied for symbols, where possible:
Parameters are mainly denoted in lower case (capitals indicating separate words), which indicate the type of the parameter.
Specification of the parameter and compartment for which the parameter is specified in subscript.
Specification of the scale is shown as a subscript in capital.

As an example, the symbol $Frac_{aers,a[S]}$ means the fraction (*Frac*) aerosol solids (*aers*) in air (*a*) 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.

Table 2. Parameters with a default value used in the model.

Parameter name	Description	Default value	Reference
$Aerosol_{dep,[S]}$	deposition velocity of regional, continental and global aerosol particles	$0.001 \ m \cdot s^{-1}$	Mackay (2001)
$AreaFrac_{wA}$	area fraction arctic ocean	0.6	
$AreaFrac_{wM}$	area fraction moderate ocean	0.5	
$AreaFrac_{wT}$	area fraction tropical ocean	0.7	
$Bact_{test}$	concentration bacteria in test water	$40000 \ CFU \cdot ml^{-1}$	
$Bact_{w[S]}$	concentration bacteria in regional, continental and global waters	$40000 \ CFU \cdot ml^{-1}$	

Parameter name	Description	Default value	Reference
$C_{OHrad,a[S]}$	OH radical concentration	500000 cm^{-3}	Den Hollander et al., (2004)
$Collect_{eff[S]}$	aerosol collection efficiency representing the volume of air efficiently scavenged by rain of its aerosol content, per unit volume of rain.	200000	Mackay (2001)
$Col_{w[S]}$	concentration of colloidal organic matter in regional and continental lake, fresh and sea water	0.001 kg·m^{-3}	
Corg	standard mass fraction organic carbon in soil/sediment	0.02	Den Hollander & Van de Meent (2004)
$Corg_{aers}$	mass fraction organic carbon in aerosol	0.1	
$Corg_{s[S]}$	mass fraction organic carbon in regional and continental natural and agricultural soil	0.02	Den Hollander & Van de Meent (2004)
$Corg_{sd[S]}$	mass fraction organic carbon in regional and continental lake, fresh and sea water sediment	0.05	
$Corg_{susp[S]}$	mass fraction organic carbon in regional and continental lake, fresh and sea water suspended matter	0.1	
$Depth_{s[S]}$	mixing depth regional, continental and global soils	0.05 m for regional and continental natural land, other soils, and global soils; 0.2 m for the regional and continental agricultural soils	Den Hollander & Van de Meent (2004)
$Depth_{sd[S]}$	mixed depth regional, continental and global water sediments	0.03 m	

Parameter name	Description	Default value	Reference
Depth$_{w[S]}$	mixed depth of regional, continental and global sea waters	10 m for regional sea water; 200m for continental sea water; 100 m for global surface sea water; 3000 m for global deep sea water	
Ea$_{Ohrad}$	Activation energy OH radical reaction	6000 J·mol^{-1}	
Erosion$_{s[S]}$	Erosion of global soils	0.000000000000951 m·s^{-1}	
Frac$_{a,s[S]}$	volume fraction air in regional, continental and global soils	0.2	
Frac$_{aers,a[S]}$	Volume fraction solid particles in regional, continental and global airs	0.00000000002	
Frac$_{aerw,a[S]}$	Volume fraction aqueous phase aerosols in regional, continental and global airs	0.00000000002	
Frac$_{inf,s[S]}$	Volume fraction of precipitation infiltrating into global soils	0.25	
Frac$_{run,s[S]}$	Volume fraction of precipitation running off to global waters	0.25	
Frac$_{w,s[S]}$	volume fraction water in regional, continental and global soils	0.2	
Frac$_{w,sd[S]}$	volume fraction water in regional, continental and global sediments	0.8	Paterson & Mackay (1994)
HO$_{sol}$	enthalpy of dissolution	described in substance data,if not: 10000 J.mol^{-1}	
Height$_{a[S]}$	mixed height of the regional, continental and global air	1000 m	Den Hollander & Van de Meent (2004)
k0$_{OHrad}$	frequency factor OH radical reaction	0.000000000079 cm^3·s^{-1}	

Parameter name	Description	Default value	Reference
$K_{p,col[S]}$	colloidal organic matter-water partitioning coefficient in global waters	220 L·kg^{-1}	
$k_{wsd,sed,sd[S]}$	partial mass transfer co-efficient for the sediment side of regional, continental and global water/sediment interface	0.00000002778 m.s^{-1}	Mackay (2001)
$k_{wsd,water,w[S]}$	partial mass transfer co-efficient for the water side of regional, continental and global water/sediment interface	0.000002778 m.s^{-1}	Mackay (2001)
NetSed-Rate$_{w[S]}$	Net sediment accumulation rate for regional, continental and global waters	0.0000000000868 m·s^{-1} for regional fresh water; 0.0000000000862 m·s^{-1} for continental fresh water; 0.0000000000634 m·s^{-1} for regional sea water; 0.0000000000274 m·s^{-1} for continental sea water; 0.0000000000000895 m·s^{-1} for moderate sea water; 0.0000000000000634 m·s^{-1} for arctic/tropical sea water;	
Ocean-Current	global ocean circulation current	150000000 m^3·s^{-1}	
pH$_{aerw}$	pH aerosol water	3	Franco & Trapp (2010)
pH_{cldw}	pH cloud water (average of pH of water in air before oxidation (6.5) and after oxidation (4.7))	5.6	Franco & Trapp (2010)
pH$_s$	pH of soil	5 for natural soil; 7 for agricultural and other soil	Franco & Trapp (2010)

Parameter name	Description	Default value	Reference
pH_w	pH of water	7 for fresh water; 8 for sea water	Franco & Trapp (2010)
$Prod_{susp,w[S]}$	autochthonous production of suspended matter in regional, continental and global waters	1.99 kg·s^{-1} for regional fresh water; 0.32 kg·s^{-1} for regional sea water; 32.39 kg·s^{-1} for continental fresh water; 552.52 kg·s^{-1} for continental sea water; 1229.88 kg·s^{-1} for moderate sea water; 808.6 kg·s^{-1} for arctic sea water; 2830.1 kg·s^{-1} for tropical sea water	Den Hollander & Van de Meent (2004)
Q_{10}	rate increase factor per 10°C	2	
$RainRate_{[S]}$	global annual precipitation	2.22E-08 m·s^{-1} forthe moderate scale; 4.12E-08 m·s^{-1} for the tropic scale; 7.93E-09 m·s^{-1} for the arctic scale	
$Settl\text{-}Velocity_{[S]}$	settling velocity of suspended particles	0.0000289 m·s^{-1}	Den Hollander & Van de Meent, 2004
$Susp_{w[S]}$	concentration of suspended matter in regional and continental lake, fresh and sea water	0.0005 kg·m^{-3} for lake water; 0.015 kg·m^{-3} for fresh water; 0.005 kg·m^{-3} for sea water	Asselman (1997)
$System\text{-}Area_A$	area arctic scale	4250000000000 m^2	
$System\text{-}Area_T$	area tropical scale	127500000000000 m^2	
$Temp_{[S]}$	temperature global scale	263 K for the arctic zone; 285 K for the moderate zone; 298 K for the tropical zone	
$Wind\text{-}Speed_{[S]}$	average global wind speed	3 m.s^{-1}	

Parameter name	Description	Default value	Reference
ρ_{aers}	dry density of aerosol solids	2000 kg·m^{-3}	
ρ_{solid}	mineral density of sediment and soil	2500 kg·m^{-3}	

3.2 Characteristics of the landscape

The landscape data in Table 3 contain values for the regional and continental landscape characteristics: area land and sea; fraction lake, fresh and sea water; fraction natural, agricultural and other soil; wind speed; rain rate; depth of lake and fresh water; river flow; fraction runoff; fraction infiltration; erosion and the emission scenario.

In its default settings, SimpleBox represents the Earth's northern hemisphere: continents surrounded by oceans in three climatic zones, and continents composed of river catchments, one of which is detailed as regional environment. In addition to this default landscape, specific landscapes can be selected from SimpleBox's database, such as the standard EUSES landscape and 17 sub-continental landscapes, based on the REIMSEA model proposed by Wegener Sleeswijk et al. (2003).

Table 3. Default values for landscape characteristics.

Variable name	Default value regional scale	Default value continental scale	Unit
$Area_{land[S]}$	228570000000	3714410000000	m^2
$Area_{sea[S]}$	1000000000	3714410000000	m^2
$Frac_{w0[S]}$	0.0025	0.0025	-
$Frac_{w1[S]}$	0.0275	0.0275	-
$Frac_{s1[S]}$	0.27	0.27	-
$Frac_{s2[S]}$	0.6	0.6	-
$Frac_{s3[S]}$	0.1	0.1	-
$Temp_{[S]}$	285	285	K
$WindSpeed_{[S]}$	3	3	$m·s^{-1}$
$RainRate_{[S]}$	0.0000000222	0.0000000222	$m·s^{-1}$
$Depth_{w0[S]}$	100	100	m
$Depth_{w1[S]}$	3	3	m
$Frac_{w1R \to w1C}$/ $Frac_{w1C \to w1R}$	0	0	-
$Frac_{run[S]}$	0.25	0.25	-
$Frac_{inf[S]}$	0.25	0.25	-
$Erosion_{[S]}$	0.000000000000951	0.000000000000951	$m·s^{-1}$
$Emission_{a[S]}$	2.157	0	$mol·s^{-1}$
$Emission_{w0[S]}$	0	0	$mol·s^{-1}$
$Emission_{w1[S]}$	2.157	0	$mol·s^{-1}$
$Emission_{w2[S]}$	0	0	$mol·s^{-1}$
$Emission_{s1[S]}$	0	0	$mol·s^{-1}$
$Emission_{s2[S]}$	2.157	0	$mol·s^{-1}$
$Emission_{s3[S]}$	0	0	$mol·s^{-1}$

3.3 Characteristics of the chemical

The substance data describes the physical-chemical characteristics and degradation rates of 267 high production volume chemicals (HPVC; supporting information from Harbers et al., 2006). In SimpleBox 4.0, these characteristics are used for conversion of units, calculations of partitioning coefficients, and degradation of the substances. This section describes the physical-chemical characteristics used in the fate calculation of SimpleBox 4.0.

3.3.1 Molecular weight
Molecular weight is used to calculate the gas and water diffusion coefficients and the partial mass transfer coefficients between air and water. In addition, molecular weight is used to convert the units of water solubility, emissions and output. If the molecular weight is not mentioned in the substance data, the median of all substances is used as default, 0.138 kilogram per mol.

3.3.2 Solid-water partitioning coefficient

The solid-water partitioning coefficient is used to calculate the partitioning coefficients of the suspended solids, sediment and soil to water and for estimating the degradation rate in sediment and soil. If the solid-water partitioning coefficient is not mentioned in the substance data, it can be obtained by means of QSARs (Franco & Trapp, 2008):

For acids (original species):

$$K_{sw} = 10^{0.54 \cdot \log K_{ow} + 1.11} \cdot Corg \cdot \frac{\rho_{solid}}{1000} \tag{2}$$

For acids (alternate form):

$$K_{sw,alt} = 10^{0.11 \cdot \log K_{ow} + 1.54} \cdot Corg \cdot \frac{\rho_{solid}}{1000} \tag{3}$$

For bases (original species):

$$K_{sw} = 10^{0.37 \cdot \log K_{ow} + 1.7} \cdot Corg \cdot \frac{\rho_{solid}}{1000} \tag{4}$$

For bases (alternate form):

$$K_{sw,alt} = 10^{pK_a^{0.65} \cdot \frac{K_{ow}}{1+K_{ow}}^{0.14}} \cdot Corg \cdot \frac{\rho_{solid}}{1000} \tag{5}$$

For metals, solids-water partition coefficients need to be entered by users as model input. By default, a K_p value of 1000 is used:

$$K_{sw} = 1000 \cdot Corg \cdot \frac{\rho_{solid}}{1000} \tag{6}$$

For other chemical classes:

$$K_{sw} = a \cdot K_{ow}{}^{b} \cdot Corg \cdot \frac{\rho_{solid}}{1000} \tag{7}$$

with
K_{sw}: dimensionless solids-water partitioning coefficient of the original species [-]
$K_{sw,alt}$: dimensionless solids-water partitioning coefficient of the alternate form [-]
K_{ow}: octanol-water partitioning coefficient of the original species [-]
Corg: standard mass fraction organic carbon in soil/sediment [-]
ρ_{solid}: mineral density in soil/sediment [kg·m⁻³]
pK_a: dissociation constant of (conjugated) acid [-]
1000: conversion factor [m³·kg⁻¹]

Where a and b values for the other chemical classes can be found in Table 4.

Table 4. Solid-water partitioning coefficient QSAR values for other chemical classes described by the European Commission (2003a).

Chemical class	a	b
Neutral/Hydrophobics	1.26	0.81
Non hydrophobics	10.47	0.52
Phenols, anilines, benzonitriles, nitrobenzenes	7.94	0.63
Acetanilides, carbamates, esters, phenylureas, phosphates, triazines, triazoles, uracils	12.30	0.47
Alcohols, organic acids	3.16	0.47
Acetanilides	13.18	0.40
Alcohols	3.16	0.39
Amides	17.78	0.33
Anilines	7.08	0.62
Carbamates	13.80	0.37
Dinitroanilines	83.18	0.38
Esters, Phenylureas	11.22	0.49
Nitrobenzenes	3.55	0.77
Organic acids	2.09	0.60
Phenols, benzonitriles	12.02	0.57
Phosphates	14.79	0.49
Triazines	31.62	0.30
Triazoles	25.70	0.47

3.3.3 Gas-water partitioning coefficient

The air-water partitioning coefficient is used to calculate the scale specific air-water partitioning coefficient and the scale specific aerosol solids-water partitioning coefficient. If the air-water partitioning coefficient is not mentioned in the substance data, it can be obtained from:

For $P_{vap25} > 100000$:

$$K_{aw} = \frac{\frac{100000}{Sol_{25}}}{8.31 \cdot 298} \tag{8}$$

For $P_{vap25} < 100000$:

$$K_{aw} = \frac{\frac{P_{vap25}}{Sol_{25}}}{8.31 \cdot 298} \tag{9}$$

with

K_{aw}: dimensionless gas-water partition coefficient of the original species [-]

P_{vap25}: vapour pressure of original species at 25°C [Pa]

Sol_{25}: water solubility of original species at 25°C [mol·m^{-3}]

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

298: temperature [K]

100000: maximum vapour pressure of original species at 25°C [Pa]

This estimation cannot be used for metals, and therefore the air-water partitioning coefficient is considered to be 1.0E-20.

3.3.4 Octanol-water partitioning coefficient

The octanol-water partitioning coefficient is used to estimate the water solubility, the apparent octanol-water partitioning coefficient, the organic carbon-water partitioning coefficient (original species and alternate form) and the aerosol solids-water partitioning coefficient. If no octanol-water partitioning coefficient is listed in the substance data, and the user does not specify one as model input, the median value of all substances in the database is used by default.

The octanol-water partitioning coefficient of the alternate form may be obtained from:

$$K_{ow,alt} = 10^{\log K_{ow} - 3.5} \tag{10}$$

with
$K_{ow,alt}$: octanol-water partitioning coefficient of the alternate form [-]
K_{ow}: octanol-water partitioning coefficient of the original species [-]

The apparent octanol-water partitioning coefficient is described by Trapp & Horobin (2005) and can be obtained from:

For acids:
$$D = \left(\frac{1}{1 + 10^{7 - pK_a}}\right) \cdot K_{ow} + \left(1 - \left(\frac{1}{1 + 10^{7 - pK_a}}\right) \cdot K_{ow,alt}\right) \tag{11}$$

For bases:
$$D = \left(\frac{1}{1 + 10^{pK_a - 7}}\right) \cdot K_{ow} + \left(1 - \left(\frac{1}{1 + 10^{pK_a - 7}}\right) \cdot K_{ow,alt}\right) \tag{12}$$

For neutrals:
$$D = 1 \cdot K_{ow} + (1 - 1) \cdot K_{ow,alt} \tag{13}$$

with
D: apparent octanol/water partition coefficient at neutral pH [-]
pK_a: dissociation constant of (conjugated) acid [-]
K_{ow}: octanol/water partition coefficient of the original species [-]
$K_{ow,alt}$: octanol/water partition coefficient of the alternate form [-]
7: neutral pH [-]

3.3.5 pKa

The dissociation constant of (conjugated) acid (pKa) is used to determine the fraction of original species in waters, sediments and soils and to calculate the apparent octanol-water partitioning coefficient. For substances that may occur to a significant extent in their alternate (i.e. non-neutral) forms, it is essential that a pKa value is available. By default, a 50-50 split between original and alternate forms at neutral pH is assumed using a pKa value of 7.

3.3.6 Fraction original species

The fraction original species in aerosol water, in fresh water, in sea water, in sediments, in soils and in soil pore water are calculated in SimpleBox 4.0 in order to correct for ionisable compounds. These fraction original species for aerosol, fresh, sea and soil pore water can be determined using the Henderson-Hasselbalch equation (Henderson, 1908):

For acids:

$$Fr_{orig,w} = \frac{1}{1 + 10^{pH_w - pK_a}} \tag{14}$$

For bases:

$$Fr_{orig,w} = \frac{1}{1 + 10^{pK_a - pH_w}}$$

For neutrals:
$$Fr_{orig,w} = 1$$

with
$Fr_{orig,w}$:   fraction original species in aerosol, fresh, sea and soil pore waters [-]
pH_w: pH aerosol, fresh, sea and soil pore waters [-]
pK_a: dissociation constant of (conjugated) acid [-]

The fraction original species in sediments and soil can be determined using equations proposed by Franco and Trapp (2008), which are derived from the Henderson-Hasselbalch equation (Henderson, 1908):

For acids:

$$Fr_{orig,s/sd} = \frac{1}{1 + 10^{pH_{s/sd} - 0.6 - pK_a}} \tag{15}$$

For bases:

$$Fr_{orig,s/sd} = \frac{1}{1 + 10^{pK_a - 4.5}} \tag{16}$$

For neutrals:
$$Fr_{orig,s/sd} = 1 \tag{17}$$

with
$Fr_{orig,s/sd}$:   fraction original species in sediment and soil [-]
$pH_{s/sd}$:   pH sediment and soil [-]
pK_a: dissociation constant of (conjugated) acid [-]

3.3.7 Vapour pressure

The vapour pressure is used to calculate Henry's constant for both the original and the alternate form and the enthalpy of vaporization. If the vapour pressure is not mentioned in the substance data, the median of all substances is used as default; 4.7 Pascal.

3.3.8 Enthalpy of vaporization

The enthalpy of vaporization is used to calculate the scale specific air-water partitioning coefficients. The enthalpy of vaporization is substance dependent and is described by MacLeod *et al.* (2007):

With $T_m > 298$:

$$H0_{vap} = \left(-3.82 \cdot LN\left(P_{vap25} \cdot e^{-6.79 \cdot \left(1 - \frac{T_m}{298}\right)}\right) + 70\right) \cdot 1000 \qquad (18)$$

With $T_m \leq 298$:

$$H0_{vap} = \left(-3.82 \cdot LN\left(P_{vap25}\right) + 70\right) \cdot 1000 \qquad (19)$$

with
$H0_{vap}$: enthalpy of vaporization [J·mol^{-1}]
P_{vap25}: vapour pressure of original species at 25°C [Pa]
T_m: melting point [K]
298:   temperature [K]
1000: conversion factor [J·kJ^{-1}]

3.3.9 Solubility

The solubility is used to calculate the Henry's Law constant for both the original and the alternate form:

$$Sol_{25} = 10^{-1.214\log K_{ow}+0.85} \cdot 1000 \qquad (20)$$

with
Sol_{25}: water solubility of neutral species at 25°C [mol·m^{-3}]
K_{ow}:   octanol-water partitioning coefficient of the original species [mol·L^{-1}]
1000: conversion factor [dm^3·m^{-3}]

3.3.10 Enthalpy of dissolution

The enthalpy of dissolution is used to calculate the scale specific air-water partitioning coefficient and has a default value of 10000 Joules per mol.

3.3.11 Melting point

The melting point of a substance is used to calculate the enthalpy of vaporization. If the melting point is not mentioned in the substance data, the median of all substances is used as default; 276 Kelvin.

3.3.12 Degradation rates

The degradation rates in air, water, sediment and soil are used to derive the scale specific removal rates in the air, water, sediment and soil compartments. If the degradation rate in air is not listed in the substance data, it can be obtained from (Wania & Daly, 2002):

$$k_{deg,air} = C_{OHrad,a[S]} \cdot k0_{OHrad} \cdot e^{\frac{-Ea_{OHrad}}{8.314 \cdot 298}} \qquad (21)$$

with

$k_{deg,air}$:   gas phase degradation rate constant at 25°C [s^{-1}]

$C_{OHrad,a[S]}$:   OH radical concentration [cm^{-3}]

$k0_{OHrad}$: frequency factor OH radical reaction [$cm^3 \cdot s^{-1}$]

Ea_{OHrad}: activation energy OH radical reaction [$J \cdot mol^{-1}$]

8.314:   gas constant [$Pa \cdot m^{-3} \cdot mol^{-1} \cdot K^{-1}$]

298:     temperature [K]

where the OH radical concentration, the frequency factor and the activation energy OH radical reaction are given in Table 2.

If degradation rate constants in water are not listed in the substance data, default half-lives for substances of which results from standard (OECD) tests are available can be used (European Commission, 2003a):

For ready-biodegradable (r) substances:

$$k_{deg,water} = \frac{\frac{\ln 2}{15} \cdot Q_{10}^{\frac{13}{10}}}{3600 \cdot 24} \tag{22}$$

with

$k_{deg,water}$: dissolved phase degradation rate constant at 25°C [s^{-1}]

Q_{10}:   rate increase factor per 10°C [-]

where the rate increase factor per 10°C is given in Table 2.

For ready-biodegradable (r-) substances failing the ten-day window (see REACH TGD, European Commission 2003 a):

$$k_{deg,water} = \frac{\frac{\ln 2}{50} \cdot Q_{10}^{\frac{13}{10}}}{3600 \cdot 24} \tag{23}$$

with

$k_{deg,water}$: dissolved phase degradation rate constant at 25°C [s^{-1}]

Q_{10}:   rate increase factor per 10°C [-]

where the rate increase factor per 10°C is given in Table 2.

For inherently biodegradable (i) substances:

$$k_{deg,water} = \frac{\frac{\ln 2}{150} \cdot Q_{10}^{\frac{13}{10}}}{3600 \cdot 24} \tag{24}$$

with

$k_{deg,water}$: dissolved phase degradation rate constant at 25°C [s^{-1}]

Q_{10}:   rate increase factor per 10°C [-]

where the rate increase factor per 10°C is given in Table 2.

For persistent (p) substances, the degradation rate in water is assumed to be 1.0E-20.

If the degradation rate in sediment is not mentioned in the substance data, it can be obtained from (European Commission, 2003a):

$$k_{deg,sed} = \frac{\frac{0.1 \cdot Q_{10}^{\frac{13}{10}} \cdot \ln(2)}{a}}{3600 \cdot 24} \tag{25}$$

with

$k_{deg,sed}$: bulk degradation rate constant standard sediment at 25°C [s⁻¹]
Q_{10}: rate increase factor per 10°C [-]

where the rate increase factor per 10°C is given in Table 2 and 'a' is derived from the biodegradation class and the partitioning from organic carbon in sediment to the water (Table 5).

Table 5. Half-lives (days) for sediment and soil based on biodegradation test results. Adapted from the European Commission (2003b).

$K_{sw}/Corg \cdot \rho_{solid}/1000$ is	r	r-	i/p
≤100	30	90	300
≤1000	300	900	3000
≤10000	3000	9000	30000
>100000	30000	90000	300000

If the degradation rate in soil is not mentioned in the substance data, it can be obtained from (European Commission, 2003a):

$$k_{deg,soil} = \frac{\frac{Q_{10}^{\frac{13}{10}} \cdot \ln(2)}{a}}{3600 \cdot 24} \tag{26}$$

with

$k_{deg,sed}$: bulk degradation rate constant standard sediment at 25°C [s⁻¹]
Q_{10}: rate increase factor per 10°C [-]

where the rate increase factor per 10°C is given in Table 2 and 'a' in Table 5.

3.4 Intermedia partitioning processes

Intermedia equilibrium constants (air-water; aerosol-water; sediment-water; soil-water) or partition coefficients are required for various purposes, but principally for estimating intermedia mass transfer coefficients. The coefficients represent concentration ratios. Partition coefficients are available from experimental data or field measurements. More often, however, this information is not available. In these cases, the estimation methods described below can 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.

3.4.1 Air-water

The air-water partition coefficient differs across the different scales of the SimpleBox model. The scale specific air-water partition coefficient can be obtained from:

$$K_{aw[S]} = K_{aw} \cdot e^{\frac{H0_{vap}}{8.314}\left(\frac{1}{298} - \frac{1}{Temp[S]}\right)} \cdot e^{-\frac{H0_{sol}}{8.314}\left(\frac{1}{298} - \frac{1}{Temp[S]}\right)} \cdot \frac{298}{Temp[S]} \qquad (27)$$

with

$K_{aw[S]}$: dimensionless air-water partition coefficient of the original species at regional, continental and global temperature [-]

K_{aw}: dimensionless gas-water partition coefficient of the original species [-]

$H0_{vap}$: enthalpy of vaporization [J·mol⁻¹]

$Temp_{[S]}$: temperature [K]

$H0_{sol}$: enthalpy of dissolution [J·mol⁻¹]

8.31: gas constant [Pa·m⁻³·mol⁻¹·K⁻¹]

298: temperature [K]

Where the dimensionless gas-water partition coefficient of the original species, the enthalpy of vaporization and the dissolution are described in Section 3.3.8; the regional and continental scale temperatures are described in Table 3; and the global scale temperature in Table 2.

3.4.2 Aerosol solids-air

The aerosol solids-water partitioning coefficient is calculated as described by Harner & Bidleman (1998; adjusted according to Götz *et al.*, 2007):

$$K_{aers,a[S]} = 0.54 \cdot \frac{K_{ow}}{K_{aw}} \cdot Corg_{aers} \cdot \frac{\rho_{aers}}{1000} \qquad (28)$$

with

$K_{aers,a[S]}$: regional, continental and global dimensionless aerosol solids-water partitioning coefficient [-]

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

K_{aw}: dimensionless gas-water partitioning coefficient of the original species at 25°C [-]

$Corg_{aers}$: mass fraction organic carbon in aerosol [-]

ρ_{aers}: dry density of aerosol solids [kg·m⁻³]

1000: conversion factor [m³·kg⁻¹]

Where the octanol-water partitioning coefficient and the gas-water partitioning coefficient are described in Sections 3.3.4 and 3.3.4, respectively. The mass fraction organic carbon in aerosol and the dry density of aerosol solids are described in Table 2.

3.4.3 Aerosol water-air

The aerosol water-water partitioning coefficient can be obtained from:

$$k_{aerw,a[S]} = \frac{1}{K_{aw} \cdot Fr_{orig,aerw}} \tag{29}$$

with

$k_{aerw,a[S]}$: regional, continental and global dimensionless aerosol water-water partitioning coefficient [-]

K_{aw}: dimensionless gas-water partitioning coefficient of the original species at 25°C [-]

$Fr_{orig,aerw}$: fraction original species in aerosol water [-]

Where the gas-water partitioning coefficient and the fraction original species in aerosol water are described in Section 3.3.6.

3.4.4 Suspended solids-water

The suspended solids-water partitioning coefficient can be obtained from:

$$K_{p,susp[S]} = (Fr_{orig,w} \cdot K_{sw} + (1 - Fr_{orig,w}) \cdot K_{sw,alt}) \cdot \frac{\frac{1000}{\rho_{solid}}}{Corg} \cdot Corg_{susp[S]} \tag{30}$$

with

$k_{p,susp[S]}$: regional, continental and global suspended solids-water partitioning coefficient [-]

$Fr_{orig,w}$: fraction original species in water [-]

K_{sw}: dimensionless solids-water partitioning coefficient of the original species [-]

$K_{sw,alt}$: dimensionless solids-water partitioning coefficient of the alternate form [-]

Corg: standard mass fraction organic carbon in soil/sediment [-]

$Corg_{susp[S]}$: mass fraction organic carbon in regional, continental and global suspended matter [-]

ρ_{solid}: mineral density of soil/sediment [kg·m^{-3}]

1000: conversion factor [m^3·kg^{-1}]

Where the fraction original species in water and the solids-water partitioning coefficients are described in Section 3.3.6 and 3.3.2, respectively. The standard mass fraction organic carbon in soil/sediment, the mass fraction organic carbon in suspended matter, and the mineral density of soil/sediment are described in Table 2.

3.4.5 Soil-water

The soil-water partitioning coefficient may be derived from:

$$K_{p,s[S]} = (Fr_{orig,s} \cdot K_{sw} + (1 - Fr_{orig,s}) \cdot K_{sw,alt}) \cdot \frac{\frac{1000}{\rho_{solid}}}{Corg} \cdot Corg_{s[S]} \tag{31}$$

with

$K_{p,s[S]}$: regional, continental and global soil-water partitioning coefficient [-]

$Fr_{orig,s}$: fraction original species in soil [-]

K_{sw}: dimensionless solids-water partitioning coefficient of the original species [-]

$K_{sw,alt}$: dimensionless solids-water partitioning coefficient of the alternate form [-]

Corg: standard mass fraction organic carbon in soil/sediment [-]

$Corg_{s[S]}$: mass fraction organic carbon in regional, continental and global soil [-]

ρ_{solid}: mineral density of soil/sediment [kg·m^{-3}]

1000: conversion factor [m^3·kg^{-1}]

Where the fraction of original species in soil and the solids-water partitioning coefficients are described in Section 3.3.6. and 3.3.2, respectively. The standard mass fraction organic carbon in soil/sediment, the mass fraction organic carbon in soil, and the mineral density of soil/sediment are described in Table 2.

The dimensionless soil-water partitioning coefficient can be derived from:

$$K_{slw[S]} = Frac_{a,s[S]} \cdot (K_{aw[S]} \cdot Fr_{orig,sw}) + Frac_{w,s[S]} + Frac_{s,s[S]} \cdot K_{p,s[S]} \cdot \frac{\rho_{solid}}{1000} \quad (32)$$

with

$K_{slw[S]}$: regional, continental and global dimensionless soil-water partitioning coefficient [-]

$Frac_{a,s}$: volume fraction air in regional, continental and global soil [-]

$K_{aw[S]}$: dimensionless air-water partitioning coefficient of the original species at regional, continental and global temperature [-]

$Fr_{orig,sw}$: fraction original species in soil porewater [-]

$Frac_{w,s[S]}$: volume fraction water in regional, continental and global soil [-]

$Frac_{s,s[S]}$: volume fraction solids in regional, continental and global soil [-]

$K_{p,s[S]}$: regional, continental and global soil-water partitioning coefficient [-]

ρ_{solid}: mineral density of soil/sediment [kg·m^{-3}]

1000: conversion factor [m^3·kg^{-1}]

Where the volume fraction air in soil, water in soil, and the mineral density of soil/sediment are described in Table 2. The volume fraction solid in soil is described in Equation 75. The fraction original species in soil pore water is described in Section 3.3.6. The air-water partitioning coefficient and the soil-water partitioning coefficient are described in Equation 27 and 31, respectively.

3.4.6 Sediment-water

The sediment-water partitioning coefficient can be derived from:

$$K_{p,sd[S]} = (Fr_{orig,sd} \cdot K_{sw} + (1 - Fr_{orig,sd}) \cdot K_{sw,alt}) \cdot \frac{\frac{1000}{\rho_{solid}}}{Corg} \cdot Corg_{sd[S]} \tag{33}$$

with

$K_{p,sd[S]}$:   regional, continental and global sediment-water partitioning coefficient [-]

$Fr_{orig,sd}$:   fraction original species in sediment [-]

K_{sw}:   dimensionless solids-water partitioning coefficient of the original species [-]

$K_{sw,alt}$:   dimensionless solids-water partitioning coefficient of the alternate form [-]

$Corg$:   standard mass fraction organic carbon in soil/sediment [-]

$Corg_{sd[S]}$: mass fraction organic carbon in regional, continental and global sediment [-]

ρ_{solid}:   mineral density of soil/sediment [kg·m^{-3}]

1000:   conversion factor [m^3·kg^{-1}]

Where the fraction original species in sediment and the solids-water partitioning coefficients are described in Section 3.3.6. and 3.3.2, respectively. The standard mass fraction organic carbon in soil/sediment, the mass fraction organic carbon in soil, and the mineral density of soil/sediment are described in Table 2.

The dimensionless sediment-water partitioning coefficient can be derived from:

$$K_{sdw[S]} = Frac_{w,sd[S]} + Frac_{s,sd[S]} \cdot K_{p,sd[S]} \cdot \frac{\rho_{solid}}{1000} \tag{34}$$

with

$K_{sdw[S]}$:   regional, continental and global dimensionless sediment-water partitioning coefficient [-]

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

$Frac_{s,sd[S]}$: volume fraction solids in regional, continental and global sediment [-]

$K_{p,sd[S]}$:   regional, continental and global sediment-water partitioning coefficient [-]

ρ_{solid}:   mineral density of soil/sediment [kg·m^{-3}]

1000:   conversion factor [m^3·kg^{-1}]

Where the volume fraction water in sediment and the mineral density of soil/sediment are described in Table 2. The volume fraction solids in sediment and the sediment-water partitioning coefficient are described in Equation 71 and 33, respectively.

3.4.7 Colloidal organic matter-water

The colloidal organic matter-water partitioning coefficient is described by Burkhard (2000) and can be obtained from:

$$K_{p,col[S]} = 0.08 \cdot D \tag{35}$$

with
$K_{p,col[S]}$: colloidal organic matter-water partitioning coefficient [-]
D: apparent octanol-water partitioning coefficient at neutral pH [-]

Where the apparent octanol-water partitioning coefficient is described in Section 3.3.4.

3.5 Characteristics of the environment

The default settings for SimpleBox 4.0 are the Earth's northern hemisphere with three climate zones ('moderate', 'arctic' and 'tropic'), one continental scale (within 'moderate') and one regional scale (within 'continental'). The regional system area can be obtained from:

$$SystemArea_R = Area_{land,R} + Area_{sea,R})$$ (36)

with
$SystemArea_R$: regional system area [m^2]
$Area_{land,R}$: area regional land [m^2]
$Area_{sea,R}$: area regional sea [m^2]

Where the areas land and sea are described in Table 3.

The continental system area can be obtained from:

$$SystemArea_C = Area_{land,C} + Area_{sea,C} - SystemArea_R$$ (37)

with
$SystemArea_C$: continental system area [m^2]
$Area_{land,C}$: area continental land [m^2]
$Area_{sea,C}$: area continental sea [m^2]
$SystemArea_R$: regional system area [m^2]

Where the areas land and sea are described in Table 3.

The moderate system area can be obtained from:

$$SystemArea_M = 85000000000000 - (SystemArea_C + SystemArea_R)$$ (38)

with
$SystemArea_M$: moderate system area [m^2]
8.5E13: area of the moderate zone [m^2]
$SystemArea_C$: continental system area [m^2]
$SystemArea_R$: regional system area [m^2]

The arctic and the tropic system areas have default values, which can be found in Table 2.

3.5.1 Air

Air is treated in SimpleBox as a homogeneous compartment, consisting of a gas phase, an aerosol water phase, an aerosol solids 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 as wind blows air from a larger scale into the system, and from the system to a larger

scale. The wind blows from the regional scale, through the continental scale to the moderate zone and vice versa. From the moderate zone, the wind blows to the arctic and the tropical zones and vice versa. 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 2. The refreshment rate is characterised by the atmospheric residence time.
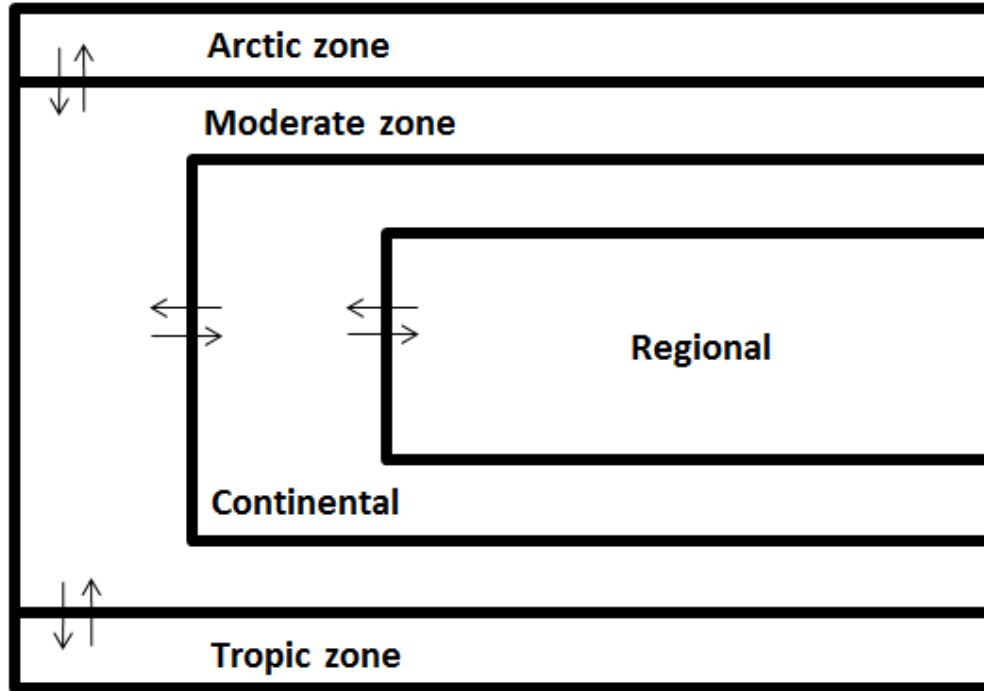
Figure 2: Air flows between the scales in SimpleBox 4.0.

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

$$Volume_{a[S]} = SystemArea_{[S]} \cdot Height_{a[S]} \tag{39}$$

with
$Volume_{a[S]}$:   volume of the regional, continental and global air [m^3]
$SystemArea_{[S]}$: regional, continental and global system area [m^2]
$Height_{a[S]}$:   height of regional, continental and global air [m]

Where the height of the air compartment is described in Table 2.

The fraction of the chemical in the aerosol solids phase can be obtained from:

$$Fr_{aers,a[S]} = \frac{Frac_{aers,a[S]} \cdot K_{aers,a[S]}}{1 + Frac_{aerw,a[S]} \cdot K_{aerw,a[S]} + Frac_{aers,a[S]} \cdot K_{aers,a[S]}} \tag{40}$$

with
$Fr_{aers,a[S]}$:   fraction of chemical in the aerosol solid phase [-]
$Frac_{aers,a[S]}$: volume fraction solid particles in air [-]
$K_{aers,a[S]}$:   dimensionless aerosol solid-air partitioning coefficient [-]
$Frac_{aerw,a[S]}$: volume fraction aqueous phase aerosols in air [-]

$K_{aerw,a[S]}$:   dimensionless aerosol water-air partitioning coefficient [-]

Where the volume fraction solid particles in air and the volume fraction aqueous phase aerosols in air are described in Table 2. The dimensionless aerosol solid-air and aerosol water-air partitioning coefficients are described in Equations 28 and 29, respectively.

The fraction of the chemical in the aerosol water phase can be obtained from:

$$Fr_{aerw,a[S]} = \frac{Frac_{aerw,a[S]} \cdot K_{aerw,a[S]}}{1 + Frac_{aerw,a[S]} \cdot K_{aerw,a[S]} + Frac_{aers,a[S]} \cdot K_{aers,a[S]}} \tag{41}$$

with

$Fr_{aerw,a[S]}$: fraction of chemical in the aerosol water phase [-]
$Frac_{aerw,a[S]}$:   volume fraction aqueous phase aerosols in air [-]
$K_{aerw,a[S]}$: dimensionless aerosol water-air partitioning coefficient [-]
$Frac_{aers,a[S]}$:   volume fraction solid particles in air [-]
$K_{aers,a[S]}$: dimensionless aerosol solid-air partitioning coefficient [-]

Where the volume fraction solid particles in air and the volume fraction aqueous phase aerosols in air are described in Table 2. The dimensionless aerosol solid-air and aerosol water-air partitioning coefficients are described in Equations 28 and 29, respectively.

The fraction of the chemical in the gas phase can be obtained from:

$$Fr_{gas,a[S]} = 1 - Fr_{aerw,a[S]} - Fr_{aers,a[S]} \tag{42}$$

with

$Fr_{gas,a[S]}$: fraction of chemical in the gas phase [-]
$Fr_{aerw,a[S]}$: fraction of chemical in the aerosol water phase [-]
$Fr_{aers,a[S]}$: fraction of chemical in the aerosol solids phase [-]

Air flows
Magnitudes of air flows are derived in SimpleBox from the residence times of air masses in air compartments. To estimate these residence times, it is assumed that air compartments are continuously refreshed by wind that blows at a constant speed of 3 ms^{-1} through a well-mixed air box:

$$\tau_{a[S]} = 0.75 \cdot \frac{\sqrt{SystemArea_{[S]}}}{WindSpeed_{[S]}} \tag{43}$$

with

$\tau_{a[S]}$:   residence time in urban and continental air [s]
SystemArea$_{[S]}$: regional, continental and global system area [m^2]
WindSpeed$_{[S]}$: regional, continental and global wind speed [ms^{-1}]
0.75:   empirical proportionality constant, according to Benarie (1980)

Where the regional and continental wind speeds are described in Table 3 and the global wind speed in Table 2.

The air flows from the regional scale to the continental scale and back, from the continental scale to the moderate zone and back, and from the moderate zone to the arctic and tropic zones and back. The airflows are obtained from:

$$k_{aR \to aC} = \frac{1}{\tau_{aR}}$$

(44)

with
$k_{aR \to aC}$: transfer rate of regional air to continental air [s⁻¹]
τ_{aR}:   residence time in regional air [s]

$$k_{aC \to aR} = k_{aR \to aC} \cdot \frac{Volume_{aR}}{Volume_{aC}}$$

(45)

with
$k_{aC \to aR}$:   transfer rate of continental air to regional air [s⁻¹]
$k_{aR \to aC}$:   transfer rate of regional air to continental air [s⁻¹]
$Volume_{aR}$: volume of the regional air [m³]
$Volume_{aC}$: volume of the continental air [m³]

Where the volumes of air compartments are described in Equation 39.

$$k_{aC \to aM} = \frac{1}{\tau_{aC}} - k_{aC \to aR}$$

(46)

with
$k_{aC \to aM}$: transfer rate of continental air to moderate air [s⁻¹]
τ_{aC}:   residence time in continental air [s]
$k_{aC \to aR}$: transfer rate of continental air to regional air [s⁻¹]

$$k_{aM \to aC} = k_{aC \to aM} \cdot \frac{Volume_{aC}}{Volume_{aM}}$$

(47)

with
$k_{aM \to aC}$:   transfer rate of moderate air to continental air [s⁻¹]
$k_{aC \to aM}$:   transfer rate of continental air to moderate air [s⁻¹]
$Volume_{aC}$: volume of the continental air [m³]
$Volume_{aM}$: volume of the moderate air [m³]

Where the volumes of air compartments are described in Equation 39.

$$k_{aA \to aM} = \frac{1}{\tau_{aA}}$$

(48)

with
$k_{aA \to aM}$: transfer rate of arctic air to moderate air [s⁻¹]
τ_{aA}:   residence time in arctic air [s]

$$k_{aM \to aA} = k_{aA \to aM} \cdot \frac{Volume_{aA}}{Volume_{aM}} \tag{49}$$

with

$k_{aM \to aA}$:   transfer rate of moderate air to arctic air [s^{-1}]
$k_{aA \to aM}$:   transfer rate of arctic air to moderate air [s^{-1}]
$Volume_{aA}$: volume of the arctic air [m^3]
$Volume_{aM}$: volume of the moderate air [m^3]

Where the volumes of air compartments are described in Equation 39.

$$k_{aT \to aM} = \frac{1}{\tau_{aT}} \tag{50}$$

with

$k_{aT \to aM}$:   transfer rate of tropic air to moderate air [s^{-1}]
τ_{aT}:   residence time in tropic air [s]

$$k_{aM \to aT} = k_{aT \to aM} \cdot \frac{Volume_{aT}}{Volume_{aM}} \tag{51}$$

with

$k_{aM \to aT}$:   transfer rate of moderate air to tropic air [s^{-1}]
$k_{aT \to aM}$:   transfer rate of tropic air to moderate air [s^{-1}]
$Volume_{aT}$: volume of the tropic air [m^3]
$Volume_{aM}$: volume of the moderate air [m^3]

Where the volumes of air compartments are described in Equation 39.

3.5.2 Water

At the regional and continental scale, three water compartments are present: lake water, fresh water and sea water. At the global scale, only sea water is present, which includes a surface sea water and a deep-sea water compartment. In SimpleBox, the water compartments are treated as homogeneous boxes, consisting of a suspended matter phase and a colloidal organic matter phase. The presence of suspended matter and colloidal organic matter influences the fate of chemicals in a very similar way to that of aerosol solids and aerosol water in the atmosphere. These phases bind the chemical, thus inhibiting it from taking part in the mass transfer and degradation processes that occur in the water phase. Suspended matter acts as a physical carrier of the chemical across the sediment-water interface. The colloidal organic matter only causes the chemical to be inhibited from taking part in mass transfer and degradation processes. Concentration ratios among suspended matter, colloidal organic matter and water are often close to equilibrium. For multimedia fate modelling, the water compartment is treated the same way as the air, sediment and soil compartments: equilibrium is assumed among water, suspended matter and colloidal organic matter at all times. The water compartments at all scales are continuously flushed with water from outside that scale.

The volume of the lake, fresh and sea water compartments can be obtained from:

$$Volume_{w[S]} = SystemArea_{[S]} \cdot AreaFrac_{w[S]} \cdot Depth_{w[S]} \tag{52}$$

with

$Volume_{w[S]}$:   volume of the regional, continental and global waters [m^3]

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

$AreaFrac_{w[S]}$:   area fraction regional, continental and global waters [-]

$Depth_{w[S]}$:   depth of regional, continental and global waters [m]

Where the system areas are described in Equations 36 to 38, the depth of the lake and fresh water in Table 3, and the depth of the sea waters in Table 2.

The area fraction regional and continental lake and fresh water can be obtained from:

$$AreaFrac_{w[S]} = \frac{Area_{land[S]} \cdot Frac_{w[S]}}{SystemArea[S]} \tag{53}$$

with

$AreaFrac_{w[S]}$:   area fraction regional and continental lake and fresh water [-]

$Area_{land[S]}$:   area regional and continental land [m^2]

$Frac_{w[S]}$:   fraction regional and continental lake and fresh water [-]

$SystemArea_{[S]}$: regional and continental system area [m^2]

Where the area land and fraction lake and fresh water are described in Table 3, and the system areas are described in Equations 36 to 38.

The area fraction regional and continental sea water can be obtained from:

$$\begin{aligned} AreaFrac_{w2[S]} = {} & 1 - AreaFrac_{w0[S]} - AreaFrac_{w1[S]} - Areafrac_{s1[S]} \\ & - AreaFrac_{s2[S]} - AreaFrac_{s3[S]} \end{aligned} \tag{54}$$

with

$AreaFrac_{w2[S]}$: area fraction regional and continental sea water [-]

$AreaFrac_{w[S]}$:   area fraction regional and continental lake and fresh water [-]

$AreaFrac_{s[S]}$:   area fraction regional and continental natural, agricultural and other soil [-]

Where the area fraction water is described in Equation 53, and the area fractions soil in Equation 73.

The fraction of chemical truly dissolved in the water can be obtained from:

$$Fr_{w,w[S]} = \frac{1}{1 + K_{p,susp[S]} \cdot \dfrac{Susp_{w[S]}}{1000} + K_{p,col[S]} \cdot \dfrac{Col_{w[S]}}{1000}} \tag{55}$$

with

$Fr_{w,w[S]}$:   fraction of chemical truly dissolved in the regional, continental and global waters [-]

$K_{p,susp[S]}$:   regional, continental and global suspended solids-water partitioning coefficient [L·kg^{-1}]

$Susp_{w[S]}$:   concentration suspended matter in regional, continental and global water [kg·m^3]

$K_{p,col[S]}$:   regional, continental and global colloidal organic matter-water partitioning coefficient [L·kg^{-1}]

$Col_{w[S]}$:   concentration of colloidal organic matter in regional, continental and global waters [kg·m^3]

Where the suspended solids-water and the colloidal organic matter-water partitioning coefficient are described in Equations 30 and 35, respectively. The concentrations suspended matter and colloidal organic matter in water are described in Table 2.

Water flows
The water flows from the lake water to the freshwater to the sea water at the regional and continental scale, and between the sea waters of all scales. At the global scale, the surface water flows from the moderate zone to the arctic zone, and from the tropic zone to the moderate zone. The deep-sea water flows from the arctic to the moderate zone, and from the moderate to the tropic zone. The water flows from the continental fresh water to the regional freshwater, from the moderate deep-sea to the arctic deep-sea, and from the tropic deep-sea to the moderate deep-sea are, by default, zero. The flow rates for all surface water flows can be obtained from:

$$k_{wa \to wb} = \frac{WaterFlow_{wa \to wb}}{Volume_{wa}} \tag{56}$$

with

$k_{wa \to wb}$:   transfer rate source water compartment to receiving water compartment [s^{-1}]

$WaterFlow_{wa \to wb}$:   water flow of water from the source compartment to the receiving compartment [m^3·s^{-1}]

$Volume_{wa}$:   volume of the source water compartment [m^3]

Where the water flows are described in Equations 59 to 69 and the volume is described in Equation 52.

The flow rate from continental fresh water to continental sea water can be obtained from:

$$k_{w1C \to w2C} = \frac{WaterFlow_{w1C \to w2C} \cdot (1 - Frac_{w1C \to w1R})}{Volume_{w1C}} \tag{57}$$

with

$k_{w1C \to w2C}$:   transfer rate from continental fresh water to the continental sea water [s^{-1}]

WaterFlow $_{w1C \to w2C}$: water flow from continental fresh water to the continental sea water [m^3·s^{-1}]

$Frac_{w1C \to w1R}$:   fraction discharge continental fresh water to the regional scale [-]

Volume$_{w1C}$:   volume of the receiving water compartment [m^3]

Where the water flow is described in Equation 61, the fraction discharge in Table 3, and the volume is described in Equation 52.

The flow rate for all deep-sea water flows can be obtained from:

$$k_{wa \to wb} = \frac{OceanCurrent}{Volume_{wa}} \tag{58}$$

with

$k_{wa \to wb}$:   transfer rate source water compartment to receiving water compartment [s^{-1}]

OceanCurrent: global ocean circulation current [m^3·s^{-1}]

Volume$_{wa}$:   volume of the source water compartment [m^3]

Where the global ocean circulation current is described in Table 2 and the volume in Equation 52.

The water flows from lake water to sea water, from freshwater back to lake water, from arctic surface water to moderate surface water and from moderate surface water to tropic surface water are by default zero. All other water flows may be obtained from:

$$WaterFlow_{w0R \to w1R} = 0.1 \cdot WaterFlow_{w2R \to w2C} \tag{59}$$

$$
\begin{aligned}
WaterFlow_{w1C \to w1R} \\
= ((AreaFrac_{w1C} + AreaFrac_{s1C} \cdot Frac_{run,s1C} \\
+ AreaFrac_{s2C} \cdot Frac_{run,s2C} + AreaFrac_{s3C} \cdot Frac_{run,s3C}) \\
\cdot RainRate_{[S]} \cdot SystemArea_{[S]} + WaterFlow_{w0C \to w1C}) \\
\cdot Frac_{w1C \to w1R}
\end{aligned} \tag{60}
$$

$$
\begin{aligned}
WaterFlow_{w1C \to w2C} \\
= \Big((AreaFrac_{w1C} + AreaFrac_{s1C} \cdot Frac_{run,s1C} \\
+ AreaFrac_{s2C} \cdot Frac_{run,s2C} + AreaFrac_{s3C} \cdot Frac_{run,s3C}) \\
\cdot RainRate_{[S]} \cdot SystemArea_{[S]}\Big) \cdot (1 - Frac_{w1C \to w1R})
\end{aligned} \tag{61}
$$

$$
\begin{aligned}
WaterFlow_{w1R \to w2R} \\
= \Big((AreaFrac_{w1R} + AreaFrac_{s1R} \cdot Frac_{run,s1R} \\
+ AreaFrac_{s2R} \cdot Frac_{run,s2R} + AreaFrac_{s3R} \cdot Frac_{run,s3R}) \\
\cdot RainRate_{[S]} \cdot SystemArea_{[S]} + WaterFlow_{w1C \to w1R}\Big) \cdot (1 \\
- Frac_{w1R \to w1C})
\end{aligned} \tag{62}
$$

$$WaterFlow_{w0C \to w1C} = 0.1 \cdot WaterFlow_{w1C \to w2C} \tag{63}$$

$$WaterFlow_{w2C \to w2M} = \frac{Volume_{w2C}}{\tau_{w2C}} - WaterFlow_{w2R \to w2C} \tag{64}$$

$$WaterFlow_{w2C \to w2R} = (10 - 1) \cdot WaterFlow_{w1R \to w2R} \tag{65}$$

$$WaterFlow_{w2M \to w2A} = OceanCurrent \tag{66}$$

$$WaterFlow_{w2M \to w2C} = WaterFlow_{w2C \to w2M} \tag{67}$$

$$WaterFlow_{w2R \to w2C} = WaterFlow_{w1R \to w2R} + WaterFlow_{w2C \to w2R} \tag{68}$$

$$WaterFlow_{w2T \to w2M} = OceanCurrent \tag{69}$$

with

WaterFlow$_{wa \to wb}$:	water flow of water from the source compartment to the receiving compartment [m^3·s^{-1}]
AreaFrac$_{w1[S]}$:	area fraction regional and continental fresh water [-]
AreaFrac$_{s[S]}$:	area fraction regional and continental regional and continental natural, agricultural and other soil [-]
Frac$_{run,s[S]}$:	volume fraction of precipitation on regional and continental natural, agricultural and other soil run off to surface water [-]
RainRate$_{[S]}$:	regional and continental average precipitation [m·s^{-1}]
SystemArea$_{[S]}$:	regional and continental system area [m^2]
Frac$_{w1C \to w1R}$:	fraction discharge continental fresh water to the regional scale [-]
Frac$_{w1R \to w1C}$:	fraction discharge regional fresh water to the continental scale [-]
Volume$_{w2C}$:	volume of the continental sea water [m^3]
τ_{w2C}:	residence time of sea water on the continental shelf [s]
OceanCurrent:	global ocean circulation current [m^3·s^{-1}]

Where the area fractions fresh water and the volume continental sea water are described in Equations 53 and 52, respectively and the system areas are described in Equations 36 to 38. The average precipitation and the fraction discharge are described in Table 3 and the residence time in sea water, the volume fraction run off, and the global ocean circulation current in Table 2.

3.5.3 Sediment
In SimpleBox, sediments are 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 soil pore water and solid sub-phases of the sediment phase.
The top layer of the sediment is assumed 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 refreshed. The older sediment layer and the chemicals associated with the sediment, are buried under freshly deposited material.

The volume of the regional and continental fresh and sea water sediment compartments and the global sea water compartments can be obtained from:

$$Volume_{sd[S]} = SystemArea_{[S]} \cdot AreaFrac_{w[S]} \cdot Depth_{sd[S]} \qquad (70)$$

with

$Volume_{sd[S]}$: volume of regional and continental fresh and sea water and global sea water sediment [m^3]

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

$AreaFrac_{w[S]}$: area fraction regional, continental and global water [-]

$Depth_{sd[S]}$: depth of regional, continental and global sediment [m]

Where the system areas are described in Equations 36 to 38, the area fractions water in Equation 53, and the depth of the sediment in Table 2.

The fraction solids in sediments can be obtained from:

$$Frac_{s,sd[S]} = 1 - Frac_{w,sd[S]} \qquad (71)$$

with

$Frac_{s,sd[S]}$: volume fraction solids in regional, continental and global sediment [-]

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

Where the fraction solids in sediment is described in Table 2.

3.5.4 Soil

Soil is the most stationary and, as a result, the most spatially inhomogeneous of all environmental compartments. There are many different soil types and differences in soil use. Unfortunately, the fate of chemicals is determined largely by those characteristics that vary so much (porosity, water content, and organic matter content). In addition, soil use is 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, includes three separate soil compartments. The first of these may be considered to be "natural soil"; the second as "agricultural soil"; and the third may be used to reflect the existence of "urban" or "industrially used" soil.

Only the top layer of the soil is considered in this modelling concept. Soil is treated as a homogeneous compartment, consisting of a gas phase, a water phase and a solid phase; the concentration in soil is a total concentration. The different soil phases are assumed to be in equilibrium at all times. Chemical flow from the soil to the air is dependent on the penetration depth of the chemical into the soil. Therefore, volatilization processes, runoff and leaching from the soil are corrected for a penetration depth of 0.1 m. Removal of the chemical from the soil occurs through leaching from the soil into the groundwater.

The volume of the soil compartments can be obtained from:

$$Volume_{s[S]} = SystemArea_{[S]} \cdot AreaFrac_{s[S]} \cdot Depth_{s[S]} \tag{72}$$

with

Volume$_{s[S]}$: volume of regional and continental natural, agricultural and other soil and global soil [m^3]

SystemArea$_{[S]}$: regional, continental and global system area [m^2] (Equations 36 to 38)

AreaFrac$_{s[S]}$: area fraction regional, continental and global soil [-] (Equations 73 and 74)

Depth$_{s[S]}$: depth of regional, continental and global soil [m] (Table 2)

The regional and continental area fraction soil can be obtained from:

$$AreaFrac_{s[S]} = \frac{Area_{land[S]} \cdot Frac_{soil[S]}}{SystemArea[S]} \tag{73}$$

with

AreaFrac$_{s[S]}$: area fraction regional, continental and global natural, agricultural and other soil [-]

Area$_{land[S]}$: area regional and continental land [m^2] (Table 3)

Frac$_{soil[S]}$: fraction regional and continental natural, agricultural and other soil [-] (Table 3)

SystemArea$_{[S]}$: regional and continental system area [m^2] (Equations 36 to 38)

The global area fraction soil can be obtained from:

$$AreaFrac_{s[S]} = 1 - AreaFrac_{w[S]} \tag{74}$$

with

AreaFrac$_{s[S]}$: area fraction global soil [-]

AreaFrac$_{w[S]}$: area fraction global water [-] (Equation 53)

The volume fraction solids in soil can be obtained from:

$$Frac_{s,s[S]} = 1 - Frac_{a,s[S]} - Frac_{w,s[S]} \tag{75}$$

with

Frac$_{s,s[S]}$: volume fraction solids in regional, continental and global soils [-]

Frac$_{a,s[S]}$: volume fraction air in regional, continental and global soils [-] (Table 2)

Frac$_{w,s[S]}$: volume fraction water in regional, continental and global soils [-] (Table 2)

The fraction of chemical in the solid phase of soil can be obtained from:

$$Fr_{s,s[S]} = \frac{Frac_{s,s[S]}}{\dfrac{Frac_{a,s[S]} \cdot K_{aw[S]} \cdot Fr_{orig,sw}}{\dfrac{K_{p,s[S]} \cdot \rho_{solid}}{1000}} + \dfrac{Frac_{w,s[S]}}{\dfrac{K_{p,s[S]} \cdot \rho_{solid}}{1000}} + Frac_{s,s[S]}} \tag{76}$$

with

$Fr_{s,s[S]}$: fraction of chemical in solid phase of regional, continental and global soil [-]

$Frac_{s,s[S]}$: volume fraction solids in regional, continental and global soils [-] (Equation 75)

$Frac_{a,s[S]}$: volume fraction air in regional, continental and global soils [-](Table 2)

$K_{aw[S]}$: dimensionless regional, continental and global air-water partitioning coefficient [-] (Equation 27)

$Fr_{orig,sw}$: fraction original species in porewater of soil [-] (Equation 14)

$K_{p,s[S]}$: soil-water partitioning coefficient of soil [-] (Equation 31)

ρ_{solid}: mineral density of sediment and soil [kg·m^{-3}] (Table 2)

1000: conversion factor [m^3·kg^{-1}]

$Frac_{w,s[S]}$: volume fraction water in regional, continental and global soils [-](Table 2)

The fraction of chemical in water phase of soil can be obtained from:

$$Fr_{w,s[S]} = \frac{Frac_{w,s[S]}}{Frac_{a,s[S]} \cdot K_{aw[S]} \cdot Fr_{orig,sw} + Frac_{w,s[S]} + Frac_{s,s[S]} \cdot \frac{K_{p,s[S]} \cdot \rho_{solid}}{1000}} \quad (77)$$

with

$Fr_{w,s[S]}$: fraction of chemical in water phase of regional, continental and global soil [-]

$Frac_{w,s[S]}$: volume fraction water in regional, continental and global soils [-](Table 2)

$Frac_{a,s[S]}$: volume fraction air in regional, continental and global soils [-](Table 2)

$K_{aw[S]}$: dimensionless regional, continental and global air-water partitioning coefficient [-](Equation 27)

$Fr_{orig,sw}$: fraction original species in pore water of soil [-](Equation 14)

$Frac_{s,s[S]}$: volume fraction solids in regional, continental and global soils [-](Equation 75)

$K_{p,s[S]}$: soil-water partitioning coefficient of soil [-](Equation 31)

ρ_{solid}: mineral density of sediment and soil [kg·m^{-3}] (Table 2)

1000: conversion factor [m^3·kg^{-1}]

3.6 Loss processes

3.6.1 Degradation in air

The removal from the air is caused by temperature dependent degradation in the air, and by escape of the substance from the air to the stratosphere. The temperature correction reaction rate in air can be obtained from:

$$TempFactor_{a[S]} = e^{\frac{Ea_{OHrad}}{8.314} \frac{Temp_{[S]} - 298}{298^2}} \quad (78)$$

with

$TempFactor_{a[S]}$: temperature correction reaction rate regional, continental and global air [-]

Ea_{OHrad}: activation energy OH radical reaction [J·mol^{-1}](Table 2)

$Temp_{[S]}$: continental temperature [K](Table 3)

298: temperature [K]

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

The degradation in air can be obtained from:

$$KDeg_{a[S]} = Fr_{gas,a[S]} \cdot k_{deg,air} \cdot \frac{C_{OHrad,a[S]}}{C_{OHrad}} \cdot TempFactor_{a[S]} \tag{79}$$

with
$KDeg_{a[S]}$:   degradation in regional, continental and global air [s^{-1}]
$Fr_{gas,a[S]}$:   fraction of chemical in the gas phase in regional, continental and global air [-](Equation 42)
$k_{deg,air}$:   gas phase degradation rate constant at 25°C [s^{-1}] (Equation 21)
$C_{OHrad,a[S]}$:   regional, continental and global OH-radical concentration [cm^{-3}](Table 2)
C_{OHrad}:   OH-radical concentration [cm^{-3}] (Table 2)
$TempFactor_{a[S]}$: temperature correction reaction rate regional, continental and global air [-]

The escape from air to the stratosphere can be obtained from:

$$k_{esc,a[S]} = \frac{LN(2)}{60 \cdot 365 \cdot 24 \cdot 3600} \tag{80}$$

with
$k_{esc,a[S]}$:   escape from regional, continental and global air to stratosphere [s^{-1}]
60:             half life time in air [yr]
365·24·3600:   conversion factor [s·yr^{-1}]

The removal from the air can be obtained from:

$$k_{a[S]} = k_{esc,a[S]} + KDeg_{a[S]} \tag{81}$$

with
$k_{a[S]}$:   removal from the regional, continental and global air [s^{-1}]
$k_{esc,a[S]}$:   escape from regional, continental and global air to stratosphere [s^{-1}]
$KDeg_{a[S]}$: degradation in regional, continental and global air [s^{-1}]

3.6.2 *Degradation in water*
The removal from water is caused by temperature dependent degradation in the water. The degradation in water can be obtained using the scaling procedure proposed by Struijs & 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. The temperature correction reaction rate in water can be obtained from:

$$TempFactor_{wsds[S]} = Q_{10}^{\frac{Temp_{[S]}-298}{10}} \tag{82}$$

with
$TempFactor_{wsds[S]}$: temperature correction reaction rate regional, continental and global water/sediment/soil [-]
Q_{10}:   rate increase factor per 10°C [-](Table 2)

Temp[S]:	continental temperature [K](Table 3)
298:	temperature [K]
10:	temperature factor [K]

The degradation in water can be obtained from:

$$KDeg_{w[S]} = Fr_{w,w[S]} \cdot k_{deg,water} \cdot \frac{Bact_{w[S]}}{Bact_{test}} \cdot TempFactor_{wsds[S]} \qquad (83)$$

with

KDeg$_{w[S]}$:	degradation in regional, continental and global waters [s^{-1}]
Fr$_{w,w[S]}$:	fraction of chemical truly dissolved in regional, continental and global waters [-](Equation 55)
k$_{deg,water}$:	dissolved phase degradation rate constant at 25°C [s^{-1}] (Equations 22-24)
Bact$_{w[S]}$:	concentration bacteria in regional, continental and global water [CFU·ml^{-1}] (Table 2)
Bact$_{test}$:	concentration bacteria in test water [CFU·ml^{-1}] (Table 2)
TempFactor$_{wsds[S]}$:	temperature correction reaction rate regional, continental and global water/sediment/soil [-]

The overall removal from the water can be obtained from:

$$k_{w[S]} = KDeg_{w[S]} \qquad (84)$$

with

k$_{w[S]}$:	removal from the regional, continental and global water [s^{-1}]
KDeg$_{w[S]}$:	degradation in regional, continental and global water [s^{-1}]

3.6.3 *Degradation in sediment*
The removal from sediment is caused by temperature dependent degradation in sediment and burial processes. The degradation rate in sediment is calculated from the degradation rate stated in the substance data and can be obtained from:

$$KDeg_{sd[S]} = TempFactor_{wsds[S]} \cdot k_{deg,sed} \qquad (85)$$

with

KDeg$_{sd[S]}$:	degradation in regional, continental and global sediments [s^{-1}]
TempFactor$_{wsds[S]}$:	temperature correction reaction rate regional, continental and global water/sediment/soil [-]
k$_{deg,sed}$:	bulk degradation rate constant at 25°C [s^{-1}] (Equations 25)

The removal from the sediment can be obtained from the degradation in sediments and the burial rate:

$$k_{sd[S]} = KDeg_{sd[S]} + \frac{NetSedRate_{w[S]}}{Depth_{sd[S]}} \qquad (86)$$

with

$k_{sd[S]}$: removal from the regional, continental and global sediments [s^{-1}]

$KDeg_{sd[S]}$: degradation in regional, continental and global sediments [s^{-1}]

$NetSedRate_{w[S]}$: net sediment accumulation rate in regional, continental and global water [m·s^{-1}](Table 2)

$Depth_{sd[S]}$: depth of regional, continental and global sediments [m] (Table 2)

3.6.4 *Degradation in soil*

The removal from soil is caused by temperature dependent degradation in sediment and leaching of the chemical from the soil into ground water. The correction factor for depth dependent soil concentration can be obtained from Hollander *et al.* (2004):

$$Corr_{leach,s[S]} = \frac{e^{\left(-\frac{1}{0.1}·0.5\right)} · \frac{1}{0.1} · Depth_{s[S]}}{1 - e^{\left(\frac{-1}{0.1}·Depth_{s[S]}\right)}} \tag{87}$$

with

$Corr_{leach,s[S]}$: regional, continental and global correction factor depth dependent soil concentration [-]

$Depth_{s[S]}$: depth of regional, continental and global soils [m] (Table 2)

The degradation rate in soil is calculated from the degradation rate stated in the substance data and can be obtained from:

$$KDeg_{s[S]} = TempFactor_{wsds[S]} · k_{deg,soil} \tag{88}$$

with

$KDeg_{s[S]}$: degradation in regional, continental and global soils [s^{-1}]

$TempFactor_{wsds[S]}$: temperature correction reaction rate regional, continental and global water/sediment/soil [-]

$k_{deg,soil}$: bulk degradation rate constant at 25°C [s^{-1}] (Equations 25)

The removal from the soil can be obtained from:

$$k_{s[S]} = KDeg_{s[S]} + \frac{Frac_{inf,s[S]} · RainRate[S] · Corr_{leach,s[S]}}{K_{slw[S]} · Depth_s[S]} \tag{89}$$

with

$k_{s[S]}$: removal from the regional, continental and global soils [s^{-1}]

$KDeg_{s[S]}$: degradation in regional, continental and global soils [s^{-1}]

$Frac_{inf,s[S]}$: volume fraction of precipitation infiltrating into regional, continental and global soils [-](Table 2)

$RainRate[S]$: regional, continental and global annual precipitation [m·s^{-1}] (Table 2)

$Corr_{leach,s[S]}$: regional, continental and global correction factor depth dependent soil concentration [-]

$K_{slw[S]}$: regional, continental and global dimensionless soil/water partitioning coefficient in soil [-] (Equation 32)

Depth$_{s[S]}$:   depth of regional, continental and global soils [m] (Table 2)

3.7   Intermedia transfer processes

3.7.1   *Deposition*

In SimpleBox 4.0, dry and wet deposition occurs through dry aerosol deposition, and through wet aerosol and gas washout; mass-flows are derived by means of the approach described by Jolliet and Hauschild (2006). The dry aerosol deposition rate can be obtained from:

$$DryDep_{aerosol[S]} = Aerosol_{deprate[S]} \cdot (Fr_{aerw,a[S]} + Fr_{aers,a[S]}) \qquad (90)$$

with

DryDep$_{aerosol[S]}$:   regional, continental and global dry aerosol deposition rate [m·s^{-1}]

Aerosol$_{deprate[S]}$:   deposition velocity aerosol particles [m·s^{-1}] (Table 2)

Fr$_{aerw,a[S]}$:   volume fraction aqueous phase aerosols in regional, continental and global air [-](Equation 41)

Fr$_{aers,a[S]}$:   volume fraction solids particles in regional, continental and global air [-] (Equation 40)

The aerosol washout can be obtained from:

$$AerosolWashout[S] = \frac{Fr_{aers,a[S]} \cdot (t_{dry[S]} + t_{wet[S]})}{t_{wet[S]}} \cdot RainRate[S] \cdot Collect_{eff[S]} \qquad (91)$$

with

AerosolWashout$_{[S]}$:   regional, continental and global aerosol washout [m·s^{-1}]

Fr$_{aers,a[S]}$:   volume fraction solids particles in regional, continental and global air [-] (Equation 40)

t$_{dry[S]}$:   duration dry episode [s] (Table 2)

t$_{wet[S]}$:   duration wet episode [s] (Equation 95)

RainRate$_{[S]}$:   regional, continental and global annual precipitation [m·s^{-1}] (Table 2; Table 3)

Collect$_{eff[S]}$:   regional, continental and global aerosol collection efficiency [-] (Table 2)

The gas washout can be obtained from:

$$GasWashout[S] = \frac{Fr_{gas,a[S]} \cdot (t_{dry[S]} + t_{wet[S]})}{t_{wet[S]}} \cdot \frac{RainRate[S]}{K_{aw[S]} \cdot Fr_{orig,aerw}} \qquad (92)$$

with

GasWashout$_{[S]}$:   regional, continental and global gas washout [m·s^{-1}]

Fr$_{gas,a[S]}$:   fraction of chemical in gas phase regional, continental and global air [-] (Equation 42)

t$_{dry[S]}$:   duration dry episode [s] (Table 2)

t$_{wet[S]}$:   duration wet episode [s] (Equation 95)

RainRate$_{[S]}$:   regional, continental and global annual precipitation [m·s^{-1}] (Table 2; Table 3)

$K_{aw[S]}$: regional, continental and global dimensionless air/water partitioning coefficient [-] (Equation 27)

$Fr_{orig,aerw}$: fraction original species in aerosol water [-] (Equation 14)

The deposition pattern consists of dry and wet periods of dry and wet deposition, respectively. The dry deposition contains dry deposition from the aerosol phase of the air and gas absorption from the air to the soil and water compartments, and can be obtained from:

$$k_{dry[S]}$$
$$= \frac{DryDep_{aerosol[S]}}{Height_{a[S]}}$$
$$+ \left(\frac{\sum_i GasAbs_{a \to wi[S]} \cdot AreaFrac_{wi[S]} + \sum_j GasAbs_{a \to sj[S]} \cdot AreaFrac_{sj[S]}}{Height_{a[S]}} \right. \tag{93}$$
$$\left. + KDeg_{a[S]} + k_{a \to a,out} \right)$$

with

$k_{dry[S]}$: total removal rate constant from regional, continental and global atmosphere during dry episodes [s⁻¹]

$DryDep_{aerosol[S]}$: regional, continental and global dry aerosol deposition rate [m·s⁻¹]

$Height_{a[S]}$: height of regional, continental and global air compartment [m] (Table 2)

$GasAbs_{a \to wi[S]}$: gas absorption flux to regional, continental and global "i" water [m·s⁻¹] (Equation 104) where "i" is lake, fresh and (surface) sea water

$AreaFrac_{wi[S]}$: regional, continental and global area fraction "i" water [-] (Equation 53)

$GasAbs_{a \to sj[S]}$: gas absorption flux to regional, continental and global "j" soil [m·s⁻¹] (Equation 100) where "j" is natural, agricultural or urban/industrial soil

$AreaFrac_{sj[S]}$: regional, continental and global area fraction "j" soil [-](Equation 73-74)

$KDeg_{a[S]}$: degradation in regional, continental and global air [s⁻¹] (Equation 79)

$k_{a \to a,out}$: air flow from the scale into another scale [s⁻¹] (Section 0)

The wet deposition contains chemical washout from the aerosol and gas phase of the air, and from gas absorption from the air to the soil and water compartments; it can be obtained from:

$$k_{wet[S]}$$
$$= \frac{AerosolWashout_{[S]} + GasWashout_{[S]}}{Height_{a[S]}}$$
$$+ \left(\frac{\sum_i GasAbs_{a \to wi[S]} \cdot AreaFrac_{wi[S]} + \sum_j GasAbs_{a \to sj[S]} \cdot AreaFrac_{sj[S]}}{Height_{a[S]}} \right. \tag{94}$$
$$\left. + KDeg_{a[S]} + k_{a \to a,out} \right)$$

with

$k_{wet[S]}$:	total removal rate constant from regional, continental and global atmosphere during dry episodes [s^{-1}]
AerosolWashout$_{[S]}$:	regional, continental and global aerosol washout [$m \cdot s^{-1}$]
GasWashout$_{[S]}$:	regional, continental and global gas washout [$m \cdot s^{-1}$]
Height$_{a[S]}$:	height of regional, continental and global air compartment [m] (Table 2)
GasAbs$_{a \to wi[S]}$:	gas absorption flux to regional, continental and global "i" water [$m \cdot s^{-1}$] (Equation 104) where "i" is lake, fresh and (surface) sea water
AreaFrac$_{wi[S]}$:	regional, continental and global area fraction "i" water [-] (Equation 53)
GasAbs$_{a \to sj[S]}$:	gas absorption flux to regional, continental and global "j" soil [$m \cdot s^{-1}$] (Equation 100) where "j" is natural, agricultural or urban/industrial soil
AreaFrac$_{sj[S]}$:	regional, continental and global area fraction "j" soil [-] (Equation 73-74)
KDeg$_{a[S]}$:	degradation in regional, continental and global air [s^{-1}] (Equation 79)
$k_{a \to a,out}$:	air flow from the scale into another scale [s^{-1}] (Section 0)

The duration of the dry episode is given in Table 2 and the duration of the wet episode can be obtained from:

$$t_{wet[S]} = 3.3 \cdot 24 \cdot 3600 \cdot \frac{0.06}{1 - 0.06} \tag{95}$$

with

$t_{wet[S]}$:	duration wet episode [s]
3.3·24·3600:	duration dry episode [s]
0.06:	percentage of time with rain > 0.3mm per hour [-]

The mean removal rate constant from atmosphere can be obtained from:

$$MeanRem_{a[S]} = \left(\left(\left(\frac{1}{k_{dry[S]}} \right) \cdot \frac{t_{dry[S]}}{t_{dry[S]} + t_{wet[S]}} + \left(\frac{1}{k_{wet[S]}} \right) \cdot \frac{t_{wet[S]}}{t_{dry[S]} + t_{wet[S]}} \right. \right.$$
$$\left. - \left(\frac{\left(\frac{1}{k_{wet[S]}} - \frac{1}{k_{dry[S]}} \right)^2}{t_{dry[S]} + t_{wet[S]}} \right) \cdot \left(1 - e^{-k_{dry[S]} \cdot t_{dry[S]}} \right) \right.$$
$$\left. \cdot \frac{1 - e^{-k_{wet[S]} \cdot t_{wet[U]}}}{1 - e^{-k_{dry[S]} \cdot t_{dry[S]} - k_{wet[S]} \cdot t_{wet[S]}}} \right)^{-1} \tag{96}$$

with

$MeanRem_{a[S]}$:   mean removal rate constant from regional, continental and global atmosphere [s^{-1}]

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

$t_{dry[S]}$:   duration dry episode [s] (Table 2)

$t_{wet[S]}$:   duration wet episode [s]

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

The mean atmospheric deposition rate constant can be obtained from:

$$MeanDep_{[S]}$$
$$= MeanRem_{a[S]}$$
$$- \left(\frac{\sum_i GasAbs_{a \rightarrow wi[S]} \cdot AreaFrac_{wi[S]} + \sum_j GasAbs_{a \rightarrow sj[S]} \cdot AreaFrac_{sj[S]}}{Height_{a[S]}} \right. \tag{97}$$
$$\left. + KDeg_{a[S]} + k_{a \rightarrow a,out} \right)$$

with

$MeanDep_{[S]}$:   mean regional, continental and global atmospheric deposition rate constant [s^{-1}]

$MeanRem_{a[S]}$:   mean removal rate constant from regional, continental and global atmosphere [s^{-1}]

$GasAbs_{a \rightarrow wi[S]}$:   gas absorption flux to regional, continental and global "i" water [$m \cdot s^{-1}$] (Equation 104) where "i" is lake, fresh and (surface) sea water

$AreaFrac_{wi[S]}$:   regional, continental and global area fraction "i" water [-] (Equation 53)

$GasAbs_{a \rightarrow sj[S]}$:   gas absorption flux to regional, continental and global "j" soil [$m \cdot s^{-1}$] (Equation 100) where "j" is natural, agricultural or urban/industrial soil

$AreaFrac_{sj[S]}$:   regional, continental and global area fraction "j" soil [-] (Equation 73-74)

$KDeg_{a[S]}$:   degradation in regional, continental and global air [s^{-1}] (Equation 79)

$Height_{a[S]}$:   height of regional, continental and global air compartment [m] (Table 2)

$k_{a \rightarrow a,out}$:   air flow from the scale into another scale [s^{-1}] (Section 0)

3.7.2   *Air to water and soil*

The deposition flow from the air to water and soils consists of a deposition and gas absorption of the chemical. The overall mass transfer coefficient for gas absorption can be estimated using the classical two-film resistance model (Schwarzenbach *et al.*, 1993). In the case of transport across the air/water interface, the overall transfer coefficients follow from summation of the resistances at the water and air sides of the interface. In the case of transport across the air/soil interface, the soil-side of the interface is treated as a pair of parallel resistances (air phase and water phase of the soil).

The partial mass transfer coefficient at the air side of the air/soil interface can be obtained from:

$$MTC_{as,air,a[S]} = \frac{\frac{0.43}{24 \cdot 3600}}{0.00475} \tag{98}$$

with

$MTC_{as,air,a[S]}$: regional, continental and global partial mass transfer coefficient at the air side of the air/soil interface [m·s^{-1}]

0.43: constant described by Mackay (2001) [m·d^{-1}]

0.00475: constant described by Mackay (2001) [-]

24·3600: conversion factor [s·d^{-1}]

The partial mass transfer coefficient at the soil side of the air/soil interface can be obtained from:

$$MTC_{as,soil,s[S]} = 0.1 \cdot KDeg_{s[S]} \tag{99}$$

with

$MTC_{as,soil,s[S]}$: regional, continental and global partial mass transfer coefficient at the soil side of the air/soil interface [m·s^{-1}]

0.1: constant described by Mackay (2001) [m]

$KDeg_{s[S]}$: degradation in regional, continental and global soils [s^{-1}] (Equation 88)

as described by Hollander et al. (2004, 2007a).

The gas absorption from air to soils can be obtained from:

$$GasAbs_{a \to s[S]} = Fr_{gas,a[S]} \cdot MTC_{as,air,a[S]}$$
$$\cdot \frac{MTC_{as,soil,s[S]}}{MTC_{as,air,a[S]} \cdot \frac{K_{aw[S]} \cdot Fr_{orig,sw}}{K_{slw[S]}} + MTC_{as,soil,s[S]}} \tag{100}$$

with

$GasAbs_{a \to s[S]}$: gas absorption flux from regional, continental and global air to soils [m·s^{-1}]

$Fr_{gas,a[S]}$: fraction of chemical in the gas phase [-] (Equation 42)

$MTC_{as,air,a[S]}$: regional, continental and global partial mass transfer coefficient at the air side of the air/soil interface [m·s^{-1}]

$MTC_{as,soil,s[S]}$: regional, continental and global partial mass transfer coefficient at the soil side of the air/soil interface [m·s^{-1}]

$K_{aw[S]}$: dimensionless air-water partition coefficient of the original species at regional, continental and global temperature [-] (Equation 27)

$Fr_{orig,sw}$: fraction original species in soil pore water [-] (Equation 14)

$K_{slw[S]}$: regional, continental and global dimensionless soilwater partitioning coefficient [-] (Equation 32)

The transfer rate from air to soil can be obtained from:

$$k_{a \to s[S]} = MeanDep_{[S]} + \frac{GasAbs_{a \to s[S]}}{Height_{a[S]}} \cdot AreaFrac_{s[S]} \tag{101}$$

with

$k_{a \to s[S]}$: transfer rate from regional, continental and global air to soils [s^{-1}]

$MeanDep_{[S]}$: mean regional, continental and global atmospheric deposition rate constant [s^{-1}] (Equation 97)

$GasAbs_{a \to s[S]}$: gas absorption flux from regional, continental and global air to soils [$m \cdot s^{-1}$]

$Height_{a[S]}$: height of regional, continental and global air [m] (Table 2)

$AreaFrac_{s[S]}$: area fraction regional, continental and global natural, agricultural and other soil [-] (Equation 73-74)

The partial mass transfer coefficient at the air side of the air/water interface can be obtained from:

$$MTC_{aw,air,a[S]} = 0.01 \cdot (0.3 + 0.2 \cdot WindSpeed_{[S]}) \cdot \frac{0.018^{0.67 \cdot 0.5}}{MW} \qquad (102)$$

with

$MTC_{aw,air,a[S]}$: regional, continental and global partial mass transfer coefficient at the air side of the air/water interface [$m \cdot s^{-1}$]

0.01/0.3/0.2/
0.018/0.67/0.5: constants described by Mackay (2001)

$Windspeed_{[S]}$: regional, continental and global wind speed [$m \cdot s^{-1}$] (Table 2; Table 3)

MW: molecular weight [$kg \cdot mol^{-1}$] (Section 3.3.1)

The partial mass transfer coefficient at the water side of the air/water interface can be obtained from:

$$MTC_{aw,water,w[S]} = 0.01 \cdot (0.0004 + 0.00004 \cdot WindSpeed_{[S]}^{2}) \cdot \frac{0.032^{0.5 \cdot 0.5}}{MW} \qquad (103)$$

with

$MTC_{aw,water,w[S]}$: regional, continental and global partial mass transfer coefficient at the water side of the air/water interface [$m \cdot s^{-1}$]

0.01/0.0004/
0.00004/0.032/0.5: constants described by Mackay (2001)

$Windspeed_{[S]}$: regional, continental and global wind speed [$m \cdot s^{-1}$] (Table 2; Table 3)

MW: molecular weight [$kg \cdot mol^{-1}$] (Section 3.3.1)

The gas absorption from air to soils can be obtained from:

$$GasAbs_{a \to w[S]} = Fr_{gas,a[S]} \cdot MTC_{aw,air,a[S]} \\ \cdot \frac{MTC_{aw,water,w[S]}}{MTC_{aw,air,a[S]} \cdot K_{aw[S]} \cdot Fr_{orig,w} + MTC_{aw,water,w[S]}} \qquad (104)$$

with

$GasAbs_{a \to w[S]}$: gas absorption flux from regional, continental and global air to waters [$m \cdot s^{-1}$]

$Fr_{gas,a[S]}$: fraction of chemical in the gas phase [-] (Equation 42)

$MTC_{aw,air,a[S]}$:   regional, continental and global partial mass transfer coefficient at the air side of the air/water interface [m·s^{-1}]

$MTC_{aw,water,w[S]}$:   regional, continental and global partial mass transfer coefficient at the water side of the air/water interface [m·s^{-1}]

$K_{aw[S]}$:   dimensionless air-water partition coefficient of the original species at regional, continental and global temperature [-] (Equation 27)

$Fr_{orig,w}$:   fraction original species in water [-] (Equation 14)

The transfer rate from air to soil can be obtained from:

$$k_{a \to w[S]} = \frac{MeanDep_{[S]} + GasAbs_{a \to w[S]}}{Height_{a[S]}} \cdot AreaFrac_{w[S]} \tag{105}$$

with

$k_{a \to w[S]}$:   transfer rate from regional, continental and global air to waters [s^{-1}]

$MeanDep_{[S]}$:   mean regional, continental and global atmospheric deposition rate constant [s^{-1}] (Equation 97)

$GasAbs_{a \to w[S]}$:   gas absorption flux from regional, continental and global air to waters [m·s^{-1}]

$Height_{a[S]}$:   height of regional, continental and global air [m] (Table 2)

$AreaFrac_{w[S]}$:   area fraction regional, continental and global natural, agricultural and other water [-] (Equation 53)

3.7.3 *Water and soil to air*

The overall mass transfer coefficient for volatilization can be estimated using the classical two-film resistance model described in section 3.7.2. 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 volatilization processes from the soils to the air are corrected for the soil depth dependent concentration with a correction factor.

The correction factor for the depth dependent soil concentration can be obtained from:

$$Corr_{volat,s[S]} = \frac{\frac{1}{0.1} \cdot Depth_{s[S]}}{1 - e^{(-\frac{1}{0.1} \cdot Depth_{s[S]})}} \tag{106}$$

with

$Corr_{volat,s[S]}$:   correction factor for the regional, continental and global depth dependent soil concentration [-]

0.1:   soil penetration depth [m]

$Depth_{s[S]}$:   depth of regional, continental and global soil [m] (Table 2)

The volatilization from soils to air can be obtained from:

$$\text{Volat}_{s \to a\{S\}} = \frac{\text{MTC}_{as,air,a[S]} \cdot \text{MTC}_{as,soil,s[S]}}{\text{MTC}_{as,air,a[S]} + \dfrac{\text{MTC}_{as,soil,s[S]}}{\dfrac{K_{aw[S]} \cdot \text{Fr}_{orig,sw}}{K_{slw[S]}}}} \cdot \text{CorrVolat}_{s[S]} \qquad (107)$$

with

$\text{Volat}_{s \to a[S]}$:   volatilization from regional, continental and global soils to air [m.s^{-1}]

$\text{MTC}_{as,air,a[S]}$:   regional, continental and global partial mass transfer coefficient at the air side of the air/soil interface [m·s^{-1}]

$\text{MTC}_{as,soil,s[S]}$:   regional, continental and global partial mass transfer coefficient at the soil side of the air/soil interface [m·s^{-1}]

$K_{aw[S]}$:   dimensionless air-water partition coefficient of the original species at regional, continental and global temperature [-] (Equation 27)

$\text{Fr}_{orig,sw}$:   fraction original species in soil pore water [-] (Equation 14)

$K_{slw[S]}$:   regional, continental and global dimensionless soil-water partitioning coefficient [-] (Equation 32)

$\text{Corr}_{volat,s[S]}$:   correction factor for the regional, continental and global depth dependent soil concentration [-]

The transfer rate from soils to the air can be obtained from:

$$k_{s \to a[S]} = \frac{\text{Volat}_{s \to a[S]}}{\text{Depth}_{s[S]}} \qquad (108)$$

with

$k_{s \to a[S]}$:   transfer rate from regional, continental and global soils to air [s^{-1}]

$\text{Volat}_{s \to a[S]}$:   volatilization from regional, continental and global soils to air [m.s^{-1}]

$\text{Depth}_{s[S]}$:   depth of regional, continental and global soil [m] (Table 2)

The volatilization from soils to air can be obtained from:

$$\text{Volat}_{w \to a\{S\}} = \frac{\text{MTC}_{aw,air,a[S]} \cdot \text{MTC}_{aw,water,w[S]}}{\text{MTC}_{aw,air,a[S]} \cdot K_{aw[S]} \cdot \text{Fr}_{orig,w} + \text{MTC}_{aw,water,w[S]}} \cdot K_{aw[S]} \qquad (109)$$
$$\cdot \text{Fr}_{orig,w} \cdot \text{Fr}_{w,w[S]}$$

with

$\text{Volat}_{w \to a[S]}$:   volatilization from regional, continental and global waters to air [m.s^{-1}]

$\text{MTC}_{aw,air,a[S]}$:   regional, continental and global partial mass transfer coefficient at the air side of the air/water interface [m·s^{-1}]

$\text{MTC}_{aw,water,w[S]}$:   regional, continental and global partial mass transfer coefficient at the water side of the air/water interface [m·s^{-1}]

$K_{aw[S]}$:   dimensionless air-water partition coefficient of the original species at regional, continental and global temperature [-] (Equation 27)

$\text{Fr}_{orig,w}$:   fraction original species in water [-] (Equation 14)

$Fr_{w,w[S]}$: fraction of chemical truly dissolved in regional, continental and global waters [-] (Equation 55)

The transfer rate from soils to the air can be obtained from:

$$k_{w \to a[S]} = \frac{Volat_{w \to a[S]}}{Depth_{w[S]}}$$

(110)

with

$k_{w \to a[S]}$: transfer rate from regional, continental and global waters to air [s^{-1}]

$Volat_{w \to a[S]}$: volatilization from regional, continental and global waters to air [$m.s^{-1}$]

$Depth_{w[S]}$: depth of regional, continental and global waters [m] (Table 2)

3.7.4 *Soil to water transfer*
The runoff processes from the soils to fresh water are corrected for the soil depth dependent concentration with a correction factor.

The correction factor for the depth dependent soil concentration can be obtained from:

$$Corr_{runoff,s[S]} = \frac{\frac{1}{0.1} \cdot Depth_{s[S]}}{1 - e^{\left(-\frac{1}{0.1} \cdot Depth_{[S]s}\right)}}$$

(111)

with

$Corr_{runoff,s[S]}$: correction factor for the regional, continental and global depth dependent soil concentration [-]

0.1: soil penetration depth [m]

$Depth_{s[S]}$: depth of regional, continental and global soil [m] (Table 2)

The transfer rate from the soils to the fresh water can be obtained from:

$$k_{s \to w[S]} = \frac{\left(\frac{RainRate[S] \cdot Frac_{run,s[S]}}{K_{slw[S]}} + Erosion_{s[S]}\right) \cdot Corr_{runoff,s[S]}}{Depth_{s[S]}}$$

(112)

with

$k_{s \to w[S]}$: transfer rate from regional, continental and global soils to the freshwater [s^{-1}]

$RainRate_{[S]}$: regional, continental and global annual precipitation [m·s^{-1}] (Table 2; Table 3)

$Frac_{run,s[S]}$: volume fraction of precipitation on regional and continental natural, agricultural and other soil run off to surface water [-] (Table 2; Table 3)

$K_{slw[S]}$: regional, continental and global dimensionless soilwater partitioning coefficient [-] (Equation 32)

$Erosion_{s[S]}$: regional, continental and global soil erosion [m·s^{-1}] (Table 2; Table 3)

$Corr_{runoff,s[S]}$: correction factor for the regional, continental and global depth dependent soil concentration [-]

$Depth_{s[S]}$: depth of regional, continental and global soil [m] (Table 2)

3.7.5 Water and sediment exchange

Values for the overall mass transfer coefficients for direct adsorption and desorption across the sediment-water interface can be obtained using the two-film resistance model, in analogy to the description of mass transfer across the air-water and air-soil interfaces (Section 3.7.2).

The gross sedimentation rate from waters can be obtained from:

For $SettlVelocity[S] \cdot \frac{Susp_{w[S]}}{Frac_{s,sd[S]} \cdot \rho_{solid}} > NetSedRate_{w[S]}$

$$GrossSedRate_{w[S]} = SettlVelocity[S] \cdot \frac{Susp_{w[S]}}{Frac_{s,sd[S]} \cdot \rho_{solid}} \qquad (113)$$

For $SettlVelocity[S] \cdot \frac{Susp_{w[S]}}{Frac_{s,sd[S]} \cdot \rho_{solid}} \leq NetSedRate_{w[S]}$

$$GrossSedRate_{w[S]} = NetSedRate_{w[S]} \qquad (114)$$

with
$GrossSedRate_{w[S]}$:   gross sedimentation rate in regional, continental and global waters [m·s^{-1}]
$SettlVelocity_{[S]}$:   regional, continental and global settling velocity of suspended particles [m·s^{-1}] (Table 2)
$Susp_{w[S]}$:   concentration suspended matter in regional, continental and global waters [kg·m^{-3}] (Table 2)
$Frac_{s,sd[S]}$:   volume fraction solids in regional, continental and global sediments [-] (Equation 71)
ρ_{solid}:   mineral density in sediment and soil [kg·m^{-3}] (Table 2)
$NetSedRate_{w[S]}$:   net sediment accumulation rate in regional, continental and global waters [m·s^{-1}] (Table 2)

The sedimentation flux from waters to water sediments can be obtained from:

$$Sed_{w \rightarrow sd[S]} = GrossSedRate_{w[S]} \cdot Frac_{s,sd[S]} \cdot \frac{K_{p,susp[S]} \cdot \rho_{solid}}{1000} \qquad (115)$$

with
$Sed_{w \rightarrow sd[S]}$:   sedimentation flux from regional, continental and global waters to the water sediment [m·s^{-1}]
$GrossSedRate_{w[S]}$: gross sedimentation rate in regional, continental and global waters [m·s^{-1}]
$Frac_{s,sd[S]}$:   volume fraction solids in regional, continental and global sediments [-] (Equation 71)
$K_{p,susp[S]}$:   regional, continental and global suspended solids-water partitioning coefficient [L.kg^{-1}] (Equation 30)
ρ_{solid}:   mineral density in sediment and soil [kg·m^{-3}] (Table 2)
1000:   conversion factor [m^3·kg^{-1}]

The adsorption flux from waters to water sediments can be obtained from:

$$Adsorb_{\text{w}\rightarrow\text{sd[S]}} = \frac{k_{wsd,water,w[S]} \cdot k_{wsd,sed,sd[S]}}{k_{wsd,water,w[S]} + k_{wsd,sed,sd[S]}} \cdot FR_{w,w[S]} \qquad (116)$$

with

Adsorb$_{\text{w}\rightarrow\text{sd[S]}}$:   adsorption flux from regional, continental and global waters to the water sediments [m·s^{-1}]

k$_{wsd,water,w[S]}$:   partial mass transfer coefficient at the water side of regional, continental and global water/sediment interface [m·s^{-1}] (Table 2)

k$_{wsd,sed,sd[S]}$:   partial mass transfer coefficient at the sediment side of regional, continental and global water/sediment interface [m·s^{-1}] (Table 2)

Fr$_{w,w[S]}$:   fraction of chemical truly dissolved in regional, continental and global waters [-] (Equation 55)

The transfer rate from waters to water sediments can be obtained from the sedimentation and adsorption fluxes:

$$k_{w\rightarrow sd[S]} = \frac{Sed_{w\rightarrow sd[S]} + Adsorb_{w\rightarrow sd[S]}}{Depth_{w[S]}} \qquad (117)$$

with

k$_{w\rightarrow sd[S]}$:   transfer rate from regional, continental and global waters to water sediments [s^{-1}]

Sed$_{w\rightarrow sd[S]}$:   sedimentation flux from regional, continental and global waters to the water sediment [m·s^{-1}]

Adsorb$_{w\rightarrow sd[S]}$:   adsorption flux from regional, continental and global waters to the water sediments [m·s^{-1}]

Depth$_{w[S]}$:   depth of regional, continental and global waters [m] (Table 2)

The resuspension flux from water sediments to waters can be obtained from:

$$Resusp_{sd\rightarrow w[S]} = GrossSedRate_{w[S]} - NetSedRate_{w[S]} \qquad (118)$$

with

Resusp$_{sd\rightarrow w[S]}$:   resuspension flux from regional, continental and global water sediments to waters [m·s^{-1}]

GrossSedRate$_{w[S]}$:   gross sedimentation rate in regional, continental and global waters [m·s^{-1}]

NetSedRate$_{w[S]}$:   net sediment accumulation rate in regional, continental and global waters [m·s^{-1}] (Table 2)

The desorption flux from water sediments to water can be obtained from:

$$Desorb_{sd\rightarrow w[S]} = \frac{\dfrac{k_{wsd,water,w[S]} \cdot k_{wsd,sed,sd[S]}}{k_{wsd,water,w[S]} + k_{wsd,sed,sd[S]}}}{K_{sdw[S]}} \qquad (119)$$

with

Desorb$_{sd \rightarrow w[S]}$:   desorption flux from regional, continental and global
  water sediments to the waters [m·s^{-1}]

k$_{wsd,water,w[S]}$:   partial mass transfer coefficient at the water side of
  regional, continental and global water/sediment interface
  [m·s^{-1}] (Table 2)

k$_{wsd,sed,sd[S]}$:   partial mass transfer coefficient at the sediment side of
  regional, continental and global water/sediment interface
  [m·s^{-1}] (Table 2)

K$_{sdw[S]}$:   dimensionless sediment-water partitioning coefficient of
  regional, continental and global waters [-] (Equation 34)

The transfer rate from water sediments to waters can be obtained from
the resuspension and desorption fluxes:

$$k_{sd \rightarrow w[S]} = \frac{ResuspRate_{sd[S]} + Desorb_{sd \rightarrow w[S]}}{Depth_{sd[S]}} \tag{120}$$

with

k$_{sd \rightarrow w[S]}$:   transfer rate from regional, continental and global water
  sediments to waters [s^{-1}]

Resusp$_{sd \rightarrow w[S]}$:   resuspension flux from regional, continental and global
  water sediments to waters [m·s^{-1}]

Desorb$_{sd \rightarrow w[S]}$:   desorption flux from regional, continental and global
  water sediments to the waters [m·s^{-1}]

Depth$_{sd[S]}$:   depth of regional, continental and global water
  sediments [m] (Table 2)

3.7.6   *Ocean mixing*

SimpleBox 4.0 adopts the ocean description of the CYCLES model, as
applied by Verbruggen et al. (1997). Vertical mixing in the global oceans
is assumed to depend on the global ocean circulation current (Table 2)
and the vertical mixing flow. The vertical mixing flow can be obtained by
dividing the volume of the mixed layer by the residence time of water in
this layer (55 days; Castro Jiménez and Van de Meent, 2011):

$$OceanMixing_{[S]} = \frac{Volume_{w2[S]}}{\tau_{surf[S]}} \tag{121}$$

with

OceanMixing$_{[S]}$:   global vertical mixing flow [m^3.s^{-1}]

Volume$_{w2[S]}$:   volume of global surface waters [m^3] (Equation 52)

τ$_{surf[S]}$:   global residence time mixed layer [s] (Table 2)

The transfer rate from surface waters to deep-sea waters can be
obtained from:

$$k_{w2 \rightarrow w3[S]} = \frac{OceanCurrent + OceanMixing[S]}{Volume_{w2[S]}} \tag{122}$$

with

OceanCurrent: global ocean circulation current [m^3.s^{-1}]

OceanMixing$_{[S]}$:   global vertical mixing flow [m^3.s^{-1}]

Volume$_{w2[S]}$:   volume of global surface waters [m^3] (Equation 52)

The transfer rate from deep-sea waters to surface waters can be obtained from:

$$k_{w3 \to w2[S]} = \frac{OceanCurrent + OceanMixing[S]}{Volume_{w3[S]}}$$ (123)

with
OceanCurrent: global ocean circulation current [$m^3.s^{-1}$]
OceanMixing[S]: global vertical mixing flow [$m^3.s^{-1}$]
Volume[w3[S]]: volume of global deep-sea waters [m^3] (Equation 52)

3.8 Mass balance equations

3.8.1 Air compartment
The air compartment receives chemical mass by means of emission, air flows from other scales, and intermedia transfer from waters and soils. The chemical mass decreases by means of air flows to other scales, intermedia transfer to waters and soils, and removal.

The mass balance equation for regional, continental and global air compartments is:

$$
\begin{aligned}
\frac{d\vec{m}_{air}(t)}{dt} &= EMIS_{air[S]} + k_{air[Sd \to Sr]} \cdot m_{air[Sr]} - k_{air[Sr \to Sd]} \cdot m_{air[Sd]} \\
&\quad + \sum_i k_{wi \to air[S]} \cdot m_{wi[S]} - \sum_i k_{air \to wi[S]} \cdot m_{air[S]} \\
&\quad + \sum_j k_{sj \to air[S]} \cdot m_{sj[S]} - \sum_j k_{air \to sj[S]} \cdot m_{air[S]} - k_{air[S]} \\
&\quad \cdot m_{air[S]}
\end{aligned}
$$ (124)

with
m_x : mass of the chemical in compartment x [mol]
t : time [s]
$EMIS_{air[S]}$: emission rate of the chemical into air compartment [mol·s-1] (Table 3)
$k_{air[Sd \to Sr]}$: transfer rate from source air compartment to receptor air compartment [s^{-1}] (Section 3.5.1)
$k_{air[Sr \to Sd]}$: transfer rate from receptor air compartment to source air compartment [s^{-1}] (Section 3.5.1)
$k_{wi \to air[S]}$: transfer rate from water compartment to air compartment [s-1] (Section 3.7.3)
$k_{air \to wi[S]}$: transfer rate from air compartment to water compartment [s-1] (Section 3.7.2)
$k_{sj \to air[S]}$: transfer rate from soil compartment to air compartment [s-1] (Section 3.7.3)
$k_{air \to sj[S]}$: transfer rate from air compartment to soil compartment [s-1] (Section 3.7.2)
$k_{air[S]}$: removal rate of the chemical from the air compartment [s-1] (Section 3.6.1)

3.8.2 Water compartment
The different water compartments have various input and output sources. The lake water compartment receives chemical mass from

emission and intermedia transfer from air, while the mass is decreased by means of intermedia transfer and removal to and from air.

For lake water compartments at the regional and continental scale the mass balance equation is:

$$\frac{d\vec{m}_{w0}(t)}{dt} = EMIS_{w0[S]} + k_{air \to w0[S]} \cdot m_{air[S]} - k_{w0 \to w1[S]} \cdot m_{w0[S]} - k_{w0 \to air[S]} \quad (125)$$
$$\cdot m_{w0[S]} - k_{w0[S]} \cdot m_{w0[S]}$$

with
m_x :   mass of the chemical in compartment x [mol]
t :   time [s]
$EMIS_{w0[S]}$: emission rate of the chemical into lake compartment [mol·s-1] (Table 3)
$k_{w0 \to w1[S]}$:   transfer rate from lake water compartment to fresh water compartment [s-1] (Section 3.5.2)
$k_{w0 \to air[S]}$:   transfer rate from lake compartment to air compartment [s-1] (Section 3.7.3)
$k_{air \to w0[S]}$:   transfer rate from air compartment to lake compartment [s-1] (Section 3.7.2)
$k_{w0[S]}$:   removal rate of the chemical from the lake compartment [s-1] (Section 3.6.1)

The fresh water compartment receives chemical mass from emission, water flows, and intermedia transfer from air, soil and sediment. The mass is decreased by means of water flows, intermedia transfer to air and sediment, and removal.

For fresh water compartments at the regional and continental scale the mass balance equation is:

$$\frac{d\vec{m}_{w1}(t)}{dt} = EMIS_{w1[S]} + k_{w0 \to w1[S]} \cdot m_{w0[S]} - k_{w1 \to w2[S]} \cdot m_{w1[S]} + k_{air \to w1[S]}$$
$$\cdot m_{air[S]} - k_{w1 \to air[S]} \cdot m_{w1[S]} + k_{sd1 \to w1[S]} \cdot m_{sd1[S]} - k_{w1 \to sd1[S]} \quad (126)$$
$$\cdot m_{w1[S]} + \sum_{j} k_{sj \to w1[S]} \cdot m_{sj[S]} - k_{w1[S]} \cdot m_{w1[S]}$$

with
m_x :   mass of the chemical in compartment x [mol]
t :   time [s]
$EMIS_{w1[S]}$: emission rate of the chemical into the fresh water compartment [mol·s- 1] (Table 3)
$k_{w0 \to w1[S]}$:   transfer rate from lake water compartment to fresh water compartment [s-1] (Section 3.5.2)
$k_{w1 \to w2[S]}$:   transfer rate from fresh water compartment to sea water compartment [s-1] (Section 3.5.2)
$k_{air \to w1[S]}$:   transfer rate from air compartment to fresh water compartment [s-1] (Section 3.7.2)
$k_{w1 \to air[S]}$:   transfer rate from fresh water compartment to air compartment [s-1] (Section 3.7.3)
$k_{sd1 \to w1[S]}$:   transfer rate from fresh water sediment compartment to fresh water compartment [s-1] (Section 3.7.5)

$k_{w1 \to sd1[S]}$: transfer rate from fresh water compartment to fresh water sediment compartment [s-1] (Section 3.7.5)

$k_{sj \to w1[S]}$: transfer rate from soil compartments to fresh water compartment [s-1] (Section 3.7.4)

$k_{w1[S]}$: removal rate of the chemical from the fresh water compartment [s-1] (Section 3.6.2)

The sea water compartment receives chemical mass from emission, water flows, and intermedia transfer from air and sediment. The mass is decreased by means of water flows, intermedia transfer to air and sediment, and removal.

For the sea water compartments at a regional and continental scale the mass balance equation is:

$$\frac{d\vec{m}_{w2}(t)}{dt} = EMIS_{w2[S]} + k_{w1 \to w2[S]} \cdot m_{w1[S]} + k_{w2[Sr \to Sd]} \cdot m_{w2[Sr]} - k_{w2[Sd \to Sr]}$$
$$\cdot m_{w2[Sd]} + k_{air \to w2[S]} \cdot m_{air[S]} - k_{w2 \to air[S]} \cdot m_{w2[S]} + k_{sd2 \to w2[S]} \quad (127)$$
$$\cdot m_{sd2[S]} - k_{w2 \to sd2[S]} \cdot m_{w2[S]} - k_{w2[S]} \cdot m_{w2[S]}$$

with

m_x : mass of the chemical in compartment x [mol]

t : time [s]

$EMIS_{w2[S]}$: emission rate of the chemical into the sea water compartment [mol·s-1] (Table 3)

$k_{w1 \to w2[S]}$: transfer rate from fresh water compartment to sea water compartment [s-1] (Section 3.5.2)

$k_{w2[Sr \to Sd]}$: transfer rate from receptor sea water compartment to source sea water compartment [s-1] (Section 3.5.2)

$k_{w2[Sd \to Sr]}$: transfer rate from source sea water compartment to receptor sea water compartment [s-1] (Section 3.5.2)

$k_{air \to w2[S]}$: transfer rate from air compartment to sea water compartment [s-1] (Section 3.7.2)

$k_{w2 \to air[S]}$: transfer rate from sea water compartment to air compartment [s-1] (Section 3.7.3)

$k_{sd2 \to w2[S]}$: transfer rate from sea water sediment compartment to sea water compartment [s-1] (Section 3.7.5)

$k_{w2 \to sd2[S]}$: transfer rate from sea water compartment to sea water sediment compartment [s-1] (Section 3.7.5)

$k_{w2[S]}$: removal rate of the chemical from the sea water compartment [s-1] (Section 3.6.2)

The surface sea water compartment receives chemical mass from emission, water flows, and intermedia transfer from air and deep-sea water. The mass is decreased by means of water flows, intermedia transfer to air and deep-sea water, and removal.

For the surface sea water compartments at the global scale the mass balance equation is:

$$
\frac{d\vec{m}_{w2}(t)}{dt} = EMIS_{w2[S]} + \sum_l k_{w2[Srl \to Sd]} \cdot m_{w2[Srl]}
$$
$$
- \sum_l k_{w2[Sd \to Srl]} \cdot m_{w2[Sd]} + k_{air \to w2[S]} \cdot m_{air[S]} - k_{w2 \to air[S]} \qquad (128)
$$
$$
\cdot m_{w2[S]} + k_{w3 \to w2[S]} \cdot m_{w3[S]} - k_{w2 \to w3[S]} \cdot m_{w2[S]} + k_{s \to w2[S]}
$$
$$
\cdot m_{s[S]} - k_{w2[S]} \cdot m_{w2[S]}
$$

with

m_x : mass of the chemical in compartment x [mol]

t : time [s]

$EMIS_{w2[S]}$: emission rate of the chemical into the surface sea water compartment [mol·s-1] (Table 3)

$k_{w2[Srl \to Sd]}$: transfer rate from receptor surface sea water compartments to source surface sea water compartment [s-1] (Section 3.5.2)

$k_{w2[Sd \to Srl]}$: transfer rate from source surface sea water compartments to receptor surface sea water compartment [s-1] (Section 3.5.2)

$k_{air \to w2[S]}$: transfer rate from air compartment to surface sea water compartment [s-1] (Section 3.7.2)

$k_{w2 \to air[S]}$: transfer rate from surface sea water compartment to air compartment [s-1] (Section 3.7.3)

$k_{w3 \to w2[S]}$: transfer rate from deep-sea water compartment to surface sea water compartment [s-1] (Section 3.7.6)

$k_{w2 \to w3[S]}$: transfer rate from surface sea water compartment to deep-sea water compartment [s-1] (Section 3.7.6)

$k_{s \to w2[S]}$: transfer rate from soil compartment to surface sea water compartment [s-1] (Section 3.7.4)

$k_{w2[S]}$: removal rate of the chemical from the surface sea water compartment [s-1] (Section 3.6.2)

The deep-sea water compartment receives chemical mass from water flows and intermedia transfer from surface sea water and sediment. The mass is decreased by means of intermedia transfer to surface sea water and sediment, and removal.

For the deep-sea water compartments at the global scale, the mass balance equation is:

$$
\frac{d\vec{m}_{w3}(t)}{dt} = \sum_l k_{w3[Srl \to Sd]} \cdot m_{w3[Srl]} - \sum_l k_{w3[Sd \to Srl]} \cdot m_{w3[Sd]} - k_{w3 \to w2[S]}
$$
$$
\cdot m_{w3[S]} + k_{w2 \to w3[S]} \cdot m_{w2[S]} + k_{sd \to w3[S]} \cdot m_{sd[S]} - k_{w3 \to sd[S]} \qquad (129)
$$
$$
\cdot m_{w3[S]} - k_{w3[S]} \cdot m_{w3[S]}
$$

with

m_x : mass of the chemical in compartment x [mol]

t : time [s]

$k_{w3[Srl \to Sd]}$: transfer rate from receptor deep-sea water compartments to source deep-sea water compartment [s-1] (Section 3.5.2

$k_{w3[Sd \to Srl]}$: transfer rate from source deep-sea water compartments to receptor deep-sea water compartment [s-1] (Section 3.5.2

$k_{w3 \to w2[S]}$: transfer rate from deep-sea water compartment to surface sea water compartment [s-1] (Section 3.7.6)

$k_{w2 \to w3[S]}$: transfer rate from surface sea water compartment to deep-sea water compartment [s-1] (Section 3.7.6)

$k_{sd \to w3[S]}$: transfer rate from sea water sediment compartment to deep-sea water compartment [s-1] (Section 3.7.5)

$k_{w3 \to sd[S]}$: transfer rate from deep-sea water compartment to sea water sediment compartment [s-1] (Section 3.7.5)

$k_{w3[S]}$: removal rate of the chemical from the deep-sea water compartment [s-1] (Section 3.6.2)

3.8.3 *Sediment compartment*

The sediment compartment receives chemical mass from intermedia transfer from waters, while the mass is decreased by means of intermedia transfer to waters, and from removal.

For regional, continental and global sediment compartments the mass balance equation is:

$$\frac{d\vec{m}_{sd}(t)}{dt} = k_{w \to sd[S]} \cdot m_{w[S]} - k_{sd \to w[S]} \cdot m_{sd[S]} - k_{sd[S]} \cdot m_{sd[S]} \qquad (130)$$

with

m_x : mass of the chemical in compartment x [mol]

t : time [s]

$k_{w \to sd[S]}$: transfer rate from water compartments to water sediment compartments [s-1] (Section 3.7.5)

$k_{sd \to w[S]}$: transfer rate from water sediment compartments to water compartments [s-1] (Section 3.7.5)

$k_{sd[S]}$: removal rate of the chemical from the water sediment compartments [s-1] (Section 3.6.3)

3.8.4 *Soil compartment*

The soil compartment receives chemical mass from emission and intermedia transfer from air, while the mass is decreased by means of intermedia transfer to air and water, and from removal.

For the regional, continental and global soil compartments the mass balance equation is:

$$\frac{d\vec{m}_{s}(t)}{dt} = EMIS_{s[S]} + k_{air \to s[S]} \cdot m_{air[S]} - k_{s \to air[S]} \cdot m_{s[S]} - k_{s \to w[S]} \cdot m_{s[S]} - k_{s[S]} \\ \cdot m_{s[S]} \qquad (131)$$

with

m_x : mass of the chemical in compartment x [mol]

t : time [s]

$EMIS_{s[S]}$: emission rate of the chemical into soil compartments [mol·s-1] (Table 3)

$k_{air \to s[S]}$: transfer rate from air compartment to soil compartments [s-1] (Section 3.7.2)

$k_{s \to air[S]}$: transfer rate from soil compartments to air compartment [s-1] (Section 3.7.3)

$k_{s \to w[S]}$:   transfer rate from soil compartments to fresh water (regional and continental) and surface sea water (global) compartments [s-1] (Section 3.7.4)

$k_{s[S]}$:   removal rate of the chemical from soil compartments [s-1] (Section 3.6.4)

4 Model output

SimpleBox 4.0 produces two sorts of output; a steady-state or "level III" output, and the quasi-dynamic or "level IV" output.

The steady-state output is developed when the conditions (loadings and environmental conditions) remain constant in time for a sufficiently long period. The mass flows and concentrations are constant in time, as 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 by means of a matrix inversion routine. The mass flows and concentrations that characterise this steady state are given in output tables.

The quasi-dynamic output is developed when, after a change in conditions (loadings or environmental conditions), the mass flows and concentrations develop toward a new steady state, according to the mass balance equations. This computation is made 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 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 4.0 consists of the mass balance equations described in Section 3.8. In SimpleBox 4.0, nine boxes are defined for the regional and the continental system; the global scales consist of five boxes. In Table 6, the box numbers are given for the compartments of the different scales.

At steady-state, all mass balance equations (Section 3.8) become zero. In this state, the system is described by a set of linear (mass balance) equations that can be described and solved by standard linear algebra as shown by Brandes *et al.* (2002). In SimpleBox 4.0, the steady-state masses for the 33 boxes (Table 6) are given in moles (mol) as the model matrix is in per second (s^{-1}) and the emission in moles per seconds ($mol \cdot s^{-1}$):

$$m_{ss,i} = EMIS_i \cdot K^{-1} \tag{132}$$

with
$m_{ss,i}$:   steady-state mass in box i [mol]
$EMIS_i$: emission to box i [$mol \cdot s^{-1}$]
K^{-1}:   inverse model matrix [s]

The mass distribution is calculated with the steady–state masses as percentages of the total system mass hold-up:

$$Distribution_i = \frac{m_{ss,i}}{\sum_i m_{ss}} \cdot 100 \tag{133}$$

Table 6. The boxes of SimpleBox 4.0.

Box	Scale	Compartment	Box	Scale	Compartment
1	Regional	Air	18	Continental	Urban/industrial soil
2	Regional	Lake water	19	Moderate	Air
3	Regional	Fresh water	20	Moderate	Surface sea water
4	Regional	Sea water	21	Moderate	Deep-sea water
5	Regional	Fresh water sediment	22	Moderate	Sea water sediment
6	Regional	Sea water sediment	23	Moderate	Soil
7	Regional	Natural soil	24	Arctic	Air
8	Regional	Agricultural soil	25	Arctic	Surface sea water
9	Regional	Urban/industrial soil	26	Arctic	Deep-sea water
10	Continental	Air	27	Arctic	Sea water sediment
11	Continental	Lake water	28	Arctic	Soil
12	Continental	Fresh water	29	Tropic	Air
13	Continental	Sea water	30	Tropic	Surface sea water
14	Continental	Fresh water sediment	31	Tropic	Deep-sea water
15	Continental	Sea water sediment	32	Tropic	Sea water sediment
16	Continental	Natural soil	33	Tropic	Soil
17	Continental	Agricultural soil			

with
Distribution$_i$: percentage mass in box i [%]
$m_{ss,i}$:   steady-state mass in box i [mol]
$\Sigma_i m_{ss}$: summation of steady-state masses [mol]

The steady-state concentrations in the 33 boxes are calculated from the steady-state masses by dividing by the volume of the box:

$$C_{ss,i} = \frac{m_{ss,i}}{V_i}$$
(134)

with
$C_{ss,i:}$: steady-state concentration in box i [mol·m^{-3}]
$m_{ss,i:}$: steady-state mass in box i [mol]
V_i: volume of box i [m^3]

In SimpleBox 4.0 the steady-state computation results are shown in the "output" sheet in output table 1 (Figure 3). The steady state masses are given in kilograms (kg); the concentrations in grams per cubic meter (g·m^{-3}), grams per litre (g·L^{-1}) or grams per kilogram wet/dry weight (g·kg(w/d)$^{-1}$); and the fugacity in Pascal (Pa).

Output table 1: Steady-state Concentrations, Fugacities, Emissions and Mass

Model	SimpleBox, vs 4.0a
Substance	diuron
Scenario	default scenario
Case	defaults only

	Masses (kg)					Concentrations						Fugacities (Pa)				
	Reg	Cont	Mod	Arct	Trop	Reg	Cont	Mod	Arct	Trop		Reg	Cont	Mod	Arct	Trop
Air	1.8E+04 (0.1%)	1.4E+04 (0.1%)	1.7E+03 (0.0%)	6.3E+01 (0.0%)	1.0E+02 (0.0%)	7.6E-08	1.9E-09	2.2E-11	1.5E-12	8.2E-13	g.m^{-3}	7.8E-07	2.0E-08	2.3E-10	1.4E-11	8.7E-12
* GAS PHASE	5.0E+03 (0.0%)	3.9E+03 (0.0%)	4.9E+02 (0.0%)	1.8E+01 (0.0%)	3.1E+01 (0.0%)	2.2E-08	5.4E-10	6.3E-12	4.2E-13	2.4E-13	g.m^{-3}	2.2E-07	5.5E-09	6.4E-11	3.9E-12	2.6E-12
* AEROSOL PHASES	1.3E+04 (0.1%)	9.9E+03 (0.1%)	1.2E+03 (0.0%)	4.5E+01 (0.0%)	7.3E+01 (0.0%)	5.5E-08	1.4E-09	1.6E-11	1.1E-12	5.7E-13	g.m^{-3}	5.6E-07	1.4E-08	1.6E-10	9.9E-12	6.1E-12
Fresh water lake	1.4E+04 (0.1%)	5.9E+04 (0.3%)				2.4E-07	6.3E-08				g.L^{-1}	2.2E-13	5.8E-14			
* DISSOLVED	1.4E+04 (0.1%)	5.9E+04 (0.3%)				2.4E-07	6.3E-08				g.L^{-1}	2.2E-13	5.8E-14			
* SUSPENDED SOLIDS	8.9E-01 (0.0%)	3.8E+00 (0.0%)				5.8E-06	1.5E-06				g.kg(d)$^{-1}$	1.4E-17	3.8E-18			
Fresh water	5.4E+06 (39.7%)	1.7E+05 (0.9%)				2.8E-04	5.6E-07				g.L^{-1}	2.6E-10	5.1E-13			
* DISSOLVED	5.4E+06 (39.6%)	1.7E+05 (0.9%)				2.8E-04	5.6E-07				g.L^{-1}	2.6E-10	5.1E-13			
* SUSPENDED SOLIDS	2.2E+03 (0.0%)	7.1E+01 (0.0%)				6.9E-03	1.4E-05				g.kg(d)$^{-1}$	1.1E-13	2.1E-16			
Fresh water sediment	4.2E+05 (3.1%)	1.3E+04 (0.1%)				1.7E-03	3.4E-06				g.kg(w)$^{-1}$	3.0E-10	5.8E-13			
* PORE WATER	3.3E+05 (2.5%)	1.1E+04 (0.1%)				3.2E-04	6.4E-07				g.L^{-1}	2.4E-10	4.7E-13			
* SOLID PHASE	8.3E+04 (0.6%)	2.7E+03 (0.0%)				3.9E-03	7.7E-06				g.kg(d)$^{-1}$	5.9E-11	1.2E-13			
Surface sea/ocean water	2.8E+05 (2.1%)	1.8E+07 (93.8%)	1.7E+07 (3.3%)	1.4E+07 (3.9%)	1.9E+07 (3.0%)	2.8E-05	2.5E-08	4.5E-09	5.4E-09	2.1E-09	g.L^{-1}	2.6E-11	2.3E-14	4.1E-15	1.1E-16	1.4E-14
* DISSOLVED	2.8E+05 (2.1%)	1.7E+07 (93.8%)	1.7E+07 (3.3%)	1.4E+07 (3.9%)	1.9E+07 (3.0%)	2.8E-05	2.5E-08	4.5E-09	5.4E-09	2.1E-09	g.L^{-1}	2.6E-11	2.3E-14	4.1E-15	1.1E-16	1.4E-14
* SUSPENDED SOLIDS	4.9E+01 (0.0%)	3.0E+03 (0.0%)	3.0E+03 (0.0%)	2.4E+03 (0.0%)	3.3E+03 (0.0%)	6.9E-04	6.1E-07	1.1E-07	1.3E-07	5.2E-08	g.kg(d)$^{-1}$	4.5E-15	4.0E-18	7.2E-19	2.0E-20	2.4E-18
Deep sea/ocean water			5.1E+08 (96.7%)	3.3E+08 (96.1%)	6.2E+08 (97.0%)			4.4E-09	4.4E-09	2.3E-09	g.L^{-1}			4.0E-15	9.2E-17	1.5E-14
* DISSOLVED			5.1E+08 (96.7%)	3.3E+08 (96.1%)	6.1E+08 (97.0%)			4.4E-09	4.4E-09	2.3E-09	g.L^{-1}			4.0E-15	9.2E-17	1.5E-14
* SUSPENDED SOLIDS			8.8E+04 (0.0%)	5.8E+04 (0.0%)	1.1E+05 (0.0%)			1.1E-07	1.1E-07	5.6E-08	g.kg(d)$^{-1}$			7.0E-19	1.6E-20	2.6E-18
Marine sediment	6.1E+03 (0.0%)	1.9E+04 (0.1%)	3.7E+04 (0.0%)	2.4E+04 (0.0%)	4.4E+04 (0.0%)	1.6E-04	1.4E-07	2.4E-08	2.4E-08	1.3E-08	g.kg(w)$^{-1}$	2.7E-11	2.4E-14	4.2E-15	9.7E-17	1.6E-14
* PORE WATER	4.9E+03 (0.0%)	1.5E+04 (0.1%)	2.9E+04 (0.0%)	1.9E+04 (0.0%)	3.5E+04 (0.0%)	3.0E-05	2.6E-08	4.6E-09	4.6E-09	2.4E-09	g.L^{-1}	2.2E-11	1.9E-14	3.4E-15	7.8E-17	1.3E-14
* SOLID PHASE	1.2E+03 (0.0%)	3.8E+03 (0.0%)	7.3E+03 (0.0%)	4.8E+03 (0.0%)	8.8E+03 (0.0%)	3.6E-04	3.2E-07	5.6E-08	5.6E-08	2.9E-08	g.kg(d)$^{-1}$	5.5E-12	4.8E-15	8.4E-16	1.9E-17	3.2E-15
Natural soil	4.7E+05 (3.5%)	2.2E+05 (1.2%)				9.0E-05	2.6E-06				g.kg(w)$^{-1}$	1.9E-11	5.4E-13			
* PORE WATER / GROUNDWATER	1.3E+04 (0.1%)	5.9E+03 (0.0%)				2.0E-05	5.9E-07				g.L^{-1}	3.8E-12	1.1E-13			
* SOLID PHASE	4.6E+05 (3.4%)	2.2E+05 (1.2%)				9.9E-05	2.9E-06				g.kg(d)$^{-1}$	1.5E-11	4.3E-13			
Agricultural soil	6.8E+06 (50.1%)	5.8E+05 (3.1%)				1.5E-04	7.7E-07				g.kg(w)$^{-1}$	3.0E-11	1.6E-13			
* PORE WATER / GROUNDWATER	1.8E+05 (1.3%)	1.6E+04 (0.1%)				3.3E-05	1.7E-07				g.L^{-1}	6.1E-12	3.2E-14			
* SOLID PHASE	6.6E+06 (48.7%)	5.7E+05 (3.0%)				1.6E-04	8.5E-07				g.kg(d)$^{-1}$	2.4E-11	1.3E-13			
Other soil	1.7E+05 (1.3%)	8.2E+04 (0.4%)	9.5E+04 (0.0%)	1.1E+04 (0.0%)	1.5E+03 (0.0%)	9.0E-05	2.6E-06	2.9E-08	7.5E-09	4.6E-10	g.kg(w)$^{-1}$	1.9E-11	5.4E-13	6.0E-15	3.6E-17	6.9E-16
* PORE WATER / GROUNDWATER	4.7E+03 (0.0%)	2.2E+03 (0.0%)	2.5E+03 (0.0%)	2.9E+02 (0.0%)	4.0E+01 (0.0%)	2.0E-05	5.9E-07	6.6E-09	1.7E-09	1.1E-10	g.L^{-1}	3.8E-12	1.1E-13	1.2E-15	7.2E-18	1.4E-16
* SOLID PHASE	1.7E+05 (1.3%)	8.0E+04 (0.4%)	9.3E+04 (0.0%)	1.1E+04 (0.0%)	1.5E+03 (0.0%)	9.9E-05	2.9E-06	3.2E-08	8.3E-09	5.1E-10	g.kg(d)$^{-1}$	1.5E-11	4.3E-13	4.8E-15	2.9E-17	5.5E-16
Total	1.4E+07 (0.9%)	1.9E+07 (1.2%)	5.3E+08 (34.1%)	3.5E+08 (22.6%)	6.3E+08 (41.2%)							7.8E-07	2.0E-08	2.3E-10	1.4E-11	8.7E-12

Figure 3. SimpleBox 4.0 spreadsheet "Output table 1" on the output sheet.

Output table 2: Steady-state mass flows (kg.s-1)

Model	SimpleBox, vs 4.0a
Substance	default substance
Scenario	default scenario
Case	defaults only

		Emission	Inflow	Outflow	Removal	Degra dation	air-water transport	water-air transport	air-soil transport	soil-air transport	soil-water transport	water-sed transport	sed-water transport	mass balance
Regional Scale														
air	aR	3.2E-01	1.6E-01	9.3E-01	3.6E-05	2.1E-02	4.8E-04	4.7E-01						*0.0E+00*
fresh water lakes	w0R		0.0E+00	3.6E-06		1.3E-05	2.4E-05	7.5E-06						*0.0E+00*
fresh water	w1R	3.2E-01	3.6E-06	1.3E-02		1.6E-02	2.6E-04	3.0E-01			1.5E-02	2.8E-03	2.5E-03	*0.0E+00*
coastal sea water	w2R	0.0E+00	1.3E-02	9.1E-03		5.8E-04	4.2E-05	3.4E-03				2.3E-05	2.0E-05	*0.0E+00*
fresh water sediment	sd1R				7.1E-05	2.4E-04						2.8E-03	2.5E-03	*0.0E+00*
coastal marine sediment	sd2R				2.2E-07	2.3E-06						2.3E-05	2.0E-05	*0.0E+00*
natural soil	s1R	0.0E+00			1.8E-08	1.1E-05			4.1E-05	2.8E-05	2.6E-06			*0.0E+00*
agricultural soil	s2R	3.2E-01			1.0E-04	1.4E-01			9.2E-05	1.6E-01	1.5E-02			*0.0E+00*
other soil	s3R	0.0E+00			6.5E-09	4.1E-06			1.5E-05	1.0E-05	9.7E-07			*0.0E+00*
Continental Scale														
air	aC	0.0E+00	1.1E+00	9.1E-01	2.0E-04	1.2E-01	2.7E-02	7.3E-03						*0.0E+00*
fresh water lakes	w0C		0.0E+00	1.2E-06		4.3E-05	6.9E-05	2.5E-05						*0.0E+00*
fresh water	w1C	0.0E+00	1.2E-06	3.1E-05		3.7E-05	7.6E-04	7.1E-04			2.3E-05	6.6E-06	5.9E-06	*-9.7E-17*
coastal sea water	w2C	0.0E+00	9.9E-03	7.9E-03		2.2E-02	2.6E-02	6.3E-03				4.2E-05	3.8E-05	*0.0E+00*
fresh water sediment	sd1C				1.6E-07	5.5E-07						6.6E-06	5.9E-06	*-1.7E-18*
coastal marine sediment	sd2C				0.0E+00	4.2E-06						4.2E-05	3.8E-05	*0.0E+00*
natural soil	s1C	0.0E+00			5.0E-08	3.1E-05			1.2E-04	7.9E-05	7.5E-06			*0.0E+00*
agricultural soil	s2C	0.0E+00			8.5E-08	1.2E-04			2.6E-04	1.3E-04	1.3E-05			*0.0E+00*
other soil	s3C	0.0E+00			1.9E-08	1.2E-05			4.4E-05	2.9E-05	2.8E-06			*0.0E+00*
Global Scale - Moderate climate zone														
air	aM	0.0E+00	1.4E+00	1.1E+00	3.5E-04	2.1E-01	4.8E-02	7.6E-03						*0.0E+00*
upper ocean water	w2M	0.0E+00	1.2E-02	4.1E-02		1.2E-02	4.7E-02	7.0E-03			4.8E-05			*0.0E+00*
deep sea	w3M		4.0E-02	3.9E-03		3.6E-02						4.7E-06	4.2E-06	*0.0E+00*
ocean sediment	sdM				1.4E-10	4.7E-07						4.7E-06	4.2E-06	*0.0E+00*
soil	sM	0.0E+00			3.2E-07	2.0E-04			7.6E-04	5.1E-04	4.8E-05			*0.0E+00*
Global Scale - Arctic climate zone														
air	aA	0.0E+00	3.7E-01	2.5E-01	1.3E-04	6.5E-02	6.8E-02	1.4E-02						*0.0E+00*
upper ocean water	w2A	0.0E+00	2.9E-02	7.7E-02		5.4E-03	6.8E-02	1.4E-02			1.2E-18			*0.0E+00*
deep sea	w3A		7.7E-02	2.8E-02		4.9E-02						2.9E-05	2.8E-05	*0.0E+00*
ocean sediment	sdA				7.0E-10	7.0E-07						2.9E-05	2.8E-05	*-2.5E-18*
soil	sA	0.0E+00			8.3E-21	3.1E-18			1.9E-04	8.0E-18	1.2E-18			*1.9E-04*
Global Scale - Tropical climate zone														
air	aT	0.0E+00	6.4E-01	3.8E-01	3.5E-04	2.3E-01	3.5E-02	3.9E-03						*0.0E+00*
upper ocean water	w2T	0.0E+00	5.6E-04	1.7E-02		1.5E-02	3.5E-02	3.6E-03			2.6E-05			*0.0E+00*
deep sea	w3T		1.6E-02	5.6E-04		1.6E-02						8.3E-07	6.5E-07	*0.0E+00*
ocean sediment	sdT				1.6E-11	1.8E-07						8.3E-07	6.5E-07	*0.0E+00*
soil	sT	0.0E+00			1.8E-07	1.5E-04			5.4E-04	3.7E-04	2.6E-05			*0.0E+00*
		9.5E-01			*1.2E-03*	*9.5E-01*								*1.9E-04*

Figure 4. SimpleBox 4.0 spreadsheet "Output table 2" on the output sheet.

The results are given for all phases that occur in the different boxes of SimpleBox 4.0 (Table 7).

Table 7. Phases in air, water, sediment and soil compartments of SimpleBox 4.0.

Compartment	Phases	Unit
Air	Gas	$g \cdot m^{-3}$
	Aerosol	$g \cdot m^{-3}$
Water	Dissolved	$g \cdot L^{-1}$
	Suspended solids	$g \cdot kg(d)^{-1}$
Sediment	Pore water	$g \cdot L^{-1}$
	Solids	$g \cdot kg(d)^{-1}$
Soil	Pore water/groundwater	$g \cdot L^{-1}$
	Solids	$g \cdot kg(d)^{-1}$

In output table 2, the steady-state mass flows ($kg \cdot s^{-1}$) are shown (Figure 4). All mass flows from the mass balance equation are calculated from the rates, the steady-state masses, and the molar weight.

4.2 Quasi-dynamic computation

As an option, the response of the system to changes in emissions, i.e. the development toward an eventual steady-state, may be computed. This computation is termed "quasi-dynamic" since, besides the emissions, all the model parameters are assumed to be constant in time. This is computed by a separate integration routine that numerically integrates the mass balance equations described in Section 3.8.

The numerical integration is done in R (2015), by means of a Visual Basic macro that interfaces Excel and R via the Rexcel add-in (R, 2015), as shown in in Figure 5.

```
# Initialize Excel spreadsheet
Application.ScreenUpdating = False
Calculate

# Initialize R
RInterface.StartRServer
RInterface.RRun "rm(list=objects())"
RInterface.RRun "library(deSolve)"
RInterface.RRun "library(MASS)"

# Read model inputs from spreadsheet into R
RInterface.PutArray "m0", Range(".....")        '1x33 matrix 'm0'(mol) in R
RInterface.PutArray "e1", Range(".....")      '1x33 matrix 'e1' (mol.s-1) in R
RInterface.PutArray "e2", Range(".....")      '1x33 matrix 'e2' (mol.s-1) in R
RInterface.PutArray "tend1", Range(".....")      '1x1 matrix 'tend.1' (s) in R
RInterface.PutArray "tend2", Range(".....")      '1x1 matrix 'tend.2' (s) in R
RInterface.PutArray "K", Range(".....")          '33x33 matrix 'K' (s-1) in R

# Mass balance model with default ode solver from R-package deSolve
RInterface.RRun "SimpleBoxODE <- function(t, m, Pars) {dm <- K %*% m + e;
return(list(dm))}"
RInterface.RRun "e <- t(e1)"
RInterface.RRun "m <- t(m0)"
RInterface.RRun "invMinf <- solve(-diag(as.vector(solve(K)%*%e)))"
RInterface.RRun "tset1 <- seq(from=0, to=tend1*(3600*24*365),
length.out=50)"
RInterface.RRun "out1 <-
ode(y=m,times=tset1,func=SimpleBoxODE,parms=NULL)"
RInterface.RRun "Mt1 <-
cbind(out1[,1]/(3600*24*365),out1[,2:34]%*%invMinf)"
RInterface.RRun "e <- t(e2)"
RInterface.RRun "m <- as.numeric(c(out1[50,2:34]),nrow=50,ncol=1)"
RInterface.RRun "tset2 <- seq(from=tend1*(3600*24*365),
to=tend2*(3600*24*365), length.out=50)"
RInterface.RRun "out2 <- ode(y=m,times=tset2,func=
SimpleBoxODE,parms=NULL)"
RInterface.RRun "Mt2 <-
cbind(out2[,1]/(3600*24*365),out2[,2:34]%*%invMinf)"

# Read R model outputs back into spreadsheet
RInterface.GetArray "Mt1", Range(".....")
RInterface.GetArray "Mt2", Range(".....")
RInterface.StopRServer

# Finalize SimpleBox spreadsheet calculation
Calculate
Application.ScreenUpdating = False
```

*Figure 5. Visual Basic/Rexcel/R script for numerical integration of SimpleBox
mass balance equations*

5   The SimpleBox model code

5.1   SimpleBox sheets

The SimpleBox 4.0 model was developed as an MS Excel spreadsheet. Previous versions all had the same basic structure, consisting of three main parts: an "input block", a "computation block" and an "output block". The latest SimpleBox model still has the same blocks with, in addition, three database sheets. The spreadsheet includes input, output, databases, definitions and computations sheets. The substance, landscape and case data described in Sections 3.2 and 3.3, can be invoked in the "input" sheet. The steady-state computation and the quasi-dynamic computation can be found in the "engine" sheet and the "dynamicR" sheet, respectively. SimpleBox 4.0 gives steady-state output in the "output" sheet and quasi-dynamic output in the "dynamicR" sheet. The individual modules are further described in the following sections. The SimpleBox variables described in the previous chapter appear in the spreadsheet as cells. The cells containing the value used for each variable, are added to the "Name Manager" in Excel with matching variable name.

5.1.1   Input
The SimpleBox 4.0 input sheet contains the "look-up table picker", in which the substance, scenario and case can be chosen from the databases. After the substance, scenario and case have been selected, the substance properties, emissions and landscape settings used in the model are presented below the "look-up table picker".

5.1.2   Output
The SimpleBox 4.0 output sheet contains the two output tables included in Section 4.1. In addition, five figures visualize the scales with their compartments, steady-state percentages, and the steady-state mass flows (Figure 6).

5.1.3   Quasi-dynamic computation ("dynamicR")
The quasi-dynamic computation consists of input block, an output block and a graphs block. The input block summarises the model version, substance, scenario and case, and the characteristic time scale of the the current model analysis - the so-called 'overall persistence in the environment, P_{OV}' of the chemical. This P_{OV} is used as a standard time scale for the dynamic computation; the P_{OV} time scale can be shortened or extended to suit the purpose of the analysis. In the output block, the molar masses over time, computed in R, are returned. In the graphs block, the percentages mass of the steady-state over time are visualised in graphs for all spatial scales. This is illustrated in Figure 7, where quasi-dynamic model output of masses at the regional scale is shown.
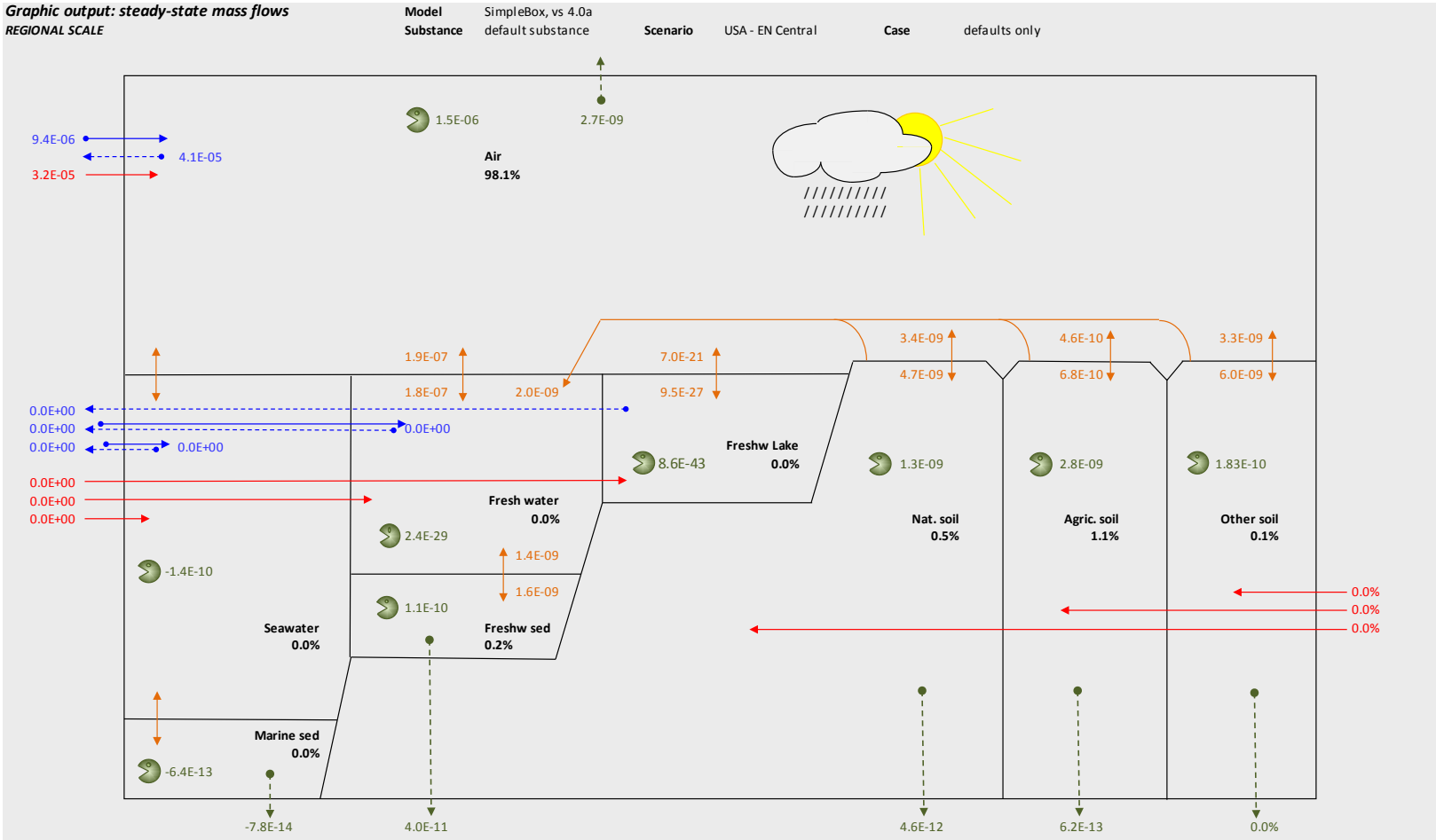
Figure 6. Part of graphic output in SimpleBox 4.0 from the "output" sheet
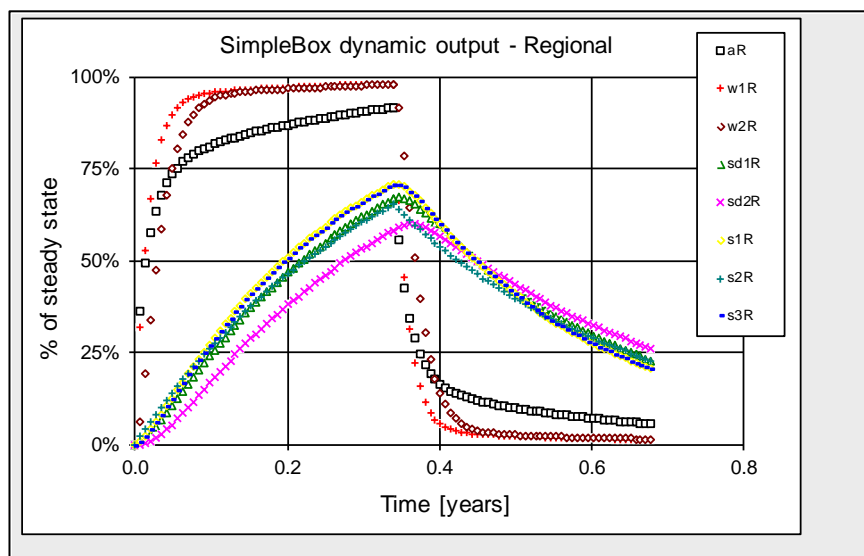
Figure 7. Part of graphs block in SimpleBox 4.0 from the "dynamicR" sheet.

5.1.4 Database

In SimpleBox 4.0 three databases are incorporated; a substance database, a scenario database and an archive of previously studied cases. Currently, the cases database lists the step-wise evolution of SimpleBox 4.01 (20150331) as described by Hollander et al. (2015). The cases database is designed to store model analyses, ready to be recalled in future work. The substance database and the scenario database contain the 276 HPVCs (Section 3.3) and the settings for a default, EUSES and 17 sub-continental landscapes (Section 3.2), respectively.

5.1.5 Definition ("regional", "continental" and "global")

The three scales in SimpleBox 4.0 are defined separately in the three sheets; "regional", "continental" and "global". Each scale/zone definition is divided into four blocks, each of which describes the environment, intermedia partitioning, intermedia transfer and removal from system.

REGIONAL SCALE MODEL DEFINITION

ENVIRONMENT	Variable Name	Unit	User input	LookUp	Default	Used	
VOLUME air compartment	VOLUME.aR	[m^3]			7.8E+14	7.8E+14	m^3
VOLUME lake water compartment	VOLUME.w0R	[m^3]			7.8E-29	7.8E-29	m^3
VOLUME fresh water compartment	VOLUME.w1R	[m^3]			1.5E-09	1.5E-09	m^3
VOLUME sea water compartment	VOLUME.w2R	[m^3]			-1.1E+10	-1.1E+10	m^3
VOLUME fresh water sediment compartment	VOLUME.sd1R	[m^3]			4.5E+09	4.5E+09	m^3
VOLUME marine sediment compartment	VOLUME.sd2R	[m^3]			-3.2E+07	-3.2E+07	m^3
VOLUME natural soil compartment	VOLUME.s1R	[m^3]			1.3E+10	1.3E+10	m^3
VOLUME agricultural soil compartment	VOLUME.s2R	[m^3]			6.6E+10	6.6E+10	m^3
VOLUME other soil compartment	VOLUME.s3R	[m^3]			1.9E+09	1.9E+09	m^3
AREA regional system	SYSTEMAREA.R	[km^2]			7.8E+05	7.8E+11	m^2
AREA FRACTION lake water	AREAFRAC.w0R	[-]			1.0E-20	1.0E-20	-
AREA FRACTION fresh water	AREAFRAC.w1R	[-]			1.9E-01	1.9E-01	-
AREA FRACTION natural soil	AREAFRAC.s1R	[-]			3.3E-01	3.3E-01	-
AREA FRACTION agricultural soil	AREAFRAC.s2R	[-]			4.3E-01	4.3E-01	-
AREA FRACTION other soil	AREAFRAC.s3R	[-]			4.8E-02	4.8E-02	-
AREA FRACTION sea water	AREAFRAC.w2R	[-]			-1.4E-03	-1.4E-03	-

Figure 8. Part of variable description in SimpleBox 4.0 from the "regional" sheet.

All definition sheets follow a general lay-out; variable description, variable name used in this document, the initial unit, user input, lookup from cases, substances or landscape databases, default, and used and final unit (Figure 8). In the definition sheets, user input is required, as a value needs to be assigned to each of the SimpleBox "definition parameters". Values can be assigned in two ways:

- By entering a value into the cell to the right of the parameter name in the column labelled "User input", using the units given in square brackets to the right of the variable name.
- By accepting the value that appears in either the column labelled "LookUp" (indicating that the value is defined in the selected case), or in the column labelled "Default" (indicating that a fixed default value or an estimating formula is producing the value). This default formula or value is accepted by leaving the cell empty. Usually a number appears in only one of the columns. If both columns contain a number, the number in the column "LookUp" is used, unless the user overrides this by entering a number into the column "User input".

The default values in the column labelled "Default" depend on the values assigned to other cells in the spreadsheet. For the estimation formulas, the values of auxiliary parameters are used as input. As a rule, the auxiliary parameters used are placed in the rows immediately below the text strings that label them. The result returned by the estimation formulas changes when the value of any of the auxiliary parameters is changed, as the spreadsheet is recalculated automatically after each data entry.
A value is assigned to the cell in the column labelled "Used" by a conditional statement in this cell that takes either the user input (column "User"), the case look-up (column "LookUp") or the default value/estimating formulas (column "Default") 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.

5.1.6 *Steady-state computation ("engine")*
The computation of the steady-state solution as described in Section 4.1, is done in the engine sheet, and consists of multiple blocks. The first block summarises the volumes of all compartments and the emissions to these compartments. The second block is the model matrix, which contains all transfer and removal rates. In the third block, the steady-state masses, concentration, and fugacities are calculated as described in Section 4.1. The fourth block calculates the mass flows matrix by multiplying the model matrix with the steady-state masses. Finally, in the last block, the mass balances are checked.

5.1.7 *Operation*
For the operation of SimpleBox 4.0, MS Windows (XP or up) and MS Excel (2007 or up) are required. The Excel workbook file *SimpleBox4.01.xlsx* recalculates the steady-state ('level III') solution of the mass balance equations automatically after every change. Calculation of transient solutions ('level IV') requires the availability of R (2.15.2 or up; with packages deSolve and MASS) and the RExcel add-in. These background

tools are invoked by clicking the dynamicR button on the "dynamicR" sheet.

5.2 Running the model

The SimpleBox spreadsheet distributed with this document is an Excel spreadsheet. The spreadsheet was created originally in MS Excel 2010 version 14.0 (32-bits).
The spreadsheet, R and RExcel are freely available from:
http://www.rivm.nl/en/Topics/S/Soil_and_water/SimpleBox_4_0_tool
http://www.r-project.org/
http://rcom.univie.ac.at/download.html

To run SimpleBox, take the following steps:
1. In Windows, start Excel.
2. In Excel, open the file SimpleBox4.01 20150331.xlsx.
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 may take a while. In the Calculation Tab under Formulas it is possible to change the automatic calculation to manual calculation. In that case, use F9 to calculate the SimpleBox spreadsheet after the changes in parameter values.
4. Make your choice for the substance, scenario and case in the "input" sheet.
5. Optionally run the quasi-dynamic computation by the "dynamicR" button on the "dynamicR" sheet.
   NOTE: Depending on the model definition and the computing power available, this may take a long time.
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.

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Appendix – Landscape scenarios

Table 8. Landscape scenarios for the regional scale. The scenarios consist of two defaults (SimpleBox and EUSES), nine regions in the United States of America (USA) and eight regions in Canada (CAN).

	Default scenario	EUSES settings	USA Mid Atlantic	USA New England	USA – East North Central	USA – West North Central	USA South Atlantic	USA East South Central	USA West South Central	USA Mountain	
AREAland.R	2.3E+05	4.0E+04	2.8E+05	1.8E+05	7.8E+05	1.3E+06	7.4E+05	4.7E+05	1.1E+06	2.2E+06	**[km2]**
AREAsea.R	1.0E+03	4.0E+02	1.5E+03	1.0E+03	0.0E+00	0.0E+00	4.4E+03	1.5E+02	1.2E+04	0.0E+00	**[km2]**
FRAClake.R	2.5E-03	1.0E-10	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	**-**
FRACfresh.R	2.8E-02	3.0E-02	8.1E-02	8.6E-02	1.9E-01	2.4E-02	6.3E-02	2.4E-02	3.1E-02	8.7E-03	**-**
FRACnatsoil.R	2.7E-01	2.7E-01	5.8E-01	7.4E-01	3.3E-01	1.5E-01	6.0E-01	5.6E-01	2.8E-01	5.8E-01	**-**
FRACagsoil.R	6.0E-01	6.0E-01	2.3E-01	8.8E-02	4.3E-01	8.0E-01	2.7E-01	3.8E-01	6.6E-01	4.1E-01	**-**
FRACothersoil.R	1.0E-01	1.0E-01	1.0E-01	8.5E-02	4.8E-02	2.8E-02	7.1E-02	3.4E-02	2.5E-02	6.7E-03	**-**
TEMP.R	1.2E+01	1.2E+01	1.1E+01	6.5E+00	8.5E+00	9.2E+00	1.7E+01	1.6E+01	1.8E+01	1.1E+01	**[°C]**
WINDspeed.R	3.0E+00	3.0E+00	3.2E+00	3.9E+00	3.3E+00	3.5E+00	2.7E+00	2.4E+00	3.4E+00	3.2E+00	**m.s-1**
RAINrate.R	7.0E+02	7.0E+02	1.0E+03	1.1E+03	1.2E+03	1.1E+03	1.1E+03	1.4E+03	8.8E+02	3.1E+02	**mm.yr-1**
DEPTHlake.R	1.0E+02	1.0E-10	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	**m**
DEPTHfreshwater.R	3.0E+00	3.0E+00	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	**m**
FRAC.w1R.w1C	0.0E+00	0.0E+00	4.6E-01	0.0E+00	1.0E+00	1.0E+00	0.0E+00	9.8E-01	0.0E+00	1.0E+00	**-**
FRACrun.R	2.5E-01	2.5E-01	3.6E-01	3.2E-01	3.4E-01	6.8E-02	3.5E-01	3.8E-01	2.0E-01	2.4E-01	**-**
FRACinf.R	2.5E-01	2.5E-01									**-**
EROSION.R	3.0E-02	3.0E-02	4.2E-02	4.2E-02	8.0E-02	6.7E-02	3.2E-02	4.7E-02	4.1E-02	5.1E-02	**mm.yr-1**

	USA Pacific	CAN Newfoundland and Labrador	CAN Atlantic Maritimes	CAN Québec	CAN Ontario	CAN Manitoba	CAN Saskatch-ewan	CAN Alberta	CAN British Columbia	
AREAland.R	8.5E+05	4.1E+05	1.3E+05	1.5E+06	1.1E+06	6.5E+05	6.5E+05	6.6E+05	9.4E+05	**[km2]**
AREAsea.R	4.9E+03	3.9E+03	1.3E+03	1.5E+04	3.2E+03	2.7E+03	0.0E+00	0.0E+00	5.4E+03	**[km2]**
FRAClake.R	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	**-**
FRACfresh.R	2.5E-02	7.7E-02	2.5E-02	1.1E-01	1.5E-01	1.5E-01	9.1E-02	3.0E-02	2.1E-02	**-**
FRACnatsoil.R	6.6E-01	9.2E-01	8.8E-01	8.6E-01	7.9E-01	7.4E-01	5.0E-01	6.5E-01	9.5E-01	**-**
FRACagsoil.R	2.8E-01	1.0E-03	7.9E-02	2.2E-02	5.1E-02	1.2E-01	4.0E-01	3.2E-01	2.7E-02	**-**
FRACothersoil.R	3.4E-02	1.8E-03	1.3E-02	4.9E-03	7.1E-03	1.4E-03	1.3E-03	5.0E-03	4.6E-03	**-**
TEMP.R	1.3E+01	-3.1E-01	5.5E+00	-1.1E+00	5.1E-01	-2.2E+00	2.1E-01	2.4E+00	4.7E+00	**[°C]**
WINDspeed.R	2.5E+00	4.6E+00	4.5E+00	4.2E+00	3.7E+00	4.1E+00	4.0E+00	3.7E+00	3.5E+00	**m.s-1**
RAINrate.R	6.9E+02	1.0E+03	1.2E+03	8.8E+02	7.4E+02	4.9E+02	4.2E+02	4.5E+02	7.5E+02	**mm.yr-1**
DEPTHlake.R	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	**m**
DEPTHfreshwater.R	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	**m**
FRAC.w1R.w1C	0.0E+00	0.0E+00	0.0E+00	0.0E+00	3.9E-01	1.9E-03	1.0E+00	1.0E+00	3.1E-01	**-**
FRACrun.R	5.0E-01	6.8E-01	6.1E-01	6.3E-01	4.0E-01	3.1E-01	2.4E-01	2.2E-01	8.4E-01	**-**
FRACinf.R										**-**
EROSION.R	2.3E-02	1.2E-02	5.0E-02	9.2E-03	2.0E-02	5.0E-03	6.7E-03	3.3E-02	1.3E-01	**mm.yr-1**

Table 9. Landscape scenarios for the continental scale. The scenarios consist of two defaults (SimpleBox and EUSES), nine regions in the United States of America (USA) and eight regions in Canada (CAN).

	Default scenario	EUSES settings	USA Mid Atlantic	USA New England	USA – East North Central	USA – West North Central	USA South Atlantic	USA East South Central	USA West South Central	USA Mountain	
AREAland.C	3.7E+06	3.5E+06	1.5E+07	1.5E+07	1.5E+07	1.5E+07	1.5E+07	1.5E+07	1.5E+07	1.5E+07	[km2]
AREAsea.C	3.7E+06	3.5E+06	5.4E+05	5.4E+05	5.4E+05	5.4E+05	5.4E+05	5.4E+05	5.4E+05	5.4E+05	[km2]
FRAClake.C	2.5E-03	1.0E-10	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	-
FRACfresh.C	2.8E-02	3.0E-02	6.5E-02	6.5E-02	5.8E-02	6.9E-02	6.5E-02	6.6E-02	6.8E-02	7.6E-02	-
FRACnatsoil.C	2.7E-01	2.7E-01	6.0E-01	6.0E-01	6.1E-01	6.5E-01	6.0E-01	6.0E-01	6.3E-01	6.0E-01	-
FRACagsoil.C	6.0E-01	6.0E-01	3.2E-01	3.2E-01	3.1E-01	2.6E-01	3.2E-01	3.1E-01	2.9E-01	3.0E-01	-
FRACothersoil.C	1.0E-01	1.0E-01	1.7E-02	1.8E-02	1.7E-02	2.0E-02	1.6E-02	1.8E-02	1.8E-02	2.1E-02	-
TEMP.C	1.2E+01	1.2E+01	7.3E+00	7.4E+00	7.3E+00	7.2E+00	6.9E+00	7.1E+00	6.4E+00	6.7E+00	[oC]
WINDspeed.C	3.0E+00	3.0E+00	3.5E+00	3.5E+00	3.5E+00	3.5E+00	3.5E+00	3.5E+00	3.5E+00	3.5E+00	m.s-1
RAINrate.C	7.0E+02	7.0E+02	7.8E+02	7.8E+02	7.6E+02	7.4E+02	7.6E+02	7.6E+02	7.7E+02	8.7E+02	mm.yr-1
DEPTHlake.C	1.0E+02	1.0E-10	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	m
DEPTHfreshwater.C	3.0E+00	3.0E+00	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	m
FRAC.w1C.w1R	0.0E+00	3.4E-02	2.2E-02	0.0E+00	0.0E+00	4.8E-03	1.3E-03	6.7E-02	1.6E-01	0.0E+00	-
FRACinf.C	2.5E-01	2.5E-01	3.7E-01	3.7E-01	3.7E-01	4.0E-01	3.7E-01	3.7E-01	3.8E-01	3.9E-01	-
FRACrun.C	2.5E-01	2.5E-01									-
EROSION.C	3.0E-02	3.0E-02	4.2E-02	4.2E-02	4.0E-02	4.0E-02	4.3E-02	4.2E-02	4.2E-02	4.0E-02	mm.yr-1

	USA Pacific	CAN Newfoundland and Labrador	CAN Atlantic Maritimes	CAN Québec	CAN Ontario	CAN Manitoba	CAN Saskatch-ewan	CAN Alberta	CAN British Columbia	
AREAland.C	1.5E+07	1.5E+07	1.5E+07	1.5E+07	1.5E+07	1.5E+07	1.5E+07	1.5E+07	1.5E+07	**[km2]**
AREAsea.C	5.4E+05	5.4E+05	5.4E+05	5.4E+05	5.4E+05	5.4E+05	5.4E+05	5.4E+05	5.4E+05	**[km2]**
FRAClake.C	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	**-**
FRACfresh.C	6.8E-02	6.5E-02	6.5E-02	5.9E-02	5.8E-02	6.1E-02	6.4E-02	6.7E-02	6.8E-02	**-**
FRACnatsoil.C	6.0E-01	5.9E-01	6.0E-01	5.7E-01	5.8E-01	5.9E-01	6.0E-01	6.0E-01	5.7E-01	**-**
FRACagsoil.C	3.2E-01	3.2E-01	3.2E-01	3.5E-01	3.4E-01	3.2E-01	3.1E-01	3.2E-01	3.4E-01	**-**
FRACothersoil.C	1.8E-02	1.9E-02	1.9E-02	2.1E-02	2.0E-02	2.0E-02	2.0E-02	1.9E-02	2.0E-02	**-**
TEMP.C	7.0E+00	7.6E+00	7.4E+00	8.4E+00	7.9E+00	7.8E+00	7.7E+00	7.6E+00	7.6E+00	**[oC]**
WINDspeed.C	3.5E+00	3.4E+00	3.5E+00	3.4E+00	3.5E+00	3.4E+00	3.5E+00	3.5E+00	3.5E+00	**m.s-1**
RAINrate.C	7.9E+02	7.7E+02	7.8E+02	7.7E+02	7.8E+02	8.0E+02	8.0E+02	8.0E+02	7.8E+02	**mm.yr-1**
DEPTHlake.C	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	**m**
DEPTHfreshwater.C	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	1.0E-20	**m**
FRAC.w1C.w1R	4.5E-02	0.0E+00	0.0E+00	4.9E-02	0.0E+00	1.7E-02	3.2E-03	1.1E-02	0.0E+00	**-**
FRACinf.C	3.6E-01	3.6E-01	3.7E-01	3.4E-01	3.7E-01	3.7E-01	3.7E-01	3.8E-01	3.3E-01	**-**
FRACrun.C										**-**
EROSION.C	4.3E-02	4.3E-02	4.2E-02	4.6E-02	4.4E-02	4.4E-02	4.4E-02	4.3E-02	3.6E-02	**mm.yr-1**

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