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SIMPLEBOX: a generic multimedia fate evaluation model

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This work represents the spin-off of research that has been carried out in the past, most of it as part of the RIVM project no. 679102 and its predecessors. The present report was produced as part of the RIVM project no. 672720, carried out on behalf of and commissioned by the Director-General of the RIVM.

DISCLAIMER

This document has been subject to review according to the internal quality assurance procedures of the Laboratory of Ecotoxicology of the RIVM and has been approved for publication as an RIVM report. Earlier versions of the SimpleBox model have been reviewed during many years of "learning by doing". Although both the document and the model code that goes with it have been prepared with care, these materials are not claimed to be free of errors. Use of the results obtained by means of these materials is the full responsibility of the user. Use of the model is encouraged and feed back is welcomed. However, other than by means of this document, no technical support for users is being offered.

FOREWORD

This work represents the spin-off of applied research that has been carried out over the past ten years, most of it in support of the development of evaluation systems for new and existing chemicals. The SimpleBox system is the RIVM's representation of the well-known multimedia environmental fate modeling approach of the so-called Mackay-type. Earlier versions of the SimpleBox model have become known under various names. No detailed technical descriptions or user manuals have ever been produced, as these spreadsheets have been used principally by the developers themselves and a limited number of other informed users. It has recently been proposed to extend the use of this modeling concept beyond this research scope and apply this concept in support for decision making in environmental management. To serve this new purpose, the model has been reviewed. The result has been given the name SimpleBox vs 1.0 (930801). The present report is the documentation of this model.

A copy of the spreadsheet code of the model is distributed with this report in order to encourage other researchers to use and test the model. It should be emphasized that the model is meant to be used for scientific purposes only. The model is to be used in a comparative way, to explain and predict differences between different situations and differences between different chemicals, rather than to forecast concentration levels or chemical fluxes for specific situations. The environmental science on which the model is built is well established. However, to the best of my knowledge, the validity of this modeling concept to serve this general scientific purpose has never been tested adequately. Despite this, the tendency to apply this concept for decision making purposes appears to be growing. Therefore, serious attempts need to be made to specify the proper way to use this modeling concept and to identify its limitations. It is the responsibility of the scientific community to provide this guidance to users. It is hoped that the distribution of this material may be instrumental in starting the process of putting this model concept to test. Suggestions to this end are welcome.

Many individuals, inside and outside the RIVM, have contributed to the development of SimpleBox. Of these, I only name Jodi de Greef. Much of SimpleBox originated from his creative scientific thinking.
This work was completed during a sabbatical period at the US Environmental Protection Agency's Environmental Research Laboratory at Athens, Georgia. I thank the EPA for the hospitality.

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SUMMARY

This document describes the technical details of the multimedia fate model SimpleBox, version 1.0 (930801). SimpleBox is a multimedia box model of what is commonly referred to as a "Mackay-type" model; it assumes spatially homogeneous environmental compartments (air, water, suspended matter, aquatic organisms, sediment, three soil compartments). The model takes emission rates and rate constants for transport and transformation of micropollutants as input and computes concentrations in the environment as output. SimpleBox is a generic model in the sense that it can be customized to represent specific environmental situations. In its default setting, the SimpleBox computation represents the behavior of micropollutants in an open system, resembling The Netherlands. The Mackay concept of sequentially carrying out the modeling procedure at different stages of conceptual sophistication or "levels", is adopted. In SimpleBox, the lowest level is the non equilibrium, steady-state computation (level 3). In addition to this, the quasi-dynamic response to changes is the loadings (non equilibrium, non steady-state, or level 4) can be computed. Computation of mass flows and concentration levels in SimpleBox is done with concentration-based "piston velocity" type mass transfer coefficients [$m.s^{-1}$]. Transfer and transformation phenomena are treated as simple pseudo first-order processes.

SimpleBox was developed to be used as a scientific instrument --to explain why, in what way and to what extent the fate of different chemicals in a multimedia environment may be different; or to explain why, in what way and to what extent the fate of one chemical may be different in different environmental situations. The present version of the model was prepared to serve as a means to support regulatory decision making in The Netherlands:

- for estimation of real-world intermedia concentration ratios of existing chemicals, as a means to harmonize independently derived quality objectives for air, water, sediment and soil;
- for estimation of regional-scale PEC/NEC-quotients of existing chemicals, as indices for prioritization.

This report is meant to provide the technical documentation that is necessary to serve these purposes. The model is distributed on diskette, along with this document. The purpose is to encourage other researchers to use and test the multimedia modeling approach for the presently proposed decision support purposes.

1 INTRODUCTION

History

The work on SimpleBox started in 1982, when the development of a systematic procedure to evaluate the environmental risk associated with the introduction of new chemicals was initiated at RIVM. The work was inspired by the classic paper "Calculating fugacity" by Mackay and Paterson (1981). The earliest versions, Basic and Fortran codes of the "Mackay level 1 and level 2 computations", received the name "SimpleMac", after the first author. The first spreadsheet version, in Multiplan for the Apple IIe, was made in 1984. This was an exact replica of the "Mackay level 3 computation" as published earlier by Mackay (1979). This sheet received the name "SimpleSal", after the second author.

The SimpleSal sheet was found useful as an instrument to aid systematic environmental chemical reasoning. The multimedia modeling approach found its application in another area of RIVM work: the Integrated Criteria Documents for existing chemicals. Multimedia modeling became a way to generalize the fragmentary knowledge about transport and transformation processes, and to explain the field observations that were collected for the chemicals for which Integrated Criteria Documents were being produced (Van de Meent, 1987, 1990). It appears that similar developments had taken place elsewhere (Frische *et al.*, 1984; Rippen *et al.*, 1984; Cohen and Ryan, 1985; Ryan and Cohen, 1986; Travis *et al.*, 1987). The "Mackay approach" had changed the phenomenon of intermedia transfer of pollutants into something that could be understood and dealt with at the level of environmental management.

SimpleSal was also found useful as a means to direct the research in the field of environmental chemistry at the RIVM. This research is aimed at prediction of the environmental fate of chemicals. Multimedia modeling has become a way to point out if the sort of research that is needed to predict "fate". Along the same line, SimpleSal has been used often as an aid to teach environmental chemistry (Van de Meent, 1988).

In the course of time, many minor and major changes have been made to the SimpleSal sheet. A major change was the replacement, in 1986, of the original Apple/Multiplan version of SimpleSal by the present MS-DOS/Lotus123 version. This transition made it possible to take advantage of the built-in matrix inversion routine of Lotus123 to compute the general solution of a set of n mass balance equations with n unknown concentrations. It became easy to change, add or delete process formulations (atmospheric deposition, surface run-off, soil leaching, sedimentation/resuspension) or to include or delete environmental compartments. In this generic form, the spreadsheet became a framework to design multimedia box models for various purposes, rather then a specific model. This modeling framework was then called "SimpleBox" and SimpleSal became one of its applications (OECD, 1989). Other applications of the SimpleBox modeling framework have been produced under the names: "SimpleSingh", a spatially inhomogeneous multimedia box model (Singh and Van de Meent, 1989), "SimpleTreat", a model of a waste water treatment plant (Struijs and Van de Meent, 1988; OECD, 1989; Struijs *et al.* 1991) and "WaterBox", a water version of SimpleSal for teaching purposes.

Another major development was the coupling, also in 1986, of the spreadsheet-based "level 3 computation" of SimpleSal with a numeric integrator: the "level 4 computation". The "level 4 routine" made use of the "Friendly Applied Modeling Environment, FAME", a numeric integration program that had been developed earlier at RIVM (Wortelboer and Aldenberg, 1991). This way, the dynamic response of the system to changes in loadings --the development in time of concentrations towards the steady state, computed with the "level 3 routine" of SimpleSal-- could be simulated.

In 1989, a version of the SimpleSal spreadsheet was prepared to serve the purpose for which the work was started originally. Leaving the basic structure of the model unchanged, the input and output parts were set up in such a way that SimpleSal could be used on a semi-routine basis as a generic exposure estimation model to carry out risk estimations for new chemicals. This version of SimpleSal was then called "SimpleRisk" (Van de Meent, 1989). Recently, the SimpleRisk spreadsheet has found application in two areas of environmental decision making: (i) as an element of the prototype of UBS, the Uniform Substances Evaluation System (RPC, 1991) and (ii) as an element in the harmonization of environmental quality standards for air, water and soil. These applications have been named "UBS-Box" and "INS-Box", respectively.

Present

The present version of the model was prepared in response of the proposed use of this approach in support of environmental decision making in The Netherlands. The multimedia modeling approach is being proposed for two specific purposes:

- for estimation of real-world intermedia concentration ratios of existing chemicals, as a means to harmonize independently derived quality objectives for air, water, sediment and soil (Van de Meent and De Bruijn, 1993).
- for estimation of regional-scale PEC/NEC-quotients of existing chemicals, as indices for prioritization (Van de Meent and Toet, 1992);

Because none of the earlier versions of the model, for which no detailed descriptions were available, could serve these new purposes, it was decided to merge the large number of previously developed "Mackay-type" spreadsheets back into one generic modeling system: SimpleBox (version 1.0), and prepare a technical description that can serve as a user manual.

In a general sense, SimpleBox is to be considered as a "non-validated" modeling concept. In fact, validation of a body of theory or a modeling concept as general as SimpleBox should not even be attempted. Instead, effort should be made to test how well specific applications of the model described well-defined end points. Not all end points can be easily validated, however. As in the abovementioned examples:

- it will be hard, if not impossible, to test how successful the model is in predicting the intermedia concentration ratios that are to be expected as a result of the long term environmental management measures that are yet to be implemented;
- it may be impossible to test how successfully the model can be applied in predicting the relative environmental risks for a series of chemicals, as is proposed in the priority-setting procedure.

Although "non-validated", the model may be a useful tool to assist the scientific reasoning on which environmental decision-making is to be based. As long as the reasoning is made explicit and reproducible by providing proper documentation. The purpose of publication of the present version of the SimpleBox model is to document the multimedia fate modeling approach that has been applied in the past at RIVM and start the process of testing the validity of this approach to specific ends.

SimpleBox is meant as a game to be played by scientists to find out what the implications are of the knowledge that they are prepared to assume about intermedia transfer and transformation processes. Models like SimpleBox are meant to be used in a generic way --to explain why, in what way and to what extent the fate of different chemicals in a multimedia environment may differ; or to explain why, in what way and to what extent the fate of one chemical may be different in different environmental situations. Although many of the processes that are accounted for in this model may be reasonably well understood, the overall result of the simultaneous operation of these processes may not be obvious at all. It is not rare to obtain modeling results that are not understood (or even believed) initially, and yet in hindsight conclude that this is an understandable consequence of the accepted theory that the model represents and therefore reasonable. Used this way, SimpleBox may be helpful as a support for scientific reasoning. And ultimately as a means to test the "validity" of our knowledge about environmental processes. If "fate", as expressed in terms of concentration levels, intermedia fluxes and elimination rates, is consistent with our observations in real-world situations, this may be taken as an indication that we have general understanding of multimedia environmental behavior. However, testing of this kind has, to the best of the author's knowledge, not been carried out extensively.

The SimpleBox model is distributed on diskette, along with this document. The purpose is to encourage other researchers to use and test the multimedia modeling approach for the presently proposed decision support purposes. It is hoped that experience with the model that can lead to correction of the inevitable errors in the document and the model code, to better understanding of the limitations of the modeling concept, and to further improvements of the model will be fed back to the developers.

Future

It is expected that in the future the development of SimpleBox will continue as it has in the past: whenever new uses are proposed, SimpleBox will be updated with relevant new knowledge on transport and transformation processes. Further implementation of SARs to estimate process rate constants, especially transformation rate constants, is anticipated. As in the past, no formal release of documented updates is planned. However, potential users, willing to share their expertise, are welcome to contact the author and request access to the most recent version.

2 THE SIMPLEBOX MODEL

2.1 Model concept

SimpleBox can be characterized as a model of the "Mackay-type" (Mackay, 1991) in the sense that it is a multimedia fate model in which the environmental compartments are represented by homogeneous boxes. Within this main assumption of homogeneity of environmental compartments, the SimpleBox model is generic in the sense that it can be customized to represent specific environmental situations. In its default setting, the SimpleBox computation represents the behavior of micropollutants in an open system, resembling The Netherlands. This computation is similar to the computation, described recently by Mackay *et al.* (1992). Also, the Mackay concept of sequentially carrying out the modeling procedure at different stages of conceptual sophistication or "levels", is adopted. In SimpleBox, the lowest level is the non equilibrium, steady-state computation (level 3). In addition to this, the quasi-dynamic response to changes is the loadings (non equilibrium, non steady-state, or level 4) can be computed. Unlike the fugacity approach as adopted by Mackay, computation of mass flows and concentration levels in SimpleBox is done with concentration-based "piston velocity" type mass transfer coefficients [$m.s^{-1}$]. The reason for this is that, in most of the scientific literature, mass transfer is expressed in these terms, rather than in terms of the fugacity-based "conductivity" type coefficients [$mol.hr^{-1}.Pa^{-1}$]. As is done in the Mackay models, transfer and transformation phenomena are treated as simple pseudo first-order processes.

The computational basis of the SimpleBox system is illustrated in Figure 1. Environmental compartments are represented by boxes. The concentration of a chemical in these boxes is affected by processes that cause mass flows of the chemical to and from the boxes.

The chemical can be *INPUT* into a box from outside the system, *OUTPUT* from a box to outside the system, or transported by means of *ADVECTIVE* or *DIFFUSIVE* processes to and from other boxes. A mass balance equation can be written for each of the boxes. The mass balance equations have the

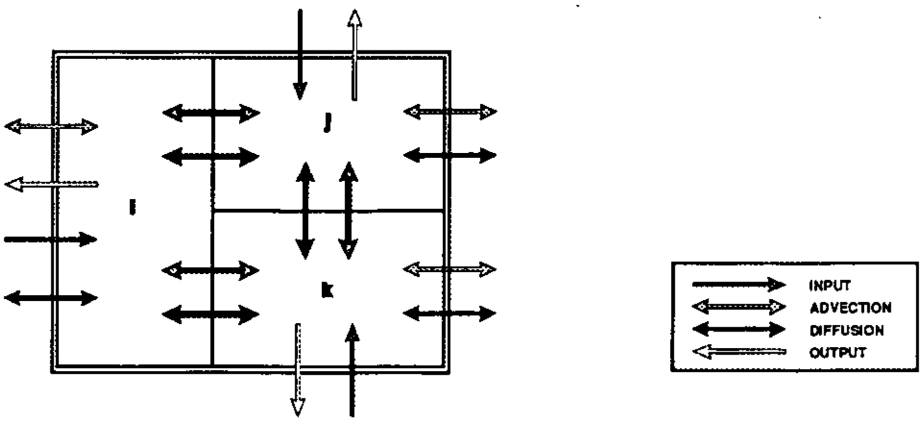


Figure 1 *SimpleBox computes n concentrations in n compartments by solving the mass balance equations for n compartments.*

following format:

$$V_i \cdot \frac{dC_i}{dt} = EMIS_i + IMP_i - EXP_i - DEGRD_i - LCH_i - BRL_i + \Sigma ADV_{ij} + \Sigma DIFF_{ij} \qquad (1)$$

with

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

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

The principal task (the scientific part of the modeling task) is to find mathematical expressions that describe the magnitude of process mass flows in terms of properties of the chemical and characteristics of the environment. Models can be written of environmental systems with few or many boxes, with few or many processes, to suit the objectives of the specific modeling exercise. Using the present day computing systems, the number of boxes that can be modeled this way is limited only by our knowledge of the processes, that is our ability to express the mass flows as simple functions of the concentrations and the system parameters.

The practical part of the modeling task is to provide a framework within which the model computations can be carried out. This part is not unimportant, as model application often requires numerous, error-prone manipulation and unit-conversion of input and output data. In SimpleBox, the user is often offered several options for entering an input data item; the selection of the manner in which way to enter the input may be made dependent on the availability of knowledge in the specific situation. In some instances, values for input parameters may be available in a format that can be readily used for computation (e.g., mass transfer coefficients in $m.s^{-1}$); in other instances, it may be more practical to estimate a value from other input data, using established estimation equations (e.g., deriving sediment-water partition coefficients from the octanol-water partition coefficient and the organic carbon content).

The SimpleBox model described in this document (Figure 2) has eight compartments: air, water, sediment, suspended particles, aquatic organisms, and three separate soil compartments. The different atmospheric phases (gas, rain, aerosol) and the different terrestrial phases (solids, water, air) are considered to be in a state of thermodynamic equilibrium at all times; air and soil are treated as bulk compartments. For the aquatic phases (water, suspended particles, biota), no equilibrium assumption

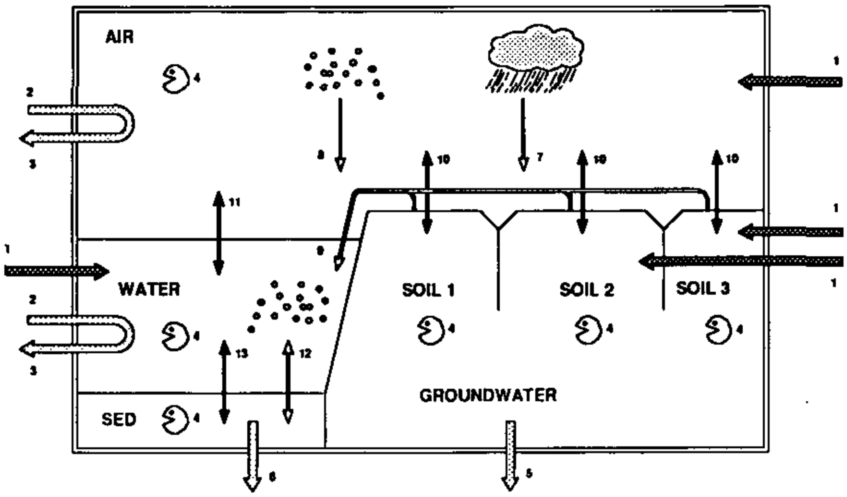


Figure 2 *Compartments and processes in SimpleBox.*

is made; the phases are treated as separate compartments. The justification for these choices is historic, rather than reasoned. The three different soil compartments can be used to define different geographic areas, different soil types or different soil use.

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

IMPORT takes place in the air, water and suspended matter compartments. Import is the result of refreshment of the air and water in the system with air and water from outside. Import may be derived from the concentrations at the system boundaries, which are externally controlled, and the atmospheric and hydraulic residence times, which are system characteristics. The residence times may be derived from windspeed, rain rate and stream flows. Import is considered to be constant in time.

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

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

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

2.2 Model parameters

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

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

2.2.1 Parameters that characterize the environment

Air

Air is treated in SimpleBox as a bulk compartment, consisting of a gas phase, an aerosol phase and a rain water phase; the concentration in air is a total concentration.

The air in the system is not stagnant; it is continuously being flushed. Wind blows air from the "outside" into the system and from the system to "outside". As the chemical is carried with these airstreams, this leads to "import" and "export" mass flows of the chemical to and from the system. The air compartment is considered to be well-mixed. The refreshment rate is characterized by the atmospheric residence time.

The volume of the air compartment may be obtained from:

$$V_{air} = VOLUME_{air} = SYSTEMAREA \,.\, HEIGHT_{air} \tag{2}$$

with

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

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

$$SYSTEMAREA = 37975\,km^2 = 3.80.10^{10}\,m^2 \qquad (3)$$

with

SYSTEMAREA : total area of the system (air/water + air/soil interfaces) [m^2] *(D)*

the area of The Netherlands;

$$HEIGHT_{air} = 1000\,m \qquad (4)$$

with

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

the thickness of the atmospheric mixing layer over The Netherlands.

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

$$TAU_{air} = \frac{\sqrt{SYSTEMAREA\,.\,\pi / 4}}{WINDSPEED}$$

with

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

SYSTEMAREA : total area of the system (air/water + air/soil interfaces) [m^2] *(D)*

WINDSPEED : average windspeed at 10 m above the surface [$m.s^{-1}$] *(A)*

in which the following may be considered as a default:

$$WINDSPEED = 5\,m.s^{-1} \qquad (6)$$

with

WINDSPEED : average windspeed at 10 m above the surface [$m.s^{-1}$] *(A)*

This is a typical windspeed at a height of 10 m for The Netherlands.

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

$$AEROSOLDEPRATE = 0.1\,cm.s^{-1} \qquad (7)$$

with

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

$$RAINRATE = 760\,mm.yr^{-1} \qquad (8)$$

with

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

This is the average annual precipitation in The Netherlands.

Water

In SimpleBox, "water" refers to the truly dissolved state. Colloidal or macromolecular materials (small organisms and their debris, "humic" material, "dissolved" organic matter, "third phase", etc.) are considered to be part of the suspended matter and biota compartments that are treated here as separate entities. The presence of suspended matter and biota influences the fate of chemicals in a

very similar way to that of aerosols and rainwater in the atmosphere. These phases bind the chemical, thus inhibiting it from taking part in mass transfer and degradation processes that occur in the water phase. Suspended matter acts as a physical carrier of the chemical across the sediment-water interface. Concentration ratios among suspended matter, biota and water are often close to equilibrium. For the purpose of multimedia fate modeling, the water compartment could be treated the same way as the air, sediment and soil compartments: that is at all times equilibrium is assumed among water, suspended matter and biota holds at all times. The reason that this is not done in SimpleBox is purely historical. It may be done in future versions.
The water compartment is continuously flushed with water (and suspended matter) from outside the system, "importing" and "exporting" the chemical to and from the system. Like air, water is also considered well-mixed. The rate of refreshment is characterized by means of a single hydraulic residence time. This assumption strongly caricaturizes reality as typically multimedia environmental situations (like the default system: "The Netherlands") contain many different water bodies with different characteristics. Naturally, the single mixed water compartment in the system cannot represent all of these. Instead, the water compartment that is modeled here is chosen to be "typical" --an exemplification of any real water body in the system.

The volume of the water compartment may be obtained from:

$$V_{water} = VOLUME_{water} = SYSTEMAREA \, . \, AREAFRAC_{water} \, . \, DEPTH_{water} \tag{9}$$

with

V_{water} : volume of the water compartment [m^3] *(I)*
$VOLUME_{water}$: volume of the water compartment [m^3] *(D)*
$SYSTEMAREA$: total area of the system (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{water}$: fraction of the system area that is water [-] *(D)*
$DEPTH_{water}$: depth of the water column [m] *(A)*

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

$$AREAFRAC_{water} = 12.5\ \% \tag{10}$$

with

$AREAFRAC_{water}$: fraction of the system area that is water [-] *(D)*

the area percentage of surface water (rivers, lakes, canals, ditches, tidal waters) in The Netherlands;

$$DEPTH_{water} = 3\ m \tag{11}$$

with

$DEPTH_{water}$: depth of the water column [m] *(A)*

a typical value for the above mentioned surface waters.

A typical hydraulic residence time may be obtained by calculating a water balance. The water compartment receives water from three sources: incoming streams, surface run-off and urban run-off. The same amount flows out of the system (into the ocean):

$$TAU_{water} = \frac{VOLUME_{water}}{STREAMS + RUNOFF + EFFLUENT_{stp}} \tag{12}$$

with

TAU_{water} : hydraulic residence time of the water compartment [s] *(D)*
$VOLUME_{water}$: volume of the water compartment [m^3] *(D)*

STREAMS : sum of the discharges of all streams crossing the system boundaries [m^3.s^{-1}] *(A)*
RUNOFF : total run off from soil 1, soil 2 and soil 3 into the water compartment [m^3.s^{-1}] *(A)*
EFFLUENT$_{stp}$: total of all STP-effluent discharges into the water compartment [m^3.s^{-1}] *(A)*

$$RUNOFF = \Sigma\,(FRACrun_{soil\,i} \,.\, AREAFRAC_{soil\,i}) \,.\, RAINRATE \,.\, SYSTEMAREA \tag{13}$$

with
RUNOFF : total run off from soil 1, soil 2 and soil 3 into the water compartment [m^3.s^{-1}] *(A)*
FRACrun$_{soil\,i}$: fraction of the wet precipitation that runs off soil i to water [-] *(A)*
AREAFRAC$_{soil\,i}$: fraction of the systemarea that is soil i [-] *(D)*
RAINRATE : rate of wet precipitation [m$_{rain}$.s^{-1}] *(A)*
SYSTEMAREA : total area of the system (air/water + air/soil interfaces) [m^2] *(D)*

$$EFFLUENT_{stp} = 0.15 \,.\, STPcapacity \,.\, (24 \,.\, 3600) \tag{14}$$

with
EFFLUENT$_{stp}$: total of all STP-effluent discharges to the water compartment [m^3.s^{-1}] *(A)*
STPcapacity : total capacity of all sewage treatment plants in the system [eq] *(A)*
0.15 : amount of water per inhabitant equivalent [m^3.eq^{-1}] *(C)*
24 · 3600 : conversion factor [s.d^{-1}] *(C)*

$$STPcapacity = 0.95 \,.\, POPULATION \tag{15}$$

with
STPcapacity : total capacity of all sewage treatment plants in the system [eq] *(A)*
POPULATION : total population of the system [inh] *(A)*
0.95 : fraction of the sewage that is treated in sewage treatment plants *(C)*

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

$$STREAMS = 2600\, m^3.s^{-1} \tag{16}$$

with
STREAMS : sum of the discharges of all streams crossing the system boundaries [m^3.s^{-1}] *(A)*
the total discharge of the major rivers, entering The Netherlands;

$$POPULATION = 350 \,.\, (SYSTEMAREA \,.\, 10^6) \tag{17}$$

with
POPULATION : total population of the system [inh] *(A)*
350 : average population density in The Netherlands [inh.km^{-2}] *(C)*
SYSTEMAREA : total area of the system (air/water + air/soil interfaces) [m^2] *(D)*
10^6 : conversion factor [m^2.km^{-2}] *(C)*

Suspended matter

In this context, "suspended matter" refers to all abiotic colloidal or macromolecular materials (debris of organisms, "humic" material, "dissolved" organic matter, "third phase", etc.) that is not truly dissolved. Treatment of suspended matter as a separate compartment has one advantage: the material balance for the suspended matter compartment, which is important for the fate of chemicals that tend to partition into this phase, can be considered very explicitly.

Suspended matter is "imported", with water, from "outside" the system, and also "exported" from the system to "outside". This transport is characterized by the flow of water and the concentrations of suspended matter in the incoming and outgoing water. Suspended matter may also be produced in the system itself, by growth of small aquatic organisms (bacteria, algae). Sewage treatment plant effluents are another source of suspended matter. Finally, there is continuous exchange of particles across the sediment-water interface by sedimentation and resuspension. The balance of these suspended matter mass flows determines the magnitude and the direction of the particle exchange between sediment and water, and thus the mass flow of the chemical that is associated with the particles.

The volume of the suspended matter compartment may be obtained from:

$$V_{susp} = VOLUME_{susp} = VOLUME_{water} \cdot \frac{SUSP_{water}}{(1 - FRwater_{susp}).RHOsolid} \tag{18}$$

with

V_{susp} : volume of the suspended matter compartment [m^3] *(I)*
$VOLUME_{susp}$: volume of the suspended matter compartment [m^3] *(D)*
$VOLUME_{water}$: volume of the water compartment [m^3] *(D)*
$SUSP_{water}$: concentration of suspended matter in the water column [$kg_{solid}.m_{water}^{-3}$] *(D)*
$FRwater_{susp}$: volume fraction water of suspended matter [-] *(A)*
$RHOsolid$: density of the solid phase of suspended matter [$kg.m^{-3}$] *(A)*

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

$$SUSP_{water} = 15\, mg(dry).l^{-1} \tag{19}$$

with

$SUSP_{water}$: concentration of suspended matter in the water column [$kg_{solid}.m_{water}^{-3}$] *(D)*

a typical value for the major bodies of surface water in The Netherlands. The bulk density of suspended particles --used in various formulas throughout the model-- is inferred from the water content and the density of solid matter, and cannot be set directly:

$$RHO_{susp} = FRwater_{susp} . 1000 + (1 - FRwater_{susp}) . RHOsolid \tag{20}$$

with

RHO_{susp} : bulk density of suspended matter [$kg_{susp}.m_{susp}^{-3}$] *(I)*
$FRwater_{susp}$: volume fraction water of suspended matter [-] *(A)*
1000 : density of water [$kg.m^{-3}$] *(C)*
$RHOsolid$: density of the solid phase of suspended matter [$kg.m^{-3}$] *(A)*

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

$$FRwater_{susp} = 0.9 \tag{21}$$

with

$FRwater_{susp}$: volume fraction water of suspended matter [-] *(A)*

on intuitive grounds;

$$RHOsolid = 2500\, kg.m^{-3} \tag{22}$$

with

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

a typical value for minerals.

Suspended matter is transported into the system with the inflowing water. The inflow of suspended matter is given by the concentration of suspended matter in the "imported" water, for which, by default, the following value may be considered:

$$SUSPimport = 37\ mg(dry).l^{-1} \tag{23}$$

with

SUSPimport : concentration of suspended matter in water that flows across the system boundaries $[kg_{solid}.m_{water}^{-3}]$ *(A)*

the average suspended matter load of the Rhine river at the point of entry in The Netherlands. The outflow of suspended matter is given by the concentration of suspended matter in the water in the system, $SUSP_{water}$.

Particle exchange between sediment and water is characterized by:

$$GROSSsedrate = \frac{SETTLEvelocity\,.\,SUSP_{water}}{(1 - FRwater_{sed})\,.\,RHOsolid} \tag{24}$$

with

GROSSsedrate : gross sedimentation rate $[m_{sed}.s^{-1}]$ *(A)*
SETTLEvelocity : settling velocity of suspended particles $[m_{water}.s^{-1}]$ *(A)*
$SUSP_{water}$: concentration of suspended matter in the water column $[kg_{solid}.m_{water}^{-3}]$ *(D)*
$FRwater_{sed}$: volume fraction water of the sediment [-] *(A)*
RHOsolid : density of the solid phase of the sediment $[kg.m^{-3}]$ *(A)*

$$RESUSPrate = GROSSsedrate - NETsedrate \tag{25}$$

with

RESUPrate : resuspension rate $[m_{sed}.s^{-1}]$ *(A)*
GROSSsedrate : gross sedimentation rate $[m_{sed}.s^{-1}]$ *(A)*
NETsedrate : net sedimentation rate $[m_{sed}.s^{-1}]$ *(A)*

$$\begin{aligned} NETsedrate = {} & (PROD_{Susp} + SUSPimport\,.\,STREAMS + SUSPeff_{stp}\,.\,EFFLUENT_{stp} \\ & + \Sigma\ EROSION_{soil\,i}.AREAFRAC_{soil\,i}\,.\,SYSTEMAREA\,.\,FRsolid_{soil\,i}\,.\,RHOsolid \\ & - SUSP_{water}\,.\,(STREAMS + EFFLUENT_{stp} + RUNOFF)) \\ & .\frac{1}{(1 - FRwater_{sed})\,.\,RHOsolid}\,.\,\frac{1}{(SYSTEMAREA\,.\,AREAFRAC_{water})} \end{aligned} \tag{26}$$

with

NETsedrate : net sedimentation rate $[m_{sed}.s^{-1}]$ *(A)*
$PROD_{susp}$: rate of production of suspended matter in the water column $[kg_{solid}.s^{-1}]$ *(A)*
SUSPimport : concentration of suspended matter in water that flows across the system boundaries $[kg_{solid}.m_{water}^{-3}]$ *(A)*
STREAMS : total of the stream water that flows across the system boundaries $[m_{water}^{3}.s^{-1}]$ *(A)*
$SUSPeff_{stp}$: concentration of suspended matter in STP-effluents $[kg_{solid}.m_{eff}^{-3}]$ *(A)*
$EFFLUENT_{stp}$: total of all STP-effluent discharges to the water compartment $[m_{eff}^{3}.s^{-1}]$ *(A)*
$EROSION_{soil\,i}$: rate of erosion of soil i $[m_{soil}.s^{-1}]$ *(A)*
$AREAFRAC_{soil\,i}$: fraction of the systemarea that is soil i [-] *(D)*
$FRsolid_{soil\,i}$: volume fraction solid of soil i [-] *(A)*
RHOsolid : density of the solid phase of the sediment $[kg.m^{-3}]$ *(A)*
SYSTEMAREA : total area of the system (air/water + air/soil interfaces) $[m^{2}]$ *(D)*
$SUSP_{water}$: concentration of suspended matter in the water column $[kg_{solid}.m_{water}^{-3}]$ *(D)*
RUNOFF : total run off from soil 1, soil 2 and soil 3 into the water compartment $[m_{water}^{3}.s^{-1}]$ *(A)*
$FRwater_{sed}$: volume fraction water of the sediment [-] *(A)*
$AREAFRAC_{water}$: fraction of the system area that is water [-] *(D)*

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

$$SETTLvelocity = 2.5\,m.d^{-1} \tag{27}$$

with

SETTLvelocity : settling velocity of suspended particles $[m_{water}.s^{-1}]$ *(A)*

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

$$PROD_{susp} = 0\ kg.s^{-1} \tag{28}$$

with

$PROD_{susp}$: rate of production of suspended matter in the water column $[kg_{solid}.s^{-1}]$ *(A)*

a value typical for the winter period in turbid waters;

$$SUSPeff_{stp} = 40\,mg(dry).l^{-1} \tag{29}$$

with

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

a typical value for communal water treatment facilities.

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

$$CORG_{susp} = 0.1 \tag{30}$$

with

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

a typical value for suspended particulate matter is Dutch surface waters.

Biota

"Biota" refers to all living organisms in water, from bacteria to mammals. The compartment biota is usually small, compared to even the suspended matter compartment. As a result, biota usually play an insignificant role with regard to the overall fate of the chemicals.

The volume of the compartment biota may be obtained from:

$$V_{bio} = VOLUME_{bio} = VOLUME_{water} . \frac{BIO_{water}}{(1 - FRwater_{bio}) . RHOsolid} \tag{31}$$

with

V_{bio} :	volume of the biota compartment $[m^3]$ *(I)*
$VOLUME_{bio}$:	volume of the biota matter compartment $[m^3]$ *(D)*
$VOLUME_{water}$:	volume of the water compartment $[m^3]$ *(D)*
BIO_{water} :	concentration of biota in the water column $[kg_{solid}.m_{water}^{-3}]$ *(D)*
$FRwater_{bio}$:	volume fraction water of biota [-] *(A)*
RHOsolid :	density of the solid phase of suspended matter $[kg.m^{-3}]$ *(A)*

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

$$BIO_{water} = 1\,mg(dry).l^{-1} \tag{32}$$

with

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

with no other rationale then that this seems to relate reasonably well to the default value of 15 mg.l^{-1}, suggested for $SUSP_{water}$. The bulk density of biota --used in various formulas throughout the model-- is inferred from the water content and the density of solid matter, and cannot be set directly:

$$RHO_{bio} = FRwater_{bio} \,.\, 1000 + (1 - FRwater_{bio}) \,.\, RHOsolid \quad (33)$$

with

RHO_{bio} : bulk density of biota $[kg_{bio}.m_{bio}^{-3}]$ *(A)*
$FRwater_{bio}$: volume fraction water of biota [-] *(A)*
1000 : density of water $[kg.m^{-3}]$
$RHOsolid$: density of the solid phase of suspended matter $[kg.m^{-3}]$ *(A)*

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

$$FRwater_{bio} = 0.95 \quad (34)$$

with

$FRwater_{bio}$: volume fraction water of biota [-] *(A)*

on intuitive grounds,

$$RHOsolid = 2500\, kg.m^{-3} \quad (35)$$

with

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

a typical value for minerals.

Sediment

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

The top layer of the sediment is considered to be well-mixed. If the sedimentation of particles from the water column is greater than the resuspension (net sedimentation), this top layer is continuously being refreshed. The older sediment layer, and the chemicals that are associated with the sediment with it, gets buried under the freshly deposited material.

The volume of the sediment compartment may be obtained from:

$$V_{sed} = VOLUME_{sed} = SYSTEMAREA \,.\, AREAFRAC_{water} \,.\, DEPTH_{sed} \quad (36)$$

with

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

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

$$DEPTH_{sed} = 3\, cm \quad (37)$$

with

$DEPTH_{sed}$: mixing depth of the sediment [m] *(A)*

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

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

$$BURIAL_{sed} = NETsedrate \tag{38}$$

with

$BURIAL_{sed}$: burial rate of old sediment under fresh deposits [$m_{sed}.s^{-1}$] *(A)*
$NETsedrate$: net sedimentation rate [$m_{sed}.s^{-1}$] *(A)*

The bulk density of sediment --used in various formulas throughout the model-- is inferred from the water content and the density of solid matter, and cannot be set directly:

$$RHO_{sed} = FRwater_{sed} . 1000 + (1 - FRwater_{sed}) . RHOsolid \tag{39}$$

with

RHO_{sed} : bulk density of the sediment [$kg_{sed}.m_{sed}^{-3}$] *(A)*
$FRwater_{sed}$: volume fraction water of the sediment [-] *(A)*
1000 : density of water [$kg.m^{-3}$] *(C)*
$RHOsolid$: density of the solid phase of the sediment [$kg.m^{-3}$] *(A)*

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

$$FRwater_{sed} = 0.8 \tag{40}$$

with

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

$$RHOsolid = 2500\ kg.m^{-3} \tag{41}$$

with

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

an typical value for minerals.

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

$$CORG_{sed} = 0.05 \tag{42}$$

with

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

a typical value for the sediments in Dutch surface waters.

Soil

Soil is the most stationary and, as a result, the most spatially inhomogeneous of all environmental compartments. There are many different soil types and differences in soil use. Unfortunately, the fate of chemicals is determined largely by just the characteristics that vary so much (porosity, water content, organic matter content). Also, soil use happens to be the key factor determining whether it may be loaded directly with a chemical. One soil compartment may not be sufficient to reflect the role of "soil" in the multimedia fate of chemicals. SimpleBox, therefore, comes with three separate soil compartments. The first soil compartment may be thought of as "natural soil". The second soil compartment may be thought of as "agricultural soil". The third soil compartment may be used to reflect the existence of "urban" or "industrially used" soil.

Only the top layer of the soil is considered in this modeling concept. The top layer is assumed to be

homogeneous in a sense that the concentration of the chemical does not vary with the depth. For agricultural soil, which is frequently reworked by mechanical action (by plowing, etc.), this may be close to the truth. For natural soil, this may be a much less realistic assumption.
Soil is treated as a bulk compartment, consisting of a gas phase, a water phase and a solid phase; the concentration in soil is a total concentration. The different soil phases are assumed to be in equilibrium at all times.

The volumes of the soil compartments may be obtained from:

$$V_{soil\,i} = VOLUME_{soil\,i} = SYSTEMAREA \,.\, AREAFRAC_{soil\,i} \,.\, DEPTH_{soil\,i} \tag{43}$$

with

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

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

$$AREAFRAC_{soil\,1} = 41.5\,\% \tag{44}$$

with

$AREAFRAC_{soil\,1}$: fraction of the system area that is soil 1 [-] *(D)*

the approximate area percentage of soil that is not in agricultural use in The Netherlands,

$$DEPTH_{soil\,1} = 5\,cm \tag{45}$$

with

$DEPTH_{soil\,1}$: mixing depth of soil 1 [m] *(A)*

the approximate thickness of the litter layer,

$$AREAFRAC_{soil\,2} = 45\,\% \tag{46}$$

with

$AREAFRAC_{soil\,2}$: fraction of the system area that is soil 2 [-] *(D)*

the approximate area percentage of agricultural land in The Netherlands,

$$DEPTH_{soil\,2} = 20\,cm \tag{47}$$

with

$DEPTH_{soil\,2}$: mixing depth of soil 2 [m] *(A)*

a typical mechanical reworking depth for agricultural soil,

$$AREAFRAC_{soil\,3} = 1\,\% \tag{48}$$

with

$AREAFRAC_{soil\,3}$: fraction of the system area that is soil 3 [-] *(D)*

with no rationale at all,

$$DEPTH_{soil\,3} = 5\,cm \tag{49}$$

with

$DEPTH_{soil\,3}$: mixing depth of soil 3 [m] *(A)*

the same value as for soil 1.

It is assumed that the sludge produced in the area considered is applied onto soil 2. The rate of production of sludge may be obtained from Struijs *et al.* (1991):

$$SOLIDS_{stp} = STPcapacity \,.\, (0.15 \,.\, 0.40 + 0.0355) \qquad (50)$$

with

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

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

$$FRrun_{soil\,i} = 0.5 \qquad (51)$$

with

$FRrun_{soil\,i}$: fraction of rain water that runs of from soil i to water [-] *(A)*

$$FRinf_{soil\,i} = 0.4 \qquad (52)$$

with

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

These values may be regarded as typical for The Netherlands.

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

$$EROSION_{soil\,i} = 0 \qquad (53)$$

with

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

typical for flat terrain.

The bulk density of soil --used in various formulas throughout the model-- is inferred from the water content and the density of solid matter, and cannot be set directly:

$$RHO_{soil} = FRair_{soil} \,.\, 1.3 + FRwater_{soil} \,.\, 1000 + FRsolid_{soil} \,.\, RHOsolid \qquad (54)$$

with

RHO_{soil} : bulk density of soil $[kg_{soil}.m_{soil}^{-3}]$ *(A)*
$FRair_{soil}$: volume fraction air of soil [-] *(A)*
1.3 : density of air $[kg.m^{-3}]$ *(C)*
$FRwater_{soil}$: volume fraction water of soil [-] *(A)*
1000 : density of water $[kg.m^{-3}]$ *(C)*
$FRsolid_{soil}$: volume fraction solid of soil [-] *(A)*
$RHOsolid$: density of the solid phase of the soil $[kg.m^{-3}]$ *(A)*

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

$$FRair_{soil} = 0.2 \tag{55}$$

with

$FRair_{soil}$: volume fraction air of soil i [-] *(A)*

$$FRwater_{soil} = 0.4 \tag{56}$$

with

$FRwater_{soil}$: volume fraction water of the sediment [-] *(A)*

$$FRsolid_{soil} = 0.4 \tag{57}$$

with

$FRsolid_{soil}$: volume fraction solid of soil [-] *(A)*

typical values for soil in The Netherlands (Linders, RIVM, personal communication).

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

$$CORG_{soil\,1} = 0.05 \tag{58}$$

with

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

$$CORG_{soil\,2} = 0.05 \tag{59}$$

with

$CORG_{soil\,2}$: organic carbon content of soil 2 [$kg_{org.\ carbon}.kg_{solid}^{-1}$] *(A)*

$$CORG_{soil\,3} = 0.05 \tag{60}$$

with

$CORG_{soil\,3}$: organic carbon content of soil 3 [$kg_{org.\ carbon}.kg_{solid}^{-1}$] *(A)*

a typical value for soil anywhere.

2.2.2 Parameters that describe the properties of the chemical

Molecular weight

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

$$MOL\ WEIGHT = 250\,g.mol^{-1} \tag{61}$$

with

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

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

Octanol-water partition coefficient

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

$$K_{ow} = 10^5 \tag{62}$$

with

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

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

Vapor pressure

The vapor pressure of the chemical, *VAPOR PRESSURE*, is also used in the formulas for estimating the fraction of the chemical that is associated with aerosol particles in air and the air-water partition coefficient. As for K_{ow}, a value for *VAPOR PRESSURE* needs to be entered if it has been decided that either one of these estimation formulas is to be used. As for K_{ow}, no estimation formula for *VAPOR PRESSURE* is provided in SimpleBox. The default value

$$VAPOR\,PRESSURE = 10^{-3}\,Pa \tag{63}$$

with

VAPOR PRESSURE : vapor pressure of the chemical [Pa] *(A)*

may be taken as a starting point; it is the value of a non-volatile chemical.

Solubility

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

$$SOL = 10^{-1.214 \,.\, \log K_{ow} \,+\, 0.85} \,.\, 1000 \tag{64}$$

with

SOL : solubility of the chemical in water [$\mathrm{mol.m_{water}^{-3}}$] *(A)*
K_{ow} : octanol-water partition coefficient of the chemical [-] *(A)*
1000 : conversion factor [$\mathrm{l.m^{-3}}$]

Biodegradability

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

$$PASSreadytest = n \tag{65}$$

with

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

Environmental Quality Standards

If quality standards for air, water, soil or groundwater have been derived for the chemical, these standards can be used as a reference. SimpleBox requires quality standards as input in order to compute quotients of the computed exposure concentrations of the chemicals and their quality standards, as an indicator for "environmental risk". If no environmental quality standards are available, an estimated minimum toxicity of the chemical for aquatic ecosystems, based on the chemical's narcotic activity (Van Leeuwen *et al.*, 1992), in combination with the Equilibrium Partitioning concept (DiToro *et al.*, 1991), may be used as a starting point to derive estimated values for water, sediment, soil and groundwater:

$$STND_{water} = 10^{-0.85 \cdot \log K_{ow} - 1.6} \cdot 1000 \tag{66}$$

with

$STND_{water}$: quality standard for water [$\text{mol.m}_{water}^{-3}$] *(A)*
K_{ow} : octanol-water partition coefficient [-] *(A)*
1000 : conversion factor [l.m^{-3}]

$$STND_{sed} = STND_{water} \cdot \frac{Kp_{sed}}{1000} \tag{67}$$

with

$STND_{sed}$: quality standard for sediment [$\text{mol.kg}_{solid}^{-1}$] *(D)*
$STND_{water}$: quality standard for water [$\text{mol.m}_{water}^{-3}$] *(D)*
Kp_{sed} sediment-water partition coefficient [$\text{l}_{water}.\text{kg}_{solid}^{-1}$] *(A)*
1000 : conversion factor [l.m^{-3}] *(C)*

$$STND_{soil} = STND_{water} \cdot \frac{Kp_{soil\,1}}{1000} \tag{68}$$

with

$STND_{soil}$: quality standard for soil [$\text{mol.kg}_{sollid}^{-1}$] *(D)*
$STND_{water}$: quality standard for water [$\text{mol.m}_{water}^{-3}$] *(D)*
$Kp_{soil\,1}$: soil-water partition coefficient [$\text{l}_{water}.\text{kg}_{solid}^{-1}$] *(A)*
1000 : conversion factor [l.m^{-3}] *(C)*

$$STND_{grndwater} = STND_{water} \tag{69}$$

with

$STND_{grndwater}$: quality standard for groundwater [$\text{mol.m}_{water}^{-3}$] *(D)*
$STND_{water}$: quality standard for water [$\text{mol.m}_{water}^{-3}$] *(D)*

For quality standards in air, no such estimation routine is available. Very tentatively, an air-analogon of the Equilibrium Partitioning concept as used for sediment and soil is proposed here as a starting point for further assessment:

$$STND_{air} = STND_{water} \cdot K_{air-water} \tag{70}$$

with

$STND_{air}$: quality standard for air [mol.m_{air}^{-3}] *(D)*

$STND_{water}$: quality standard for water [$mol.m_{water}^{-3}$] *(D)*
$K_{air-water}$: air-water equilibrium distribution constant [$mol.m_{air}^{-3}/mol.m_{water}^{-3}$] *(A)*

2.2.3 Parameters that describe intermedia partitioning of the chemical

Intermedia equilibrium constants (air/water; air/aerosol, air/soil, sediment/water; soil/water, susp/-water, bio/water) or partition coefficients are required for various purposes, but principally for estimating intermedia mass transfer coefficients. The coefficients represent concentration ratios. The concentrations can be expressed on a volume basis [$mol.m^{-3}$] or on a weight basis [$mol.kg^{-1}$].
Partition coefficients may be available from experimental data or field measurements. More often, however, this information is not available. If that is the case, the estimation methods described below may be used. It should be noted that, in general, the applicability of these estimation methods is limited to those classes of (organic) chemicals for which the relationships have been derived. Extrapolation beyond these limits may lead to errors of orders of magnitude. For metals, no generally applicable estimation methods are known.

Air-water

The air-water equilibrium distribution constant, $K_{air-water}$, also known as the "dimensionless" Henry's law constant, can be estimated from the ratio of the vapor pressure and the water solubility. Alternatively, if no reliable vapor pressure and/or solubility data are available, the bond contribution method of Meylan and Howard (1991) may be used. The estimation in SimpleBox is:

$$K_{air-water} = \frac{H}{R\,.\,TEMPERATURE} = \frac{VAPOR\,PRESSURE\,/\,SOLUBILITY}{R\,.\,TEMPERATURE} \qquad (71)$$

with

$K_{air-water}$: air-water equilibrium distribution constant [$mol.m_{air}^{-3}/mol.m_{water}^{-3}$] *(A)*
H : Henry's law constant [$Pa.m^3.mol^{-1}$]
VAPOR PRESSURE : vapor pressure of the chemical [Pa] *(A)*
SOLUBILITY : solubility of the chemical in water [$mol.m^{-3}$] *(A)*
R : gas constant, = 8.314 $Pa.m^3.mol^{-1}.K^{-1}$ *(C)*
TEMPERATURE : temperature at the air-water interface [K] *(A)*

A suggested default temperature is:

$$TEMPERATURE = 12\,°C \qquad (72)$$

with

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

the average air temperature at ground level in The Netherlands.

Air-aerosol

Air-aerosol partition coefficients are usually not known. However, some information is frequently available on the fraction of the chemical that occurs in association with the aerosol phase. SimpleBox uses this information for the computations. A value for the fraction of the chemical that is associated with the aerosol phase, $FRass_{aerosol}$, can be entered directly, or estimated on the basis of the chemical's vapor pressure, according to Junge (1977):

$$FRass_{aerosol} = \frac{CONST\,.\,\theta}{VAPOR\,PRESSURE + CONST\,.\,\theta} \tag{73}$$

with

$FRass_{aerosol}$: fraction of the chemical in air that is associated with aerosol particles [-] *(A)*
$VAPOR\ PRESSURE$: vapor pressure of the chemical [Pa] *(A)*
$CONST$: constant [Pa.m] *(C)*
θ : surface area of aerosol phase [$m_{aerosol}^{2}/m_{air}^{3}$] *(C)*

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

Air-rain

The scavenging ratio may be known from measurements or estimated:

$$SCAVratio = \frac{1 - FRass_{aerosol}}{K_{air-water}} + FRass_{aerosol}\,.\,2.10^{5} \tag{74}$$

with

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

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

Sediment-water, susp-water and soil-water

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

$$\log Kp = \log(Koc\,.\,CORG) = a \log Kow + b + \log CORG \tag{75}$$

with

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

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

$$\log Kp = \log Kow + \log CORG \qquad or \qquad Kp = CORG\,.\,Kow \tag{76}$$

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

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

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

$$K_{susp-water} = FRwater_{susp} + (1 - FRwater_{susp}) \, . \, Kp_{susp} \, . \, RHOsolid \, / \, 1000 \tag{77}$$

with

$K_{susp-water}$: suspended matter-water equilibrium distribution constant [mol.m$_{susp}^{-3}$/mol.m$_{water}^{-3}$] *(A)*
$FRwater_{susp}$: volume fraction of the water phase of suspended matter [-] *(A)*
Kp_{susp} : suspended matter-water partition coefficient [l$_{water}$.kg$_{solid}^{-1}$] *(I)*
$RHOsolid$: density of the solid phase [kg$_{solid}$.m$_{solid}^{-3}$] *(A)*
1000 : conversion factor [l.m$_{.3}$] *(C)*

$$K_{sed-water} = FRwater_{sed} + (1 - FRwater_{sed}) \, . \, Kp_{sed} \, . \, RHOsolid \, / \, 1000 \tag{78}$$

with

$K_{sed-water}$ sediment-water equilibrium distribution constant [mol.m$_{sed}^{-3}$/mol.m$_{water}^{-3}$] *(A)*
$FRwater_{sed}$: volume fraction of the water phase of sediment [-] *(A)*
Kp_{sed} : sediment-water partition coefficient [l$_{water}$.kg$_{solid}^{-1}$] *(I)*
$RHOsolid$: density of the solid phase [kg$_{solid}$.m$_{solid}^{-3}$] *(A)*
1000 : conversion factor [l.m$_{.3}$] *(C)*

$$K_{soil\,i-water} = FRwater_{soil} + FRsolid_{soil} \, . \, Kp_{soil,i} \, . \, RHOsolid \, / \, 1000 \tag{79}$$

with

$K_{soil\,i-water}$ soil-water equilibrium distribution constant [mol.m$_{soil}^{-3}$/mol.m$_{water}^{-3}$] *(A)*
$FRwater_{soil}$: volume fraction of the water phase of soil [-] *(A)*
$FRsolid_{soil}$: volume fraction of the solid phase of soil [-] *(A)*
$Kp_{soil\,i}$: soil-water partition coefficient [l$_{water}$.kg$_{solid}^{-1}$] *(I)*
$RHOsolid$: density of the solid phase [kg$_{solid}$.m$_{solid}^{-3}$] *(A)*
1000 : conversion factor [l.m$_{.3}$] *(C)*

The fraction of a chemical, present in the water phase of sediment and soil systems can be estimated on the basis of the equilibrium distribution constants and the fractions of the sub-phases:

$$FRdisslvd_{sed} = \frac{FRwater_{sed}}{K_{sed-water}} \tag{80}$$

with

$FRdisslvd_{sed}$: fraction of the chemical present in the water phase of the sediment [-] *(A)*
$FRwater_{sed}$: volume fraction of the water phase of the sediment [-] *(A)*
$K_{sed-water}$: sediment-water equilibrium distribution constant [mol.m$_{sed}^{-3}$/mol.m$_{water}^{-3}$] *(A)*

$$FRdisslvd_{soil} = \frac{FRwater_{soil}}{K_{soil\,1-water}} \tag{81}$$

with

$FRdisslvd_{soil}$: fraction of the chemical present in the water phase of the soil [-] *(A)*
$FRwater_{soil}$: volume fraction of the water phase of the soil [-] *(A)*
$K_{soil\,1-water}$: soil-water equilibrium distribution constant for soil 1 [mol.m$_{sed}^{-3}$/mol.m$_{water}^{-3}$] *(A)*

Bio-water

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

$$BCF_{fish} = \frac{FAT_{fish}}{FRwater_{bio} + (1 - FRwater_{bio}) \,.\, RHO_{solid} / 1000} \,.\, K_{ow} \tag{82}$$

with

BCF_{fish} : bioconcentration factor for fish [$l_{water}.kg_{fish}^{-1}$] *(A)*
FAT_{fish} : volume fraction of fat in fish [-] *(A)*
$FRwater_{bio}$: volume fraction of water in biota [-] *(A)*
$RHOsolid$: density of the solid phase [$kg_{solid}.m_{solid}^{-3}$] *(A)*
1000 : conversion factor [$l.m^{-3}$] *(C)*
K_{ow} : octanol-water partition coefficient of the chemical [-] *(A)*

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

$$FAT_{fish} = 5\ \% \tag{83}$$

with

FAT_{fish} : volume fraction of fat in fish [-] *(A)*

The bio-water equilibrium distribution constant may be derived from:

$$K_{bio-water} = BCF_{fish} \,.\, (FRwater_{bio} + (1 - FRwater_{bio}) \,.\, RHOsolid / 1000) \tag{84}$$

with

$K_{bio-water}$: biota-water equilibrium distribution constant [$mol.m_{bio}^{-3}/mol.m_{water}^{-3}$] *(A)*
BCF_{fish} : bioconcentration factor for fish [$l_{water}.kg_{fish}^{-1}$] *(A)*
$FRwater_{bio}$: volume fraction of water in biota [-] *(A)*
$RHOsolid$: density of the solid phase [$kg_{solid}.m_{solid}^{-3}$] *(A)*
1000 : conversion factor [$l.m^{-3}$] *(C)*

2.3 Mass balances

2.3.1 The air compartment

Mass balance

The mass balance equation for the air compartment is:

$$\begin{aligned} V_{air} \,.\, \frac{dC_{air}}{dt} = & + EMIS_{air} + IMP_{air} \\ & - FLOW_{air} \,.\, C_{air} - V_{air} \,.\, DEG_{air} \,.\, C_{air} \\ & - DEP_{water} \,.\, C_{air} - DEP_{soil\,1} \,.\, C_{air} - DEP_{soil\,2} \,.\, C_{air} - DEP_{soil\,3} \,.\, C_{air} \\ & - XCH_{air-water} \,.\, C_{air} - XCH_{air-soil\,1} \,.\, C_{air} - XCH_{air-soil\,2} \,.\, C_{air} - XCH_{air-soil\,3} \,.\, C_{air} \\ & + XCH_{water-air} \,.\, C_{water} + \Sigma XCH_{soil\,i-air} \,.\, C_{soil\,i} \end{aligned} \tag{85}$$

with

V_{air} : volume of the air compartment [m_{air}^{3}] *(I)*
C_{air} : total concentration in air (gas phase + aerosol phase + rain water phase) [$mol.m_{air}^{-3}$] *(S)*
t : time [s] *(S)*
$EMIS_{air}$: emission mass flow into the air compartment [$mol.s^{-1}$] *(I)*
IMP_{air} : import mass flow into air [$mol.s^{-1}$] *(I)*
$FLOW_{air}$: refreshment flow through the air compartment [$m_{air}^{3}.s^{-1}$] *(I)*
DEG_{air} : pseudo first order transformation rate constant in air [s^{-1}] *(I)*
DEP_{water} : transport coefficient for atmospheric deposition (wet and dry) to water [$m_{air}^{3}.s^{-1}$] *(I)*

$DEP_{soil\,1}$: transport coefficient for atmospheric deposition (wet and dry) to soil 1 [$m_{air}^3.s^{-1}$] *(I)*
$DEP_{soil\,2}$: transport coefficient for atmospheric deposition (wet and dry) to soil 2 [$m_{air}^3.s^{-1}$] *(I)*
$DEP_{soil\,3}$: transport coefficient for atmospheric deposition (wet and dry) to soil 3 [$m_{air}^3.s^{-1}$] *(I)*
$XCH_{air\text{-}water}$: transport coefficient gas absorption to water [$m_{air}^3.s^{-1}$] *(I)*
$XCH_{air\text{-}soil\,1}$: transport coefficient gas absorption to soil 1 [$m_{air}^3.s^{-1}$] *(I)*
$XCH_{air\text{-}soil\,2}$: transport coefficient gas absorption to soil 2 [$m_{air}^3.s^{-1}$] *(I)*
$XCH_{air\text{-}soil\,3}$: transport coefficient gas absorption to soil 3 [$m_{air}^3.s^{-1}$] *(I)*
$XCH_{water\text{-}air}$: transport coefficient volatilization from water [$m_{water}^3.s^{-1}$] *(I)*
C_{water} : concentration in water (dissolved) [$mol.m_{water}^{-3}$] *(S)*
$XCH_{soil\,i\text{-}air}$: transport coefficient volatilization from soil i [$m_{soil}^3.s^{-1}$] *(I)*
$C_{soil\,i}$: concentration in soil i [$mol.m_{soil}^{-3}$] *(S)*

Emission

The emission mass flow to air is obtained from:

$$EMIS_{air} = Edirect_{air} + Estp_{air} \tag{86}$$

with

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

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

$$Edirect_{air} = PRODUCTION \,.\, EMISfact_{air} \tag{87}$$

with

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

$$Estp_{air} = STPload \,.\, ACTIVEtime \,.\, FR_{volatstp} \tag{88}$$

with

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

The following defaults may be considered:

$$PRODUCTION = 1 mg.inh^{-1}.d^{-1} = (10^{-6}/MOL\ WEIGHT) \,.\, (24.3600) \,.\, POPULATION \tag{89}$$

with

$PRODUCTION$: total amount produced or imported in the system [$mol.s^{-1}$] *(A)*
$MOL\ WEIGHT$: molecular weight of the chemical [$kg.mol^{-1}$] *(A)*
24·3600 : conversion factor [$s.d^{-1}$]
$POPULATION$: total population of the system [inh] *(A)*

as a starting point;

$$EMISfact_{air} = 0.1\ \% \tag{90}$$

with

$EMISfact_{air}$: emission factor for air: the fraction of the production volume that is released to the air compartment [-] *(A)* as a starting point;

$$STPload = PRODUCTION \,.\, EMISfact_{water} \tag{91}$$

with

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

as a starting point;

$$EMISfact_{water} = 0.1\ \% \tag{92}$$

with

EMISfact$_{water}$: emission factor for water: the fraction of the production volume that is released to the water compartment [-] *(A)*

as a starting point;

$$ACTIVEtime = 365\, d.yr^{-1} = 1 \tag{93}$$

with

ACTIVEtime : fraction of the time that the sewage treatment plant is loaded with the chemical [-] *(A)*

assuming continuous activity;

$$FR_{volatstp} = 0.1 \tag{94}$$

with

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

as a starting point.

Import

The import mass flow into air is obtained from:

$$IMP_{air} = IMPORT_{air} \tag{95}$$

with

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

A value for *IMPORT*$_{air}$ may be derived as follows:

$$IMPORT_{air} = AIRinflow \,.\, CONCimp_{air} \tag{96}$$

with

IMPORT$_{air}$: transport of the chemical with air (wind) across the system boundaries [mol.s^{-1}] *(D)*
AIRinflow : rate of air flow across the system boundaries [$m_{air}^3.s^{-1}$] *(A)*
CONCimp$_{air}$: concentration of the chemical in the imported air [mol.m_{air}^{-3}] *(A)*

AIRinflow may be estimated as:

$$AIRinflow = \frac{VOLUME_{air}}{TAU_{air}} \tag{97}$$

with

AIRinflow : rate of air flow across the system boundaries into the system [$m_{air}^3.s^{-1}$] *(A)*
VOLUME$_{air}$: volume of the air compartment [m^3] *(D)*
TAU$_{air}$: residence time of air in the system [s] *(D)*

It should be noted that *AIRinflow* is an auxiliary parameter that is meant to be used for estimating the import mass flow of the chemical. The significance of this is that *AIRinflow* can be set to a value that serves this purpose more realistically than the ratio of volume and residence time. The export mass flow is always computed from equation (97), on the basis of the ratio of the definition parameters $VOLUME_{air}$ and TAU_{air}, no matter the value of *AIRinflow*.

For the concentration in air at the system boundary, the following default may be considered:

$$CONCimp_{air} = STND_{air} \tag{98}$$

with

$CONCimp_{air}$: concentration of the chemical in the imported air [mol.m_{air}^{-3}] *(A)*
$STND_{air}$: quality standard for air [mol.m_{air}^{-3}] *(D)*

Export

The export mass flow from air is obtained from:

$$EXP_{air} = FLOW_{air} \,.\, C_{air} \tag{99}$$

with

EXP_{air} : export mass flow from the air compartment [mol.s^{-1}] *(I)*
$FLOW_{air}$: refreshment flow through the air compartment [$m_{air}^{3}.s^{-1}$] *(I)*
C_{air} : total concentration in air (gas phase + aerosol phase + rain water phase) [mol.m_{air}^{-3}] *(S)*

$$FLOW_{air} = VOLUME_{air} / TAU_{air} \tag{100}$$

with

$FLOW_{air}$: refreshment flow through the air compartment [$m_{air}^{3}.s^{-1}$] *(I)*
$VOLUME_{air}$: volume of the air compartment [m^3] *(D)*
TAU_{air} : residence time of air in the system [s] *(D)*

Degradation

The apparent degradation mass flow from air is obtained from:

$$DEGRD_{air} = V_{air} \,.\, DEG_{air} \,.\, C_{air} \tag{101}$$

with

$DEGRD_{air}$: degradation mass flow from the air compartment [mol.s^{-1}] *(I)*
V_{air} : volume of the air compartment [m^3] *(I)*
DEG_{air} : pseudo first order transformation rate constant in air [s^{-1}] *(I)*
C_{air} : total concentration in air (gas phase + aerosol phase + rain water phase) [mol.m_{air}^{-3}] *(S)*

$$DEG_{air} = kdeg_{air} \tag{102}$$

with

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

A value for $kdeg_{air}$ may be obtained as follows:

$$kdeg_{air} = (1 - FRass_{aerosol}) \,.\, krad_{OH} \tag{103}$$

with

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

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

$$krad_{OH} = \frac{\ln 2}{160}\ d^{-1} \tag{104}$$

with

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

may be taken as a minimum reactivity.

Advective transport

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

$$ADV_{air-water} = DEP_{water} \,.\, C_{air} \tag{105}$$

with

$ADV_{air\text{-}water}$: advective mass flow from air to water by atmospheric deposition [mol.s^{-1}] *(I)*
DEP_{water} : transport coefficient for atmospheric deposition (wet and dry) to water [m$_{air}^{3}$.s^{-1}] *(I)*
C_{air} : total concentration in air (gas phase + aerosol phase + rain water phase) [mol.m$_{air}^{-3}$] *(S)*

$$ADV_{air-soil\,i} = DEP_{soil\,i} \,.\, C_{air} \tag{106}$$

with

$ADV_{soil\,i}$: advective mass flow from air to soil i by atmospheric deposition [mol.s^{-1}] *(I)*
$DEP_{soil\,i}$: transport coefficient for atmospheric deposition (wet and dry) to soil i [m$_{air}^{3}$.s^{-1}] *(I)*
C_{air} : total concentration in air (gas phase + aerosol phase + rain water phase) [mol.m$_{air}^{-3}$] *(S)*

$$DEP_{water} = (DRYDEP_{aerosol} + WASHOUT) \,.\, SYSTEMAREA \,.\, AREAFRAC_{water} \tag{107}$$

with

DEP_{water} : transport coefficient for atmospheric deposition (wet and dry) to water [m$_{air}^{3}$.s^{-1}] *(I)*
$DRYDEP_{aerosol}$: mass transfer coefficient for dry deposition of aerosol-associated chemical [m$_{air}$.s^{-1}] *(D)*
$WASHOUT$: mass transfer coefficient for wet atmospheric deposition [m$_{air}$.s^{-1}] *(D)*
$SYSTEMAREA$: total area of the system (air/water + air/soil interfaces) [m^{2}] *(D)*
$AREAFRAC_{water}$: fraction of the system area that is water [-] *(D)*

$$DEP_{soil\,i} = (DRYDEP_{aerosol} + WASHOUT) \,.\, SYSTEMAREA \,.\, AREAFRAC_{soil\,i} \tag{108}$$

with

$DEP_{soil\,i}$: transport coefficient for atmospheric deposition (wet and dry) to soil i [m$_{air}^{3}$.s^{-1}] *(I)*
$DRYDEP_{aerosol}$: mass transfer coefficient for dry deposition of aerosol-associated chemical [m$_{air}$.s^{-1}] *(D)*
$WASHOUT$: mass transfer coefficient for wet atmospheric deposition [m$_{air}$.s^{-1}] *(D)*
$SYSTEMAREA$: total area of the system (air/water + air/soil interfaces) [m^{2}] *(D)*
$AREAFRAC_{soil\,i}$: fraction of the system area that is soil i [-] *(D)*

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

$$DRYDEP_{aerosol} = AEROSOLDEPRATE \,.\, FRass_{aerosol} \tag{109}$$

with

$DRYDEP_{aerosol}$: mass transfer coefficient for dry deposition of aerosol-associated chemical [m$_{air}$.s^{-1}] *(D)*
$AEROSOLDEPRATE$: deposition velocity of the aerosol particles with which the chemical is associat-

ed [$m.s^{-1}$] *(A)*

$FRass_{aerosol}$: fraction of the chemical in air that is associated with aerosol particles [-] *(A)*

$$WASHOUT = RAINRATE \, . \, SCAVratio \tag{110}$$

with

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

Diffusive transport

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

$$DIFF_{air-water} = XCH_{air-water} \, . \, C_{air} \tag{111}$$

with

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

$$DIFF_{air-soil\,i} = XCH_{air-soil\,i} \, . \, C_{air} \tag{112}$$

with

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

$$XCH_{air-water} = GASABS_{water} \, . \, SYSTEMAREA \, . \, AREAFRAC_{water} \tag{113}$$

with

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

$$XCH_{air-soil\,i} = GASABS_{soil\,i} \, . \, SYSTEMAREA \, . \, AREAFRAC_{soil\,i} \tag{114}$$

with

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

The volatilization mass flows are obtained from:

$$DIFF_{water-air} = XCH_{water-air} \, . \, C_{water} \tag{115}$$

with

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

$$DIFF_{soil\,i-air} = XCH_{soil\,i-air} \, . \, C_{soil\,i} \tag{116}$$

with

$DIFF_{soil\,i-air}$: diffusive mass flow from soil i to air by volatilization [$mol.s^{-1}$] *(I)*

$XCH_{soil\,i\text{-}air}$: transport coefficient for volatilization from soil i [$m_{soil}^3.s^{-1}$] *(I)*
$C_{soil\,i}$: total concentration in soil i (gas phase + water phase + solid phase) [$mol.m_{soil}^{-3}$] *(S)*

$$XCH_{water\text{-}air} = VOLAT_{water} \,.\, SYSTEMAREA \,.\, AREAFRAC_{water} \tag{117}$$

with

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

$$XCH_{soil\,i\text{-}air} = VOLAT_{soil\,i} \,.\, SYSTEMAREA \,.\, AREAFRAC_{soil\,i} \tag{118}$$

with

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

Values for the overall mass transfer coefficients for gas absorption and volatilization may be estimated using the classical two-film resistance model. In the case of transport across the air-water interface, the overall transfer coefficients follow from summation of the resistances at the water- and air sides of the interface. In the case of transport across the air-soil interface, the soil-side of the interface is treated as a pair of parallel resistances (air phase and water phase of the soil). The following equations may be used:

$$GASABS_{water} = \frac{kaw_{air} \,.\, kaw_{water}}{kaw_{air} \,.\, K_{air-water} + kaw_{water}} \,.\, (1 - FRass_{aerosol}) \tag{119}$$

with

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

$$GASABS_{soil} = \frac{kasl_{air} \,.\, kasl_{soilair} + kasl_{air} \,.\, kasl_{soilwater} / K_{air-water}}{kasl_{air} + kasl_{soilair} + kasl_{soilwater} / K_{air-water}} \,.\, (1 - FRass_{aerosol}) \tag{120}$$

with

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

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

$$VOLAT_{water} = \frac{GASABS_{water}}{1 - FRass_{aerosol}} \cdot K_{air-water} \tag{121}$$

with

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

$$VOLAT_{soil\,i} = \frac{GASABS_{soil\,i}}{1 - FRass_{aerosol}} \cdot \frac{K_{air-water}}{K_{soil\,i-water}} \tag{122}$$

with

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

A value for the partial mass transfer coefficient at the air-side of the air-water interface may be derived from Southworth's equation (Lyman *et al.*, 1982):

$$kaw_{air} = 3.16.10^{-3} . WINDSPEED . \sqrt{\frac{0.018}{MOL\ WEIGHT}} \tag{123}$$

with

kaw_{air} : partial mass transfer coefficient at the air side of the air-water interface [$m_{air}.s^{-1}$] *(A)*
$WINDSPEED$: average windspeed at 10 m above the surface [$m.s^{-1}$] *(A)*
$MOL\ WEIGHT$: molecular weight of the chemical [$kg.mol^{-1}$] *(A)*
$3.16 \cdot 10^{-3}$: proportionality constant *(C)*
0.018 : molecular weight of water *(C)*

Alternatively, following the example of Mackay *et al.* (1992), a fixed value may be chosen for all chemicals and all circumstances:

$$kaw_{air} = 1.39.10^{-3}\,m.s^{-1} \tag{124}$$

with

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

For the partial mass transfer coefficient at the water side of the air-water interface, Cohen's recipe (Lyman *et al.*, 1982) may be used:

$$\begin{aligned} kaw_{water} = &+7.10^{-6}\,m.s^{-1} \quad \textit{if} \quad WINDSPEED < 3\ m.s^{-1} \\ &+5.10^{-5}\,m.s^{-1} \quad \textit{if} \quad 3\,m.s^{-1} < WINDSPEED < 10\,m.s^{-1} \\ &+1.10^{-4}\,m.s^{-1} \quad \textit{if} \quad WINDSPEED > 10\,m.s^{-1} \end{aligned} \tag{125}$$

with

kaw_{water} : partial mass transfer coefficient at the water-side of the air-water interface [$m_{water}.s^{-1}$] *(A)*
$WINDSPEED$: average windspeed at 10 m above the surface [$m.s^{-1}$] *(A)*

Or, after Mackay *et al.* (1992), a fixed value may be preferred:

$$kaw_{water} = 1.39.10^{-5}\,m.s^{-1} \tag{126}$$

with

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

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

$$kasl_{air} = kaw_{air} \tag{127}$$

with

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

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

$$kasl_{soilair} = 5.56.10^{-6}\,m.s^{-1} \tag{128}$$

with

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

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

$$kasl_{soilwater} = 5.56.10^{-10}\,m.s^{-1} \tag{129}$$

with

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

2.3.2 The water compartment

Mass balance

The mass balance equation for the water compartment is:

$$\begin{aligned}
V_{water}.\frac{dC_{water}}{dt} = & + EMIS_{water} + IMP_{water} \\
& - FLOW_{water}.C_{water} - V_{water}.DEG_{water}.C_{water} \\
& + DEP_{water}.C_{air} + \Sigma RUN\text{-}OFF_{soil\,i}.C_{soil\,i} \\
& - XCH_{water-air}.C_{water} - XCH_{water-susp}.C_{water} - XCH_{water-bio}.C_{water} - XCH_{water-sed}.C_{water} \\
& + XCH_{air-water}.C_{air} + XCH_{susp-water}.C_{susp} + XCH_{bio-water}.C_{bio} + XCH_{sed-water}.C_{sed}
\end{aligned} \tag{130}$$

with

V_{water} : volume of the water compartment [m_{water}^3] *(I)*
C_{water} : concentration in water (dissolved) [$mol.m_{water}^{-3}$] *(S)*
t : time [s] *(S)*

$EMIS_{water}$: emission to the water compartment [mol.s^{-1}] *(I)*
IMP_{water} : import in water [mol.s^{-1}] *(I)*
$FLOW_{water}$: refreshment flow through the water compartment [m$_{water}^{3}$.s^{-1}] *(I)*
DEG_{water} : pseudo first order transformation rate constant in water [s^{-1}] *(I)*
DEP_{water} : transport coefficient for atmospheric deposition (wet and dry) to water [m$_{air}^{3}$.s^{-1}] *(I)*
$RUN\text{-}OFF_{soil\,i}$: transport coefficient for run off from soil i to water [m$_{soil}^{3}$.s^{-1}] *(I)*
$C_{soil\,i}$: concentration in soil i [mol.m$_{soil}^{-3}$] *(S)*
$XCH_{water\text{-}air}$: transport coefficient for volatilization from water [m$_{water}^{3}$.s^{-1}] *(I)*
$XCH_{water\text{-}susp}$: transport coefficient for adsorption to suspended matter [m$_{water}^{3}$.s^{-1}] *(I)*
$XCH_{water\text{-}bio}$: transport coefficient for biosorption to biota [m$_{water}^{3}$.s^{-1}] *(I)*
$XCH_{water\text{-}sed}$: transport coefficient for uptake by sediment [m$_{water}^{3}$.s^{-1}] *(I)*
$XCH_{air\text{-}water}$: transport coefficient for gas absorption from air [m$_{air}^{3}$.s^{-1}] *(I)*
C_{air} : concentration in air [mol.m$_{air}^{-3}$] *(S)*
$XCH_{susp\text{-}water}$: transport coefficient for desorption from suspended matter [m$_{susp}^{3}$.s^{-1}] *(I)*
C_{susp} : concentration in suspended matter [mol.m$_{susp}^{-3}$] *(S)*
$XCH_{bio\text{-}water}$: transport coefficient for elimination from biota [m$_{bio}^{3}$.s^{-1}] *(I)*
C_{bio} : concentration in biota [mol.m$_{bio}^{-3}$] *(S)*
$XCH_{sed\text{-}water}$: transport coefficient for release from sediment [m$_{sed}^{3}$.s^{-1}] *(I)*
C_{sed} : concentration in sediment [mol.m$_{sed}^{-3}$] *(S)*

Emissions

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

$$EMIS_{water} = Edirect_{water} + Estp_{water} \tag{131}$$

with

$EMIS_{water}$: total emission mass flow into the water compartment [mol.s^{-1}] *(I)*
$Edirect_{water}$: sum of all direct emissions to the water compartment [mol.s^{-1}] *(D)*
$Estp_{water}$: indirect emission to water with effluent from sewage treatment [mol.s^{-1}] *(D)*

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

$$Edirect_{water} = PRODUCTION \,.\, EMISfact_{water} \tag{132}$$

with

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

$$Estp_{water} = ACTIVEtime \,.\, EFFLUENT_{stp} \,.\, CONCstp_{water} \tag{133}$$

with

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

$$CONCstp_{water} = \frac{STPload \,.\, FR_{effstp}}{EFFLUENT_{stp} \,.\, (1 + Kp_{susp} \,.\, SUSPeff_{stp} / 1000)} \tag{134}$$

with

$CONCstp_{water}$: concentration of the chemical, dissolved in STP-effluent [mol.m$_{water}^{-3}$] *(A)*
$STPload$: load of the sewage treatment plant during release episodes [mol.s^{-1}] *(A)*
FR_{effstp} : fraction of the load that is rerouted to the water compartment with effluent (water + particles) upon sewage treatment [-] *(A)*
$EFFLUENT_{stp}$: amount of STP-effluent discharged into the water compartment [m$_{water}^{3}$.s^{-1}] *(A)*
Kp_{susp} : suspended matter-water partition coefficient [l$_{water}$.kg$_{solid}^{-1}$] *(A)*

$SUSPeff_{stp}$: concentration of suspended matter in STP-effluents $[kg_{solid}.m_{eff}^{-3}]$ *(A)*
1000 : conversion factor $[l.m^{-3}]$ *(C)*

In addition to the values mentioned earlier in equations (89), (91), (92) and (93), by default, the following values may be considered as starting points:

$$\boldsymbol{EFFLUENT_{stp} = STPcapacity\,.\,0.15} \tag{135}$$

with

$EFFLUENT_{stp}$: amount of STP-effluent discharged into the water compartment $[m_{water}^{3}.s^{-1}]$ *(A)*
$STPcapacity$: total capacity of all sewage treatment plants in the system [eq] *(A)*
0.15 : sewage production $[m_{water}^{3}.eq^{-1}]$ *(C)*

$$\boldsymbol{FR_{effstp} = 0.2} \tag{136}$$

with

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

$$\boldsymbol{SUSPeff_{stp} = 40\,mg\,.\,l^{-1}} \tag{137}$$

with

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

Import

The import mass flow into water is obtained from:

$$\boldsymbol{IMP_{water} = IMPORT_{water}} \tag{138}$$

with

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

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

$$\boldsymbol{IMPORT_{water} = WATERinflow\,.\,CONCimp_{water}} \tag{139}$$

with

$IMPORT_{water}$: transport of the chemical with water across the system boundaries $[mol.s^{-1}]$ *(D)*
$WATERinflow$: rate of water flow across the system boundaries $[m_{water}^{3}.s^{-1}]$ *(A)*
$CONCimp_{water}$: concentration of the chemical in the imported water $[mol.m_{water}^{-3}]$ *(A)*

By default, a value for $WATERinflow$ may be taken as:

$$\boldsymbol{WATERinflow = STREAMS} \tag{140}$$

with

$WATERinflow$: rate of water flow across the system boundaries into the system $[m_{water}^{3}.s^{-1}]$ *(A)*
$STREAMS$: sum of the discharges of all streams crossing the system boundaries $[m_{water}^{3}.s^{-1}]$ *(A)*

and $CONCimp_{water}$ as:

$$\boldsymbol{CONCimp_{water} = STND_{water}} \tag{141}$$

with

$CONCimp_{water}$: concentration of the chemical in the imported water $[mol.m_{water}^{-3}]$ *(A)*
$STND_{water}$: quality standard for water $[mol.m_{water}^{-3}]$ *(D)*

Export

The export mass flow from water is obtained from:

$$EXP_{water} = FLOW_{water} \cdot C_{water} \tag{142}$$

with

EXP_{water} : export mass flow from the water compartment [mol.s^{-1}] *(I)*
$FLOW_{water}$: refreshment flow through the water compartment [m$_{water}^{3}$.s^{-1}] *(I)*
C_{water} : dissolved concentration in water [mol.m$_{water}^{-3}$] *(S)*

$$FLOW_{water} = VOLUME_{water} / TAU_{water} \tag{143}$$

with

$FLOW_{water}$: refreshment flow through the water compartment [m$_{water}^{3}$.s^{-1}] *(I)*
$VOLUME_{water}$: volume of the water compartment [m^3] *(D)*
TAU_{water} : residence time of water in the system [s] *(D)*

Degradation

The apparent degradation mass flow from water is obtained from:

$$DEGRD_{water} = V_{water} \cdot DEG_{water} \cdot C_{water} \tag{144}$$

with

$DEGRD_{water}$: degradation mass flow from the water compartment [mol.s^{-1}] *(I)*
V_{water} : volume of the water compartment [m$_{water}^{3}$] *(I)*
DEG_{water} : pseudo first order transformation rate constant in water [s^{-1}] *(I)*
C_{water} : dissolved concentration in water [mol.m$_{water}^{-3}$] *(S)*

$$DEG_{water} = kdeg_{water} \tag{145}$$

with

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

A value for $kdeg_{water}$ may be obtained by means of the scaling procedure proposed by Struijs and Van den Berg (1993). This procedure assumes that the pseudo first order rate constant for degradation in water is proportional to the concentration of bacteria in the water. The rate constant for surface water may be deduced from the rate constant observed in laboratory tests by scaling:

$$kdeg_{water} = kdeg_{test} \cdot \frac{BACT_{water}}{BACT_{test}} \tag{146}$$

with

$kdeg_{water}$: pseudo first order degradation rate constant in water [s^{-1}] *(D)*
$kdeg_{test}$: pseudo first order degradation rate constant in laboratory test [s^{-1}] *(A)*
$BACT_{water}$: concentration of bacteria in the water compartment [cfu.ml$_{water}^{-1}$] *(A)*
$BACT_{test}$: concentration of bacteria in the laboratory test water [cfu.ml$_{test\ water}^{-1}$] *(A)*

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

$$kdeg_{test} = \frac{\ln 2}{5}\ d^{-1} \quad if \quad PASSreadytest = y$$
$$kdeg_{test} = \frac{\ln 2}{1000}\ d^{-1} \quad if \quad PASSreadytest = n \tag{147}$$

with

$kdeg_{test}$: pseudo first order degradation rate constant in laboratory test [d^{-1}] *(A)*

PASSreadytest : the result of a standard screening test; expressed as "y" if the chemical is "readily biodegradable" and "n" if the chemical is not "readily biodegradable"

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

$$BACT_{test} = 4.10^{4}\ cfu.ml^{-1} \tag{148}$$

with

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

$$BACT_{water} = 4.10^{4}\ cfu.ml^{-1} \tag{149}$$

with

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

Advective transport

Advective transport from air to water takes place by wet and dry atmospheric deposition, as described in paragraph 2.3.1. See equations (105), (107), (109) and (110).

Advective transport from soil to water by run-off is described in paragraph 2.3.6, equations (211)-(213).

Diffusive transport

Diffusive transport between air and water takes place by gas absorption and volatilization. The formulas for this have been given in paragraph 2.3.1, equations (111), (113), (115), (117), (119), (121), (123)-(126).

Diffusive transport between water and suspended particles by means of adsorption and desorption is described in paragraph 2.3.3, equations (163)-(169).

Diffusive transport between water and aquatic organisms by means of passive uptake and elimination is described in paragraph 2.3.4, equations (171)-(177).

Diffusive transport across the sediment-water interface by means of adsorption and desorption is described in paragraph 2.3.5, equations (185)-(192).

2.3.3 The suspended matter compartment

Mass balance

The mass balance equation for the suspended matter compartment is:

$$
\begin{aligned}
V_{susp} \cdot \frac{dC_{susp}}{dt} = & + EMIS_{susp} + IMP_{susp} \\
& - FLOW_{susp} \cdot C_{susp} \\
& - SEDIMENTATION \cdot C_{susp} \\
& + RESUSPENSION \cdot C_{sed} \\
& - XCH_{susp\text{-}water} \cdot C_{susp} \\
& + XCH_{water\text{-}susp} \cdot C_{water}
\end{aligned}
\qquad (150)
$$

with

V_{susp} : volume of the suspended matter compartment $[\mathrm{m}_{susp}^{3}]$ *(I)*
C_{susp} : concentration in suspended matter $[\mathrm{mol.m}_{susp}^{-3}]$ *(S)*
t : time [s] *(S)*
$EMIS_{susp}$: emission to the suspended matter compartment $[\mathrm{mol.s}^{-1}]$ *(I)*
IMP_{susp} : import in the suspended matter water compartment $[\mathrm{mol.s}^{-1}]$ *(I)*
$FLOW_{susp}$: refreshment flow through compartment suspended matter compartment $[\mathrm{m}_{susp}^{3}.\mathrm{s}^{-1}]$ *(I)*
$SEDIMENTATION$: transport coefficient for sedimentation $[\mathrm{m}_{susp}^{3}.\mathrm{s}^{-1}]$ *(I)*
C_{sed} : concentration in sediment $[\mathrm{mol.m}_{sed}^{-3}]$ *(S)*
$RESUSPENSION$: transport coefficient for resuspension $[\mathrm{m}_{sed}^{3}.\mathrm{s}^{-1}]$ *(I)*
$XCH_{susp\text{-}water}$: transport coefficient for desorption from suspended matter $[\mathrm{m}_{susp}^{3}.\mathrm{s}^{-1}]$ *(I)*
$XCH_{water\text{-}susp}$: transport coefficient for adsorption to suspended matter $[\mathrm{m}_{water}^{3}.\mathrm{s}^{-1}]$ *(I)*
C_{water} : concentration in water $[\mathrm{mol.m}_{water}^{-3}]$ *(S)*

Emission

The emission mass flow to suspended matter is obtained from:

$$
EMIS_{susp} = Estp_{susp} \qquad (151)
$$

with

$EMIS_{susp}$: total emission mass flow into the suspended matter compartment $[\mathrm{mol.s}^{-1}]$ *(I)*
$Estp_{susp}$: indirect emission to suspended matter with particulate matter present in effluent of sewage treatment $[\mathrm{mol.s}^{-1}]$ *(D)*

$Estp_{susp}$ may be derived by means of:

$$
Estp_{susp} = ACTIVEtime \cdot EFFLUENT_{stp} \cdot \frac{SUSPeff_{stp}}{(1 - FRwater_{susp}) \cdot RHOsolid} \cdot \frac{CONCstp_{susp} \cdot K_{susp\text{-}water}}{Kp_{susp} / 1000} \qquad (152)
$$

with

$Estp_{susp}$: indirect emission to suspended matter with particulate matter present in effluent of sewage treatment $[\mathrm{mol.s}^{-1}]$ *(D)*
$ACTIVEtime$: fraction of the time that the sewage treatment plant is loaded with the chemical [-] *(A)*
$EFFLUENT_{stp}$: amount of STP-effluent discharged into the water compartment $[\mathrm{m}_{water}^{3}.\mathrm{s}^{-1}]$ *(A)*
$SUSPeff_{stp}$: concentration of particulate matter present in STP-effluent $[\mathrm{kg}_{solid}.\mathrm{m}_{water}^{-3}]$ *(A)*
$FRwater_{susp}$: volume fraction water of suspended matter [-] *(A)*
$RHOsolid$: density of the solid phase of suspended matter $[\mathrm{kg.m}^{-3}]$ *(A)*
$CONCstp_{susp}$: concentration of the chemical in suspended particles of STP-effluent $[\mathrm{mol.kg}_{solid}^{-1}]$ *(A)*
$K_{susp\text{-}water}$: suspended matter-water equilibrium distribution constant $[\mathrm{mol.m}_{susp}^{-3}/\mathrm{mol.m}_{water}^{-3}]$ *(A)*
Kp_{susp} : suspended matter-water partition coefficient $[\mathrm{l}_{water}.\mathrm{kg}_{solid}^{-1}]$ *(A)*
1000 : conversion factor $[\mathrm{l.m}_{-3}]$ *(C)*

$$CONCstp_{susp} = CONCstp_{water} \cdot \frac{Kp_{susp-water}}{1000} \tag{153}$$

with

$CONCstp_{susp}$: concentration of the chemical in suspended particles of STP-effluent [$mol.kg_{solid}^{-1}$] *(A)*
$CONCstp_{water}$: concentration of the chemical, dissolved in STP-effluent [$mol.m_{water}^{-3}$] *(A)*
$Kp_{susp-water}$: suspended matter-water partition coefficient [$l_{water}.kg_{solid}^{-1}$]
1000 : conversion factor [$l.m^{-3}$] *(C)*

Import

The import mass flow into the suspended matter compartment is obtained from:

$$IMP_{susp} = IMPORT_{susp} \tag{154}$$

with

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

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

$$IMPORT_{susp} = WATERinflow \cdot \frac{SUSP_{import}}{(1 - FRwater_{susp}) \cdot RHOsolid} \cdot \frac{CONCimp_{susp} \cdot K_{susp-water}}{Kp_{susp} / 1000} \tag{155}$$

with

$IMPORT_{susp}$: transport of the chemical, associated with suspended particles in water across the system boundaries [$mol.s^{-1}$] *(D)*
$WATERinflow$: rate of water flow across the system boundaries [$m_{water}^{3}.s^{-1}$] *(A)*
$SUSP_{import}$: concentration of particulate matter present in "imported" water [$kg_{solid}.m_{water}^{-3}$] *(A)*
$FRwater_{susp}$: volume fraction water of suspended matter [-] *(A)*
$RHOsolid$: density of the solid phase of suspended matter [$kg.m^{-3}$] *(A)*
$CONCstp_{susp}$: concentration of the chemical in suspended particles of STP-effluent [$mol.kg_{solid}^{-1}$] *(A)*
$K_{susp-water}$: suspended matter-water equilibrium distribution constant [$mol.m_{susp}^{-3}/mol.m_{water}^{-3}$] *(A)*
Kp_{susp} : suspended matter-water partition coefficient [$l_{water}.kg_{solid}^{-1}$] *(A)*
1000 : conversion factor [$l.m^{-3}$] *(C)*

$$CONCimp_{susp} = CONCimp_{water} \cdot \frac{Kp_{susp-water}}{1000} \tag{156}$$

with

$CONCimp_{susp}$: concentration of the chemical in the imported suspended particles [$mol.kg_{susp}^{-1}$] *(A)*
$CONCimp_{water}$: concentration of the chemical in the imported water [$mol.m_{water}^{-3}$] *(A)*
$Kp_{susp-water}$: suspended matter-water partition coefficient [$l_{water}.kg_{solid}^{-1}$]
1000 : conversion factor [$l.m^{-3}$] *(C)*

Export

The export mass flow from the suspended matter compartment is obtained from:

$$EXP_{susp} = FLOW_{susp} \cdot C_{susp} \tag{157}$$

with

EXP_{susp} : export mass flow from the suspended matter compartment [$mol.s^{-1}$] *(I)*
$FLOW_{susp}$: refreshment flow through the suspended matter compartment [$m_{susp}^{3}.s^{-1}$] *(I)*
C_{susp} : concentration in suspended particles [$mol.m_{susp}^{-3}$] *(S)*

$$FLOW_{susp} = \frac{VOLUME_{susp}}{TAU_{water}} \tag{158}$$

with

$FLOW_{susp}$: refreshment flow through the suspended matter compartment $[m_{susp}^3.s^{-1}]$ *(I)*
$VOLUME_{susp}$: volume of the suspended matter compartment $[m^3]$ *(D)*
TAU_{water} : residence time of water (and suspended matter) in the system [s] *(D)*

Degradation

Degradation is modeled as taking place in the water phase only.

Advective transfer

Advective mass flows between the suspended matter compartment and sediment compartment by means of sedimentation and resuspension are obtained from:

$$ADV_{susp\text{-}sed} = SEDIMENTATION \,.\, C_{susp} \tag{159}$$

with

$ADV_{susp\text{-}sed}$: advective mass flow suspended matter to sediment by sedimentation $[mol.s^{-1}]$ *(I)*
$SEDIMENTATION$: transport coefficient for sedimentation $[m_{susp}^3.s^{-1}]$ *(I)*
C_{susp} : concentration in suspended matter $[mol.m_{susp}^{-3}]$ *(S)*

$$SEDIMENTATION = GROSSsedrate \,.\, \frac{1 - FRwater_{sed}}{1 - FRwater_{susp}} \,.\, SYSTEMAREA \,.\, AREAFRAC_{water} \tag{160}$$

with

$SEDIMENTATION$: transport coefficient for sedimentation $[m_{susp}^3.s^{-1}]$ *(I)*
$GROSSsedrate$: gross sedimentation rate $[m_{sed}.s^{-1}]$ *(A)*
$FRwater_{sed}$: volume fraction of the water phase of the sediment [-] *(A)*
$FRwater_{susp}$: volume fraction water of suspended matter [-] *(A)*
$SYSTEMAREA$: total area of the system (air/water + air/soil interfaces) $[m^2]$ *(D)*
$AREAFRAC_{water}$: fraction of the system area that is water [-] *(D)*

$$ADV_{sed\text{-}susp} = RESUSPENSION \,.\, C_{sed} \tag{161}$$

with

$ADV_{sed\text{-}susp}$: advective mass flow from sediment to suspended matter by resuspension $[mol.s^{-1}]$ *(I)*
$RESUSPENSION$: transport coefficient for resuspension $[m_{sed}^3.s^{-1}]$ *(I)*
C_{sed} : concentration in sediment matter $[mol.m_{sed}^{-3}]$ *(S)*

$$RESUSPENSION = RESUSPrate \,.\, SYSTEMAREA \,.\, AREAFRAC_{water} \tag{162}$$

with

$RESUSPENSION$: transport coefficient for resuspension $[m_{sed}^3.s^{-1}]$ *(I)*
$RESUSPrate$: resuspension rate $[m_{sed}.s^{-1}]$ *(A)*
$SYSTEMAREA$: total area of the system (air/water + air/soil interfaces) $[m^2]$ *(D)*
$AREAFRAC_{water}$: fraction of the system area that is water [-] *(D)*

Diffusive transport

Diffusive mass flows between suspended particles and water by means of adsorption and desorption are obtained from:

$$DIFF_{susp-water} = XCH_{susp-water} \cdot C_{susp} \tag{163}$$

with
$DIFF_{susp-water}$: diffusive mass flow from suspended matter to water [$mol.s^{-1}$] *(I)*
$XCH_{susp-water}$: transport coefficient for desorption from suspended matter [$m_{susp}^{3}.s^{-1}$] *(I)*
C_{susp} : concentration in suspended matter [$mol.m_{susp}^{-3}$] *(S)*

$$XCH_{susp-water} = TRANS_{susp-water} \tag{164}$$

with
$XCH_{susp-water}$: transport coefficient for desorption from suspended matter [$m_{susp}^{3}.s^{-1}$] *(I)*
$TRANS_{susp-water}$: transport coefficient for desorption from suspended matter [$m_{susp}^{3}.s^{-1}$] *(D)*

$$TRANS_{susp-water} = \frac{\ln 2}{EQUtime_{susp}} \cdot V_{susp} \tag{165}$$

with
$TRANS_{susp-water}$: transport coefficient for desorption from suspended matter [$m_{susp}^{3}.s^{-1}$] *(D)*
$EQUtime_{susp}$: equilibration half-time for water and suspended particles [s] *(A)*
V_{susp} : volume of the suspended matter compartment [m_{susp}^{3}] *(D)*

$$DIFF_{water-susp} = XCH_{water-susp} \cdot C_{water} \tag{166}$$

with
$DIFF_{water-susp}$: diffusive mass flow to suspended matter from water [$mol.s^{-1}$] *(I)*
$XCH_{water-susp}$: transport coefficient for adsorption to suspended matter [$m_{water}^{3}.s^{-1}$] *(I)*
C_{water} : concentration in suspended matter [$mol.m_{water}^{-3}$] *(S)*

$$XCH_{water-susp} = TRANS_{water-susp} \tag{167}$$

with
$XCH_{water-susp}$: transport coefficient for adsorption to suspended matter [$m_{water}^{3}.s^{-1}$] *(I)*
$TRANS_{water-susp}$: transport coefficient for adsorption to suspended matter [$m_{water}^{3}.s^{-1}$] *(D)*

$$TRANS_{water-susp} = TRANS_{susp-water} \cdot K_{susp-water} \tag{168}$$

with
$TRANS_{water-susp}$: transport coefficient for adsorption to suspended matter [$m_{susp}^{3}.s^{-1}$] *(D)*
$TRANS_{susp-water}$: transport coefficient for desorption from suspended matter [$m_{susp}^{3}.s^{-1}$] *(D)*
$K_{susp-water}$: suspended matter-water equilibrium distribution constant [$mol.m_{susp}^{-3}/mol.m_{water}^{-3}$] *(A)*

By default, the following value for $EQUtime_{susp}$ may be considered:

$$EQUtime_{susp} = 10\,hr = 3.6 \cdot 10^{4}\,s \tag{169}$$

with
$EQUtime_{susp}$: equilibration half-time for water and suspended particles [s] *(A)*

2.3.4 The compartment biota

Mass balance

The mass balance equation for the compartment biota is:

$$V_{bio} \cdot \frac{dC_{bio}}{dt} = - XCH_{bio-water} \cdot C_{bio} + XCH_{water-bio} \cdot C_{water} \tag{170}$$

with

V_{bio} : volume of the compartment biota [m_{bio}^{3}] *(I)*
C_{bio} : concentration in biota [$mol.m_{bio}^{-3}$] *(S)*
t : time [s] *(S)*
$XCH_{bio-water}$: transport coefficient for elimination from biota [$m_{bio}^{3}.s^{-1}$] *(I)*
$XCH_{water-bio}$: transport coefficient for biosorption to biota [$m_{water}^{3}.s^{-1}$] *(I)*
C_{water} : concentration in water [$mol.m_{water}^{-3}$] *(S)*

In SimpleBox, the compartment biota is modeled as being in passive, non-equilibrium exchange with water. No mechanisms other than diffusive exchange are considered.

Diffusive transport

Diffusive mass flows between biota and water by means of passive uptake and elimination are obtained from:

$$DIFF_{bio-water} = XCH_{bio-water} \cdot C_{bio} \tag{171}$$

with

$DIFF_{bio-water}$: diffusive mass flow from biota to water [$mol.s^{-1}$] *(I)*
$XCH_{bio-water}$: transport coefficient for elimination from biota matter [$m_{bio}^{3}.s^{-1}$] *(I)*
C_{bio} : concentration in biota [$mol.m_{bio}^{-3}$] *(S)*

$$XCH_{bio-water} = TRANS_{bio-water} \tag{172}$$

with

$XCH_{bio-water}$: transport coefficient for elimination from biota [$m_{bio}^{3}.s^{-1}$] *(I)*
$TRANS_{bio-water}$: transport coefficient for elimination from biota [$m_{bio}^{3}.s^{-1}$] *(D)*

$$TRANS_{bio-water} = \frac{\ln 2}{EQUtime_{bio}} \cdot V_{bio} \tag{173}$$

with

$TRANS_{bio-water}$: transport coefficient for elimination from biota [$m_{bio}^{3}.s^{-1}$] *(D)*
$EQUtime_{bio}$: equilibration half-time for water and biota [s] *(A)*
V_{bio} : volume of the compartment biota [m_{bio}^{3}] *(D)*

$$DIFF_{water-bio} = XCH_{water-bio} \cdot C_{water} \tag{174}$$

with

$DIFF_{water-bio}$: diffusive mass flow to biota from water [$mol.s^{-1}$] *(I)*
$XCH_{water-bio}$: transport coefficient for uptake by biota [$m_{water}^{3}.s^{-1}$] *(I)*
C_{water} : concentration in water [$mol.m_{water}^{-3}$] *(S)*

$$XCH_{water-bio} = TRANS_{water-bio} \tag{175}$$

with

$XCH_{water-bio}$: transport coefficient for uptake by biota [$m_{water}^{3}.s^{-1}$] *(I)*
$TRANS_{water-bio}$: transport coefficient for uptake by biota [$m_{water}^{3}.s^{-1}$] *(D)*

$$TRANS_{water-bio} = TRANS_{bio-water} \cdot K_{bio-water} \tag{176}$$

with

$TRANS_{water-bio}$: transport coefficient for uptake by biota [$m_{bio}^{3}.s^{-1}$] *(D)*
$TRANS_{bio-water}$: transport coefficient for elimination from biota [$m_{bio}^{3}.s^{-1}$] *(D)*

$K_{bio\text{-}water}$: biota-water equilibrium distribution constant [$mol.m_{bio}^{-3}/mol.m_{water}^{-3}$] *(A)*

An indication for $EQUtime_{bio}$ may be obtained from Mackay's equation (Mackay, 1982):

$$EQUtime_{bio} = 100 + \frac{K_{ow}}{1000} \tag{177}$$

with

$EQUtime_{bio}$: equilibration half-time for water and biota [hr] *(A)*
K_{ow} : octanol-water partition coefficient of the chemical [-] *(A)*

2.3.5 The sediment compartment

Mass balance

The mass balance equation for the sediment compartment is:

$$\begin{aligned} V_{sed} \cdot \frac{dC_{sed}}{dt} = & - V_{sed} \cdot DEG_{sed} \cdot C_{sed} - SEDBURIAL \cdot C_{sed} \\ & - RESUSPENSION \cdot C_{sed} \\ & + SEDIMENTATION \cdot C_{susp} \\ & - XCH_{sed\text{-}water} \cdot C_{sed} \\ & + XCH_{water\text{-}sed} \cdot C_{water} \end{aligned} \tag{178}$$

with

V_{sed} : volume of the sediment compartment [m_{sed}^3] *(I)*
C_{sed} : total concentration in sediment (water phase + solid phase) [$mol.m_{sed}^{-3}$] *(S)*
t : time [s] *(S)*
DEG_{sed} : pseudo first order transformation rate constant in sediment [s^{-1}] *(I)*
$SEDBURIAL$: transport coefficient for sediment burial [$m_{sed}^3.s^{-1}$] *(I)*
$RESUSPENSION$: transport coefficient for resuspension [$m_{sed}^3.s^{-1}$] *(I)*
$SEDIMENTATION$: transport coefficient for sedimentation [$m_{susp}^3.s^{-1}$] *(I)*
C_{susp} : concentration in suspended matter [$mol.m_{susp}^{-3}$] *(S)*
$XCH_{sed\text{-}water}$: transport coefficient for release from sediment [$m_{sed}^3.s^{-1}$] *(I)*
$XCH_{water\text{-}sed}$: transport coefficient for uptake by sediment [$m_{water}^3.s^{-1}$] *(I)*
C_{water} : concentration in water [$mol.m_{water}^{-3}$] *(S)*

Degradation

The apparent degradation mass flow from sediment is obtained from:

$$DEGRD_{sed} = V_{sed} \cdot DEG_{sed} \cdot C_{sed} \tag{179}$$

with

$DEGRD_{sed}$: degradation mass flow from the sediment compartment [$mol.s^{-1}$] *(I)*
V_{sed} : volume of the sediment compartment [m_{sed}^3] *(I)*
DEG_{sed} : pseudo first order transformation rate constant in sediment [s^{-1}] *(I)*
C_{sed} : bulk concentration in sediment [$mol.m_{sed}^{-3}$] *(S)*

$$DEG_{sed} = kdeg_{sed} \tag{180}$$

with

DEG_{sed} : pseudo first order transformation rate constant in sediment [s^{-1}] *(I)*
$kdeg_{sed}$: pseudo first order transformation rate constant in sediment [s^{-1}] *(D)*

A value for $kdeg_{sed}$ may be obtained by means of the scaling procedure proposed by Struijs and Van den Berg (1993). As with degradation in water (paragraph 2.3.2), it is assumed that the degradation rate is related to the degradation rate constant observed in standard tests for (aerobic) ready degradability in water. Degradation in sediment is treated as disappearance from the water phase of the sediment. The concentration of bacteria, present in the pore water or at the surface of the solid phase (or both), in the sediment compartment is expressed on a pore water volume basis:

$$kdeg_{sed} = kdeg_{test} \cdot \frac{BACT_{sed}}{BACT_{test}} \cdot FRdisslvd_{sed} \tag{181}$$

with

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

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

$$BACT_{sed} = \frac{1.8 . 10^{9}}{FRwater_{sed}} \tag{182}$$

with

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

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

Burial

The apparent mass flow from the sediment as a result of burial is obtained from:

$$BRL_{sed} = SEDBURIAL \, . \, C_{sed} \tag{183}$$

with

BRL_{sed} : apparent burial mass flow from the sediment compartment [mol.s^{-1}] *(I)*
$SEDBURIAL$: transport coefficient for sediment burial [$m_{sed}^{3}.s^{-1}$] *(I)*
C_{sed} : bulk concentration in sediment [mol.m_{sed}^{-3}] *(S)*

$$SEDBURIAL = BURIAL_{sed} \, . \, SYSTEMAREA \, . \, AREAFRAC_{water} \tag{184}$$

with

$SEDBURIAL$: transport coefficient for sediment burial [$m_{sed}^{3}.s^{-1}$] *(I)*
$BURIAL_{sed}$: sediment burial rate [$m_{sed}.s^{-1}$] *(D)*
$SYSTEMAREA$: total area of the system (air/water + air/soil interfaces) [m^{2}] *(D)*
$AREAFRAC_{water}$: fraction of the system area that is water [-] *(D)*

Advective transport

Advective transport between sediment and suspended matter by sedimentation and resuspension is described in paragraph 2.3.3, equations (159)-(162).

Diffusive transport

Diffusive mass flows between sediment and water, by direct adsorption and desorption across the sediment-water interface, are obtained from:

$$DIFF_{sed\text{-}water} = XCH_{sed\text{-}water} \cdot C_{sed} \tag{185}$$

with

$DIFF_{sed\text{-}water}$: diffusive desorption mass flow from sediment to water [$mol.s^{-1}$] *(I)*
$XCH_{sed\text{-}water}$: transport coefficient for desorption from sediment [$m_{sed}^{3}.s^{-1}$] *(I)*
C_{sed} : concentration in sediment [$mol.m_{sed}^{-3}$] *(S)*

$$XCH_{sed\text{-}water} = DESORB_{sed} \, . \, SYSTEMAREA \, . \, AREAFRAC_{water} \tag{186}$$

with

$XCH_{sed\text{-}water}$: transport coefficient for desorption from sediment [$m_{sed}^{3}.s^{-1}$] *(I)*
$DESORB_{sed}$: overall mass transfer coefficient for desorption across the sediment-water interface, referenced to sediment [$m_{sed}.s^{-1}$] *(D)*
$SYSTEMAREA$: total area of the system (air/water + air/soil interfaces) [m^{2}] *(D)*
$AREAFRAC_{water}$: fraction of the system area that is water [-] *(D)*

$$DIFF_{water\text{-}sed} = XCH_{water\text{-}sed} \cdot C_{water} \tag{187}$$

with

$DIFF_{water\text{-}sed}$: diffusive adsorption mass flow to sediment to water [$mol.s^{-1}$] *(I)*
$XCH_{water\text{-}sed}$: transport coefficient for adsorption to sediment [$m_{water}^{3}.s^{-1}$] *(I)*
C_{water} : concentration in water [$mol.m_{water}^{-3}$] *(S)*

$$XCH_{water\text{-}sed} = ADSORB_{sed} \, . \, SYSTEMAREA \, . \, AREAFRAC_{water} \tag{188}$$

with

$XCH_{water\text{-}sed}$: transport coefficient for adsorption to sediment [$m_{water}^{3}.s^{-1}$] *(I)*
$ADSORB_{sed}$: overall mass transfer coefficient for adsorption across the sediment-water interface, referenced to water [$m_{water}.s^{-1}$] *(D)*
$SYSTEMAREA$: total area of the system (air/water + air/soil interfaces) [m^{2}] *(D)*
$AREAFRAC_{water}$: fraction of the system area that is water [-] *(D)*

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

$$ADSORB_{sed} = \frac{kws_{water} \cdot kws_{sed}}{kws_{water} + kws_{sed}} \tag{189}$$

with

$ADSORB_{sed}$: overall mass transfer coefficient for adsorption across the sediment-water interface, referenced to water [$m_{water}.s^{-1}$] *(D)*
kws_{water} : partial mass transfer coefficient at the water side of the sediment-water interface [$m_{water}.s^{-1}$] *(A)*
kws_{sed} : partial mass transfer coefficient at the pore water side of the sediment-water interface [$m_{pore\ water}.s^{-1}$] *(A)*

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

$$DESORB_{sed} = \frac{ADSORB_{sed}}{K_{sed-water}} \tag{190}$$

with

$DESORB_{sed}$: overall mass transfer coefficient for desorption across the sediment-water interface, referenced to sediment [$m_{sed}.s^{-1}$] *(D)*

$ADSORB_{sed}$: overall mass transfer coefficient for adsorption across the sediment-water interface, referenced to water [$m_{water}.s^{-1}$] *(D)*

$K_{sed-water}$ sediment-water equilibrium distribution constant [$mol.m_{sed}^{-3}/mol.m_{water}^{-3}$] *(A)*

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

$$kws_{water} = 2.78 \,.\, 10^{-6}\, m.s^{-1} \tag{191}$$

with

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

Mass transfer at the pore water side of the sediment-water interface is treated, according to Mackay's reasoning (Mackay *et al.*, 1992), as molecular diffusion in the aqueous phase of a porous solid material, characterized by an effective diffusivity of $2 \cdot 10^{-6}$ $m^2.hr^{-1}$ and a diffusion path length of 2 cm. This leads to:

$$kws_{sed} = 2.78 \,.\, 10^{-8}\, m.s^{-1} \tag{192}$$

with

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

2.3.6 The soil compartments

Mass balances

The mass balance equations for the soil compartments are:

$$\begin{aligned} V_{soil\,i} \cdot \frac{dC_{soil\,i}}{dt} = &+ EMIS_{soil\,i} \\ &- V_{soil\,i} \cdot DEG_{soil\,i} \cdot C_{soil\,i} - LEACHING_{soil\,i} \cdot C_{soil\,i} \\ &- \Sigma RUN\text{-}OFF_{soil\,i} \cdot C_{soil\,i} + DEP_{soil\,i} \cdot C_{air} \\ &- XCH_{soil\,i\text{-}air} \cdot C_{soil\,i} \\ &+ XCH_{air\text{-}soil\,i} \cdot C_{air} \end{aligned} \tag{193}$$

with

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

$C_{soil\,i}$: total concentration in soil i (gas phase + water phase + solid phase) [$mol.m_{soil}^{-3}$] *(S)*

t : time [s] *(S)*

$EMIS_{soil\,i}$: emission to soil i [$mol.s^{-1}$] *(I)*

$DEG_{soil\,i}$: pseudo first order transformation rate constant in soil i [s^{-1}] *(I)*

$LEACHING_{soil\,i}$: transport coefficient for leaching from soil i [$m_{soil}^3.s^{-1}$] *(I)*

$RUN\text{-}OFF_{soil\,i}$: transport coefficient for run off from soil i to water [$m_{soil}^3.s^{-1}$] *(I)*

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

C_{air} : total concentration in air [$mol.m_{air}^{-3}$] *(S)*

$XCH_{soil\,i\text{-}air}$: transport coefficient volatilization from soil i [$m_{soil}^3.s^{-1}$] *(I)*

$XCH_{air\text{-}soil\,i}$: transport coefficient gas absorption to soil i [$m_{air}^3.s^{-1}$] *(I)*

Emission

Soil 1 and soil 3 only receive direct emissions. In addition to this, soil 2 may receive indirect emission through application of the sludge that is produced upon sewage treatment. Emission mass flows to soil are obtained from:

$$EMIS_{soil\,1} = Edirect_{soil\,1} \tag{194}$$

$$EMIS_{soil\,2} = Edirect_{soil\,2} + Estp_{soil\,2} \tag{195}$$

$$EMIS_{soil\,3} = Edirect_{soil\,3} \tag{196}$$

with

$EMIS_{soil\,i}$: total emission mass flow to soil i [$mol.s^{-1}$] *(I)*
$Edirect_{soil\,i}$: sum of all direct emissions to soil i [$mol.s^{-1}$] *(D)*
$Estp_{soil\,2}$: indirect emission to soil 2, resulting from application of sewage sludge [$mol.s^{-1}$] *(D)*

$Edirect_{soil\,i}$ and $Estp_{soil\,2}$ may be derived by means of:

$$Edirect_{soil\,i} = PRODUCTION\,.\,EMISfact_{soil\,i} \tag{197}$$

with

$Edirect_{soil\,i}$: sum of all direct emissions to soil i [$mol.s^{-1}$] *(D)*
$PRODUCTION$: total amount produced or imported in the system [$mol.s^{-1}$] *(A)*
$EMISfact_{soil\,i}$: *emission factor for soil i: the fraction of the production volume that is released to soil i* [-] *(A)*

$$Estp_{soil\,2} = ACTIVEtime\,.\,SOLIDS_{stp}\,.\,CONCstp_{sludge} \tag{198}$$

with

$Estp_{soil\,2}$: indirect emission to soil 2, resulting from application of sewage sludge [$mol.s^{-1}$] *(D)*
$ACTIVEtime$: fraction of the time that the sewage treatment plant is loaded with the chemical [-] *(A)*
$SOLIDS_{stp}$: rate of sewage sludge production [$kg_{solid}.s^{-1}$] *(A)*
$CONCstp_{sludge}$: concentration of the chemical in sewage sludge [$mol.kg_{solid}^{-1}$] *(A)*

$$CONC_{sludge} = \frac{STPload\,.\,FR_{sludgestp}}{SOLIDS_{stp}} \tag{199}$$

with

$CONCstp_{sludge}$: concentration of the chemical in the solid phase of STP-sludge [$mol.kg_{solid}^{-1}$] *(A)*
$STPload$: load of the sewage treatment plant during release episodes [$mol.s^{-1}$] *(A)*
$FR_{sludgestp}$: fraction of the load that is rerouted to the soil compartment with sludge upon sewage treatment [-] *(A)*
$SOLIDS_{stp}$: rate of sewage sludge production [$kg_{solid}.s^{-1}$] *(A)*

The following default values may serve as a starting point:

$$EMISfact_{soil\,1} = 0 \tag{200}$$

$$EMISfact_{soil\,2} = 0.1\ \% \tag{201}$$

$$EMISfact_{soil3} = 0.1\ \% \tag{202}$$

with

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

$$FR_{sludgestp} = 0.6 \tag{203}$$

with

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

Degradation

The apparent degradation mass flows from soil are obtained from:

$$DEGRD_{soil\,i} = V_{soil\,i} \cdot DEG_{soil\,i} \cdot C_{soil\,i} \tag{204}$$

with

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

$$DEG_{soil\,i} \approx kdeg_{soil} \tag{205}$$

with

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

A value for $kdeg_{soil}$ may be obtained by means of the scaling procedure proposed by Struijs and Van den Berg (1993), in analogy with the derivation of $kdeg_{sed}$ (paragraph 2.3.5).

$$kdeg_{soil} = kdeg_{test} \cdot \frac{BACT_{soil}}{BACT_{test}} \cdot FRdisslvd_{soil} \tag{206}$$

with

$kdeg_{soil}$: pseudo first order degradation rate constant in soil [s^{-1}] *(D)*
$kdeg_{test}$: pseudo first order degradation rate constant in laboratory test [s^{-1}] *(A)*
$BACT_{soil}$: concentration of bacteria in soil, expressed on a pore water basis [cfu.ml$_{pore\ water}^{-1}$] *(A)*
$BACT_{test}$: concentration of bacteria in the laboratory test water [cfu.ml$_{test\ water}^{-1}$] *(A)*
$FRdisslvd_{soil}$: fraction of the chemical in soil, present in the pore water phase [-]

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

$$BACT_{soil} \approx \frac{10^6 / 1.4}{FRwater_{soil}} \tag{207}$$

with

$BACT_{soil}$: concentration of bacteria in soil, expressed on a pore water basis [cfu.ml$_{pore\ water}^{-1}$] *(A)*
10^6 : concentration of bacteria reported in aerobic soil [cfu.g$_{soil}$]
1.4 : bulk density of soil [kg$_{soil}$.m$_{soil}^{-3}$] *(A)*
$FRwater_{soil}$: volume fraction water of the soil [-] *(A)*

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

Leaching

The mass flows for removal from soil by leaching are obtained from:

$$LCH_{soil\,i} = LEACHING_{soil\,i} \cdot C_{soil\,i} \tag{208}$$

with

$LCH_{soil\,i}$: leaching mass flow from the soil i [mol.s^{-1}] *(I)*
$LEACHING_{soil\,i}$: transport coefficient for leaching from soil i [m_{soil}^{3}.s^{-1}] *(I)*
$C_{soil\,i}$: bulk concentration in soil i [mol.m_{soil}^{-3}] *(S)*

$$LEACHING_{soil\,i} = LEACH_{soil\,i} \cdot SYSTEMAREA \cdot AREAFRAC_{soil\,i} \tag{209}$$

with

$LEACHING_{soil\,i}$: transport coefficient for leaching from soil i [m_{soil}^{3}.s^{-1}] *(I)*
$LEACH_{soil\,i}$: mass transfer coefficient for leaching from soil i [m_{soil}.s^{-1}] *(D)*
$SYSTEMAREA$: total area of the system (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{soil\,i}$: fraction of the system area that is soil i [-] *(D)*

$$LEACH_{soil\,i} = \frac{FRACinf_{soil\,i} \cdot RAINrate}{K_{soil\,i-water}} \tag{210}$$

with

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

Advection

The mass flows for advective transport from soil to water by run-off are obtained from:

$$ADV_{soil\,i-water} = RUN\text{-}OFF_{soil\,i} \cdot C_{soil\,i} \tag{211}$$

with

$ADV_{soil\,i-water}$: run-off mass flow from the soil i to water [mol.s^{-1}] *(I)*
$RUN\text{-}OFF_{soil\,i}$: transport coefficient for run-off from soil i [m_{soil}^{3}.s^{-1}] *(I)*
$C_{soil\,i}$: bulk concentration in soil i [mol.m_{soil}^{-3}] *(S)*

$$RUN\text{-}OFF_{soil\,i} = RUNOFF_{soil\,i} \cdot SYSTEMAREA \cdot AREAFRAC_{soil\,i} \tag{212}$$

with

$RUN\text{-}OFF_{soil\,i}$: transport coefficient for run-off from soil i [m_{soil}^{3}.s^{-1}] *(I)*
$RUNOFF_{soil\,i}$: mass transfer coefficient for run-off from soil i [m_{soil}.s^{-1}] *(D)*
$SYSTEMAREA$: total area of the system (air/water + air/soil interfaces) [m^2] *(D)*
$AREAFRAC_{soil\,i}$: fraction of the system area that is soil i [-] *(D)*

$$RUNOFF_{soil\,i} = \frac{FRACrun_{soil\,i} \cdot RAINrate}{K_{soil\,i-water}} + EROSION_{soil\,i} \tag{213}$$

with

$RUNOFF_{soil\,i}$: mass transfer coefficient for run-off from soil i [m_{soil}.s^{-1}] *(D)*
$FRACrun_{soil\,i}$: fraction of rain water that infiltrates into soil i [-] *(A)*
$RAINRATE$: rate of wet precipitation [m_{rain}.s^{-1}] *(A)*
$K_{soil\,i-water}$: soil i-water equilibrium distribution constant [m_{water}^{3}.m_{solid}^{-3}] *(A)*
$EROSION_{soil\,i}$: rate at which soil is washed from soil i into surface water [m_{soil}.s^{-1}] *(A)*

Advective transport from air to soil by atmospheric deposition has been described in paragraph 2.3.1, equations (105), (108)-(110).

Diffusion

Diffusive transport between air and soil by means of gas absorption and volatilization has been described in paragraph 2.3.1, equations (112), (114), (116), (118), (120), (122), (123)-(129).

2.4 Model output

SimpleBox produces two sorts of output:

1. Steady-state or "level 3" output. If the conditions (loadings and environmental conditions) remain constant in time for a sufficiently long period of time, eventually a steady state, in which all mass flows and concentrations are constant in time, will develop. At steady state, the sum of the mass balance equation terms is equal to zero for all boxes, and the n steady-state concentrations can be solved from the n linear mass balance equations. This steady-state solution is obtained in SimpleBox by means of a matrix inversion routine. The mass flows and concentrations that characterize this steady state are written by SimpleBox in output tables.
2. Quasi-dynamic or "level 4" output. After a change in conditions (loadings or environmental conditions), mass flows and concentrations develop toward a new steady state, according to the mass balance equations. The "level 4" computation is done by numerical integration of the set of mass balance equations from time zero, with all concentrations at zero, to infinite time with all concentrations constant at steady state.

The standard procedure in SimpleBox is to compute the steady-state solution first and carry out the dynamic response computation afterwards, as an option.

2.4.1 Steady-state computation

The model description in SimpleBox consists of the eight mass balance equations described in the previous paragraphs. Air is represented by "box 1", water by "box 2", sediment by "box 3", soil 1 by "box 4", soil 2 by "box 5", soil 3 by "box 6", suspended matter by "box 7" and biota by "box 8". At steady state, all balances become equal to zero:

$$V_i \cdot \frac{dC_i}{dt} = EMIS_i + IMP_i - EXP_i - LCH_i - BRL_i - DEGRD_i + \Sigma ADV_{i\text{-}j} + \Sigma DIFF_{i\text{-}j} = 0 \tag{214}$$

with

V_i : volume of box i [m^3] *(I)*
C_i : concentration in box i [mol.m^{-3}] *(S)*
$EMIS_i$: emission mass flow into box i [mol.s^{-1}] *(I)*
t : time [s] *(S)*
IMP_i : import mass flow into box i [mol.s^{-1}] *(I)*
EXP_i : export mass flow from box i [mol.s^{-1}] *(I)*
LCH_i : leaching mass flow from box i [mol.s^{-1}] *(I)*
BRL_i : apparent burial mass flow from box i [mol.s^{-1}] *(I)*
$DEGRD_i$: apparent degradation mass flow from box i [mol.s^{-1}] *(I)*
$ADV_{i\text{-}j}$: advective mass flows to and from box i [mol.s^{-1}] *(I)*
$DIFF_{i\text{-}j}$: diffusive mass flows to and from box i [mol.s^{-1}] *(I)*

The mass balances (214) are rewritten as:

$$CNST_i = CF_{ii}.Css_i + \Sigma(CF_{ij}.Css_j) \tag{215}$$

with

$CNST_i$: constant term in mass balance of box i [$\mathrm{mol.s^{-1}}$] *(I)*
CF_{ii} : sum of coefficients for (apparent) transport from box i to elsewhere [$\mathrm{m^3_{medium\ i}.s^{-1}}$] *(I)*
CF_{ij} : sum of coefficients for transport from compartment j to box i [$\mathrm{m^3_{medium\ i}.s^{-1}}$] *(I)*
Css_i : steady-state concentration in box i [$\mathrm{mol.m_{medium\ i}^{-3}}$] *(I)*
Css_j : steady-state concentration in compartment j [$\mathrm{mol.m_{medium\ j}^{-3}}$] *(I)*

where

$$CNST_i = -EMIS_i - IMP_i \tag{216}$$

with

$CNST_i$: constant term in mass balance of box i [$\mathrm{mol.s^{-1}}$] *(I)*
$EMIS_i$: emission mass flow into box i [$\mathrm{mol.s^{-1}}$] *(I)*
IMP_i : import mass flow into box i [$\mathrm{mol.s^{-1}}$] *(I)*

In matrix-format, the set of eight mass balances reads:

$$\overline{CNST} = CF.\overline{Css} \tag{217}$$

with

$\overline{CNST}$: vector of constant terms of mass balance equations *(I)*
CF : matrix of coefficients *(I)*
$\overline{Css}$: vector of steady-state concentrations *(I)*

As the product of a matrix and its inverse is equals to 1, the solution of the set of mass balances can be obtained by multiplying the left and right parts of (217) by the inverse of the matrix of coefficients:

$$CF^{-1}.CF.\overline{Css} = \overline{Css} = CF^{-1}.\overline{CNST} \tag{218}$$

SimpleBox uses this matrix-inversion method to produce the steady-state output. The steady-state computation procedure produces the following output:

Steady-state concentrations in "standard units"

The elements Css_1-Css_8 of the vector *Css*, computed as described above, are expressed in the internal SimpleBox-dimensions of $\mathrm{mol.m_{medium}^{-3}}$. These variables are only used internally; they are not shown in the SimpleBox output tables.

Steady-state fugacities

For easy evaluation of the departure from (thermodynamic) equilibrium of the steady-state solution, steady-state fugacities of the chemical are computed by multiplying the steady-state concentrations with the fugacity capacities of the media. (In case of thermodynamic equilibrium, the chemical's fugacities in different compartments have the same value.) The result is a vector *Fss*, with elements Fss_1-Fss_8; shown in the output table 1.

$$Fss_{air} = Fss_1 = Css_1 \,.\, R \,.\, TEMPERATURE \tag{219}$$

with

Fss_{air} : steady-state fugacity in air [Pa] *(O)*
Fss_1 : steady-state fugacity in box 1 [Pa] *(I)*
Css_1 : steady-state concentration in box 1 [mol.m^{-3}] *(I)*
R : gas constant [8.314 Pa.m^3.mol^{-1}.K^{-1}] *(C)*
$TEMPERATURE$: temperature at air-water and air-soil interfaces [K] *(A)*

$$Fss_{water} = Fss_2 = Css_2 \,.\, R \,.\, TEMPERATURE \,.\, K_{air-water} \tag{220}$$

with

Fss_{water} : steady-state fugacity in water [Pa] *(O)*
Fss_2 : steady-state fugacity in box 2 [Pa] *(I)*
Css_2 : steady-state concentration in box 2 [mol.m^{-3}] *(I)*
R : gas constant [8.314 Pa.m^3.mol^{-1}.K^{-1}] *(C)*
$TEMPERATURE$: temperature at air-water and air-soil interfaces [K] *(A)*
$K_{air\text{-}water}$: air-water equilibrium distribution constant [m$_{water}^{3}$.m$_{air}^{-3}$] *(A)*

$$Fss_{sed} = Fss_3 = Css_3 \,.\, R \,.\, TEMPERATURE \,.\, \frac{K_{air-water}}{K_{sed-water}} \tag{221}$$

with

Fss_{sed} : steady-state fugacity in sediment [Pa] *(O)*
Fss_3 : steady-state fugacity in box 3 [Pa] *(I)*
Css_3 : steady-state concentration in box 3 [mol.m^{-3}] *(I)*
R : gas constant [8.314 Pa.m^3.mol^{-1}.K^{-1}] *(C)*
$TEMPERATURE$: temperature at air-water and air-soil interfaces [K] *(A)*
$K_{air\text{-}water}$: air-water equilibrium distribution coefficient [m$_{water}^{3}$.m$_{air}^{-3}$] *(A)*
$K_{sed\text{-}water}$: sediment-water equilibrium distribution coefficient [m$_{water}^{3}$.m$_{sed}^{-3}$] *(A)*

$$Fss_{pw\,sed} = Fss_{sed} \tag{222}$$

with

$Fss_{pw\,sed}$: steady-state fugacity in pore water of sediment [Pa] *(O)*
Fss_{sed} : steady-state fugacity in sediment [Pa] *(I)*

$$Fss_{soil\,i} = Fss_i = Css_i \,.\, R \,.\, TEMPERATURE \,.\, \frac{K_{air-water}}{K_{soil\,i-water}} \tag{223}$$

with

$Fss_{soil\,i}$: steady-state fugacity in soil i [Pa] *(O)*
Fss_i : steady-state fugacity in box i (4, 5 or 6) [Pa] *(I)*
Css_i : steady-state concentration in box i (4, 5 or 6) [mol.m^{-3}] *(I)*
R : gas constant [8.314 Pa.m^3.mol^{-1}.K^{-1}] *(C)*
$TEMPERATURE$: temperature at air-water and air-soil interfaces [K] *(A)*
$K_{air\text{-}water}$: air-water equilibrium distribution coefficient [m$_{water}^{3}$.m$_{air}^{-3}$] *(A)*
$K_{soil\,i\text{-}water}$: soil i-water equilibrium distribution coefficient [m$_{water}^{3}$.m$_{soil}^{-3}$] *(A)*

$$Fss_{pw\,soil\,i} = Fss_{soil\,i} \tag{224}$$

with

$Fss_{pw\,soil\,i}$: steady-state fugacity in pore water of soil i [Pa] *(O)*
$Fss_{soil\,i}$: steady-state fugacity in soil i [Pa] *(I)*

$$Fss_{susp} = Fss_7 = Css_7 \,.\, R \,.\, TEMPERATURE \,.\, \frac{K_{air-water}}{K_{susp-water}} \tag{225}$$

with

Fss_{susp} : steady-state fugacity in suspended matter [Pa] *(O)*

Fss_7 : steady-state fugacity in box 7 [Pa] *(I)*
Css_7 : steady-state concentration in box 7 [$mol.m^{-3}$] *(I)*
R : gas constant [8.314 $Pa.m^3.mol^{-1}.K^{-1}$] *(C)*
TEMPERATURE : temperature at air-water and air-soil interfaces [K] *(A)*
$K_{air\text{-}water}$: air-water equilibrium distribution coefficient [$m_{water}^3.m_{air}^{-3}$] *(A)*
$K_{susp\text{-}water}$: sediment-water equilibrium distribution coefficient [$m_{water}^3.m_{sed}^{-3}$] *(A)*

$$Fss_{bio} = Fss_8 = Css_8 \, . \, R \, . \, TEMPERATURE \, . \, \frac{K_{air-water}}{K_{bio-water}} \tag{226}$$

with
Fss_{bio} : steady-state fugacity in biota [Pa] *(O)*
Fss_8 : steady-state fugacity in box 8 [Pa] *(I)*
Css_8 : steady-state concentration in box 8 [$mol.m^{-3}$] *(I)*
R : gas constant [8.314 $Pa.m^3.mol^{-1}.K^{-1}$] *(C)*
TEMPERATURE : temperature at air-water and air-soil interfaces [K] *(A)*
$K_{air\text{-}water}$: air-water equilibrium distribution coefficient [$m_{water}^3.m_{air}^{-3}$] *(A)*
$K_{bio\text{-}water}$: sediment-water equilibrium distribution coefficient [$m_{water}^3.m_{sed}^{-3}$] *(A)*

Steady-state hold-up

The amount of the chemical present in each of the compartments at steady state is computed by:

$$HOLD\text{-}UP_i = Css_i \, . \, V_i \tag{227}$$

with
$HOLD\text{-}UP_i$: amount of the chemical in box i at steady state [mol] *(I)*
Css_i : steady-state concentration in box i [$mol.m^{-3}$] *(I)*
V_i : volume of box i [m^3] *(I)*

The total hold-up in the system is obtained by summation:

$$SYSTEM\ HOLD\text{-}UP = \Sigma\, HOLD\text{-}UP_i \tag{228}$$

with
SYSTEM HOLD-UP : total amount of the chemical in the system at steady state [mol] *(I)*
$HOLD\text{-}UP_i$: hold-up at steady state in box i [mol] *(I)*

These variables are not shown in the SimpleBox output tables.

Steady-state distribution

The steady-state distribution of the chemical is obtained by expressing the steady-state hold-ups as a percentage of the *SYSTEM HOLD-UP*:

$$DISTRIBUTION_i = \frac{HOLD\text{-}UP_i}{SYSTEM\ HOLD\text{-}UP} \, . \, 100 \tag{229}$$

with
$DISTRIBUTION_i$: percentage of the chemical in box i at steady state [%] *(O)*
$HOLD\text{-}UP_i$: amount of the chemical in box i at steady state [mol] *(I)*
SYSTEM HOLD-UP : total amount of the chemical in the system at steady state [mol] *(I)*

The distribution percentages are shown in the SimpleBox output table 3.

Steady-state mass flows

The steady-state mass flows of the chemical, i.e. the terms of equation (214), are computed by means of the equations described in the previous paragraphs. As a check for the integrity of the steady-state computation, the mass flows are summed for each of the boxes:

$$INPUT_i = EMIS_i + IMP_i + \Sigma ADV_{j\text{-}i} + \Sigma DIFF_{j\text{-}i} \qquad (230)$$

$$OUTPUT_i = EXP_i + LCH_i + BRL_i + DEGRD_i + \Sigma ADV_{i\text{-}j} + \Sigma DIFF_{i\text{-}j} \qquad (231)$$

with

$INPUT_i$: sum of the mass flows into box i [mol.s^{-1}] *(I)*
$EMIS_i$: emission mass flow into box i [mol.s^{-1}] *(I)*
IMP_i : import mass flow into box i [mol.s^{-1}] *(I)*
$ADV_{j\text{-}i}$: advective mass flows to box i [mol.s^{-1}] *(I)*
$DIFF_{j\text{-}i}$: diffusive mass flows to box i [mol.s^{-1}] *(I)*
$OUTPUT_i$: sum of the mass flows out of box i [mol.s^{-1}] *(I)*
EXP_i : export mass flow from box i [mol.s^{-1}] *(I)*
LCH_i : leaching mass flow from box i [mol.s^{-1}] *(I)*
BRL_i : apparent burial mass flow from box i [mol.s^{-1}] *(I)*
$DEGRD_i$: apparent degradation mass flow from box i [mol.s^{-1}] *(I)*
$ADV_{i\text{-}j}$: advective mass flows from box i [mol.s^{-1}] *(I)*
$DIFF_{i\text{-}j}$: diffusive mass flows from box i [mol.s^{-1}] *(I)*

At steady state, *INPUT* and *OUTPUT* for each of the boxes as well as in total, should be equal:

$$THROUGHPUT = \Sigma INPUT_i = \Sigma OUTPUT_i \qquad (232)$$

with

$THROUGHPUT$: sum of all mass flows into or out of the system [mol.s^{-1}] *(I)*
$INPUT_i$: sum of the mass flows into box i [mol.s^{-1}] *(I)*
$OUTPUT_i$: sum of the mass flows out of box i [mol.s^{-1}] *(I)*

A full mass balance checking table is produced; this is not shown as part of the SimpleBox output. Instead, a separate table of mass flows is produced as SimpleBox output table 2. This table can be displayed in different units to suit the demands of the specific analysis. To do so, the mass flows are expressed as the product of the mass flow in standard units (mol.s^{-1}) and a conversion factor:

$$FLOW_{shown} = FLOW_{standard} \cdot CONVFACTOR_i \qquad (233)$$

with

$FLOW_{shown}$: mass flow in chosen units *(I)*
$FLOW_{standard}$: mass flow in standard units [mol.s^{-1}] *(I)*
$CONVFACTOR_i$: conversion factor of choice *(I)*

There are four options:

$$CONVFACTOR_1 = 1 \qquad (234)$$

To express the mass flows in table 2 as mol.s^{-1}.

$$CONVFACTOR_2 = \frac{100}{THROUGHPUT} \qquad (235)$$

To express the mass flows in table 2 as percentages of the total mass flow through the system at steady state. The most characteristic mass flows (*$EMIS_i$, IMP_i, LCH_i, BRL_i, $DEGRD_i$*) are shown in this unit in SimpleBox output table 1.

$$CONVFACTOR_3 = (MOLWEIGHT/1000).(3600.24.365) \quad (236)$$

To express the mass flows in table 2 as $t.y^{-1}$.

$$CONVFACTOR_4 = MOLWEIGHT.(3600.24) \quad (237)$$

To express the mass flows in table 2 as $kg.d^{-1}$.

Steady-state concentrations in "common units"

Steady-state concentrations expressed in "common" units are shown in SimpleBox output table 1. The values are obtained by conversion of the elements of vector *Css*:

$$Css_{air} = Css_1 . MOLWEIGHT . 1000 \quad (238)$$

with

Css_{air} : steady-state concentration in air [$g.m^{-3}$] *(O)*
Css_1 : steady-state concentration in box 1 [$mol.m^{-3}$] *(I)*
MOL WEIGHT : molecular weight of the chemical [$kg.mol^{-1}$] *(D)*
1000 : conversion factor [$g.kg^{-1}$]

$$Css_{water} = Css_2 . MOLWEIGHT \quad (239)$$

with

Css_{water} : steady-state concentration in water [$g.l^{-1}$] *(O)*
Css_2 : steady-state concentration in box 2 [$mol.m^{-3}$] *(I)*
MOL WEIGHT : molecular weight of the chemical [$kg.mol^{-1}$] *(D)*

$$Css_{sed} = Css_3 . \frac{MOLWEIGHT . Kp_{sed}}{K_{sed-water}} \quad (240)$$

with

Css_{sed} : steady-state concentration in sediment [$g.kg_{solid}^{-1}$] *(O)*
Css_3 : steady-state concentration in box 3 [$mol.m^{-3}$] *(I)*
MOL WEIGHT : molecular weight of the chemical [$kg.mol^{-1}$] *(D)*
Kp_{sed} : sediment-water partition coefficient [$l_{water}.kg_{solid}^{-1}$] *(I)*
$K_{sed-water}$: sediment-water equilibrium distribution coefficient [$m_{water}^3.m_{sed}^{-3}$] *(A)*

$$Css_{pw\,sed} = Css_3 . \frac{MOLWEIGHT}{K_{sed-water}} \quad (241)$$

with

$Css_{pw\,sed}$: steady-state concentration in pore water of sediment [$g.l^{-1}$] *(O)*
Css_3 : steady-state concentration in box 1 [$mol.m^{-3}$] *(I)*
MOL WEIGHT : molecular weight of the chemical [$kg.mol^{-1}$] *(D)*
$K_{sed-water}$: sediment-water equilibrium distribution coefficient [$m_{water}^3.m_{sed}^{-3}$] *(A)*

$$Css_{soil\,i} = Css_i . \frac{MOLWEIGHT . Kp_{soil\,i}}{K_{soil\,i-water}} \quad (242)$$

with

$Css_{soil\,i}$: steady-state concentration in soil i [$g.kg_{solid}^{-1}$] *(O)*
Css_i : steady-state concentration in box i (4, 5 or 6) [$mol.m^{-3}$] *(I)*
MOL WEIGHT : molecular weight of the chemical [$kg.mol^{-1}$] *(D)*
$Kp_{soil\,i}$: soil i-water partition coefficient [$l_{water}.kg_{solid}^{-1}$] *(I)*
$K_{soil\,i-water}$: soil i-water equilibrium distribution coefficient [$m_{water}^3.m_{soil}^{-3}$] *(A)*

$$Css_{pw\,soil\,i} = Css_i \cdot \frac{MOL\,WEIGHT}{K_{soil\,i\text{-}water}} \tag{243}$$

with
$Css_{pw\,soil\,i}$: steady-state concentration in pore water of soil i [g.l^{-1}] *(O)*
Css_i : steady-state concentration in box i (4, 5 or 6) [mol.m^{-3}] *(S)*
$MOL\ WEIGHT$: molecular weight of the chemical [kg.mol^{-1}] *(D)*
$K_{soil\,i\text{-}water}$: soil i-water equilibrium distribution constant [m$_{water}^{3}$.m$_{soil}^{-3}$]*(A)*

$$Css_{susp} = Css_7 \cdot \frac{MOL\,WEIGHT \cdot Kp_{susp}}{K_{susp\text{-}water}} \tag{244}$$

with
Css_{susp} : steady-state concentration in suspended matter [g.kg$_{solid}^{-1}$] *(O)*
Css_7 : steady-state concentration in box 7 [mol.m^{-3}] *(I)*
$MOL\ WEIGHT$: molecular weight of the chemical [kg.mol^{-1}] *(D)*
Kp_{susp} : suspended matter-water partition coefficient [l$_{water}$.kg$_{solid}^{-1}$] *(I)*
$K_{susp\text{-}water}$: suspended matter-water equilibrium distribution coefficient [m$_{water}^{3}$.m$_{susp}^{-3}$] *(A)*

$$Css_{bio} = Css_8 \cdot \frac{MOL\,WEIGHT \cdot BCF_{fish}}{K_{bio\text{-}water}} \tag{245}$$

with
Css_{bio} : steady-state concentration in biota [g.kg$_{solid}^{-1}$] *(O)*
Css_8 : steady-state concentration in box 8 [mol.m^{-3}] *(I)*
$MOL\ WEIGHT$: molecular weight of the chemical [kg.mol^{-1}] *(D)*
BCF_{fish} : biota-water partition coefficient [l$_{water}$.kg$_{fish}^{-1}$] *(I)*
$K_{bio\text{-}water}$: biota-water equilibrium distribution coefficiG15
ent [m$_{water}^{3}$.m$_{bio}^{-3}$] *(A)*

Steady-state "risk quotients"

The term "risk quotient" is used here to indicate the quotient of a computed concentration and the quality standard set for the compartment. "Risk quotients" are displayed in SimpleBox output table 1. The values are obtained from:

$$Qss_{air} = \frac{Css_1}{STND_{air}} \tag{246}$$

with
Qss_{air} : steady-state "risk quotient" for air [-] *(O)*
Css_1 : steady-state concentration in box 1 [mol.m^{-3}] *(I)*
$STND_{air}$: quality standard for air [mol.m^{-3}] *(D)*

$$Qss_{water} = \frac{Css_2}{STND_{water}} \tag{247}$$

with
Qss_{water} : steady-state "risk quotient" for water [-] *(O)*
Css_2 : steady-state concentration in box 2 [mol.m^{-3}] *(I)*
$STND_{water}$: quality standard for water [mol.m^{-3}] *(D)*

$$Qss_{sed} = \frac{Css_3 \cdot \dfrac{Kp_{sed}/1000}{K_{sed\text{-}water}}}{STND_{sed}} \tag{248}$$

with
Qss_{sed} : steady-state "risk quotient" for sediment [-] *(O)*
Css_3 : steady-state concentration in box 3 [mol.m^{-3}] *(I)*

Kp_{sed} : sediment-water partition coefficient [$l_{water}.kg_{solid}^{-1}$] *(I)*
1000 : conversion factor [$l.m^{-3}$] *(C)*
$K_{sed\text{-}water}$: sediment-water equilibrium distribution coefficient [$m_{water}^{3}.m_{sed}^{-3}$] *(A)*
$STND_{sed}$: quality standard for sediment [$mol.kg_{solid}^{-1}$] *(D)*

$$Qss_{soil\,i} = \frac{Css_i \,.\, \dfrac{Kp_{soil\,i} / 1000}{K_{soil\,i\text{-}water}}}{STND_{soil}} \tag{249}$$

with

$Qss_{soil\,i}$: steady-state "risk quotient" for soil i [-] *(O)*
Css_i : steady-state concentration in box i (4, 5 or 6) [$mol.m^{-3}$] *(I)*
$Kp_{soil\,i}$: soil i-water partition coefficient [$l_{water}.kg_{solid}^{-1}$] *(I)*
1000 : conversion factor [$l.m^{-3}$] *(C)*
$K_{soil\,i\text{-}water}$: soil i-water equilibrium distribution coefficient [$m_{water}^{3}.m_{soil}^{-3}$] *(A)*
$STND_{soil}$: quality standard for soil [$g.kg_{solid}^{-1}$] *(D)*

$$Qss_{pw\,soil\,i} = \frac{Css_i / K_{soil\,i\text{-}water}}{STND_{grndwater}} \tag{250}$$

with

$Qss_{pw\,soil\,i}$: steady-state "risk quotient" for groundwater in soil i [-] *(O)*
Css_i : steady-state concentration in box i (4, 5 or 6) [$mol.m^{-3}$] *(I)*
$K_{soil\,i\text{-}water}$: soil i-water equilibrium distribution coefficient [$m_{water}^{3}.m_{soil}^{-3}$] *(A)*
$STND_{grndwater}$: quality standard for groundwater [$g.kg_{solid}^{-1}$] *(D)*

2.4.2 Quasi-dynamic computation

As an option, the response of the system to changes in loadings (emissions or imports), i.e., the development toward an eventual steady state, may be computed. This computation is called "quasi-dynamic" since, besides the loadings, all the model parameters are assumed to be constant in time. The computation is done by a separate integration routine that numerically integrates the mass balance equations described in the previous paragraphs. To this end, the mass balances are rewritten in the following format:

$$\frac{dc(i)}{dt} = \frac{emis(i) + imp(i) + cf(i1).c(1) + cf(i2).c(2) + \ldots\ldots\ldots\ldots + cf(i8).c(8)}{v(i)} \tag{251}$$

with

$c(i)$: concentration in box i [$mol.m^{-3}$] *(S)*
t : time [s] *(S)*
$emis(i)$: emission mass flow into box i [$mol.s^{-1}$] *(I)*
$imp(i)$: import mass flow into box i [$mol.s^{-1}$] *(I)*
$cf(ij)$: sum of coefficients for (apparent) transport to and from box i [$m^{3}_{medium\,i}.s^{-1}$] *(I)*
$v(i)$: volume of box i [m^3] *(I)*

In these mass balance equations, the parameters *v(i)* and *cf(ij)* have the same values as their equivalents V_i and CF_{ij} in equations (214) and (215), used for computation of the steady-state solution. These parameter values are written into a settings table, which is read by the integration routine. The parameters *emis(i)* and *imp(i)* are read by the integration routine from a scenario table. The most commonly used loadings scenario is a "block scenario", in which the loadings have the value used in the steady-state computation for a period of time, long enough to approach the steady state, followed by the value zero for an equally long period of time. Using this scenario, both the development toward the steady state that has been computed and the recovery upon elimination of sources are computed. This computation is known in "Mackay-nomenclature" as "level 4 computation". The quasi-dynamic computation routine produces the following output:

Concentration-time series

Concentrations at pre-set time intervals are written by the integration routine into SimpleBox output table 4. The concentrations are expressed as percentages of the steady-state concentration, computed earlier:

$$C_i = \frac{c(i)}{Css_i} \cdot 100 \tag{252}$$

with

C_i : concentration in box i at time t, referenced to the steady-state concentration [%] *(O)*
$c(i)$: concentration in box i at time t [$\mathrm{mol.m^{-3}}$] *(S)*
Css_i : steady-state concentration in box i [$\mathrm{mol.m^{-3}}$] *(I)*

Amount-time series

Also, the total amount of the chemical present in the whole system is saved:

$$TOTAL = \frac{\Sigma\, c(i) \cdot v(i)}{\Sigma\, Css_i \cdot v(i)} \cdot 100 \tag{253}$$

with

$TOTAL$: amount of the chemical in the system at time t, referenced to the hold-up at steady-state [%] *(O)*
$c(i)$: concentration in box i at time t [$\mathrm{mol.m^{-3}}$] *(S)*
$v(i)$: volume of box i [$\mathrm{m^3}$] *(I)*
Css_i : steady-state concentration in box i [$\mathrm{mol.m^{-3}}$] *(I)*

"Risk quotient"-time series

"Risk-quotients" at the same time intervals are computed as:

$$Q_i = \frac{c(i)}{stnd(i)} \tag{254}$$

with

Q_i : "risk quotient" for box i [-] *(O)*
$c(i)$: concentration in box i at time t [$\mathrm{mol.m^{-3}}$] *(S)*
$stnd(i)$: quality standard for box i [$\mathrm{mol.m^{-3}}$] *(D)*

The parameters *stnd(i)* have the same values as the equivalents $STND_i$ in the steady-state computation, after conversion of the solids-based values (sediment, soil) to volume-base.

3 THE SIMPLEBOX MODEL CODE

3.1 SimpleBox modules

The SimpleBox model was developed as a spreadsheet. The various versions that have been produced in the past all had the same basic structure, consisting of three main parts: an "input block", a "computation block" and an "output block". The computation block was common to all; modifications were made to the input- and output blocks (Figure 3).

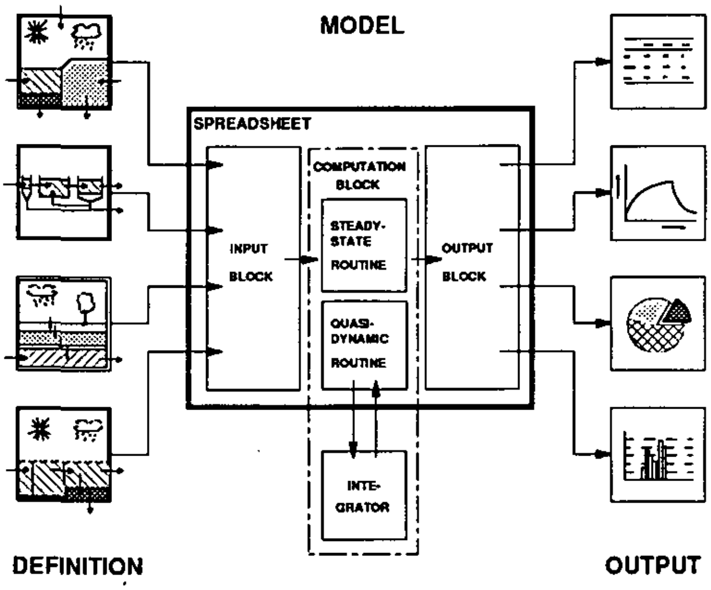


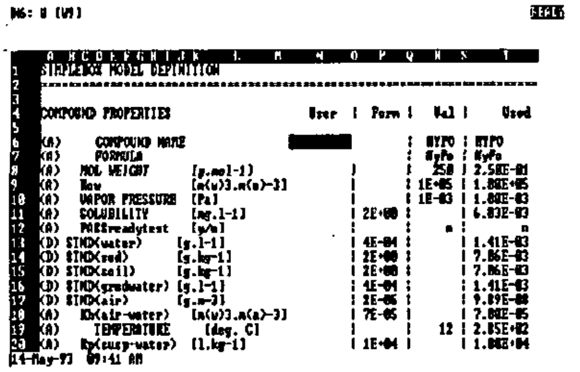
Figure 3 SimpleBox spreadsheet lay-out

The present SimpleBox model still has the same basic modular structure. The spreadsheet consists of the following modules: definition blocks (2), steady-state computation block, quasi-dynamic computation blocks (3), output blocks (4), macro block and start-up screen. A navigation plan and a print-out of the contents of each of these blocks, as it appears on the screen while in SimpleBox, is given as an appendix (A-1); the individual modules are further described in the following paragraphs.

The SimpleBox variables as described in the previous chapter appear in the spreadsheet as cells. As a general rule, these cells are placed directly to the right of a cell containing a text string that corresponds as closely as possible to the variable names used in this document. The cells are usually named with this text string ("label" in Lotus123). The cell names defined in the SimpleBox spreadsheet are listed in the appendix (A-23).

Definition

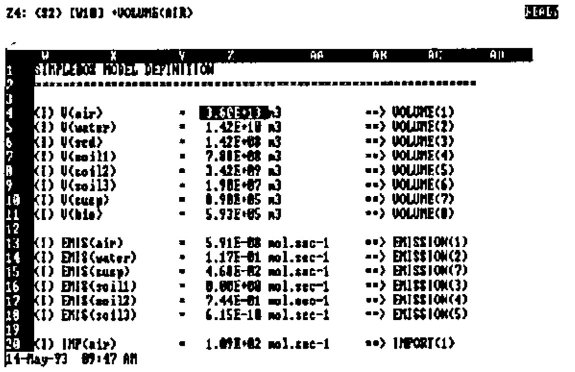
The definition module consists of two blocks, *DEFINITION1* (Figure 4) and *DEFINITION2* (Figure 5). The block *DEFINITION1* is where the actual model definition is entered into the spreadsheet; this is the first of the few places in the spreadsheet where user input is required. A



```
N6: 0 (W9)                                                    READY

   A B C D E F G H I J K    L     M     N     O   P   Q   R   S    T
1  SIMPLEBOX MODEL DEFINITION
2  ====================================================================
3
4  COMPOUND PROPERTIES                       User  | Form |  Val |    Used
5
6  (A)      COMPOUND NAME                                 ! HYPO ! HYPO
7  (A)      FORMULA                                       ! HyPo ! HyPo
8  (A)    MOL WEIGHT      [g.mol-1]           |          !  250 | 2.50E+02
9  (A)    Kow             [m(w)3.m(o)-3]      |          ! 1E+05 | 1.00E+05
10 (A)    VAPOR PRESSURE  [Pa]                |          ! 1E-03 | 1.00E-03
11 (A)    SOLUBILITY      [mg.l-1]            | 2E+00 !          | 6.83E-03
12 (A)    PASSreadytest   [y/n]               !       !      n !        n
13 (D) STND(water)       [g.l-1]              | 4E-04 !          | 1.41E-03
14 (D) STND(sed)         [g.kg-1]             | 2E+00 !          | 7.86E-03
15 (D) STND(soil)        [g.kg-1]             | 2E+00 !          | 7.86E-03
16 (D) STND(grndwater)   [g.l-1]              ! 4E-04 !          ! 1.41E-03
17 (D) STND(air)         [g.m-3]              ! 2E-06 !          ! 9.89E-08
18 (A)    Kh(air-water)   [m(w)3.m(a)-3]      | 7E-05 |          | 7.00E-05
19 (A)      TEMPERATURE     [deg. C]          |       |       12 ! 2.85E+02
20 (A)    Kp(susp-water)  [l.kg-1]            | 1E+04 |          | 1.00E+04
14-May-93  09:41 AM
```

Figure 4 *First screen of the spreadsheet block "DEFINITION1"; see also appendix (A-3)*



```
Z4: (S2) [W10] +VOLUME(AIR)                                   READY

   W          X        Y       Z             AA       AB       AC       AD
1  SIMPLEBOX MODEL DEFINITION
2  ==============================================================
3
4  (I) V(air)          =   3.60E+13 m3              --> VOLUME(1)
5  (I) V(water)        =   1.42E+10 m3              --> VOLUME(2)
6  (I) V(sed)          =   1.42E+08 m3              --> VOLUME(3)
7  (I) V(soil1)        =   7.80E+08 m3              --> VOLUME(4)
8  (I) V(soil2)        =   3.42E+09 m3              --> VOLUME(5)
9  (I) V(soil3)        =   1.90E+07 m3              --> VOLUME(6)
10 (I) V(susp)         =   8.90E+05 m3              --> VOLUME(7)
11 (I) V(bio)          =   5.93E+05 m3              --> VOLUME(8)
12
13 (I) EMIS(air)       =   5.91E-08 mol.sec-1       --> EMISSION(1)
14 (I) EMIS(water)     =   1.17E-01 mol.sec-1       --> EMISSION(2)
15 (I) EMIS(susp)      =   4.60E-02 mol.sec-1       --> EMISSION(7)
16 (I) EMIS(soil1)     =   0.00E+00 mol.sec-1       --> EMISSION(3)
17 (I) EMIS(soil2)     =   7.44E-01 mol.sec-1       --> EMISSION(4)
18 (I) EMIS(soil3)     =   6.15E-10 mol.sec-1       --> EMISSION(5)
19
20 (I) IMP(air)        =   1.09E+02 mol.sec-1       --> IMPORT(1)
14-May-93  09:47 AM
```

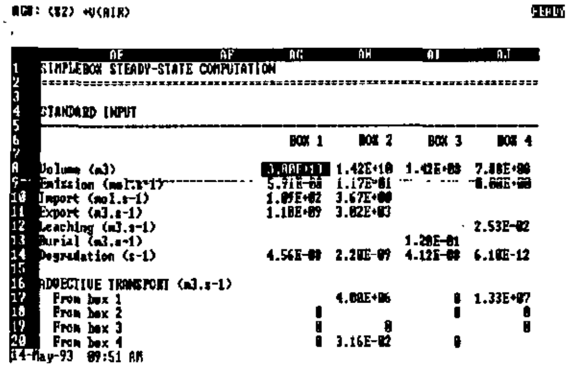
Figure 5 *First screen of the spreadsheet block "DEFINITION2"; see also appendix (A-5)*

value needs to be assigned by the user to each of the SimpleBox "definition parameters". The definition parameters are labeled "(D)" in the first column. Values can be assigned in two ways:

1. By entering a value into the cell to the right of the parameter name in the column labeled "User", using the units that are given in square brackets to the right of the variable name.
2. By accepting the value that appears in either the column labeled "Form" (indicating that an estimation formula is producing the number shown) or the column labeled "Val" (indicating that a fixed default value is producing the number). This default formula or value is accepted by entering nothing (or the value zero, which is equivalent) into the cell. Usually a number appears in one of the columns only. When both columns contain a number, the number in the column "Form" is used, unless the user overrides this by entering the number that appears in the column "Def" into the column "User".

The numbers that appear in the column labeled "Def" do not depend on the values assigned to other cells in the spreadsheet. The numbers in the column labeled "Form" do. The estimation formulas that produce the numbers take the values of auxiliary parameters as input. As a rule, the auxiliary parameters used are placed in the rows immediately below, the text strings that label them indented. The result returned by the estimation formulas changes when the value of any of the used auxiliary parameters are changed, as the spreadsheet is recalculated automatically after each data entry.

This way a value is assigned to the cell in the column labeled "Used". This is done by a conditional statement in this cell that takes either the user input (column "User"), the estimation formula (column "Form") or the default value (column "Def") as input and converts this into internal SimpleBox units (MKS). The values in the column "Used" are used as the SimpleBox model definition. The cells in this column carry the names of the corresponding variable names. The second definition block serves as an interface between the input block and the actual computation. *DEFINITION2* uses the values of the definition parameters set in *DEFINITION1* to produce the internal variables that are to be used in the mass balance equations. The output of this block is the full model definition. The values are used in the SimpleBox computation block; the box numbers used are indicated in the last column of this block.



```
AG8: (S2) +V(AIR)                                                READY

       AE                    AF          AG         AH         AI         AJ
1   SIMPLEBOX STEADY-STATE COMPUTATION
2   ========================================================================
3
4   STANDARD INPUT
5   ------------------------------------------------------------------------
6                                      BOX 1      BOX 2      BOX 3      BOX 4
7
8   Volume (m3)                    [illegible]  1.42E+10   1.42E+08   7.88E+08
9   Emission (mol.s-1)              5.71E-08   1.17E+01              8.60E+00
10  Import (mol.s-1)                1.09E+02   3.67E+00
11  Export (m3.s-1)                 1.18E+09   3.02E+03
12  Leaching (m3.s-1)                                                2.53E-02
13  Burial (m3.s-1)                                       1.20E-01
14  Degradation (s-1)               4.56E-08   2.20E-09   4.12E-08   6.10E-12
15
16  ADVECTIVE TRANSPORT (m3.s-1)
17    From box 1                               4.00E+06          0   1.33E+07
18    From box 2                           0                     0          0
19    From box 3                           0          0                     0
20    From box 4                           0   3.16E-02          0
14-May-93  09:51 AM
```

Figure 6 *First screen of the spreadsheet block "SSCOMPUTATION"; see also appendix (A-6)*

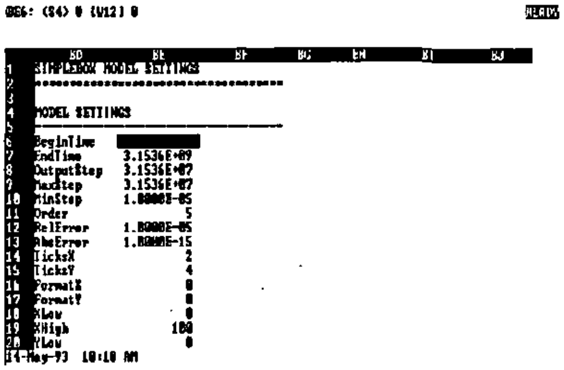
Steady-state computation

The computation of the steady-sate solution as described in paragraph 2.4.1, is done in the block *SSCOMPUTATION* (Figure 6). The values of the internal model parameters from *DEFINITION2* are assigned to numbered boxes. The output of this block consists of the steady-state concentrations in standard units, shown in the row labeled "CONCENTRATION (mol.m^{-3})"; the steady-state fugacities, shown in the row labeled "FUGACITIES (Pa)"; the total amount of chemical present in the total system at steady state, shown in the row labeled "HOLD-UP (mol)"; the percentual distribution at steady state, shown in the row labeled "DISTRIBUTION (%)"; and the throughput at steady state, shown in the row labeled "THROUGHPUT". There are two rows labeled "THROUGHPUT"; the first is computed as the sum of all inputs, the second is the sum of all outputs. These numbers are used in the development stage of new model definitions only; the two numbers should be equal for correctly defined models. Differences greater than the rounding error of the spreadsheet program indicate errors in the model definition.

The steady-state computation requires inversion of the matrix in mass balance coefficients, *CF*, multiplication of the inverse matrix, CF^{-1}, with the vector of constants, *CNST* and recalculation of the spreadsheet. In the Lotus123-code of SimpleBox, this is done by a series of instructions in the macro *COMPUTE* or *ALT-C*.

Quasi-dynamic computation

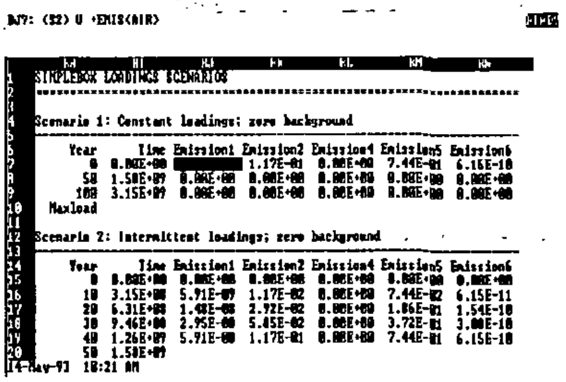
This part of the model code is discussed only briefly here. The integration is done on the basis of Wortelboer and Aldenberg's Friendly Applied Modeling Environment FAME, version 3.0. Discussion of this process is beyond the scope of this document. For further information, the reader is referred to the FAME program documentation (Wortelboer and Aldenberg, 1991).



```
BE6: (S4) U [W12] 0                                    READY

         BD         BE        BF     BG     BH     BI     BJ
1   SIMPLEBOX MODEL SETTINGS
2   ****************************************
3
4   MODEL SETTINGS
5   ----------------------------------------
6   BeginTime
7   EndTime      3.1536E+09
8   OutputStep   3.1536E+07
9   MaxStep      3.1536E+07
10  MinStep      1.0000E-05
11  Order                 5
12  RelError     1.0000E-05
13  AbsError     1.0000E-15
14  TicksX                2
15  TicksY                4
16  FormatX               0
17  FormatY               0
18  XLow                  0
19  XHigh               100
20  YLow                  0
14-May-93  10:10 AM
```

Figure 7 *First screen of the spreadsheet block "DYNCOMPUTATION2"; see also appendix (A-11)*



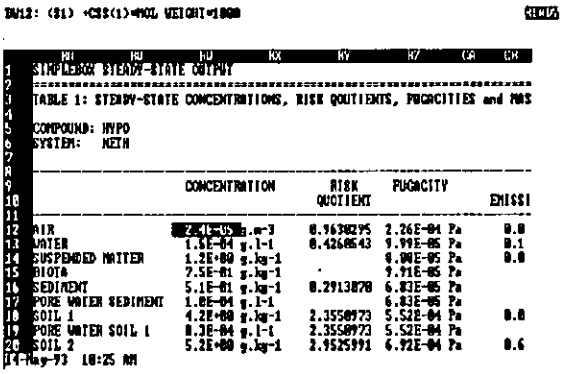
```
KJ7: (S2) U +EMIS(AIR)

          KH        KI        KJ        KK        KL        KM        KN
1   SIMPLEBOX LOADINGS SCENARIOS
2   ***********************************************************************
3
4   Scenario 1: Constant loadings; zero background
5   -----------------------------------------------------------------------
6         Year      Time Emission1 Emission2 Emission4 Emission5 Emission6
7            0  0.00E+00           1.17E-01  0.00E+00  7.44E-01  6.15E-10
8           50  1.50E+09  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00
9          100  3.15E+09  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00
10     Maxload
11
12  Scenario 2: Intermittent loadings; zero background
13  -----------------------------------------------------------------------
14        Year      Time Emission1 Emission2 Emission4 Emission5 Emission6
15           0  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00
16          10  3.15E+08  5.91E-09  1.17E-02  0.00E+00  7.44E-02  6.15E-11
17          20  6.31E+08  1.48E-08  2.72E-02  0.00E+00  1.86E-01  1.54E-10
18          30  9.46E+08  2.95E-08  5.45E-02  0.00E+00  3.72E-01  3.00E-10
19          40  1.26E+09  5.91E-08  1.17E-01  0.00E+00  7.44E-01  6.15E-10
20          50  1.50E+09
14-May-93  10:21 AM
```

Figure 8 *First screen of the spreadsheet block "DYNCOMPUTATION3"; see also appendix (A-13)*

The quasi-dynamic computation consists of three spreadsheet blocks plus the external integration program. The first block of the dynamic computation module, *DYNCOMPUTATION1*, contains the model code of the integration routine. This text has been used once, in the development stage, to compile the integrator, *SIMINT.exe*. A print-out of *DYNCOMPUTATION1* can be found in the appendix. The second and third block of the dynamic computation module, *DYNCOMPUTATION2* (Figure 7) and *DYNCOMPUTATION3* (Figure 8), produce the texts that are read by the integrator as a settings-file and a scenario file, respectively, any time the integration routine is carried out. The integration process can be controlled by editing these blocks of the spreadsheet. For standard operation, it suffices to accept the settings and standard loadings scenario. Calling the integration routine then results in computation of the development towards a steady state with the same model definition as was used for computation of the steady-sate solution. The computation starts from time zero

concentrations. A block scenario is assumed for the loadings: at time zero the constant loadings as used for the steady-state computation are applied for a period of 50 years, followed by a period of 50 years with zero loadings. It is suggested that only experienced users attempt to set custom integration scenarios after consulting the FAME-documentation (Wortelboer and Aldenberg, 1991).
The quasi-dynamic computation is carried out by the macro *INTEGRATE* or *ALT-I*. This macro first creates the DOS-files that are necessary to externally perform the integration: it prints the contents of the block *INTEGRAT.bat* to a text file with the same name to create a DOS integration batch and it prints the contents of the blocks *DYNCOMPUTATION2* and *DYNCOMPUTATION3* to the text files *SIMINT.set* and *SIMINT.scn*, respectively. The macro then starts a new DOS-environment and calls the newly created DOS-batch *INTEGRAT.bat*. The integration batch then starts the integrator, *SIMINT.exe*, which reads the model definition and loadings scenario from the files *SIMINT.set* and *SIMINT.scn* and carries out the integration, producing a raw output file *SIMINT.res*. The FAME-utility *SPLITRES.exe* is then called by *INTEGRAT.bat* to convert the raw output into the spreadsheet-readable output file *INTEGRAT.dat*. The DOS-batch *INTEGRAT.bat* ends and control is returned to the spreadsheet macro. The macro then reads the integration results from the file *INTEGRAT.dat* and produces a graph of these data on screen, using the spreadsheet graphing functions.



```
BW12: ($1) +C$$(1)*MOL WEIGHT*1000                                          READY

      BU         BV         BW          BX          BY          BZ       CA    CB
1   SIMPLEBOX STEADY-STATE OUTPUT
2   ========================================================================
3   TABLE 1: STEADY-STATE CONCENTRATIONS, RISK QOUTIENTS, FUGACITIES and MAS
4
5   COMPOUND: HYPO
6   SYSTEM:   NETH
7
8   ------------------------------------------------------------------------
9                             CONCENTRATION     RISK      FUGACITY
10                                            QUOTIENT                  EMISSI
11  ------------------------------------------------------------------------
12  AIR                      2.4E-05 g.m-3   0.9630295  2.26E-04 Pa      0.0
13  WATER                    1.5E-04 g.l-1   0.4260543  9.99E-05 Pa      0.1
14  SUSPENDED MATTER         1.2E+00 g.kg-1             9.00E-05 Pa      0.0
15  BIOTA                    7.5E-01 g.kg-1             9.91E-05 Pa
16  SEDIMENT                 5.1E-01 g.kg-1  0.2913878  6.83E-05 Pa
17  PORE WATER SEDIMENT      1.0E-04 g.l-1              6.83E-05 Pa
18  SOIL 1                   4.2E+00 g.kg-1  2.3550973  5.52E-04 Pa      0.0
19  PORE WATER SOIL 1        8.3E-04 g.l-1   2.3550973  5.52E-04 Pa
20  SOIL 2                   5.2E+00 g.kg-1  2.9525991  6.92E-04 Pa      0.6
14-May-93  10:25 AM
```

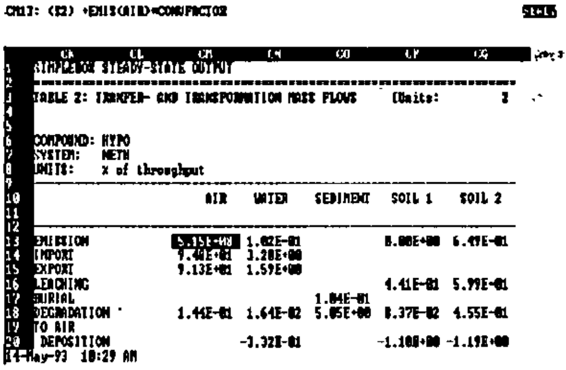
Figure 9 *First screen of the spreadsheet block "SSOUTPUT1"; see also appendix (A-14)*

Output

The SimpleBox output consists of four blocks. The first block, *SSOUTPUT1*, is a table listing the steady-state concentrations in "common" units, the steady-state "risk quotients", the steady-state fugacities and the main characteristics of the steady-state mass balance, as described in paragraph 2.4.1. The second output block, *SSOUTPUT2*, is a extensive listing of all steady-state mass flows. The mass flows can be read out in four different units:

1: moles per second [$mol.s^{-1}$]
2: % of THROUGHPUT [%]
3: metric tons per year [$t.yr^{-1}$]
4: kilograms per day [$kg.d^{-1}$]

This is controlled by the number in the cell right of the label "Units:" in the top line of the table. This number can be changed by the user.
The third output block, *SSOUTPUT3*, is a table that is designed to be used to document the exposure



```
CM17: (S2) +EMIS(AIR)*CONVFACTOR

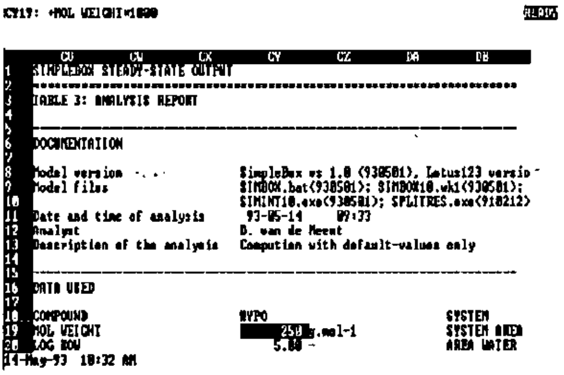
SIMPLEBOX STEADY-STATE OUTPUT
=================================================================
TABLE 2: TRANSFER- AND TRANSFORMATION MASS FLOWS     (Units:        %


COMPOUND: HYPO
SYSTEM:   METH
UNITS:    % of throughput
-----------------------------------------------------------------
                        AIR      WATER    SEDIMENT  SOIL 1    SOIL 2

-----------------------------------------------------------------
EMISSION              5.15E+00 1.02E-01            8.00E+00 6.49E-01
IMPORT                9.40E+01 3.20E+00
EXPORT                9.13E+01 1.59E+00
LEACHING                                           4.41E-01 5.99E-01
BURIAL                                   1.04E-01
DEGRADATION           1.44E-01 1.64E-02 5.05E+00  8.37E-02 4.55E-01
TO AIR
 DEPOSITION                   -3.32E-01           -1.10E+00 -1.19E+00
14-May-93  10:29 AM
```

Figure 10   First screen of the spreadsheet block "SSOUTPUT2"; see also appendix (A-15)

analysis that is carried out using SimpleBox. To this end, it specifies the model version and model files, that produced the output, the name of the analyst and the date and time that the results were produced. The user has the option to further document the analysis with some comments. It further echoes the values that were assigned to the most important model parameters. It finally lists the results of the steady-state computation.



```
CY19: +MOL WEIGHT*1000

SIMPLEBOX STEADY-STATE OUTPUT
*****************************************************************
TABLE 3: ANALYSIS REPORT

-----------------------------------------------------------------
DOCUMENTATION

Model version               SimpleBox vs 1.0 (930501), Lotus123 versio
Model files                 SIMBOX.bat(930501); SIMBOX10.wk1(930501);
                            SIMINT10.exe(930501); SPLITRES.exe(910212)
Date and time of analysis    93-05-14     09:33
Analyst                     D. van de Meent
Description of the analysis Compution with default-values only

-----------------------------------------------------------------
DATA USED

COMPOUND                    HYPO                        SYSTEM
MOL WEIGHT                       250 g.mol-1            SYSTEM AREA
LOG KOW                         5.00 -                  AREA WATER
14-May-93  10:32 AM
```

Figure 11   First screen of the spreadsheet block "SSOUTPUT3"; see also appendix (A-16)

The fourth output block, *DYNOUTPUT*, lists the results of the integration that was carried out last.

Operation

The operation of SimpleBox is controlled by the following DOS-batch files and spreadsheet macro-instructions:

- The start-up DOS-batch file *SIMBOX.bat*. SimpleBox modeling sessions are started from this batch that performs two tasks only: (i) start the SimpleBox spreadsheet and (ii) delete the intermediate results files upon finishing.
- The integration batch file *INTEGRAT.bat* described in the previous paragraph

- The six spreadsheet macros contained in the block *MACROS*.
    - The start-up macro. Labeled *START* and *\0*. In normal spreadsheet operation, this macro is carried out upon starting the spreadsheet. It may also be started with *ALT-Z*. It shows the spreadsheet block *STARTSCREEN*, pauses for reading of the welcome message and moves the cell pointer to the model definition block.
    - The computation macro. Labeled *COMPUTE* and *\C*, to be started with *ALT-C*. Recalculates the spreadsheet, carries out the steady-state computation and recalculates the sheet once more.
    - The integration macro. Labeled *INTEGRATE* and *\I*, to be started with *ALT-I*. Described in the previous paragraph.
    - The postscript print macro. Labeled *REPORT PP* and *\P*, to be started with *ALT-P*. If the spreadsheet is in the WYSIWYG-mode (available in Lotus123 version 2.3 and up), this macro prints a full report to the postscript printer. The spreadsheet blocks *DEFINITION1*, *DEFINITION2*, *SCOMPUTATION*, *SSOUTPUT1*, *SSOUTPUT2* and *SSOUTPUT3* are printed with proper headers and footers.
    - The laser print macro. Labeled *REPORT LP* and *\L*, to be started with *ALT-L*. For printing to laser printers of the HP-laserjet type. Prints *DEFINITION1* and *SSOUTPUT3* with headers and footers.
    - The matrix print macro. Labeled *REPORT MP* and *\M*, to be started with ALT-M. For printing to dot matrix printers. Prints *DEFINITION1* and *SSOUTPUT3* with headers and footers.

3.2 Running the model

The SimpleBox spreadsheet that is distributed with this document is a so-called "compiled spreadsheet". The spreadsheet was created originally in Lotus123 version 2.2 as *SIMBOX10.wk1*. A "compiled executable" of the Lotus-Simbox couple was created using the spreadsheet-compiler software Baler Express version 1.0. All Lotus123 menu-options that are not essential to the operation of the SimpleBox sheet have been disabled in this compilation. The product, *SIMBOX10.exe*, is a spreadsheet that can be run as a stand-alone, without the original spreadsheet software installed, on IBM-PC compatible computers. The formulas in the compiled spreadsheet cannot be changed, neither accidently nor on purpose. Data can only be entered into the cells that are unprotected.

This SimpleBox code has been tested on a limited number of computers; no limitations other then the requirement of as much free memory space as possible have been found so far. The printing macros have hardly been tested at all; they functioned properly in the author's computer environment. It may be necessary to adjust the Lotus123 printing options. These menu options are enabled in the compiled spreadsheet.

The distribution diskette contains the following files:
- *SIMBOX.bat (930501)*
- *SIMBOX10.wkb (930501)*

- *SIMBOX10.exe (930501)*
- *SIMINT.exe (930501)*
- *SPLITRES.exe (910212)*

These files may be copied to the hard disk.

To run SimpleBox, take the following steps:

- from the DOS-prompt,

  type "SIMBOX" to start *SIMBOX.bat*
- in the spreadsheet,
  - Define a model by assigning values to the SimpleBox definition parameters. Some knowledge of the operation of Lotus123 is required to do this.

    NOTE: entering the number zero, or leaving the cell blank leads to acceptance of the default estimation or default value
  - Compute the steady-state solution by typing *ALT-C*
  - Read the results from the output tables, change model definition and re-run the computation
  - Complete the documentation of the analysis by typing the analyst's name and comments into the designated area of output table 4
  - Print the results by typing *ALT-P*, *ALT-L* or *ALT-M*
  - Optionally run the quasi-dynamic computation by typing *ALT-I*

    NOTE 1: Depending on the model definition and the computing power available, this may take a long time; use of 80386, preferably equipped with mathematical co-processor, or better is advised.

    NOTE 2: Running the integrator with the model program in memory requires more conventional memory than is commonly available; freeing as much of conventional memory as possible, and making at least 128 Kbytes of expanded memory available is, to the best of the author's knowledge, the only way to achieve this.
  - Optionally save the model definition by typing */f(ile), s(ave)*, followed by entering a file name at the program prompt
  - End the SimpleBox session by typing */q(uit)*, and *y(es)* at the program prompt

REFERENCES

Cohen, Y. and Ryan, P.A. (1985). Multimedia modeling of environmental transport: trichloroethylene test case. Environ. Sci. Technol. 19, 412-417.

DiToro, D.M., Zarba, C.S., Hansen, D.J., Berry, W.J., Swartz, R.C., Cowan, C.E., Pavlou, S.P., Allen, H.E., Thomas, N.A. and Paquin, P.R. (1991). Technical basis for establishing sediment quality criteria for nonionic organic chemicals using equilibrium partitioning. Environ. Toxicol. Chem., 10, 1541-1583.

Frische, R., Klopffer, W., Rippen, G. and Gunther, K-L. (1984). The environmental model segment approach for estimating potential environmental concentrations. I. The model. Ecotoxicol. Environ. Safety, 8, 352-362.

Hansch, C., Quinlan, J.E. and Lawrence, G.L. (1968). The linear free-energy relationships between partition coefficients and the aquaeous solubility of organic liquids. J. Org. Chem., 33, 347-350.

Junge, C.E. (1977). In: Fate of pollutants in the air and water environment (I.H. Suffet, ed.), pp. 7-25, Wiley-Interscience.

Lyman, W.J., Rheel, W.F. and Rosenblatt, D.H. (1982). Handbook of environmental property estimation. McGraw-Hill.

Mackay, D. (1979). Finding fugacity feasible. Environ. Sci. Technol., 13, 1218.

Mackay, D. (1982). Correlation of bioconcentration factors. Environ. Sci. Technol., 16, 274-278.

Mackay, D. (1991). Multimedia environmental models. Lewis, Chelsea, MI.

Mackay, D. and Paterson, S. (1981). Calculating fugacity. Environ. Sci. Technol., 15, 1006-1014.

Mackay, D., Paterson, S., Cheung, B. and Neely, W.B. (1985). Evaluating the environmental behavior of chemicals with a level III model. Chemosphere, 14, 335-374.

Mackay, D., Paterson, S. and Shiu, W.Y. (1992). Generic models for evaluating the regional fate of chemicals. Chemosphere, 24, 695-717.

Meylan, W.M. and Howard, P.H. (1991). Bond contribution method for estimating Henry's law constants. Environ. Toxicol. Chem., 10, 1283-1293.

OECD (1989). Compedium of environmental exposure assessment methods for chemicals. Method 604: SIMPLEBOX (pp. 333-338); Method 506: SIMPLESAL (pp. 278-288); Method 109: SIMPLETREAT (pp. 51-58). OECD Environmental Monographs No. 27, Paris, July 1989, 350 pp.

Rippen, G., Klopffer, W., Frische, R. and Gunther, K.O. (1984). The environmental model segment approach for estimating potential environmental concentrations. II. Application of the model to p-dichlorobenzene and trichlorobenzene. Ecotoxicol. Environ. Safety, 8, 363-377.

RPC (1991). Prototype model uniform substances evaluation system (UBS); a decision support system. Delft, Resources Planning Consultants, April 1991 [in Dutch].

Ryan, P.A. and Cohen, Y. (1986). Multimedia transport of particle-bound organics: benzo(a)pyrene test case. Chemosphere, 15, 21-47.

Singh, K.P. and Van de Meent, D. (1989). Mathematical modeling of transfer, transport and transformation of chemicals in the environment. SimpleSingh, a spacially inhomogeneous box modeling system. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report nr. 768803 002.

Struijs, J. and Van de Meent, D. (1988). The use of a multimedia box model to predict the emission patterns of xenobiotics in a waste water treatment plant. In: Proceedings of the CEC-COST 641 workshop on "Behaviour of organic micropollutants in biological waste water treatment", pp 181-184, Commission of the European Communities Report EUR 11356 (1987).

Struijs, J. and Van den Berg, R. (1993). Standardized biodegradability tests: extrapolation to aerobic environments. Water Res., submitted for publication.

Struijs, J., Stoltenkamp, J. and Van de Meent, D. (1991). SimpleTreat, a box model of the behavior of micropollutants during waste water treatment. Water Research, 25, 891-900.

Travis, C.C., Dennison, J.W. and Arms, A.D. (1987). The extend of multimedia partitioning of organic chemicals. Chemosphere, 16, 117-125.

Van de Meent, D. (1987). Intercompartment transfer of pollutants: The case of lead. Discussion paper presented at the ECE-Workshop "Transfer of pollutants from one compartment to another", Como, Italy, March 1987.

Van de Meent, D. (1988). Exposure modeling I: Principles, and Exposure modeling II: The use of simple box models. In: Manual on Aquatic Ecotoxicology (H.A.M. de Kruijf, D. de Zwart, P.K. Ray and P.N. Viswanathan, eds.), pp. 77-81, and pp. 82-87, Allied Publishers Pvt. Ltd., New Delhi.

Van de Meent, D. (1989). Evaluation System New Chemicals. SIMPLERISK, a model to estimate local concentrations in water and soil. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report nr. 718706 001 [in Dutch].

Van de Meent, D. (1990). Modelling intercompartment transfer of pollutants: the case of lead. Sci. Total Environ., 90, 41-54.

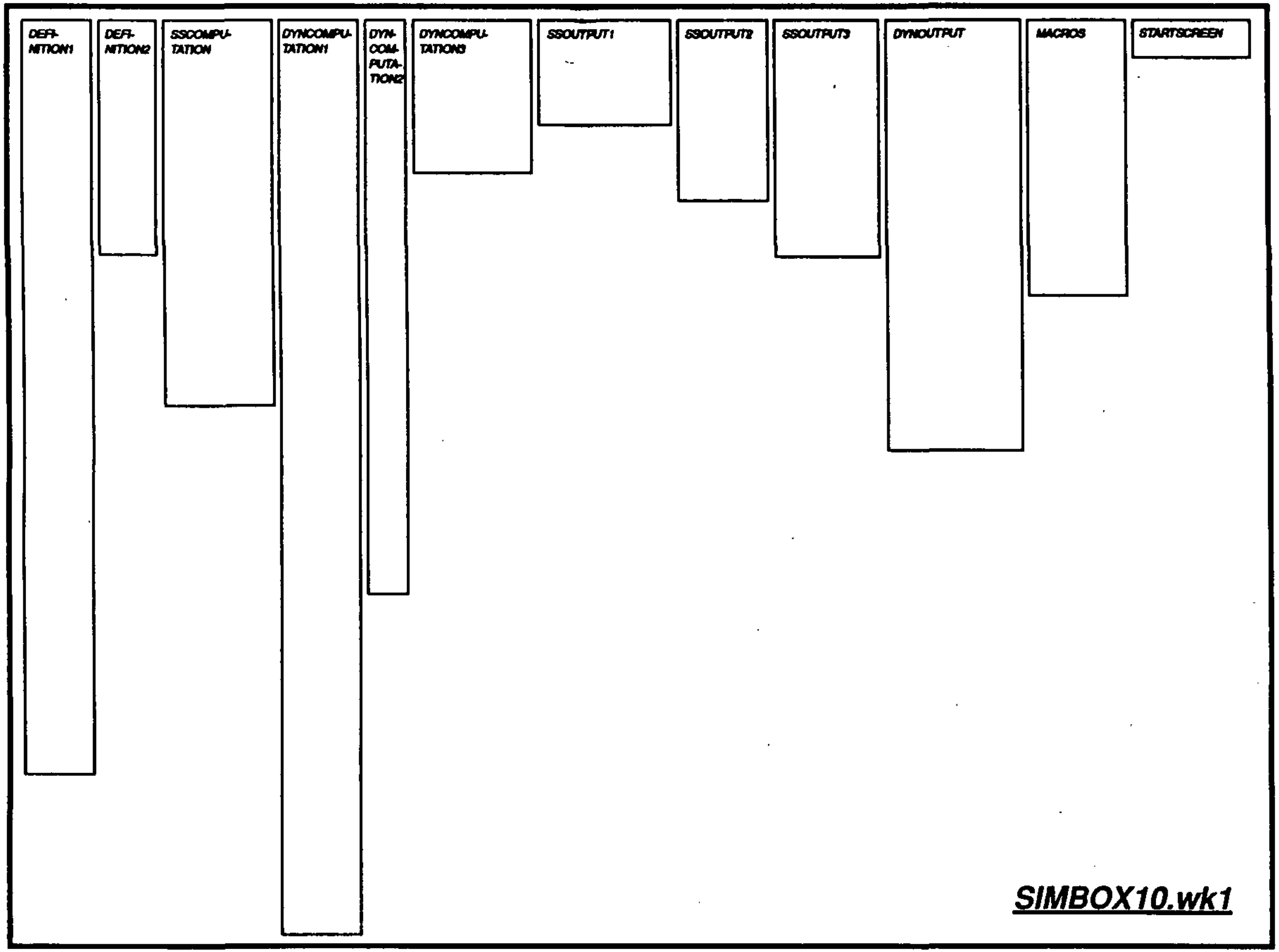
Van de Meent, D. and De Bruijn, J.H.M. (1993). A modeling procedure to evaluate the coherence of independently derived environmental quality objectives for air, water and soil. Environ. Toxicol. Chem., submitted for publication.

Van de Meent, D. and Toet, C. (1992) Dutch Priority Setting System for Existing Chemicals, a systematic procedure for ranking chemicals according to increasing environmental hazard. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM), Report nr. 679120 001.

Van Leeuwen, C.J., P.T.J. van der Zandt, T. Aldenberg, H.J.M. Verhaar and J.L.M. Hermens (1992). The application of QSARs, extrapolation and equilibrium partitioning in aquatic effects assessment for narcotic pollutants. Environ. Toxicol. Chem., 11, 267-282.

Wortelboer, F.G. and Aldenberg, T. (1991) FAME, Friendly Applied Modelling Environment. Version 3.0 User Manual. Bilthoven, National Institute of Public Health and Environmental Protection (RIVM).

APPENDIX


DEFI-NITION1
DEFI-NITION2
SSCOMPU-TATION
DYNCOMPU-TATION1
DYN-COM-PUTA-TION2
DYNCOMPU-TATION3
SSOUTPUT1
SSOUTPUT2
SSOUTPUT3
DYNOUTPUT
MACROS
STARTSCREEN
SIMBOX10.wk1

SIMPLEBOX MODEL DEFINITION

COMPOUND PROPERTIES			User	Form	Val	Used
(A)	COMPOUND NAME				HYPO	HYPO
(A)	FORMULA				HyPo	HyPo
(A)	MOL WEIGHT	[g.mol-1]			250	2.50E-01 kg.mol-1
(A)	Kow	[m(w)3.m(o)-3]			1E+05	1.00E+05 -
(A)	VAPOR PRESSURE	[Pa]			1E-03	1.00E-03 Pa
(A)	SOLUBILITY	[mg.l-1]		2E+00		6.03E-03 mol.m-3
(A)	PASSreadytest	[y/n]			n	n
(D)	STND(water)	[g.l-1]		4E-04		1.41E-03 mol.m-3
(D)	STND(sed)	[g.kg(d)-1]		2E+00		7.06E-03 mol.kg-1
(D)	STND(soil)	[g.kg(d)-1]		2E+00		7.06E-03 mol.kg-1
(D)	STND(grndwater)	[g.l-1]		4E-04		1.41E-03 mol.m-3
(D)	STND(air)	[g.m-3]		2E-05		9.89E-08 mol.m-3
(A)	K(air-water)	[-]		7E-05		7.00E-05 -
(A)	TEMPERATURE	[deg. C]			12	2.85E+02 K
(A)	K(susp-water)	[-]		3E+03		2.50E+03 -
(A)	Kp(susp)	[l.kg(d)-1]		1E+04		1.00E+04 l.kg-1
(A)	CORG(susp)	[% C]			10	1.00E-01 -
(A)	K(bio-water)	[-]		5E+03		5.00E+03 -
(A)	BCF(fish)	[l.kg(w)-1]		5E+03		4.65E+03 l.kg-1
(A)	FAT(fish)	[vol %]			5	5.00E-02 -
(A)	K(sed-water)	[-]		3E+03		2.50E+03 -
(A)	Kp(sed)	[l.kg(d)-1]		5E+03		5.00E+03 l.kg-1
(A)	CORG(sed)	[% C]			5	5.00E-02 -
(A)	K(soil1-water)	[-]		5E+03		5.00E+03 -
(A)	Kp(soil1)	[l.kg(d)-1]		5E+03		5.00E+03 l.kg-1
(A)	CORG(soil1)	[% C]			5	5.00E-02 -
(A)	K(soil2-water)	[-]		5E+03		5.00E+03 -
(A)	Kp(soil2)	[l.kg(d)-1]		5E+03		5.00E+03 l.kg-1
(A)	CORG(soil2)	[% C]			5	5.00E-02 -
(A)	K(soil3-water)	[-]		5E+03		5.00E+03 -
(A)	Kp(soil3)	[l.kg(d)-1]		5E+03		5.00E+03 l.kg-1
(A)	CORG(soil3)	[% C]			5	5.00E-02 -

ENVIRONMENT CHARACTERISTICS			User	Form	Val	Used
(A)	SYSTEM NAME				NETH	NETH
(D)	VOLUME(air)	[m3]		4E+13		3.80E+13 m3
(D)	VOLUME(water)	[m3]		1E+10		1.42E+10 m3
(D)	VOLUME(susp)	[m3]		9E+05		8.54E+05 m3
(D)	VOLUME(bio)	[m3]		1E+05		1.14E+05 m3
(D)	VOLUME(sed)	[m3]		1E+08		1.42E+08 m3
(D)	VOLUME(soil1)	[m3]		8E+08		7.88E+08 m3
(D)	VOLUME(soil2)	[m3]		3E+09		3.42E+09 m3
(D)	VOLUME(soil3)	[m3]		2E+07		1.90E+07 m3
(D)	SYSTEMAREA	[km2]			37975	3.80E+10 m2
(D)	AREAFRAC(water)	[%]			12.5	1.25E-01 -
(D)	AREAFRAC(soil1)	[%]			41.5	4.15E-01 -
(D)	AREAFRAC(soil2)	[%]			45	4.50E-01 -
(D)	AREAFRAC(soil3)	[%]			1	1.00E-02 -
(A)	HEIGHT(air)	[m]			1000	1.00E+03 m
(A)	DEPTH(water)	[m]			3	3.00E+00 m
(A)	SUSP(water)	[mg.l-1]			15	1.50E-02 kg.m-3
(A)	FRwater(susp)	[-]			0.9	9.00E-01 -
(A)	BIO(water)	[mg.l-1]			1	1.00E-03 kg.m-3
(A)	FRwater(bio)	[-]			0.95	9.50E-01 -
(A)	DEPTH(sed)	[cm]			3	3.00E-02 m
(A)	FRwater(sed)	[-]			0.8	8.00E-01 -
(A)	DEPTH(soil1)	[cm]			5	5.00E-02 m
(A)	DEPTH(soil2)	[cm]			20	2.00E-01 m
(A)	DEPTH(soil3)	[cm]			5	5.00E-02 m
(A)	FRair(soil)	[-]			0.2	2.00E-01 -
(A)	FRwater(soil)	[-]			0.4	4.00E-01 -
(A)	FRsolid(soil)	[-]			0.4	4.00E-01 -
(A)	RHOsolid	[kg.m-3]			2500	2.50E+03 kg.m-3
(D)	TAU(air)	[d]		4E-01		3.45E+04 s
(A)	WINDspeed	[m.s-1]			5	5.00E+00 m.s-1
(D)	TAU(water)	[d]		5E+01		4.71E+06 s
(A)	STREAMS	[m3.s-1]			2600	2.60E+03 m3.s-1
(A)	RUNOFF	[m3.s-1]		4E+02		4.00E+02 m3.s-1

LOADING PARAMETERS			User	Form	Val	Used
DIRECT EMISSIONS						
(D)	Edirect(air)	[t.y-1]		5E-03		6.15E-07 mol.s-1
(D)	Edirect(water)	[t.y-1]		5E-03		6.15E-07 mol.s-1
(D)	Edirect(soil1)	[t.y-1]		0E+00		0.00E+00 mol.s-1
(D)	Edirect(soil2)	[t.y-1]		5E-03		6.15E-07 mol.s-1
(D)	Edirect(soil3)	[t.y-1]		5E-03		6.15E-07 mol.s-1

(A)	PRODUCTION	[t.y-1]		5E+00		6.15E-04 mol.s-1
(A)	POPULATION	[inh]		1E+07		1.33E+07 inh
(A)	EMISfact(air)	[%]			0.1	1.00E-03 -
(A)	EMISfact(water)	[%]			0.1	1.00E-03 -
(A)	EMISfact(soil1)	[%]			0	0.00E+00 -
(A)	EMISfact(soil2)	[%]			0.1	1.00E-03 -
(A)	EMISfact(soil3)	[%]			0.1	1.00E-03 -

EMISSIONS VIA SEWAGE TREATMENT PLANT

(D)	Estp(air)	[t.y-1]		5E-04		6.15E-08 mol.s-1
(D)	Estp(water)	[t.y-1]		7E-04		8.79E-08 mol.s-1
(D)	Estp(susp)	[t.y-1]		3E-04		3.52E-08 mol.s-1
(D)	Estp(soil2)	[t.y-1]		3E-03		3.69E-07 mol.s-1
(A)	CONCstp(water)	[g.l-1]		1E-09		4.01E-09 mol.m-3
(A)	CONCstp(susp)	[g.kg(d)-1]		1E-05		4.01E-08 mol.kg-1
(A)	CONCstp(sludge)	[g.kg(d)-1]		7E-06		2.65E-08 mol.kg-1
(A)	EFFLUENT(stp)	[m3.d-1]		2E+06		2.19E+01 m3.s-1
(A)	SOLIDS(stp)	[kg(d).d-1]		1E+06		1.40E+01 kg.s-1
(A)	SUSPeff(stp)	[mg.l-1]		40		4.00E-02 kg.m-3
(A)	STPcapacity	[eq]		1E+07		1.26E+07 eq
(A)	STPload	[kg.d-1]		1E-02		6.15E-07 mol.s-1
(A)	ACTIVEtime	[d.y-1]			365	1.00E+00 -
(A)	FR(effstp)	[-]			0.2	2.00E-01 -
(A)	FR(sludgestp)	[-]			0.6	6.00E-01 -
(A)	FR(volatstp)	[-]			0.1	1.00E-01 -

IMPORT

(D)	IMPORT(air)	[t.y-1]		9E+05		1.09E+02 mol.s-1
(A)	AIRinflow	[m3.s-1]		1E+09		1.10E+09 m3.s-1
(A)	CONCimp(air)	[g.m-3]		2E-05		9.89E-08 mol.m-3
(D)	IMPORT(water)	[t.y-1]		3E+04		3.67E+00 mol.s-1
(A)	WATERinflow	[m3.s-1]		3E+03		2.60E+03 m3.s-1
(A)	CONCimp(water)	[g.l-1]		4E-04		1.41E-03 mol.m-3
(D)	IMPORT(susp)	[t.y-1]		1E+04		1.36E+00 mol.s-1
(A)	SUSPimport	[mg.l-1]			4E+01	3.70E-02 kg.m-3
(A)	CONCimp(susp)	[g.kg(d)-1]		4E+00		1.41E-02 mol.kg-1

TRANSFORMATION PROCESSES			User	Form	Val	Used
(D)	kdeg(air)	[d-1]		4E-03		4.56E-08 s-1
(A)	krad(OH)	[d-1]			4E-03	5.01E-08 s-1
(D)	kdeg(water)	[d-1]		7E-04		8.02E-09 s-1
(A)	kdeg(test)	[d-1]		7E-04		6.93E-04 d-1
(A)	BACT(test)	[cfu.ml-1]			4E+04	4.00E+04 cfu.ml-1
(A)	BACT(water)	[cfu.ml-1]			4E+04	4.00E+04 cfu.ml-1
(D)	kdeg(sed)	[d-1]		1E-02		1.44E-07 s-1
(A)	BACT(sedwater)	[cfu.ml-1]		2E+09	5E+09	2.25E+09 cfu.ml-1
(A)	FRdisslvd(sed)	[mol %]		3E-02		3.20E-04 -
(D)	kdeg(soil1)	[d-1]		5E-06		5.62E-11 s-1
(D)	kdeg(soil2)	[d-1]		5E-06		5.62E-11 s-1
(D)	kdeg(soil3)	[d-1]		5E-06		5.62E-11 s-1
(A)	BACT(soilwater)	[cfu.ml-1]		3E+06	2E+06	3.50E+06 cfu.ml-1
(A)	FRdisslvd(soil)	[mol %]		8E-03		8.00E-05 -

INTERMEDIA TRANSFER PROCESSES			User	Form	Val	Used
AIR/WATER and AIR/SOIL EXCHANGE						
(D)	DRYDEPaerosol	[m(air).s-1]		9E-05		9.09E-05 m.s-1
(A)	FRass(aerosol)	[-]		9E-02		9.09E-02 -
(A)	AEROSOLdeprate	[cm.s-1]			1E-01	1.00E-03 m.s-1
(D)	WASHOUT	[m(air).s-1]		8E-04		7.51E-04 m.s-1
(A)	RAINrate	[mm.y-1]			8E+02	2.41E-08 m.s-1
(A)	SCAVratio	[-]		3E+04		3.12E+04 -
(D)	GASABS(water)	[m(air).s-1]		4E-03		3.83E-03 m.s-1
(D)	VOLAT(water)	[m(water).s-1]		3E-07		2.95E-07 m.s-1
(A)	kaw(air)	[m.s-1]		4E-03	1E-03	4.24E-03 m.s-1
(A)	kaw(water)	[m.s-1]		5E-05	1E-05	5.00E-05 m.s-1
(D)	GASABS(soil1)	[m(air).s-1]		1E-05		1.22E-05 m.s-1
(D)	VOLAT(soil1)	[m(soil).s-1]		2E-13		1.88E-13 m.s-1
(D)	GASABS(soil2)	[m(air).s-1]		1E-05		1.22E-05 m.s-1
(D)	VOLAT(soil2)	[m(soil).s-1]		2E-13		1.88E-13 m.s-1
(D)	GASABS(soil3)	[m(air).s-1]		1E-05		1.22E-05 m.s-1
(D)	VOLAT(soil3)	[m(soil).s-1]		2E-13		1.88E-13 m.s-1
(A)	kasl(air)	[m.s-1]		4E-03	1E-03	4.24E-03 m.s-1
(A)	kasl(soilair)	[m.s-1]			6E-06	5.56E-06 m.s-1
(A)	kasl(soilwater)	[m.s-1]			6E-10	5.56E-10 m.s-1
SUSP/WATER and BIO/WATER PARTITIONING						
(D)	TRANS(susp-wat)	[m(susp)3.s-1]		2E+01		1.65E+01 m3.s-1
(D)	TRANS(wat-susp)	[m(wat)3.s-1]		4E+04		4.11E+04 m3.s-1
(A)	EQUtime(susp)	[hr]			1E+01	3.60E+04 s
(D)	TRANS(bio-wat)	[m(bio)3.s-1]		1E-01		1.10E-01 m3.s-1
(D)	TRANS(wat-bio)	[m(wat)3.s-1]		5E+02		5.48E+02 m3.s-1

(A)	EQUtime(bio)	[hr]	2E+02		7.20E+05 s
WATER/SEDIMENT EXCHANGE					
(D)	GROSSsedrate	[m(sed).s-1]	9E-10		8.68E-10 m.s-1
(A)	SETTLvelocity	[m(water).s-1]		3E-05	2.89E-05 m.s-1
(D)	RESUSPrate	[m(sed).s-1]	8E-10		8.46E-10 m.s-1
(A)	PROD(susp)	[kg(d).d-1]		0E+00	0.00E+00 kg.s-1
(A)	NETsedrate	[m.s-1]	2E-11		2.18E-11 m.s-1
(D)	ADSORB(sed)	[m(water).s-1]	3E-08		2.75E-08 m.s-1
(D)	DESORB(sed)	[m(sed).s-1]	1E-11		1.10E-11 m.s-1
(A)	kws(water)	[m.s-1]		3E-06	2.78E-06 m.s-1
(A)	kws(sed)	[m.s-1]		3E-08	2.78E-08 m.s-1
SOIL TO WATER TRANSFER					
(D)	RUNOFF(soil1)	[m(soil).s-1]	2E-12		2.41E-12 m.s-1
(D)	RUNOFF(soil2)	[m(soil).s-1]	2E-12		2.41E-12 m.s-1
(D)	RUNOFF(soil3)	[m(soil).s-1]	2E-12		2.41E-12 m.s-1
(A)	FRACrun(soil1)	[-]		5E-01	5.00E-01 -
(A)	FRACrun(soil2)	[-]		5E-01	5.00E-01 -
(A)	FRACrun(soil3)	[-]		5E-01	5.00E-01 -
(A)	EROSION(soil1)	[mm.y-1]		0E+00	0.00E+00 m.s-1
(A)	EROSION(soil2)	[mm.y-1]		0E+00	0.00E+00 m.s-1
(A)	EROSION(soil3)	[mm.y-1]		0E+00	0.00E+00 m.s-1
TRANSPORT FROM SYSTEM					
(D)	BURIAL(sed)	[m(sed).s-1]	2E-11		2.18E-11 m.s-1
(D)	LEACH(soil1)	[m(soil).s-1]	2E-12		1.93E-12 m.s-1
(D)	LEACH(soil2)	[m(soil).s-1]	2E-12		1.93E-12 m.s-1
(D)	LEACH(soil3)	[m(soil).s-1]	2E-12		1.93E-12 m.s-1
(A)	FRACinf(soil1)	[-]		4E-01	4.00E-01 -
(A)	FRACinf(soil2)	[-]		4E-01	4.00E-01 -
(A)	FRACinf(soil3)	[-]		4E-01	4.00E-01 -

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SIMPLEBOX MODEL DEFINITION
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(I)  V(air)              =   3.80E+13 m3          ==> VOLUME(1)
(I)  V(water)            =   1.42E+10 m3          ==> VOLUME(2)
(I)  V(sed)              =   1.42E+08 m3          ==> VOLUME(3)
(I)  V(soil1)            =   7.88E+08 m3          ==> VOLUME(4)
(I)  V(soil2)            =   3.42E+09 m3          ==> VOLUME(5)
(I)  V(soil3)            =   1.90E+07 m3          ==> VOLUME(6)
(I)  V(susp)             =   8.54E+05 m3          ==> VOLUME(7)
(I)  V(bio)              =   1.14E+05 m3          ==> VOLUME(8)

(I)  EMIS(air)           =    6.77E-07 mol.s-1    ==> EMISSION(1)
(I)  EMIS(water)         =    7.03E-07 mol.s-1    ==> EMISSION(2)
(I)  EMIS(susp)          =    3.52E-08 mol.s-1    ==> EMISSION(7)
(I)  EMIS(soil1)         =   0.00E+00 mol.s-1     ==> EMISSION(3)
(I)  EMIS(soil2)         =    9.85E-07 mol.s-1    ==> EMISSION(4)
(I)  EMIS(soil3)         =    6.15E-07 mol.s-1    ==> EMISSION(5)

(I)  IMP(air)            =   1.09E+02 mol.s-1     ==> IMPORT(1)
(I)  IMP(water)          =   3.67E+00 mol.s-1     ==> IMPORT(2)
(I)  IMP(susp)           =   1.36E+00 mol.s-1     ==> IMPORT(7)

(I)  FLOW(air)           =   1.10E+09 m3.s-1      ==> OUTFLOW(1)
(I)  FLOW(water)         =   3.02E+03 m3.s-1      ==> OUTFLOW(2)
(I)  FLOW(susp)          =    1.81E-01 m3.s-1     ==> OUTFLOW(7)
(I)  SEDBURIAL           =    1.03E-01 m3.s-1     ==> OUTFLOW(3)
(I)  LEACHING(soil1)     =   3.04E-02 m3.s-1      ==> OUTFLOW(4)
(I)  LEACHING(soil2)     =   3.29E-02 m3.s-1      ==> OUTFLOW(5)
(I)  LEACHING(soil3)     =   7.32E-04 m3.s-1      ==> OUTFLOW(6)

(I)  DEG(air)            =    4.56E-08 s-1        ==> DEGRADATION
(I)  DEG(water)          =    8.02E-09 s-1        ==> DEGRADATION
(I)  DEG(sed)            =    1.44E-07 s-1        ==> DEGRADATION
(I)  DEG(soil1)          =    5.62E-11 s-1        ==> DEGRADATION
(I)  DEG(soil2)          =    5.62E-11 s-1        ==> DEGRADATION
(I)  DEG(soil3)          =    5.62E-11 s-1        ==> DEGRADATION

(I)  DEP(water)          =   4.00E+06 m3.s-1      ==> ADVEC(1,2)
(I)  DEP(soil1)          =   1.33E+07 m3.s-1      ==> ADVEC(1,3)
(I)  DEP(soil2)          =   1.44E+07 m3.s-1      ==> ADVEC(1,4)
(I)  DEP(soil3)          =   3.20E+05 m3.s-1      ==> ADVEC(1,5)
(I)  SEDIMENTATION       =   8.24E+00 m3.s-1      ==> ADVEC(7,3)
(I)  RESUSPENSION        =   4.02E+00 m3.s-1      ==> ADVEC(3,7)
(I)  RUN-OFF(soil1)      =    3.80E-02 m3.s-1     ==> ADVEC(4,2)
(I)  RUN-OFF(soil2)      =    4.12E-02 m3.s-1     ==> ADVEC(5,2)
(I)  RUN-OFF(soil3)      =    9.15E-04 m3.s-1     ==> ADVEC(6,2)

(I)  XCH(air-water)      =   1.82E+07 m3.s-1      ==> DIFF(1,2)
(I)  XCH(water-air)      =   1.40E+03 m3.s-1      ==> DIFF(2,1)
(I)  XCH(air-soil1)      =   1.93E+05 m3.s-1      ==> DIFF(1,4)
(I)  XCH(soil1-air)      =    2.97E-03 m3.s-1     ==> DIFF(4,1)
(I)  XCH(air-soil2)      =   2.09E+05 m3.s-1      ==> DIFF(1,5)
(I)  XCH(soil2-air)      =    3.22E-03 m3.s-1     ==> DIFF(5,1)
(I)  XCH(air-soil3)      =   4.65E+03 m3.s-1      ==> DIFF(1,6)
(I)  XCH(soil3-air)      =    7.16E-05 m3.s-1     ==> DIFF(6,1)
(I)  XCH(susp-water)     =   1.65E+01 m3.s-1      ==> DIFF(7,2)
(I)  XCH(water-susp)     =   4.11E+04 m3.s-1      ==> DIFF(2,7)
(I)  XCH(bio-water)      =    1.10E-01 m3.s-1     ==> DIFF(8,2)
(I)  XCH(water-bio)      =   5.48E+02 m3.s-1      ==> DIFF(2,8)
(I)  XCH(sed-water)      =    5.22E-02 m3.s-1     ==> DIFF(3,2)
(I)  XCH(water-sed)      =   1.31E+02 m3.s-1      ==> DIFF(2,3)

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SIMPLEBOX STEADY-STATE COMPUTATION

STANDARD INPUT

	BOX 1	BOX 2	BOX 3	BOX 4	BOX 5	BOX 6	BOX 7	BOX 8
Volume (m3)	3.80E+13	1.42E+10	1.42E+08	7.86E+08	3.42E+09	1.90E+07	6.54E+05	1.14E+05
Emission (mol.s-1)	6.77E-07	7.03E-07		0.00E+00	9.85E-07	6.15E-07	3.52E-08	
Import (mol.s-1)	1.09E+02	3.67E+00					1.36E+00	
Export (m3.s-1)	1.10E+09	3.02E+03					1.81E-01	
Leaching (m3.s-1)				3.04E-02	3.29E-02	7.32E-04		
Burial (m3.s-1)			1.03E-01					
Degradation (s-1)	4.56E-08	8.02E-09	1.44E-07	5.62E-11	5.62E-11	5.62E-11	0	0

ADVECTIVE TRANSPORT (m3.s-1)

	BOX 1	BOX 2	BOX 3	BOX 4	BOX 5	BOX 6	BOX 7	BOX 8
From box 1		4.00E+06	0	1.33E+07	1.44E+07	3.20E+05	0	0
From box 2	0		0	0	0	0	0	0
From box 3	0	0		0	0	0	4.02E+00	0
From box 4	0	3.80E-02	0		0	0	0	0
From box 5	0	4.12E-02	0	0		0	0	0
From box 6	0	9.15E-04	0	0	0		0	0
From box 7	0	0	8.24E+00	0	0	0		0
From box 8	0	0	0	0	0	0	0	

DIFFUSIVE TRANSPORT (m3.s-1)

	BOX 1	BOX 2	BOX 3	BOX 4	BOX 5	BOX 6	BOX 7	BOX 8
From box 1		1.82E+07	0	1.93E+05	2.09E+05	4.65E+03	0	0
From box 2	1.40E+03		1.31E+02	0	0	0	4.11E+04	5.48E+02
From box 3	0	5.22E-02		0	0	0	0	0
From box 4	2.97E-03	0	0		0	0	0	0
From box 5	3.22E-03	0	0	0		0	0	0
From box 6	7.16E-05	0	0	0	0		0	0
From box 7	0	1.65E+01	0	0	0	0		0
From box 8	0	1.10E-01	0	0	0	0	0	

MASS BALANCE COEFFICIENTS

	CONSTANT	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)	C(8)
BALANCE 1	-1.09E+02	-1.15E+09	1.40E+03	0.00E+00	2.97E-03	3.22E-03	7.16E-05	0.00E+00	0.00E+00
BALANCE 2	-3.67E+00	2.22E+07	-4.64E+04	5.22E-02	3.80E-02	4.12E-02	9.15E-04	1.65E+01	1.10E-01
BALANCE 3	0.00E+00	0.00E+00	1.31E+02	-2.47E+01	0.00E+00	0.00E+00	0.00E+00	8.24E+00	0.00E+00
BALANCE 4	0.00E+00	1.35E+07	0.00E+00	0.00E+00	-1.16E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
BALANCE 5	-9.85E-07	1.46E+07	0.00E+00	0.00E+00	0.00E+00	-2.69E-01	0.00E+00	0.00E+00	0.00E+00
BALANCE 6	-6.15E-07	3.24E+05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-2.78E-03	0.00E+00	0.00E+00
BALANCE 7	-1.36E+00	0.00E+00	4.11E+04	4.02E+00	0.00E+00	0.00E+00	0.00E+00	-2.49E+01	0.00E+00
BALANCE 8	0.00E+00	0.00E+00	5.48E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-1.10E-01

INTERMEDIATE RESULTS

9.50E-08	-8.70E-10	-7.17E-11	-8.30E-12	-4.59E-11	-2.14E-11	-4.59E-11	-5.02E-11	-7.17E-11
4.34E-04	-1.48E-06	-5.89E-05	-6.82E-06	-1.94E-05	-9.03E-06	-1.94E-05	-4.12E-05	-5.89E-05
2.74E-01	-8.71E-04	-3.47E-02	-4.67E-02	-1.14E-02	-5.31E-03	-1.14E-02	-3.84E-02	-3.47E-02
1.11E+01	-1.01E-01	-8.35E-03	-9.67E-04	-8.66E+00	-2.49E-03	-5.35E-03	-5.84E-03	-8.35E-03
5.15E+00	-4.72E-02	-3.89E-03	-4.50E-04	-2.49E-03	-3.72E+00	-2.49E-03	-2.72E-03	-3.89E-03
1.11E+01	-1.01E-01	-8.35E-03	-9.67E-04	-5.35E-03	-2.49E-03	-3.59E+02	-5.84E-03	-8.35E-03
8.16E-01	*-2.59E-03*	*-1.03E-01*	*-1.88E-02*	*-3.39E-02*	*-1.58E-02*	*-3.39E-02*	*-1.15E-01*	*-1.03E-01*
2.17E+00	-7.41E-03	-2.95E-01	-3.41E-02	-9.70E-02	-4.51E-02	-9.70E-02	-2.06E-01	-9.41E+00

STANDARD STEADY-STATE OUTPUT

		BOX 1	BOX 2	BOX 3	BOX 4	BOX 5	BOX 6	BOX 7	BOX 8
CONCENTRATION (mol.m-3)		9.50E-08	4.34E-04	2.74E-01	1.11E+01	5.15E+00	1.11E+01	8.16E-01	2.17E+00
FUGACITY (Pa)		2.25E-04	7.20E-05	1.82E-05	3.67E-04	1.71E-04	3.67E-04	5.42E-05	7.20E-05
HOLP-UP (mol)	2.66E+10	3.61E+06	6.17E+06	3.91E+07	8.72E+09	1.76E+10	2.10E+08	6.97E+05	2.47E+05
DISTRIBUTION (%)	100.0	0.0	0.0	0.1	32.8	66.2	0.8	0.0	0.0

STEADY-STATE MASS FLOWS (mol.s-1)

	SUM	BOX 1	BOX 2	BOX 3	BOX 4	BOX 5	BOX 6	BOX 7	BOX 8
EMISSION	3.02E-06	6.77E-07	7.03E-07		0.00E+00	9.85E-07	6.15E-07	3.52E-08	
IMPORT	1.14E+02	1.09E+02	3.67E+00					1.36E+00	
INTERMEDIA transport									
from 1			2.11E+00	0.00E+00	1.28E+00	1.39E+00	3.08E-02	0.00E+00	0.00E+00
from 2		6.08E-01		5.66E-02	0.00E+00	0.00E+00	0.00E+00	1.78E+01	2.38E-01
from 3		0.00E+00	1.43E-02		0.00E+00	0.00E+00	0.00E+00	1.10E+00	0.00E+00
from 4		3.29E-02	4.20E-01	0.00E+00		0.00E+00	0.00E+00	0.00E+00	0.00E+00
from 5		1.66E-02	2.12E-01	0.00E+00	0.00E+00		0.00E+00	0.00E+00	0.00E+00
from 6		7.92E-04	1.01E-02	0.00E+00	0.00E+00	0.00E+00		0.00E+00	0.00E+00
from 7		0.00E+00	1.34E+01	6.73E+00	0.00E+00	0.00E+00	0.00E+00		0.00E+00
from 8		0.00E+00	2.38E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
THROUGHPUT	1.14E+02	1.09E+02	2.01E+01	6.78E+00	1.28E+00	1.39E+00	3.08E-02	2.03E+01	0.2377777

EXPORT	1.06E+02	1.04E+02	1.31E+00					1.48E-01	
BURIAL	2.84E-02			2.84E-02					
LEACHING	5.14E-01				3.36E-01	1.70E-01	8.10E-03		
DEGRADATION	7.34E+00	1.64E-01	4.95E-02	5.64E+00	4.90E-01	9.88E-01	1.18E-02	0.00E+00	0.00E+00
INTERMEDIA transport									
to 1			6.08E-01	0.00E+00	3.29E-02	1.66E-02	7.92E-04	0.00E+00	0.00E+00
to 2		2.11E+00		1.43E-02	4.20E-01	2.12E-01	1.01E-02	1.34E+01	2.38E-01
to 3		0.00E+00	5.66E-02		0.00E+00	0.00E+00	0.00E+00	6.73E+00	0.00E+00
to 4		1.28E+00	0.00E+00	0.00E+00		0.00E+00	0.00E+00	0.00E+00	0.00E+00
to 5		1.39E+00	0.00E+00	0.00E+00	0.00E+00		0.00E+00	0.00E+00	0.00E+00
to 6		3.08E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00		0.00E+00	0.00E+00
to 7		0.00E+00	1.78E+01	1.10E+00	0.00E+00	0.00E+00	0.00E+00		0.00E+00
to 8		0.00E+00	2.38E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
THROUGHPUT	1.14E+02	1.09E+02	2.01E+01	6.78E+00	1.28E+00	1.39E+00	3.08E-02	2.03E+01	2.38E-01
BALANCE (mol.s-1)	0.0E+00	0.0E+00	0.0E+00	0.0E+00	2.2E-16	2.2E-16	-3.5E-18	0.0E+00	0.0E+00

SIMPLEBOX QUASI-DYNAMIC COMPUTATION

MODEL FORMULATION

```
Environment
  BeginTime     =     0.0000E+00                                        (* [s] *)
  EndTime       =     3.1536E+07                                        (* [s] *)
  OutputStep    =     8.6400E+04                                        (* [s] *)
  RelError      =      1.0000E-03                                       (* [-] *)
  AbsError      =      1.0000E-15                                       (* [mol.m-3] *)

Measurement
  m[memis1]     =   ReadFile('Simint.scn','Time','Emission1')           (* [mol.s-1] *)
  m[memis2]     =   ReadFile('Simint.scn','Time','Emission2')           (* [mol.s-1] *)
  m[memis4]     =   ReadFile('Simint.scn','Time','Emission4')           (* [mol.s-1] *)
  m[memis5]     =   ReadFile('Simint.scn','Time','Emission5')           (* [mol.s-1] *)
  m[memis6]     =   ReadFile('Simint.scn','Time','Emission6')           (* [mol.s-1] *)
  m[memis7]     =   ReadFile('Simint.scn','Time','Emission7')           (* [mol.s-1] *)
  m[mimp1]      =   ReadFile('Simint.scn','Time','Import1')             (* [mol.s-1] *)
  m[mimp2]      =   ReadFile('Simint.scn','Time','Import2')             (* [mol.s-1] *)
  m[mimp7]      =   ReadFile('Simint.scn','Time','Import7')             (* [mol.s-1] *)
  m[mload]      =   ReadFile('Simint.scn','Time','Totload')             (* [mol.s-1] *)

Constant
  c[maxload]    =      1.1380E+02                                       (* [mol.s-1] *)
  c[stnd1]      =      9.8934E-08                                       (* [mol.m-3] *)
  c[stnd2]      =      1.4125E-03                                       (* [mol.m-3] *)
  c[stnd3]      =     3.5313E+00                                        (* [mol.m-3] *)
  c[stnd4]      =     7.0627E+00                                        (* [mol.m-3] *)
  c[css1]       =      9.5013E-08                                       (* [mol.m-3] *)
  c[css2]       =      4.3360E-04                                       (* [mol.m-3] *)
  c[css3]       =      2.7426E-01                                       (* [mol.m-3] *)
  c[css4]       =     1.1066E+01                                        (* [mol.m-3] *)
  c[css5]       =     5.1503E+00                                        (* [mol.m-3] *)
  c[css6]       =     1.1066E+01                                        (* [mol.m-3] *)
  c[css7]       =      8.1615E-01                                       (* [mol.m-3] *)
  c[css8]       =     2.1680E+00                                        (* [mol.m-3] *)
  c[init1]      =     0.0000E+00                                        (* [mol.m-3] *)
  c[init2]      =     0.0000E+00                                        (* [mol.m-3] *)
  c[init3]      =     0.0000E+00                                        (* [mol.m-3] *)
  c[init4]      =     0.0000E+00                                        (* [mol.m-3] *)
  c[init5]      =     0.0000E+00                                        (* [mol.m-3] *)
  c[init6]      =     0.0000E+00                                        (* [mol.m-3] *)
  c[init7]      =     0.0000E+00                                        (* [mol.m-3] *)
  c[init8]      =     0.0000E+00                                        (* [mol.m-3] *)
  c[v1]         =     3.7975E+13                                        (* [m3] *)
  c[v2]         =     1.4241E+10                                        (* [m3] *)
  c[v3]         =     1.4241E+08                                        (* [m3] *)
  c[v4]         =     7.8798E+08                                        (* [m3] *)
  c[v5]         =     3.4178E+09                                        (* [m3] *)
  c[v6]         =     1.8988E+07                                        (* [m3] *)
  c[v7]         =     8.5444E+05                                        (* [m3] *)
  c[v8]         =     1.1392E+05                                        (* [m3] *)
  c[cf11]       =    -1.1517E+09                                        (* [s-1] *)
  c[cf12]       =     1.4012E+03                                        (* [s-1] *)
  c[cf13]       =     0.0000E+00                                        (* [s-1] *)
  c[cf14]       =      2.9702E-03                                       (* [s-1] *)
  c[cf15]       =      3.2207E-03                                       (* [s-1] *)
  c[cf16]       =      7.1571E-05                                       (* [s-1] *)
  c[cf17]       =     0.0000E+00                                        (* [s-1] *)
  c[cf18]       =     0.0000E+00                                        (* [s-1] *)
  c[cf21]       =     2.2184E+07                                        (* [s-1] *)
  c[cf22]       =    -4.6360E+04                                        (* [s-1] *)
  c[cf23]       =      5.2204E-02                                       (* [s-1] *)
  c[cf24]       =      3.7977E-02                                       (* [s-1] *)
  c[cf25]       =      4.1180E-02                                       (* [s-1] *)
  c[cf26]       =      9.1510E-04                                       (* [s-1] *)
  c[cf27]       =     1.6451E+01                                        (* [s-1] *)
  c[cf28]       =      1.0968E-01                                       (* [s-1] *)
  c[cf31]       =     0.0000E+00                                        (* [s-1] *)
  c[cf32]       =     1.3055E+02                                        (* [s-1] *)
  c[cf33]       =    -2.4730E+01                                        (* [s-1] *)
  c[cf34]       =     0.0000E+00                                        (* [s-1] *)
  c[cf35]       =     0.0000E+00                                        (* [s-1] *)
  c[cf36]       =     0.0000E+00                                        (* [s-1] *)
  c[cf37]       =     8.2411E+00                                        (* [s-1] *)
  c[cf38]       =     0.0000E+00                                        (* [s-1] *)
  c[cf41]       =     1.3461E+07                                        (* [s-1] *)
  c[cf42]       =     0.0000E+00                                        (* [s-1] *)
  c[cf43]       =     0.0000E+00                                        (* [s-1] *)
  c[cf44]       =    -1.1558E-01                                        (* [s-1] *)
  c[cf45]       =     0.0000E+00                                        (* [s-1] *)
  c[cf46]       =     0.0000E+00                                        (* [s-1] *)
  c[cf47]       =     0.0000E+00                                        (* [s-1] *)
```

```
  c[cf48]      =     0.0000E+00                          (* [s-1] *)
  c[cf51]      =     1.4596E+07                          (* [s-1] *)
  c[cf52]      =     0.0000E+00                          (* [s-1] *)
  c[cf53]      =     0.0000E+00                          (* [s-1] *)
  c[cf54]      =     0.0000E+00                          (* [s-1] *)
  c[cf55]      =    -2.6926E-01                          (* [s-1] *)
  c[cf56]      =     0.0000E+00                          (* [s-1] *)
  c[cf57]      =     0.0000E+00                          (* [s-1] *)
  c[cf58]      =     0.0000E+00                          (* [s-1] *)
  c[cf61]      =     3.2435E+05                          (* [s-1] *)
  c[cf62]      =     0.0000E+00                          (* [s-1] *)
  c[cf63]      =     0.0000E+00                          (* [s-1] *)
  c[cf64]      =     0.0000E+00                          (* [s-1] *)
  c[cf65]      =     0.0000E+00                          (* [s-1] *)
  c[cf66]      =    -2.7850E-03                          (* [s-1] *)
  c[cf67]      =     0.0000E+00                          (* [s-1] *)
  c[cf68]      =     0.0000E+00                          (* [s-1] *)
  c[cf71]      =     0.0000E+00                          (* [s-1] *)
  c[cf72]      =     4.1143E+04                          (* [s-1] *)
  c[cf73]      =     4.0171E+00                          (* [s-1] *)
  c[cf74]      =     0.0000E+00                          (* [s-1] *)
  c[cf75]      =     0.0000E+00                          (* [s-1] *)
  c[cf76]      =     0.0000E+00                          (* [s-1] *)
  c[cf77]      =    -2.4874E+01                          (* [s-1] *)
  c[cf78]      =     0.0000E+00                          (* [s-1] *)
  c[cf81]      =     0.0000E+00                          (* [s-1] *)
  c[cf82]      =     5.4838E+02                          (* [s-1] *)
  c[cf83]      =     0.0000E+00                          (* [s-1] *)
  c[cf84]      =     0.0000E+00                          (* [s-1] *)
  c[cf85]      =     0.0000E+00                          (* [s-1] *)
  c[cf86]      =     0.0000E+00                          (* [s-1] *)
  c[cf87]      =     0.0000E+00                          (* [s-1] *)
  c[cf88]      =    -1.0968E-01                          (* [s-1] *)

Initial
  s[c1]        =   c[init1]                              (* [mol.m-3] *)
  s[c2]        =   c[init2]                              (* [mol.m-3] *)
  s[c3]        =   c[init3]                              (* [mol.m-3] *)
  s[c4]        =   c[init4]                              (* [mol.m-3] *)
  s[c5]        =   c[init5]                              (* [mol.m-3] *)
  s[c6]        =   c[init6]                              (* [mol.m-3] *)
  s[c7]        =   c[init7]                              (* [mol.m-3] *)
  s[c8]        =   c[init8]                              (* [mol.m-3] *)

Derivative
  a[emis1]     =   forcing(s[Time],m[memis1],FALSE)      (* [mol.s-1] *)
  a[imp1]      =   forcing(s[Time],m[mimp1],FALSE)       (* [mol.s-1] *)
  d[c1]        = (( a[emis1]    + a[imp1]      +
                    c[cf11]     * s[c1]        +
                    c[cf12]     * s[c2]      ) +
                 (  c[cf13]     * s[c3]        +
                    c[cf14]     * s[c4]        +
                    c[cf15]     * s[c5]        +
                    c[cf16]     * s[c6]      ) +
                 (  c[cf17]     * s[c7]        +
                    c[cf18]     * s[c8]     )) /  c[v1]  (* [mol.m-3.s-1] *)
  a[emis2]     =   forcing(s[Time],m[memis2],FALSE)      (* [mol.s-1] *)
  a[imp2]      =   forcing(s[Time],m[mimp2],FALSE)       (* [mol.s-1] *)
  d[c2]        = (( a[emis2]    + a[imp2]      +
                    c[cf21]     * s[c1]        +
                    c[cf22]     * s[c2]      ) +
                 (  c[cf23]     * s[c3]        +
                    c[cf24]     * s[c4]        +
                    c[cf25]     * s[c5]        +
                    c[cf26]     * s[c6]      ) +
                 (  c[cf27]     * s[c7]        +
                    c[cf28]     * s[c8]     )) /  c[v2]  (* [mol.m-3.s-1] *)
  d[c3]        = (( c[cf31]     * s[c1]        +
                    c[cf32]     * s[c2]        +
                    c[cf33]     * s[c3]        +
                    c[cf34]     * s[c4]      ) +
                 (  c[cf35]     * s[c5]        +
                    c[cf36]     * s[c6]        +
                    c[cf37]     * s[c7]        +
                    c[cf38]     * s[c8]     )) /  c[v3]  (* [mol.m-3.s-1] *)
  a[emis4]     =   forcing(s[Time],m[memis4],FALSE)      (* [mol.s-1] *)
  d[c4]        = (( a[emis4]                   +
                    c[cf41]     * s[c1]        +
                    c[cf42]     * s[c2]      ) +
                 (  c[cf43]     * s[c3]        +
                    c[cf44]     * s[c4]        +
                    c[cf45]     * s[c5]        +
                    c[cf46]     * s[c6]      ) +
                 (  c[cf47]     * s[c7]        +
                    c[cf48]     * s[c8]     )) /  c[v4]  (* [mol.m-3.s-1] *)
```

```
  a[emis5]     =    forcing(s[Time],m[memis5],FALSE)                        (* [mol.s-1] *)
  d[c5]        = (( a[emis5]                     +
                    c[cf51]      * s[c1]         +
                    c[cf52]      * s[c2]       ) +
                  ( c[cf53]      * s[c3]         +
                    c[cf54]      * s[c4]         +
                    c[cf55]      * s[c5]         +
                    c[cf56]      * s[c6]       ) +
                  ( c[cf57]      * s[c7]         +
                    c[cf58]      * s[c8]      )) /  c[v5]                   (* [mol.m-3.s-1] *)
  a[emis6]     =    forcing(s[Time],m[memis6],FALSE)                        (* [mol.s-1] *)
  d[c6]        = (( a[emis6]                     +
                    c[cf61]      * s[c1]         +
                    c[cf62]      * s[c2]       ) +
                  ( c[cf63]      * s[c3]         +
                    c[cf64]      * s[c4]         +
                    c[cf65]      * s[c5]         +
                    c[cf66]      * s[c6]       ) +
                  ( c[cf67]      * s[c7]         +
                    c[cf68]      * s[c8]      )) /  c[v6]                   (* [mol.m-3.s-1] *)
  a[emis7]     =    forcing(s[Time],m[memis7],FALSE)                        (* [mol.s-1] *)
  a[imp7]      =    forcing(s[Time],m[mimp7],FALSE)                         (* [mol.s-1] *)
  d[c7]        = (( a[emis7]     + a[imp7]       +
                    c[cf71]      * s[c1]         +
                    c[cf72]      * s[c2]       ) +
                  ( c[cf73]      * s[c3]         +
                    c[cf74]      * s[c4]         +
                    c[cf75]      * s[c5]         +
                    c[cf76]      * s[c6]       ) +
                  ( c[cf77]      * s[c7]         +
                    c[cf78]      * s[c8]      )) /  c[v7]                   (* [mol.m-3.s-1] *)
  d[c8]        = (( c[cf81]      * s[c1]         +
                    c[cf82]      * s[c2]         +
                    c[cf83]      * s[c3]         +
                    c[cf84]      * s[c4]       ) +
                  ( c[cf85]      * s[c5]         +
                    c[cf86]      * s[c6]         +
                    c[cf87]      * s[c7]         +
                    c[cf88]      * s[c8]      )) /  c[v8]                   (* [mol.m-3.s-1] *)

Discrete
  a[Hours]     =    s[Time]      /       3600                               (* [hr] *)
  a[Days]      =    s[Time]      /      86400                               (* [d] *)
  a[Weeks]     =    s[Time]      /     604800                               (* [wk] *)
  a[Months]    =    s[Time]      /    2635200                               (* [mth] *)
  a[Years]     =    s[Time]      /   31536000                               (* [yr] *)
  a[Cair]      = (  s[c1]        / c[css1]     ) *           100            (* [%] *)
  a[Cwater]    = (  s[c2]        / c[css2]     ) *           100            (* [%] *)
  a[Csed]      = (  s[c3]        / c[css3]     ) *           100            (* [%] *)
  a[Csoil1]    = (  s[c4]        / c[css4]     ) *           100            (* [%] *)
  a[Csoil2]    = (  s[c5]        / c[css5]     ) *           100            (* [%] *)
  a[Csoil3]    = (  s[c6]        / c[css6]     ) *           100            (* [%] *)
  a[Csusp]     = (  s[c7]        / c[css7]     ) *           100            (* [%] *)
  a[Cbio]      = (  s[c7]        / c[css7]     ) *           100            (* [%] *)
  a[Total]     = (( s[c1]        * c[v1]         +
                    s[c2]        * c[v2]         +
                    s[c3]        * c[v3]         +
                    s[c4]        * c[v4]       ) +
                  ( s[c5]        * c[v5]         +
                    s[c6]        * c[v6]         +
                    s[c7]        * c[v7]         +
                    s[c8]        * c[v8]      )) /
                 (( c[css1]      * c[v1]         +
                    c[css2]      * c[v2]         +
                    c[css3]      * c[v3]         +
                    c[css4]      * c[v4]       ) +
                  ( c[css5]      * c[v5]         +
                    c[css6]      * c[v6]         +
                    c[css7]      * c[v7]         +
                    c[css8]      * c[v8]      )) *           100            (* [%] *)
  a[Qair]      =    s[c1]        / c[stnd1]                                 (* [-] *)
  a[Qwater]    =    s[c2]        / c[stnd2]                                 (* [-] *)
  a[Qsed]      =    s[c3]        / c[stnd3]                                 (* [-] *)
  a[Qsoil1]    =    s[c4]        / c[stnd4]                                 (* [-] *)
  a[Qsoil2]    =    s[c5]        / c[stnd4]                                 (* [-] *)
  a[Qsoil3]    =    s[c6]        / c[stnd4]                                 (* [-] *)
  a[totload]   =    forcing(s[Time],m[mload],FALSE)                         (* [mol.s-1] *)
  a[Load]      =    a[totload]   / c[maxload]    *           100            (* [%] *)

------------------------------------------------------------------------------------------
```

```
SIMPLEBOX MODEL SETTINGS
========================================

MODEL SETTINGS
----------------------------------------
BeginTime       0.0000E+00
EndTime         3.1536E+09
OutputStep      3.1536E+07
MaxStep         3.1536E+07
MinStep         1.0000E-05
Order                    5
RelError        1.0000E-05
AbsError        1.0000E-15
TicksX                   2
TicksY                   4
FormatX                  0
FormatY                  0
XLow                     0
XHigh                  100
YLow                     0
YHigh                  100
ShowGraph                1
ShowResults              1
SymbolSize            0.05
MaxSymbols               1
PlotVar 0       a[Years]        a[Hours]
PlotVar 1       a[Cair]         a[Days]
PlotVar 2       a[Cwater]       a[Weeks]
PlotVar 3       a[Csed]         a[Months]
PlotVar 4       a[Csoil1]       a[Years]
PlotVar 6       a[Csoil2]       a[Cair]
PlotVar 6       a[Total]        a[Cwater]
                                a[Csed]
                                a[Csoil1]
                                a[Csoil2]
                                a[Csoil3]
                                a[Csusp]
                                a[Cbio]
                                a[Total]
                                a[Load]

ResultsFile     SimInt.res
a[Cair]         save
a[Csed]         save
a[Csoil1]       save
a[Csoil2]       save
a[Csoil3]       save
a[Cwater]       save
a[Days]
a[Hours]
a[Load]
a[Months]
a[Qair]         save
a[Qsed]         save
a[Qsoil1]       save
a[Qsoil2]       save
a[Qsoil3]       save
a[Qwater]       save
a[Total]        save
a[Weeks]
a[Years]        save
c[maxload]        1.1380E+02
c[stnd1]          9.8934E-08
c[stnd2]          1.4125E-03
c[stnd3]          3.5313E+00
c[stnd4]          7.0627E+00
c[css1]           9.5013E-08
c[css2]           4.3360E-04
c[css3]           2.7426E-01
c[css4]           1.1066E+01
c[css5]           5.1503E+00
c[css6]           1.1066E+01
c[css7]           8.1615E-01
c[css8]           2.1680E+00
c[init1]          0.0000E+00
c[init2]          0.0000E+00
c[init3]          0.0000E+00
c[init4]          0.0000E+00
c[init5]          0.0000E+00
c[init6]          0.0000E+00
c[init7]          0.0000E+00
c[init8]          0.0000E+00
c[v1]             3.7975E+13
c[v2]             1.4241E+10
c[v3]             1.4241E+08
```

c[v4]	7.8798E+08
c[v5]	3.4178E+09
c[v6]	1.8988E+07
c[v7]	8.5444E+05
c[v8]	1.1392E+05
c[cf11]	-1.1517E+09
c[cf12]	1.4012E+03
c[cf13]	0.0000E+00
c[cf14]	2.9702E-03
c[cf15]	3.2207E-03
c[cf16]	7.1571E-05
c[cf17]	0.0000E+00
c[cf18]	0.0000E+00
c[cf21]	2.2184E+07
c[cf22]	-4.6360E+04
c[cf23]	5.2204E-02
c[cf24]	3.7977E-02
c[cf25]	4.1180E-02
c[cf26]	9.1510E-04
c[cf27]	1.6451E+01
c[cf28]	1.0968E-01
c[cf31]	0.0000E+00
c[cf32]	1.3055E+02
c[cf33]	-2.4730E+01
c[cf34]	0.0000E+00
c[cf35]	0.0000E+00
c[cf36]	0.0000E+00
c[cf37]	8.2411E+00
c[cf38]	0.0000E+00
c[cf41]	1.3461E+07
c[cf42]	0.0000E+00
c[cf43]	0.0000E+00
c[cf44]	-1.1558E-01
c[cf45]	0.0000E+00
c[cf46]	0.0000E+00
c[cf47]	0.0000E+00
c[cf48]	0.0000E+00
c[cf51]	1.4596E+07
c[cf52]	0.0000E+00
c[cf53]	0.0000E+00
c[cf54]	0.0000E+00
c[cf55]	-2.6926E-01
c[cf56]	0.0000E+00
c[cf57]	0.0000E+00
c[cf58]	0.0000E+00
c[cf61]	3.2435E+05
c[cf62]	0.0000E+00
c[cf63]	0.0000E+00
c[cf64]	0.0000E+00
c[cf65]	0.0000E+00
c[cf66]	-2.7850E-03
c[cf67]	0.0000E+00
c[cf68]	0.0000E+00
c[cf71]	0.0000E+00
c[cf72]	4.1143E+04
c[cf73]	4.0171E+00
c[cf74]	0.0000E+00
c[cf75]	0.0000E+00
c[cf76]	0.0000E+00
c[cf77]	-2.4874E+01
c[cf78]	0.0000E+00
c[cf81]	0.0000E+00
c[cf82]	5.4838E+02
c[cf83]	0.0000E+00
c[cf84]	0.0000E+00
c[cf85]	0.0000E+00
c[cf86]	0.0000E+00
c[cf87]	0.0000E+00
c[cf88]	-1.0968E-01

SIMPLEBOX LOADINGS SCENARIOS

Scenario 1: Constant loadings; zero background

Year	Time	Emission1	Emission2	Emission4	Emission5	Emission6	Emission7	Import1	Import2	Import7	Totload
0	0.00E+00	6.77E-07	7.03E-07	0.00E+00	9.85E-07	6.15E-07	3.52E-08	1.09E+02	3.67E+00	1.36E+00	1.14E+02
50	1.58E+09	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
100	3.15E+09	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Maxload											1.14E+02

Scenario 2: Intermittent loadings; zero background

Year	Time	Emission1	Emission2	Emission4	Emission5	Emission6	Emission7	Import1	Import2	Import7	Totload
0	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
10	3.15E+08	6.77E-08	7.03E-08	0.00E+00	9.85E-08	6.15E-08	3.52E-09	0.00E+00	0.00E+00	0.00E+00	3.02E-07
20	6.31E+08	1.69E-07	1.76E-07	0.00E+00	2.46E-07	1.54E-07	8.79E-09	7.83E+00	9.83E-02	1.11E-02	7.94E+00
30	9.46E+08	3.38E-07	3.52E-07	0.00E+00	4.92E-07	3.08E-07	1.76E-08	2.22E+01	2.78E-01	3.14E-02	2.25E+01
40	1.26E+09	6.77E-07	7.03E-07	0.00E+00	9.85E-07	6.15E-07	3.52E-08	4.70E+01	5.90E-01	6.66E-02	4.77E+01
50	1.58E+09							9.40E+01	1.18E+00	1.33E-01	9.53E+01
60	1.89E+09							1.04E+02	1.31E+00	1.48E-01	1.06E+02
70	2.21E+09	6.77E-08	7.03E-08	0.00E+00	9.85E-08	6.15E-08	3.52E-09	1.04E+01	1.31E-01	1.48E-02	1.06E+01
80	2.52E+09										0.00E+00
90	2.84E+09										0.00E+00
100	3.15E+09										0.00E+00
110	3.47E+09										0.00E+00
120	3.78E+09										0.00E+00
130	4.10E+09										0.00E+00
140	4.42E+09										0.00E+00
150	4.73E+09										0.00E+00
160	5.05E+09										0.00E+00
170	5.36E+09										0.00E+00
180	5.68E+09										0.00E+00
190	5.99E+09										0.00E+00
200	6.31E+09										0.00E+00
210	6.62E+09										0.00E+00
220	6.94E+09										0.00E+00
230	7.25E+09										0.00E+00
240	7.57E+09										0.00E+00
250	7.88E+09										0.00E+00
Maxload											1.06E+02

```
01-Aug-93                              SimpleBox vs 1.0 (930801)                                  SIMBOX10.wk1

SIMPLEBOX STEADY-STATE OUTPUT
==============================================================================================================
TABLE 1: STEADY-STATE CONCENTRATIONS, RISK QOUTIENTS, FUGACITIES and MASS BALANCE

COMPOUNDHYPO
SYSTEM:    NETH

--------------------------------------------------------------------------------------------------------------
                        CONCENTRATION      RISK       FUGACITY                     MASS BALANCE
                                           QUOTIENT                 EMISSION   IMPORT    'EXPORT'   DEGRADATION
--------------------------------------------------------------------------------------------------------------
AIR                     2.4E-05 g.m-3      9.6E-01    2.3E-04 Pa    0.0 %      95.8 %    91.8 %     0.1 %
WATER                   1.1E-04 g.l-1      3.1E-01    7.2E-05 Pa    0.0 %       3.2 %     1.2 %     0.0 %
SUSPENDED MATTER        8.2E-01 g.kg(d)-1             5.4E-05 Pa    0.0 %       1.2 %     0.1 %
BIOTA                   5.0E-01 g.kg(w)-1             7.2E-05 Pa
SEDIMENT                1.4E-01 g.kg(d)-1  7.8E-02    1.8E-05 Pa                          0.0 %     5.0 %
PORE WATER SEDIMENT     2.7E-05 g.l-1                 1.8E-05 Pa
SOIL 1                  2.8E+00 g.kg(d)-1  1.6E+00    3.7E-04 Pa    0.0 %                           0.4 %
PORE WATER SOIL 1       5.5E-04 g.l-1      1.6E+00    3.7E-04 Pa                          0.3 %
SOIL 2                  1.3E+00 g.kg(d)-1  7.3E-01    1.7E-04 Pa    0.0 %                           0.9 %
PORE WATER SOIL 2       2.6E-04 g.l-1      7.3E-01    1.7E-04 Pa                          0.1 %
SOIL 3                  2.8E+00 g.kg(d)-1  1.6E+00    3.7E-04 Pa    0.0 %                           0.0 %
PORE WATER SOIL 3       5.5E-04 g.l-1      1.6E+00    3.7E-04 Pa                          0.0 %
--------------------------------------------------------------------------------------------------------------
                                                                    0.0 %     100.0 %    93.5 %     6.4 %
--------------------------------------------------------------------------------------------------------------

==============================================================================================================
```

SIMPLEBOX STEADY-STATE OUTPUT

TABLE 2: TRANFER- AND TRANSFORMATION MASS FLOWS [Units: 2]

COMPOUNDHYPO
SYSTEM: NETH
UNITS: % of throughput

	AIR	WATER	SEDIMENT	SOIL 1	SOIL 2	SOIL 3	SUSPENDEC MATTER	BIOTA
EMISSION	5.95E-07	6.18E-07		0.00E+00	8.65E-07	5.41E-07	3.09E-08	
IMPORT	9.56E+01	3.23E+00					1.19E+00	
EXPORT	9.18E+01	1.15E+00					1.30E-01	
LEACHING				2.95E-01	1.49E-01	7.12E-03		
BURIAL			2.49E-02					
DEGRADATION	1.44E-01	4.35E-02	4.95E+00	4.30E-01	8.69E-01	1.04E-02		
TO AIR								
DEPOSITION		-3.34E-01		-1.11E+00	-1.20E+00	-2.67E-02		
DIFFUSION		-9.85E-01		1.28E-02	-2.88E-03	3.08E-04		
TO WATER			-3.72E-02				-3.88E+00	-2.75E-18
DEPOSITION	3.34E-01							
DIFFUSION	9.85E-01							
RUN-OFF				3.69E-01	1.86E-01	8.90E-03		
TO SEDIMENT		3.72E-02					4.94E+00	
TO SOIL 1								
DEPOSITION	1.11E+00							
DIFFUSION	-1.28E-02							
RUN-OFF		-3.69E-01						
TO SOIL 2								
DEPOSITION	1.20E+00							
DIFFUSION	2.88E-03							
RUN-OFF		-1.86E-01						
TO SOIL 3								
DEPOSITION	2.67E-02							
DIFFUSION	-3.08E-04							
RUN-OFF		-8.90E-03						
TO SUSPENDED MATTER		3.88E+00	-4.94E+00					
TO BIOTA		2.75E-18						

Conversion factor used:	8.79E-01
1: 1 mol.s-1 =	1.00E+00 mol.s-1
2: 1 % =	8.79E-01 mol.s-1
3: 1 t.y-1 =	7.88E+03 mol.s-1
4: 1 kg.d-1 =	2.16E+04 mol.s-1

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SIMPLEBOX STEADY-STATE OUTPUT
==========================================================================================
TABLE 3: ANALYSIS REPORT

------------------------------------------------------------------------------------------
DOCUMENTATION

Model version                   SimpleBox vs 1.0 (930801), Lotus123 version
Model files                     SIMBOX.bat(930801); SIMBOX10.wk1(930801);
                                SIMINT10.exe(930801); SPLITRES.exe(910212)
Date and time of analysis         93-08-01       12:00
Analyst                         D. van de Meent
Description of the analysis     Compution with default values only

------------------------------------------------------------------------------------------
DATA USED

COMPOUND                        HYPO                      SYSTEM                          NETH
MOL WEIGHT                           250 g.mol-1          SYSTEM AREA                        37975 km2
LOG KOW                             5.00 -                AREA WATER                      4746.875 km2
VAPOR PRESSURE                   1.0E-03 Pa               AREA NATURAL SOIL                  15760 km2
SOLUBILITY                       1.5E-03 g.l-1            AREA AGRICULTURAL SOIL             17089 km2
HENRY'S LAW CONSTANT             1.7E-01 Pa.m3.mol-1      AREA OTHER SOIL                   379.75 km2
KP (suspended matter)              10000 l.kg-1           RESIDENCE TIME AIR                   0.4 d
KP (sediment)                       5000 l.kg-1           RESIDENCE TIME WATER                62.9 d
KP (natural soil)                   5000 l.kg-1           EFFLUENT STP                     2.8E+06 m3.d-1
KP (agricultural soil)              5000 l.kg-1           DILUTION FACTOR                      138 [-]
KP (other soil)                     5000 l.kg-1           SLUDGE PRODUCTION STP            1205849 kg.d-1
DEGRADATION RATE (air)           3.9E-03 d-1              QUALITY STANDARD (water)         3.5E-04 g.l-1
DEGRADATION RATE (water)         6.9E-04 d-1              QUALITY STANDARD (sediment)      1.8E+00 g.kg-1
DEGRADATION RATE (sediment)      1.2E-02 d-1              QUALITY STANDARD (soil)          1.8E+00 g.kg-1
DEGRADATION RATE (soil)          4.9E-06 d-1              QUALITY STANDARD (groundwater)   3.5E-04 g.l-1
------------------------------------------------------------------------------------------
FATE

 * DIRECT EMISSION TO AIR        4.9E-03 t.y-1             * EXPORT WITH AIR               8.2E+05 t.y-1
 * DIRECT EMISSION TO WATER      4.9E-03 t.y-1             * EXPORT WITH WATER             1.1E+04 t.y-1
 * DIRECT EMISSION TO SOIL       9.7E-03 t.y-1            TOTAL EXPORT                    8.35E+05 t.y-1

 * EMISSION from STP to AIR      4.9E-04 t.y-1             * BURIAL IN SEDIMENT            2.2E+02 t.y-1
 * EMISSION from STP to WATER    9.7E-04 t.y-1             * LEACHING TO GROUNDWATER       4.1E+03 t.y-1
 * EMISSION with WWTP SLUDGE     2.9E-03 t.y-1            TOTAL ACCUMULATION              4.28E+03 t.y-1
TOTAL EMISSIONS                 2.38E-02 t.y-1
                                                           * DEGRADATION in AIR            1.3E+03 t.y-1
 * IMPORT with AIR               8.6E+05 t.y-1             * DEGRADATION in WATER          3.9E+02 t.y-1
 * IMPORT with WATER             4.0E+04 t.y-1             * DEGRADATION in SEDIMENT       4.4E+04 t.y-1
TOTAL IMPORT                    8.97E+05 t.y-1             * DEGRADATION in SOIL           1.2E+04 t.y-1
                                                          TOTAL DEGRADATION               5.79E+04 t.y-1
------------------------------------------------------------------------------------------
DISTRIBUTION & RISK

                                CONCENTRATION      RISK QUOTIENT        DISTRIBUTION

AIR                              2.4E-05 g.m-3       0.9603684 -              0.0 %
WATER
 * DISSOLVED                     1.1E-04 g.l-1       0.3069652 -              0.0 %
 * PARTICULATE                   1.2E-05 g.l-1                                0.0 %
 * SEDIMENT                      1.4E-01 g.kg-1      0.0776398 -              0.1 %
SOIL
 * NATURAL SOIL                  2.8E+00 g.kg-1      1.5666509 -             32.8 %
 * AGRICULTURAL SOIL             1.3E+00 g.kg-1      0.7291724 -             66.2 %
 * OTHER SOIL                    2.8E+00 g.kg-1      1.5666822 -              0.8 %
GROUNDWATER
 * NATURAL SOIL                  5.5E-04 g.l-1       1.5666509 -

==========================================================================================
```

SIMPLEBOX QUASI-DYNAMIC OUTPUT

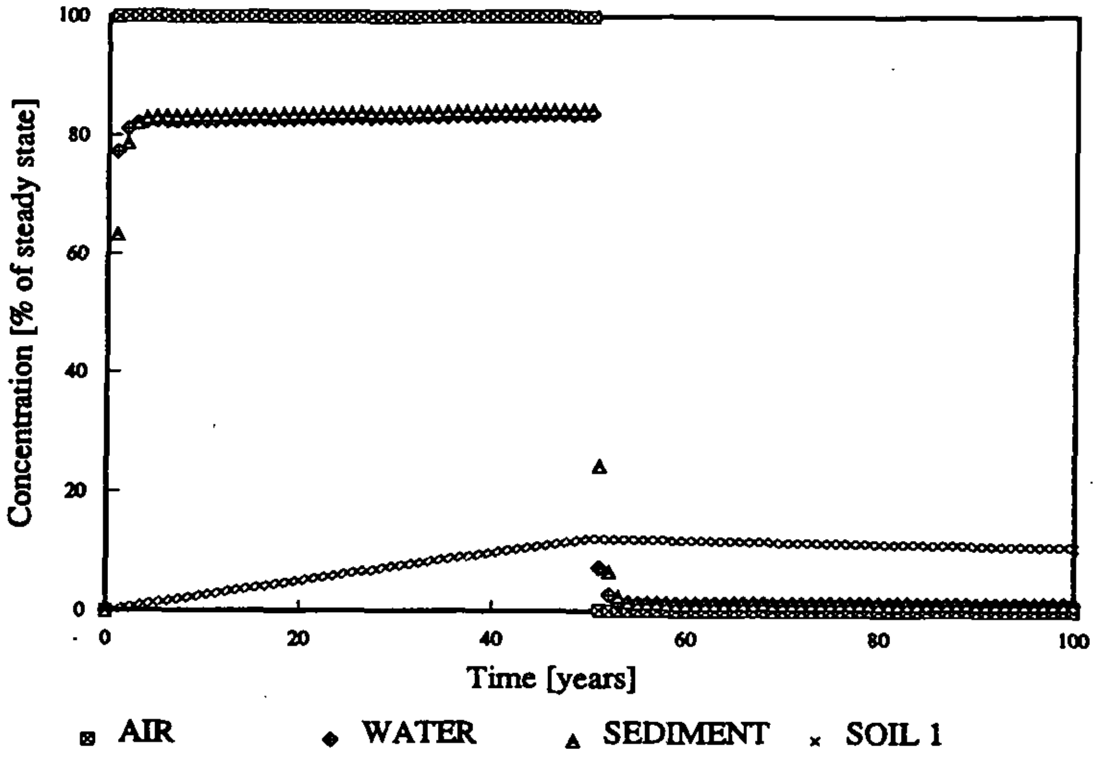
TABLE 4: RESULTS QUASI-DYNAMIC SIMULATION

COMPOUNDHYPO		AIR:	95.6 %
SYSTEM:	NETH	WATER:	4.4 %
LOADINGS:	*BLOCKSCENARIO*	*SOIL:*	0.0 %

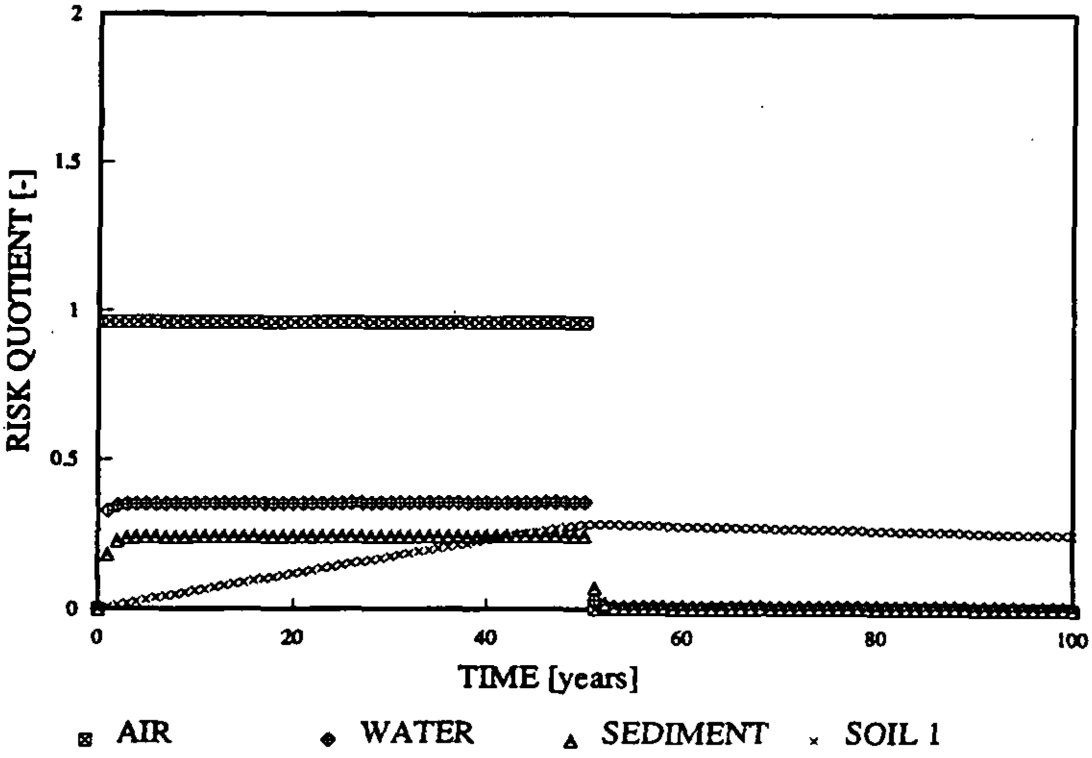
Time [y]	C(air) [%]	C(water) [%]	C(sed) [%]	C(soil1) [%]	Q(air) [-]	Q(water) [-]	Q(sed) [-]	Q(soil1) [-]
0	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1	1.00E+02	9.12E+01	9.09E+01	4.61E-01	9.61E-01	2.80E-01	7.06E-02	7.23E-03
2	1.00E+02	9.14E+01	9.19E+01	9.21E-01	9.61E-01	2.80E-01	7.14E-02	1.44E-02
3	1.00E+02	9.14E+01	9.20E+01	1.38E+00	9.62E-01	2.81E-01	7.14E-02	2.16E-02
4	1.00E+02	9.14E+01	9.20E+01	1.83E+00	9.62E-01	2.81E-01	7.15E-02	2.87E-02
5	1.00E+02	9.15E+01	9.21E+01	2.29E+00	9.62E-01	2.81E-01	7.15E-02	3.59E-02
6	1.00E+02	9.15E+01	9.21E+01	2.74E+00	9.62E-01	2.81E-01	7.15E-02	4.29E-02
7	1.00E+02	9.15E+01	9.21E+01	3.19E+00	9.62E-01	2.81E-01	7.15E-02	5.00E-02
8	1.00E+02	9.16E+01	9.21E+01	3.64E+00	9.62E-01	2.81E-01	7.16E-02	5.70E-02
9	1.00E+02	9.16E+01	9.22E+01	4.08E+00	9.62E-01	2.81E-01	7.16E-02	6.40E-02
10	1.00E+02	9.16E+01	9.22E+01	4.52E+00	9.62E-01	2.81E-01	7.16E-02	7.09E-02
11	1.00E+02	9.17E+01	9.22E+01	4.97E+00	9.62E-01	2.81E-01	7.16E-02	7.78E-02
12	1.00E+02	9.17E+01	9.23E+01	5.41E+00	9.62E-01	2.81E-01	7.17E-02	8.47E-02
13	1.00E+02	9.17E+01	9.23E+01	5.84E+00	9.62E-01	2.82E-01	7.17E-02	9.15E-02
14	1.00E+02	9.18E+01	9.23E+01	6.28E+00	9.62E-01	2.82E-01	7.17E-02	9.84E-02
15	1.00E+02	9.18E+01	9.24E+01	6.71E+00	9.62E-01	2.82E-01	7.17E-02	1.05E-01
16	1.00E+02	9.18E+01	9.24E+01	7.14E+00	9.62E-01	2.82E-01	7.18E-02	1.12E-01
17	1.00E+02	9.18E+01	9.24E+01	7.57E+00	9.62E-01	2.82E-01	7.18E-02	1.19E-01
18	1.00E+02	9.19E+01	9.24E+01	8.00E+00	9.62E-01	2.82E-01	7.18E-02	1.25E-01
19	1.00E+02	9.19E+01	9.25E+01	8.42E+00	9.62E-01	2.82E-01	7.18E-02	1.32E-01
20	1.00E+02	9.19E+01	9.25E+01	8.85E+00	9.62E-01	2.82E-01	7.18E-02	1.39E-01
21	1.00E+02	9.20E+01	9.25E+01	9.27E+00	9.62E-01	2.82E-01	7.19E-02	1.45E-01
22	1.00E+02	9.20E+01	9.26E+01	9.69E+00	9.62E-01	2.82E-01	7.19E-02	1.52E-01
23	1.00E+02	9.20E+01	9.26E+01	1.01E+01	9.62E-01	2.83E-01	7.19E-02	1.58E-01
24	1.00E+02	9.21E+01	9.26E+01	1.05E+01	9.62E-01	2.83E-01	7.19E-02	1.65E-01
25	1.00E+02	9.21E+01	9.27E+01	1.09E+01	9.62E-01	2.83E-01	7.20E-02	1.71E-01
26	1.00E+02	9.21E+01	9.27E+01	1.13E+01	9.62E-01	2.83E-01	7.20E-02	1.78E-01
27	1.00E+02	9.22E+01	9.27E+01	1.18E+01	9.62E-01	2.83E-01	7.20E-02	1.84E-01
28	1.00E+02	9.22E+01	9.27E+01	1.22E+01	9.62E-01	2.83E-01	7.20E-02	1.91E-01
29	1.00E+02	9.22E+01	9.28E+01	1.26E+01	9.62E-01	2.83E-01	7.20E-02	1.97E-01
30	1.00E+02	9.23E+01	9.28E+01	1.30E+01	9.62E-01	2.83E-01	7.21E-02	2.03E-01
31	1.00E+02	9.23E+01	9.28E+01	1.34E+01	9.62E-01	2.83E-01	7.21E-02	2.10E-01
32	1.00E+02	9.23E+01	9.29E+01	1.38E+01	9.62E-01	2.83E-01	7.21E-02	2.16E-01
33	1.00E+02	9.23E+01	9.29E+01	1.42E+01	9.62E-01	2.83E-01	7.21E-02	2.22E-01
34	1.00E+02	9.24E+01	9.29E+01	1.46E+01	9.62E-01	2.84E-01	7.22E-02	2.28E-01
35	1.00E+02	9.24E+01	9.29E+01	1.50E+01	9.62E-01	2.84E-01	7.22E-02	2.34E-01
36	1.00E+02	9.24E+01	9.30E+01	1.54E+01	9.62E-01	2.84E-01	7.22E-02	2.41E-01
37	1.00E+02	9.25E+01	9.30E+01	1.57E+01	9.62E-01	2.84E-01	7.22E-02	2.47E-01
38	1.00E+02	9.25E+01	9.30E+01	1.61E+01	9.62E-01	2.84E-01	7.22E-02	2.53E-01
39	1.00E+02	9.25E+01	9.30E+01	1.65E+01	9.62E-01	2.84E-01	7.23E-02	2.59E-01
40	1.00E+02	9.25E+01	9.31E+01	1.69E+01	9.62E-01	2.84E-01	7.23E-02	2.65E-01
41	1.00E+02	9.26E+01	9.31E+01	1.73E+01	9.62E-01	2.84E-01	7.23E-02	2.71E-01
42	1.00E+02	9.26E+01	9.31E+01	1.77E+01	9.62E-01	2.84E-01	7.23E-02	2.77E-01
43	1.00E+02	9.26E+01	9.32E+01	1.81E+01	9.62E-01	2.84E-01	7.23E-02	2.83E-01
44	1.00E+02	9.27E+01	9.32E+01	1.84E+01	9.62E-01	2.84E-01	7.24E-02	2.89E-01
45	1.00E+02	9.27E+01	9.32E+01	1.88E+01	9.62E-01	2.85E-01	7.24E-02	2.95E-01
46	1.00E+02	9.27E+01	9.32E+01	1.92E+01	9.62E-01	2.85E-01	7.24E-02	3.01E-01
47	1.00E+02	9.27E+01	9.33E+01	1.96E+01	9.62E-01	2.85E-01	7.24E-02	3.07E-01
48	1.00E+02	9.28E+01	9.33E+01	1.99E+01	9.62E-01	2.85E-01	7.24E-02	3.12E-01
49	1.00E+02	9.28E+01	9.33E+01	2.03E+01	9.62E-01	2.85E-01	7.25E-02	3.18E-01
50	1.00E+02	9.28E+01	9.33E+01	2.07E+01	9.62E-01	2.85E-01	7.25E-02	3.24E-01
51	1.76E-02	1.71E+00	3.02E+00	2.06E+01	1.69E-04	5.26E-03	2.34E-03	3.23E-01
52	1.66E-02	1.54E+00	1.45E+00	2.05E+01	1.60E-04	4.73E-03	1.12E-03	3.22E-01
53	1.66E-02	1.53E+00	1.43E+00	2.04E+01	1.59E-04	4.70E-03	1.11E-03	3.20E-01
54	1.65E-02	1.53E+00	1.42E+00	2.03E+01	1.58E-04	4.68E-03	1.10E-03	3.19E-01
55	1.64E-02	1.52E+00	1.41E+00	2.02E+01	1.58E-04	4.66E-03	1.10E-03	3.17E-01
56	1.64E-02	1.51E+00	1.41E+00	2.02E+01	1.57E-04	4.65E-03	1.09E-03	3.16E-01
57	1.63E-02	1.51E+00	1.40E+00	2.01E+01	1.56E-04	4.63E-03	1.09E-03	3.14E-01
58	1.62E-02	1.50E+00	1.40E+00	2.00E+01	1.56E-04	4.61E-03	1.08E-03	3.13E-01
59	1.62E-02	1.49E+00	1.39E+00	1.99E+01	1.55E-04	4.59E-03	1.08E-03	3.11E-01
60	1.61E-02	1.49E+00	1.39E+00	1.98E+01	1.54E-04	4.57E-03	1.08E-03	3.10E-01
61	1.60E-02	1.48E+00	1.38E+00	1.97E+01	1.54E-04	4.55E-03	1.07E-03	3.09E-01
62	1.60E-02	1.48E+00	1.37E+00	1.96E+01	1.53E-04	4.53E-03	1.07E-03	3.07E-01
63	1.59E-02	1.47E+00	1.37E+00	1.95E+01	1.53E-04	4.51E-03	1.06E-03	3.06E-01
64	1.58E-02	1.46E+00	1.36E+00	1.94E+01	1.52E-04	4.49E-03	1.06E-03	3.04E-01
65	1.58E-02	1.46E+00	1.36E+00	1.93E+01	1.51E-04	4.48E-03	1.05E-03	3.03E-01
66	1.57E-02	1.45E+00	1.35E+00	1.92E+01	1.51E-04	4.46E-03	1.05E-03	3.02E-01
67	1.56E-02	1.45E+00	1.35E+00	1.92E+01	1.50E-04	4.44E-03	1.04E-03	3.00E-01
68	1.56E-02	1.44E+00	1.34E+00	1.91E+01	1.49E-04	4.42E-03	1.04E-03	2.99E-01
69	1.55E-02	1.43E+00	1.33E+00	1.90E+01	1.49E-04	4.40E-03	1.04E-03	2.97E-01
70	1.54E-02	1.43E+00	1.33E+00	1.89E+01	1.48E-04	4.38E-03	1.03E-03	2.96E-01
71	1.54E-02	1.42E+00	1.32E+00	1.88E+01	1.48E-04	4.37E-03	1.03E-03	2.95E-01

72	1.53E-02	1.42E+00	1.32E+00	1.87E+01	1.47E-04	4.35E-03	1.02E-03	2.93E-01
73	1.52E-02	1.41E+00	1.31E+00	1.86E+01	1.46E-04	4.33E-03	1.02E-03	2.92E-01
74	1.52E-02	1.40E+00	1.31E+00	1.85E+01	1.46E-04	4.31E-03	1.02E-03	2.91E-01
75	1.51E-02	1.40E+00	1.30E+00	1.85E+01	1.45E-04	4.29E-03	1.01E-03	2.89E-01
76	1.51E-02	1.39E+00	1.30E+00	1.84E+01	1.45E-04	4.28E-03	1.01E-03	2.88E-01
77	1.50E-02	1.39E+00	1.29E+00	1.83E+01	1.44E-04	4.26E-03	1.00E-03	2.87E-01
78	1.49E-02	1.38E+00	1.29E+00	1.82E+01	1.43E-04	4.24E-03	9.98E-04	2.85E-01
79	1.49E-02	1.38E+00	1.28E+00	1.81E+01	1.43E-04	4.22E-03	9.94E-04	2.84E-01
80	1.48E-02	1.37E+00	1.28E+00	1.80E+01	1.42E-04	4.21E-03	9.90E-04	2.83E-01
81	1.47E-02	1.36E+00	1.27E+00	1.80E+01	1.42E-04	4.19E-03	9.86E-04	2.81E-01
82	1.47E-02	1.36E+00	1.26E+00	1.79E+01	1.41E-04	4.17E-03	9.82E-04	2.80E-01
83	1.46E-02	1.35E+00	1.26E+00	1.78E+01	1.40E-04	4.15E-03	9.78E-04	2.79E-01
84	1.46E-02	1.35E+00	1.25E+00	1.77E+01	1.40E-04	4.14E-03	9.74E-04	2.77E-01
85	1.45E-02	1.34E+00	1.25E+00	1.76E+01	1.39E-04	4.12E-03	9.70E-04	2.76E-01
86	1.44E-02	1.34E+00	1.24E+00	1.75E+01	1.39E-04	4.10E-03	9.66E-04	2.75E-01
87	1.44E-02	1.33E+00	1.24E+00	1.75E+01	1.38E-04	4.09E-03	9.62E-04	2.74E-01
88	1.43E-02	1.33E+00	1.23E+00	1.74E+01	1.38E-04	4.07E-03	9.58E-04	2.72E-01
89	1.43E-02	1.32E+00	1.23E+00	1.73E+01	1.37E-04	4.05E-03	9.54E-04	2.71E-01
90	1.42E-02	1.31E+00	1.22E+00	1.72E+01	1.36E-04	4.04E-03	9.50E-04	2.70E-01
91	1.41E-02	1.31E+00	1.22E+00	1.71E+01	1.36E-04	4.02E-03	9.46E-04	2.69E-01
92	1.41E-02	1.30E+00	1.21E+00	1.71E+01	1.35E-04	4.00E-03	9.42E-04	2.67E-01
93	1.40E-02	1.30E+00	1.21E+00	1.70E+01	1.35E-04	3.99E-03	9.39E-04	2.66E-01
94	1.40E-02	1.29E+00	1.20E+00	1.69E+01	1.34E-04	3.97E-03	9.35E-04	2.65E-01
95	1.39E-02	1.29E+00	1.20E+00	1.68E+01	1.34E-04	3.95E-03	9.31E-04	2.64E-01
96	1.39E-02	1.28E+00	1.19E+00	1.68E+01	1.33E-04	3.94E-03	9.27E-04	2.62E-01
97	1.38E-02	1.28E+00	1.19E+00	1.67E+01	1.33E-04	3.92E-03	9.23E-04	2.61E-01
98	1.37E-02	1.27E+00	1.18E+00	1.66E+01	1.32E-04	3.91E-03	9.19E-04	2.60E-01
99	1.37E-02	1.27E+00	1.18E+00	1.65E+01	1.31E-04	3.89E-03	9.16E-04	2.59E-01
100	1.36E-02	1.26E+00	1.17E+00	1.64E+01	1.31E-04	3.87E-03	9.12E-04	2.58E-01

SimpleBox quasi-dynamic output



SimpleBox quasi-dynamic output



SIMPLEBOX BATCHES & MACROS

LABEL — MACRO KEYSTROKE SEQUENCE — COMMENT

SIMBOX.bat

```
echo off
cls
simbox.exe
del integrat.bat
del simint.scn
del simint.set
del simint.log
del simint.res
del integrat.dat
cls
dir
```

Control batch; starts a SimpleBox session and deletes intermediate results upon finishing

\0 ; \Z

```
{frameoff}
{home}{goto}START~{d 16}
{?}
{home}{r 13}{d 5}
```

Start-up macro; shows welcome message, pauses, moves cell pointer to model definition

\Compute

```
{calc}
/dmiCF~CF-1~
/dmmCF-1~CNST~RES~
/rtRES~CSS~
{goto}SSOUTPUT3~
{calc}
```

Computation macro; carries out the steady-state computation by matrix inversion

INTEGRAT.bat

```
echo off
cls
set fame_outputexp2=1
echo Running the numeric integration routine may take quite a while . . .
echo Recorded integration times for the model in default settings:
echo    2  min. on 80486DX 50 MHz
echo    10 min. on 40386/87 33 MHZ
echo    4  hr. on 40386 25 MHZ
echo    1  hr. on 80286/87 12 MHz
echo    ...... on 8088 4.7 MHz
echo.
echo.
echo.
echo Press Ctrl-C to end . . .
pause
echo.
echo Running the integration routine . . .
simint %1 -r simint.res
splitres simint.res 14 1 6 2 3 7 12 8 9 >integrat.dat
```

Integration batch; sets DOS-environment for proper FAME-operation; starts integrator and processes raw integration output

\Integrate

```
{calc}
/dmiCF~CF-1~
/dmmCF-1~CNST~RES~
/rtRES~CSS~
{calc}
/ppoml0~mr240~ouqq
/pfINTEGRAT.BAT~rr{esc}INTEGRAT.BAT~agq
/pfSIMINT.SCN~rr{esc}SCENARIO1{?}~agq
/pfSIMINT.SET~rr{esc}SETTINGS~agq
{system "INTEGRAT"}
{goto}DYNOUTPUT~{d 12}
/reINTEGRATDATA~
/flnINTEGRAT.DAT~
/re{r 9}~
/gnuC-TIME~q
{goto}DYNCOMPUTATION2~
```

Integration macro; creates DOS-batch file for integration; creates input files for integrator; leaves the spreadsheet to start DOS integration job and returns; plots integration results on screen

\Report PP; \P

```
:plml1~r1~t1~b1~qcm53~qq
:plth..{esc}@|SimpleBox vs 1.0 (930801)|SIMBOX10.wk1{?}~qqq
:pltf..{esc}DEFINITION MODULE|DEFINITION1|page #~qqq
:prsDEFINITION1~g
:pltf..{esc}DEFINITION MODULE|DEFINITION2|page #~qqq
:prsDEFINITION2~g
:pltf..{esc}STEADY-STATE COMPUTATION MODULE|SSCOMPUTATI N|page #~qqq
:prsSSCOMPUTATION~g
:pltf..{esc}STEADY-STATE OUTPUT|SSOUTPUT1|page #~qqq
:prsSSOUTPUT1~g
:pltf..{esc}STEADY-STATE OUTPUT|SSOUTPUT2|page #~qqq
:prsSSOUTPUT2~g
:pltf..{esc}STEADY-STATE OUTPUT|SSOUTPUT3|page #~qqq
:prsSSOUTPUT3~g
```

Prints full report to postscriptprinter in WYSIWYG-mode

```
----------------------------------------------------------------------------------------------------------------------------------
\Report LP     /pppootml6~mr126~s..{esc}\027&l8D\027(s16.66H~p80~oaqq          Prints report to (HP) Laserjet
               /ppoh..{esc}@|SimpleBox vs 1.0 (930801)|SIMBOX10.wk1{?}~qq      in regular mode
               /ppof..{esc}DEFINITION||page #~qq
               /pprDEFINITION1~agpq
               /ppof..{esc}STEADY-STATE OUTPUT||page #~qq
               /pprSSOUTPUT3~agpq
----------------------------------------------------------------------------------------------------------------------------------
\Report MP     /pppootml6~mr126~s..{esc}\015~p66~oaqq                          Prints report to matrixprinter
               /ppoh..{esc}@|SimpleBox vs 1.0 (930801)|SIMBOX10.wk1{?}~qq      in regular mode
               /ppof..{esc}DEFINITION||page #~qq
               /pprDEFINITION1~agpq
               /ppof..{esc}STEADY-STATE OUTPUT||page #~qq
               /pprSSOUTPUT3~agpq
==================================================================================================================================
```

SIMPLEBOX START SCREEN

SIMPLEBOX version 1.0 (930801)
A REGIONAL MULTIMEDIA EXPOSURE ANALYSIS MODELING SHEET
by
D. van de Meent, RIVM, Bilthoven, The Netherlands

SimpleBox is a generic box model of the so-called "Mackay-type"; it can be run in steady state ("level 3") mode and in quasi-dynamic ("level 4") mode. SimpleBox is designed to be used by researchers as a diagnostic modeling tool; prediction of concentration levels in specific environmental situations is beyond the scope of this type of model. Required input: environmental quality standards, emission rates, partition coefficients, intermedia transfer rate constants and degradation rate constants. Output: concentrations and risk-quotients.

Information: Netherlands 030-743130; Dik van de Meent
[RETURN]

SIMPLEBOX VARIABLE NAMES

ACTIVETIME	T107
ADSORB(SED)	T179
ADVEC(1,1)	AG17
ADVEC(1,2)	AH17
ADVEC(1,3)	AI17
ADVEC(1,4)	AJ17
ADVEC(1,5)	AK17
ADVEC(1,6)	AL17
ADVEC(1,7)	AM17
ADVEC(1,8)	AN17
ADVEC(2,1)	AG18
ADVEC(2,2)	AH18
ADVEC(2,3)	AI18
ADVEC(2,4)	AJ18
ADVEC(2,5)	AK18
ADVEC(2,6)	AL18
ADVEC(2,7)	AM18
ADVEC(2,8)	AN18
ADVEC(3,1)	AG19
ADVEC(3,2)	AH19
ADVEC(3,3)	AI19
ADVEC(3,4)	AJ19
ADVEC(3,5)	AK19
ADVEC(3,6)	AL19
ADVEC(3,7)	AM19
ADVEC(3,8)	AN19
ADVEC(4,1)	AG20
ADVEC(4,2)	AH20
ADVEC(4,3)	AI20
ADVEC(4,4)	AJ20
ADVEC(4,5)	AK20
ADVEC(4,6)	AL20
ADVEC(4,7)	AM20
ADVEC(4,8)	AN20
ADVEC(5,1)	AG21
ADVEC(5,2)	AH21
ADVEC(5,3)	AI21
ADVEC(5,4)	AJ21
ADVEC(5,5)	AK21
ADVEC(5,6)	AL21
ADVEC(5,7)	AM21
ADVEC(5,8)	AN21
ADVEC(6,1)	AG22
ADVEC(6,2)	AH22
ADVEC(6,3)	AI22
ADVEC(6,4)	AJ22
ADVEC(6,5)	AK22
ADVEC(6,6)	AL22
ADVEC(6,7)	AM22
ADVEC(6,8)	AN22
ADVEC(7,1)	AG23
ADVEC(7,2)	AH23
ADVEC(7,3)	AI23
ADVEC(7,4)	AJ23
ADVEC(7,5)	AK23
ADVEC(7,6)	AL23
ADVEC(7,7)	AM23
ADVEC(7,8)	AN23
ADVEC(8,1)	AG24
ADVEC(8,2)	AH24
ADVEC(8,3)	AI24
ADVEC(8,4)	AJ24
ADVEC(8,5)	AK24
ADVEC(8,6)	AL24
ADVEC(8,7)	AM24
ADVEC(8,8)	AN24
AEROSOLDEPRATE	T147
AIRINFLOW	T114
AREAFRAC(SOIL1)	T53
AREAFRAC(SOIL2)	T54
AREAFRAC(SOIL3)	T55
AREAFRAC(WATER)	T52
BACT(SEDWATER)	T133
BACT(SOILWATER)	T138
BACT(TEST)	T130
BACT(WATER)	T131
BATCHES-MACROS	DS1..EC103
BCF(FISH)	T24
BIO(WATER)	T60
BURIAL(3)	AI13
BURIAL(SED)	T198
CF	AG40..AN47
CF(1,1)	AG40

CF(1,2)	AH40
CF(1,3)	AI40
CF(1,4)	AJ40
CF(1,5)	AK40
CF(1,6)	AL40
CF(1,7)	AM40
CF(1,8)	AN40
CF(2,1)	AG41
CF(2,2)	AH41
CF(2,3)	AI41
CF(2,4)	AJ41
CF(2,5)	AK41
CF(2,6)	AL41
CF(2,7)	AM41
CF(2,8)	AN41
CF(3,1)	AG42
CF(3,2)	AH42
CF(3,3)	AI42
CF(3,4)	AJ42
CF(3,5)	AK42
CF(3,6)	AL42
CF(3,7)	AM42
CF(3,8)	AN42
CF(4,1)	AG43
CF(4,2)	AH43
CF(4,3)	AI43
CF(4,4)	AJ43
CF(4,5)	AK43
CF(4,6)	AL43
CF(4,7)	AM43
CF(4,8)	AN43
CF(5,1)	AG44
CF(5,2)	AH44
CF(5,3)	AI44
CF(5,4)	AJ44
CF(5,5)	AK44
CF(5,6)	AL44
CF(5,7)	AM44
CF(5,8)	AN44
CF(6,1)	AG45
CF(6,2)	AH45
CF(6,3)	AI45
CF(6,4)	AJ45
CF(6,5)	AK45
CF(6,6)	AL45
CF(6,7)	AM45
CF(6,8)	AN45
CF(7,1)	AG46
CF(7,2)	AH46
CF(7,3)	AI46
CF(7,4)	AJ46
CF(7,5)	AK46
CF(7,6)	AL46
CF(7,7)	AM46
CF(7,8)	AN46
CF(8,1)	AG47
CF(8,2)	AH47
CF(8,3)	AI47
CF(8,4)	AJ47
CF(8,5)	AK47
CF(8,6)	AL47
CF(8,7)	AM47
CF(8,8)	AN47
CF-1	AG51..AN58
CNST	AF40..AF47
COMPOUND NAME	T6
CONCIMP(AIR)	T115
CONCIMP(SUSP)	T121
CONCIMP(WATER)	T118
CONCSTP(SLUDGE)	T101
CONCSTP(SUSP)	T100
CONCSTP(WATER)	T99
CONVFACTOR	CN43
CONVFACTOR1	CN44
CONVFACTOR2	CN45
CONVFACTOR3	CN46
CONVFACTOR4	CN47
CORG(SED)	T28
CORG(SOIL1)	T31
CORG(SOIL2)	T34
CORG(SOIL3)	T37
CORG(SUSP)	T22
CSS	AG64..AN64
CSS(1)	AG64
CSS(2)	AH64

CSS(3)	AI64
CSS(4)	AJ64
CSS(5)	AK64
CSS(6)	AL64
CSS(7)	AM64
CSS(8)	AN64
CSS(AIR)	BW12
CSS(BIO)	BW15
CSS(PWSED)	BW17
CSS(PWSOIL1)	BW19
CSS(PWSOIL2)	BW21
CSS(PWSOIL3)	BW23
CSS(SED)	BW16
CSS(SOIL1)	BW18
CSS(SOIL2)	BW20
CSS(SOIL3)	BW22
CSS(SUSP)	BW14
CSS(WATER)	BW13
DEFINITION1	A1..U204
DEFINITION2	W1..AC64
DEG(AIR)	Z32
DEG(SED)	Z34
DEG(SOIL1)	Z35
DEG(SOIL2)	Z36
DEG(SOIL3)	Z37
DEG(WATER)	Z33
DEGRADATION(1)	AG14
DEGRADATION(2)	AH14
DEGRADATION(3)	AI14
DEGRADATION(4)	AJ14
DEGRADATION(5)	AK14
DEGRADATION(6)	AL14
DEGRADATION(7)	AM14
DEGRADATION(8)	AN14
DEP(SOIL1)	Z40
DEP(SOIL2)	Z41
DEP(SOIL3)	Z42
DEP(WATER)	Z39
DEPTH(SED)	T62
DEPTH(SOIL1)	T64
DEPTH(SOIL2)	T65
DEPTH(SOIL3)	T66
DEPTH(WATER)	T57
DESORB(SED)	T180
DIFF(1,1)	AG27
DIFF(1,2)	AH27
DIFF(1,3)	AI27
DIFF(1,4)	AJ27
DIFF(1,5)	AK27
DIFF(1,6)	AL27
DIFF(1,7)	AM27
DIFF(1,8)	AN27
DIFF(2,1)	AG28
DIFF(2,2)	AH28
DIFF(2,3)	AI28
DIFF(2,4)	AJ28
DIFF(2,5)	AK28
DIFF(2,6)	AL28
DIFF(2,7)	AM28
DIFF(2,8)	AN28
DIFF(3,1)	AG29
DIFF(3,2)	AH29
DIFF(3,3)	AI29
DIFF(3,4)	AJ29
DIFF(3,5)	AK29
DIFF(3,6)	AL29
DIFF(3,7)	AM29
DIFF(3,8)	AN29
DIFF(4,1)	AG30
DIFF(4,2)	AH30
DIFF(4,3)	AI30
DIFF(4,4)	AJ30
DIFF(4,5)	AK30
DIFF(4,6)	AL30
DIFF(4,7)	AM30
DIFF(4,8)	AN30
DIFF(5,1)	AG31
DIFF(5,2)	AH31
DIFF(5,3)	AI31
DIFF(5,4)	AJ31
DIFF(5,5)	AK31
DIFF(5,6)	AL31
DIFF(5,7)	AM31
DIFF(5,8)	AN31
DIFF(6,1)	AG32

DIFF(6,2)	AH32
DIFF(6,3)	AI32
DIFF(6,4)	AJ32
DIFF(6,5)	AK32
DIFF(6,6)	AL32
DIFF(6,7)	AM32
DIFF(6,8)	AN32
DIFF(7,1)	AG33
DIFF(7,2)	AH33
DIFF(7,3)	AI33
DIFF(7,4)	AJ33
DIFF(7,5)	AK33
DIFF(7,6)	AL33
DIFF(7,7)	AM33
DIFF(7,8)	AN33
DIFF(8,1)	AG34
DIFF(8,2)	AH34
DIFF(8,3)	AI34
DIFF(8,4)	AJ34
DIFF(8,5)	AK34
DIFF(8,6)	AL34
DIFF(8,7)	AM34
DIFF(8,8)	AN34
DRYDEPAEROSOL	T145
DYNCOMPUTATION1	AP1..BB250
DYNCOMPUTATION2	BD1..BF156
DYNCOMPUTATION3	BH1..BS42
DYNOUTPUT	DH1..DQ116
EDIRECT(AIR)	T81
EDIRECT(SOIL1)	T83
EDIRECT(SOIL2)	T84
EDIRECT(SOIL3)	T85
EDIRECT(WATER)	T82
EFFLUENT(STP)	T102
EMIS(AIR)	Z13
EMIS(SOIL1)	Z16
EMIS(SOIL2)	Z17
EMIS(SOIL3)	Z18
EMIS(SUSP)	Z15
EMIS(WATER)	Z14
EMISFACT(AIR)	T88
EMISFACT(SOIL1)	T90
EMISFACT(SOIL2)	T91
EMISFACT(SOIL3)	T92
EMISFACT(WATER)	T89
EMISSION(1)	AG9
EMISSION(2)	AH9
EMISSION(4)	AJ9
EMISSION(5)	AK9
EMISSION(6)	AL9
EMISSION(7)	AM9
EQUTIME(BIO)	T171
EQUTIME(SUSP)	T168
EROSION(SOIL1)	T191
EROSION(SOIL2)	T192
EROSION(SOIL3)	T193
ESTP(AIR)	T95
ESTP(SOIL2)	T98
ESTP(SUSP)	T97
ESTP(WATER)	T96
EXPORT(1)	AG11
EXPORT(2)	AH11
EXPORT(7)	AM11
F(1)	AG65
F(2)	AH65
F(3)	AI65
F(4)	AJ65
F(5)	AK65
F(6)	AL65
F(7)	AM65
F(8)	AN65
FAMETEXT	AP6..BB249
FAT(FISH)	T25
FLOW(AIR)	Z24
FLOW(SUSP)	Z26
FLOW(WATER)	Z25
FORMULA	T7
FR(EFFSTP)	T108
FR(SLUDGESTP)	T109
FR(VOLATSTP)	T110
FRACINF(SOIL1)	T200
FRACINF(SOIL2)	T201
FRACINF(SOIL3)	T202
FRACRUN(SOIL1)	T188
FRACRUN(SOIL2)	T189

FRACRUN(SOIL3)	T190
FRAIR(SOIL)	T67
FRASS(AEROSOL)	T146
FRDISSLVD(SED)	T134
FRDISSLVD(SOIL)	T139
FRSOLID(SOIL)	T69
FRWATER(BIO)	T61
FRWATER(SED)	T63
FRWATER(SOIL)	T68
FRWATER(SUSP)	T59
GASABS(SOIL1)	T155
GASABS(SOIL2)	T157
GASABS(SOIL3)	T159
GASABS(WATER)	T151
GROSSSEDRATE	T174
HEIGHT(AIR)	T56
IMP(AIR)	Z20
IMP(SUSP)	Z22
IMP(WATER)	Z21
IMPORT(1)	AG10
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IMPORT(7)	AM10
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