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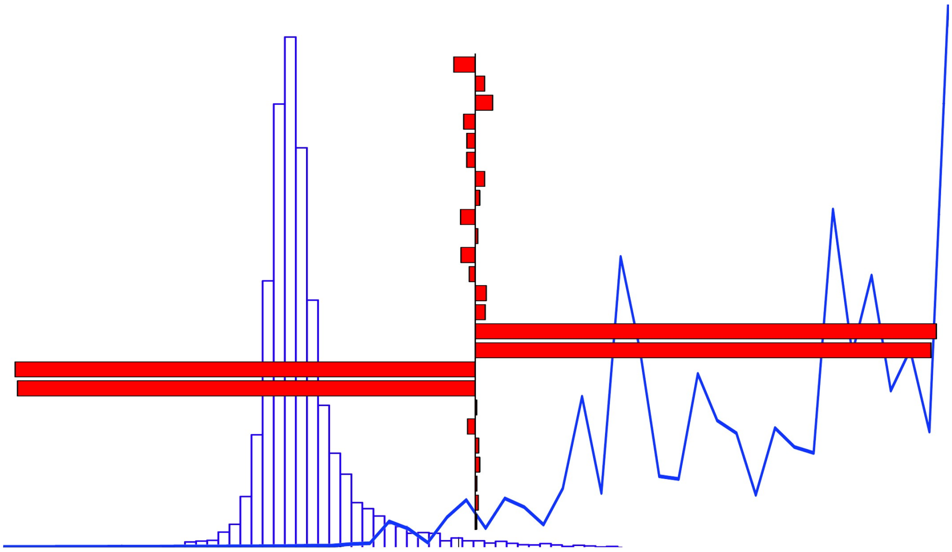

Quantitative uncertainty and sensitivity analysis of the OMNIITOX Base Model algorithm

Master of Science Thesis

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Abstract

This thesis analyzes the quantitative uncertainty and sensitivity of an intermediate parameter in the OMNIITOX Base Model algorithm which can be used for calculation of characterisation factors to carry out Life cycle assessments (LCA) and Environmental risk assessments (ERA). The quantitative uncertainty of LCA and ERA has been widely recognized, but there exists no estimation of the quantitative uncertainty of the OMNIITOX BM. The purpose of this thesis is to give an example of how large the quantitative uncertainty of an intermediate parameter of OMNIITOX BM can be and which input parameters that contributes the most to this uncertainty. This example could inspire to go further and make a quantitative uncertainty and sensitivity analysis for the complete algorithm, involving all parameters. The methodology that is used in this thesis can be modified to address the issue in more general terms.

First, the intermediate parameter *Rate coefficient from air to fresh water in Europe* was chosen for further analysis. The uncertainty analysis was limited to the nature specific parameters. For further investigation of the statistical properties of these parameters, the reference chemical Toluene was chosen for the chemical specific input parameters, provided as single point values. The distribution functions for the nature specific input parameters were estimated from information given in literature. A simulation program was implemented in *Matlab* which runs the algorithm for the chosen intermediate parameter with random numbers from the estimated input parameter distribution functions. The output data was later analyzed with the *Matlab*-tool *dfittool* to measure the uncertainty and fit a distribution function to the chosen intermediate parameter. The simulation program also measured the sensitivity of the input parameters with normalized correlation coefficients. The distribution function for the intermediate parameter was later applied to similar intermediate parameters in another simulation program which runs the complete algorithm of OMNIITOX BM. With this program, the uncertainty of the characterisation factors was estimated.

The quantitative uncertainty of the *Rate coefficient air to fresh water Europe* is remarkably high, with a 95%-confidence interval of $[-0.0130, 0.0270]$, $mean = 0.00679$ and $std = 0.01060$ if a normal distribution cut-off fit is chosen for the output data. The input parameters that contributes the most to this uncertainty is *Mixing height of air* and *Particle dry deposition velocity in air*. When randomly generating numbers from the distribution function of *Rate coefficient air to fresh water Europe* in the calculation of characterisation factors, they were insignificantly affected. If an equal distribution was assumed for all rate coefficients as the analyzed intermediate parameter, the uncertainty of the characterisation factors became extremely high.

Key words: sensitivity analysis, uncertainty analysis, OMNIITOX, characterisation factor, rate coefficient, LCA, ERA, simulation.

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1 Introduction

The OMNIITOX information system (OMNIITOX IS) is the result of an EU-project which ran from 2001 to 2004. OMNIITOX IS supports decision making regarding potentially hazardous compounds by improving methods and developing information tools necessary for impact assessment of toxic chemicals within Life Cycle Assessment (LCA) and (Environmental) Risk Assessment (E)RA. (OMNIITOX, 2008)

OMNIITOX IS contains an implementation of the OMNIITOX Base Model (OMNIITOX BM) which is a model for calculating characterisation factors for environmental impact. OMNIITOX BM is built on a matrix based modulized calculation method with a level of complexity similar to other ecotoxicity models which are used for Life Cycle Assessment (LCA). (Rosenbaum et al., 2007)

It is common that LCA studies are carried out without any quantitative estimations of the uncertainty of the result even though there is a demand and recommendation for uncertainty and sensitivity analysis in e.g. ISO 14040. With these types of analyses one can estimate the probability for making the right decision and learn how to improve this probability. These issues are addressed in, e.g., Steen (1997) and Ciroth & Srocka (2008).

There are plenty of arguments for integrating quantitative uncertainty and sensitivity analysis in Life Cycle Inventory (LCI) databases like the OMNIITOX database (see e.g. Sugiyama et al., 2005). Parameters from LCI databases are used to carry out a LCA. The uncertainty in these parameters therefore contributes to the uncertainty of the LCA results. The result from the uncertainty analysis in Hertwich et al. (1999) of the CalTOX Model, which can be used for calculating human health impact from environmental releases of chemicals, shows a great order of uncertainty in the output parameters. The CalTOX Model together with the EUSES model (EC, 1996), the Simple box model (Brandes et al., 1996), the BETR model (MacLeod et al., 2001) and IMPACT 2002 (Pennington et al., 2005) have been evaluated, compared, updated and extended to construct the OMNIITOX BM (Rosenbaum et al., 2007). The uncertainty of models like these has been widely recognized although there exist no estimation of the quantitative uncertainty in OMNIITOX BM. This leads to the problem definition of this master thesis.

This master thesis aims at answering the following questions:

1. How high is the quantitative uncertainty regarding an intermediate parameter in OMNIITOX BM?
2. Which input parameters contributes the most to this uncertainty?
3. Based on the answers to question 1 and 2, what conclusion can be made about the total uncertainty and sensitivity of the OMNIITOX BM?

The purpose of this master thesis is to improve decision making based on OMNIITOX BM by giving an example of its quantitative uncertainty and sensitivity, and show how to analyze these issues. In this way it also contributes to a more solid risk management process for OMNIITOX IS users. The goal is to give rise to an integration of quantitative uncertainty and sensitivity issues in the OMNIITOX IS.

The algorithm in OMNIITOX BM for calculating the characterisation factors contains a large number of nature and chemical specific parameters as well as equations. This master thesis focuses on the nature specific parameters in a limited part of the algorithm.

2 Characterisation factors and LCA

The OMNIITOX BM can be used to calculate the characterisation factors, *HDF-Human Damage Factors* and *EDF-Ecotoxicological Damage Factors*, describing human health impact characterisation and ecotoxicological characterisation, respectively. Combining the factors over over their compartments, exposure pathways or effect types, the framework can be expressed using matrix algebra. The matrix multiplications

$$HDM = EM \cdot XM \cdot FM$$

and

$$EDM = EEM \cdot FM,$$

represent the core of the OMNIITOX BM, where HDM is the *Human Damage Matrix*, EM the *Effect Matrix* for human impact, XM the *Exposure Matrix*, FM the *Fate factor Matrix*, EDM the *Ecotoxicological Damage Matrix* and EEM the *Ecotoxicological Effect Matrix*. Table 1 below gives a description of these matrices.

Table 1: Description of the OMNIITOX BM matrices

Matrix	Elements	Unit of elements	Size(rows, columns)
HDM	Human damage factors	$cases/kg_{emitted}$	(n_{ef}, n_i)
EM	Effect factors	$cases/kg_{intake}$	(n_{ef}, n_{xr})
XM	Exposure rates	$1/day$	(n_{xr}, n_i)
EDM	Ecotoxicological damage factors	$PAF \cdot m^3 \cdot year/kg$	(n_{es}, n_i)
EEM	Ecotoxicological effect factors	$PAF \cdot m^3 \cdot day/kg$	(n_{es}, n_i)
FM	Fate factors	$days$	(n_i, n_m)

The size of the matrices are determined by the number of final compartments, n_i, the number of initial compartments, n_m which is equal to n_i, the number of exposure routes, n_{xr}, the number of effect types, n_{ef} and the number of ecosystems, n_{es}. FM is determined from the *Rate coefficient matrix*, A by

$$FM = -A^{-1}.$$

The fate factors, $FM_{i,j}$ can be interpreted as the increase of chemical mass in compartment, i due to an emission in mass unit per day in compartment j. A row entry, i connects the fate factors to a final compartment and a column entry, j connects to an initial compartment. The human damage factors $HDM_{i,j}$ is the increase in number of cases of diseases of effect type i as a consequence of an emission in compartment j. The ecotoxicological damage factors, $EDM_{i,j}$ is the time and volume integrated increase in affected fraction of spieces, per unit of chemical mass increase in ecosystem i, due to an emission in compartment j. (Rosenbaum et al., 2007)

A characterisation factor from either HDM or EDM can be used as an input parameter in an LCA. The LCA result can be described mathematically by the following equation:

$$y = \sum_{k=1}^{N} i_k c_k v_k$$

where y is the LCA result, N is the number of emissions for the compound of interest, i_k is the inventory result of emission k, c_k is the characterisation factor for emission k and v is the valuation factor (usually discarded) for the characterized emission k. (Steen, 1997)

3 Uncertainty

The term uncertainty can be interpreted in many different ways. Uncertainty may arise from incomplete information, disagreement between information sources, interpretion issues, variability or the structure of a model. When investigating the uncertainty of a model one can choose either a parametric or a model structure perspective. (Morgan & Henrion, 1992)

3.1 Model structure uncertainty

Any model is a simplification of reality. Even the most detailed model can never be completely exact. When constructing a model, one must limit the model to a certain amount of variables. Simplifying assumptions are usually made in order to approximate the real world in a tractable model, which lends itself to empirical estimation. This leads to the conclusion: *Every model is definitely false*. However, we may be able to compare different models and decide which model that gives the most accurate results. We can choose between different approximation and estimation methods in order to make the model structure less uncertain. (Morgan & Henrion, 1992)

3.2 Parametric uncertainty

Another perspective of dealing with uncertainty is to investigate the model from within its structure, and deal with the parameters that are used for deriving the result. If M is the model one wishes to investigate then, M can be written as a function

$$Y = M(I_1, I_2, \cdots, I_n),$$

where Y is the result of the model and $I_1, I_2, \cdots, I_n$ are the parameters used to derive the result. When dealing with a quantitative parameter it is useful to understand what type of quantity the parameter represents. Table 2 illustrates some different types of quantities and gives examples of them. The table is followed by a description of each type of quantity. (Morgan & Henrion, 1992)

Table 2: Types of quantities in a model

Type of quantity	Examples
Empirical parameter	Temperature, wind speed
Defined constant	Atomic weight, π
Decision variable	financial budget, speed limit
Index variable	height, time period
Model domain parameter	Geographic region, time horizon

Empirical quantities

Empirical quantities represent measurable properties of the system being modeled. A quantity must be measurable to be called empirical. In principle, all empirical quantities are uncertain. No experiment can measure an empirical quantity with zero error. The uncertainty can however be negligible for practical reasons. (Morgan & Henrion, 1992)

Defined constants

These quantities are fundamental physical constants. Some of these constants are actually empirical quantities and therefore uncertain. However, if they are it is only to a small degree. Most of these types of quantities are certain by definition. (Morgan & Henrion, 1992)

Decision variables

The decision maker exercises direct control over decision variables. They can also be called *control variables* or *policy variables*. It can be discussed, if the decision maker is certain about the *best* value for a decision variable. But if the quantity is a decision variable, then it has no true value by definition. It is up to the decision maker to give the quantity a value. (Morgan & Henrion, 1992)

Index variables

Index variables are quantities that describes location or time, e.g., index in a matrix, set of elements or a certain time period. These quantities are independent and inherent no uncertainty. (Morgan & Henrion, 1992)

Model domain parameters

These quantities can be compared to the decision variables with the difference that they are quantities that the modeler exercise direct control over. A model domain parameter determines the boundaries of the system that is being modelled. It is up to the modeler to give the quantity a value. (Morgan & Henrion, 1992)

3.3 Probability-, density- and distribution function

Because of the uncertainty of an empirical quantity, one can, given a number of observations, investigate the probability that the quantity is equal to or lies with in an interval of a certain value. An empirical quantity can be defined as a *stochastic variable*, X and described by a *probability function* in the discrete case and a *density function* or *distribution function* in the continuous case. Definitions of these statistical terms follows. (Blom et. al., 2005)

Definition 3.1

A stochastic variable is discrete if it can be assigned to a finite or countable infinite number of values. The function

$$p_X(x) = P(X = x), x = a_1, a_2, a_3, \cdots,$$

where $a_1, a_2, a_3, \cdots$ are the possible values of X, is called *the probability function* of the stochastic variable X. (Blom et. al., 2005)

Definition 3.2

If there is a function $f_X(x)$ and a function $F_X(x)$ so that

$$P(X \leq x) = F_X(x) = \int_{-\infty}^{x} f_X(u)du$$

for every x, then X is a continuous stochastic variable, $F_X(x)$ is called the *the distribution function* and $f_X(x)$ *the density function* of X. (Blom et. al., 2005)

Random number generation

If the distribution function, $F_X(x)$ or the probability function $p_X(x)$ is known, one can randomly generate values of X through the inverse $F_X(y_1)^{-1}$ or $p_X(y_2)^{-1}$. Because $y_1 = F_X(x)$, y_1 is distributed uniformally between 0 and 1, $y_1 \sim U(0, 1)$ (see section 9.2). (Blom et. al., 2005)

4 Methodology

The methodology of this master thesis can be illustrated by the scheme given in Figure 1. Due to the limitations of this study, an output parameter and reference chemical was chosen before the algorithm was implemented. The uncertainty analysis intend to answer question 1 and 3 and the sensitivity analysis intend to answer question 2 given in section 1.

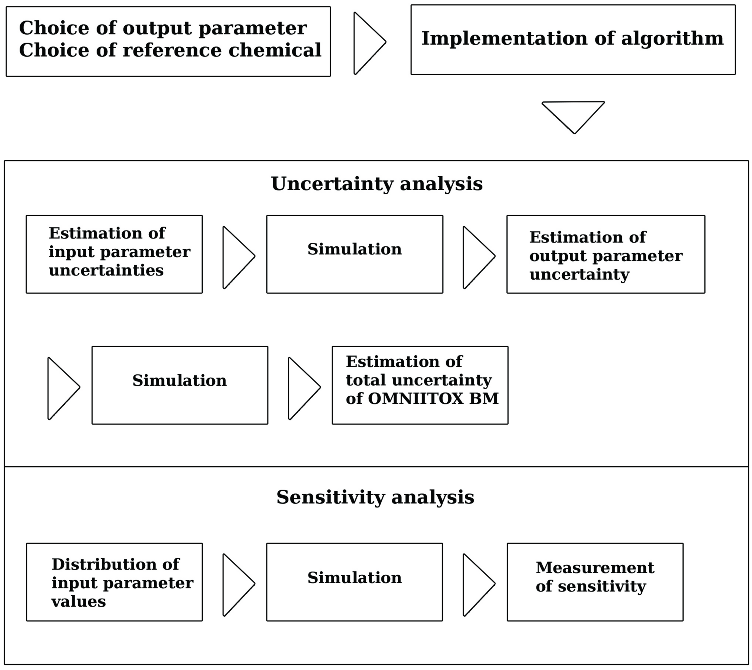

Figure 1: Methodology scheme

4.1 Choice of output parameter and reference chemical

The intermediate parameter that was chosen as output parameter for further studies was *Rate coefficient from air to fresh water in Europe*, $K_{a,fw,eur}$ (Rosenbaum & Jolliet, 2004) which is an element of the *Rate coefficient matrix A* given in section 2. The parameter is measured in the unit $days^{-1}$ and is a rate coefficient with initial compartment, air in Europe and final compartment, fresh water in Europe.

In order to estimate the uncertainty of $K_{a,fw,eur}$ contributed from the uncertainty of the nature specific input parameters, the reference chemical Toluene was chosen to represent the chemical specific input parameters. When choosing this chemical, one can estimate $K_{a,fw,eur}$ from *Rate coefficient air to fresh water dry period in Europe*, $K_{a,fw,dry,eur}$. The reason for this is that

$$K_{a,fw,eur} = K_{a,fw,dry,eur} + K_{a,fw,wet,eur},$$

where $K_{a,fw,wet,eur}$ is *Rate coefficient air to fresh water wet deposition in Europe*, and with Toluene as reference chemical $K_{a,fw,dry,eur} >> K_{a,fw,wet,eur}$.

4.2 Implementation of algorithm

At the OMNIITOX web site (OMNIITOX, 2008) you can find the parameter *Rate coefficient from air to fresh water Europe*, and get the algorithm for calculating it displayed in a tree structure showing all steps of calculation and parameters involved. Figure 2 shows a screenshot which is displaying all the intermediate parameters and some of the chemical and nature specific input parameters.

Figure 2: Screenshot of the algorithm for calculating *Rate coefficient from air to fresh water Europe*

The icons in shape of directories represent the intermediate parameters and can be considered as steps of calculation. The dashed lines illustrate the parameter dependence. When expanding the intermediate parameter icons, one can get a full view including all input parameters involved. The yellow icons represent the chemical specific input parameters and the green icons represent the nature specific input parameters. The intermediate parameters, except for *Rate coefficient from air to fresh water wet deposition Europe* have all been implemented as functions in *Matlab*. Table 3 gives the names of the Matlab function m-files. The source code for these functions are available in section 9.3. Table 4 shows all of the nature and chemical specific input parameters of the algorithm.

Intermediate parameter	File name
Volume of air compartment Europe	*vaeur.m*
Sub-cooled vapour pressure in Europe	*plseur.m*
Fraction sorbed to particles in air Europe	*frxeur.m*
Rate coefficient air to fresh water dry deposition by particles in Europe	*kafwdrypseur.m*
Henry's law constant, calc	*hc.m*
Diffusion velocity through fresh water boundary layer	*vfw.m*
Diffusion coefficient in air	*da.m*
Diffusion velocity through air boundary layer over land	*valand.m*
Diffusion velocity for air to fresh water in Europe	*vafwdiffeur.m*
Rate coefficient air to fresh water dry deposition by gases in Europe	*kafwdrypgeur.m*
Rate coefficient air to fresh water dry period in Europe	*kafwdryeur.m*

Table 3: Intermediate algorithm parameters

Input parameter	Unit
1. Diffusion coefficient for water in air	m^2/day
2. Mol weight water	$\frac{g}{mol}$
3. Mean wind speed at 10 metres over land	m/day
4. Mean air temperature in Europe	K
5. Universal gas constant	$\frac{Pa \cdot m^3}{K \cdot mol}$
6. Junge equation constant	$Pa \cdot m$
7. Specific surface area of aerosol particles	m^{-1}
8. Area of Europe	m^2
9. Mixing height of air	m
10. Particle dry deposition velocity in air	m/day
11. Surface area of fresh water compartment Europe	m^2
12. Molecular weight	$\frac{g}{mol}$
13. Vapour pressure	Pa
14. Water solubility	$\frac{kg}{m^3}$
15. Melting point	K

Table 4: Algorithm input parameters

The input parameters 1 to 11 in Table 4 are nature specific parameters and 12 to 15 are chemical specific parameters. There were also a number of unspecified parameters existing in the algorithm. Table 5 shows the values of these parameters and describes in which intermediate part of the algorithm they can be found.

Table 5: Unspecified algorithm parameters

Unspecified parameter	Found in intermediate parameter
$c_1 = 6.79$	Sub-cooled vapour pressure in Europe
$c_2 = 864$	Diffusion velocity through fresh water boundary layer
$c_3 = 32$	Diffusion velocity through fresh water boundary layer
$c_4 = 0.285$	Diffusion velocity through fresh water boundary layer
$c_5 = 0.00004$	Diffusion velocity through fresh water boundary layer
$c_6 = 86400$	Diffusion velocity through fresh water boundary layer
$c_7 = 0.0004$	Diffusion velocity through fresh water boundary layer
$c_8 = \frac{2}{3}$	Diffusion velocity through air boundary layer over land
$c_9 = 0.2$	Diffusion velocity through air boundary layer over land
$c_{10} = 0.3$	Diffusion velocity through air boundary layer over land

When refering to default parameter values and settings of the OMNIITOX BM algorithm, see section 9.1 for more information.

4.3 Uncertainty analysis

In this master thesis the uncertainty analysis will focus on parametric uncertainty of the OMNIITOX BM (see section 3.2). Among the parameters in Table 4, it is the nature specific parameters, 1 to 11 which are in focus for further analysis.

4.3.1 Estimation of input parameter uncertainty

The nature specific parameters can be considered as quantitative. One can divide these parameters into *empirical quantities* and *defined constants* (see section 3.2). The defined constants are:

1. Mol weight water
2. Universal gas constant
3. Junge equation constant

As argued in section 3.2, these parameters can be assumed to have neglible uncertainty. The empirical quantities are:

1. Diffusion coefficient for water in air
2. Mean wind speed at 10 metres over land
3. Mean air temperature in Europe
4. Specific surface area of aerosol particles
5. Area of Europe
6. Mixing height of air
7. Particle dry deposition velocity in air
8. Surface area of fresh water compartment Europe

When comparing these empirical quantities, one can assume that the relative uncertainty of *Mean wind speed at 10 metres over land*, *Mean air temperature in Europe*, *Area of Europe*, *Surface area of fresh water compartment Europe* compared the rest of the parameters are neglible. The first two mentioned are the mean value of a large number of observations through time and space.

Area measurements of the soil and fresh water of Europe are also considered as highly certain, the variance of these types of parameters are also considered as neglible. These assumptions leaves four nature specific input parameters for further investigation. Estimations have been made for these parameters' distributions based on available data and information in literature. Table 6 gives the estimated distributions and the literature sources of these estimations. A description of the estimations of each parameter's distribution function follows. For a description of the distribution functions see section 9.2.

Table 6: Estimated distribution for input parameters

Input parameter	Distribution function	Source
Diffusion coefficient for water in air	$U(1.8636, 1.1444)$	Massman, 1998
Specific surface area of aerosol particles	$U(0.42 \cdot 10^{-4}, 1.1 \cdot 10^{-3})$	Bidleman&Harner, 1998
Mixing height of air	$U(100, 2500)$	Nath&Patil, 2003
Particle dry deposition velocity in air	$N(500.8, 573.8)$	Grönholm et al., 2007

Diffusion coefficient for water in air

In Massman (1998) a review and re-analysis of historical data combined with some modeling results for the diffusion coefficient for water in air, D_w is presented. The diffusion coefficient, $D(T,p)$ is described as a function of temperature (T) and pressure (p). Near the standard temperature and pressure, STP this function can be expressed as

$$D(T,p) = D(0,1)(p_0/p)(T/T_0)^{\alpha}$$

where $T_0 = 273.15$ K, T is expressed in K, and α is limited by theory to a value between 1.5 and 2.0. The expression is valid provided that the pressure is not too near the critical pressure for the gas mixture. Therefore, all data in the study are limited to pressures well below the critical pressure. However, the study is focused on variation in $D(T,p)$ with temperature, not pressure. All data where therefore adjusted so that $p = p_0$. Furthermore, the data was fit to a regression in both a two-parameter mode (where $D(0,1)$ and α were fitted parameters) and a one-parameter mode(where only $D(0,1)$ were fit to the data and α were fixed at a value of 1.81). The results show that a fixed value of α caused no serious loss of information nor compromised the results in any significant way. The final result for $D_w(1,T)$ was

$$D_w(1,T) = 0.2178(T/273.15)^{1.81}$$

with an absolute uncertainty, (maximal difference between regressioncurve and data values) $= +-7\%$. With $T = 282.84$ K(the OMNIITOX default value of *Mean air temperature in Europe*), this information can be interpreted as

$$D_w \sim U(D_w(1,T)(1-0.07), D_w(1,T)(1+0.07)) = U(1.8636, 1.1444).$$

Specific surface area of aerosol particles

The definition of this parameter is particle surface area per volume of air. According to Bidleman & Harner (1998), a common assumption on the value of this parameter is $1.1 \cdot 10^{-3}$ m^{-1} for urban air and $(0.42 - 3.5) \cdot 10^{-4}$ m^{-1} for rural air. With only this information available, the distribution of this parameter can be assumed to be $U(0.42 \cdot 10^{-4}, 1.1 \cdot 10^{-3})$.

Mixing height of air

Mixing height is one of the fundamental parameters for determing the boundary layer structure where substances through turbulence eventually become well mixed. This is not a directly measurable parameter. It has to be estimated from advanced meteorological modelling. A specific distribution of this parameter is not given in Nath&Patil (2003), although results show that it can vary from 100 to 2500 m. The distribution can therefore assumed to be $U(100, 2500)$.

Particle dry deposition velocity in air

In Grönholm et al. (2007) measurements of particle dry deposition velocity in air, v_d is presented for the particle width, d with an interval of 10-150 nm in steps of 5-10 nm. v_d depends principally on particle size, atmospheric turbulence and stability and the collecting properties of the surface. The measurements were performed during the year 2004 at the SMEAR II station (Station for Measuring Forest Ecosystem-Atmospheric Relations), Hyytiälä, Southern Finland. To avoid seasonal variation, the measurements where normalized by multiplication with the factor $\frac{v_{30}(2004)}{v_{30}(i)}$, where $v_{30}(2004)$ is the dry deposition velocity for $d = 30$ nm measured during the whole period and $v_{30}(i)$ is the same parameter measured in month i. In all values of d, the measurements indicates a normal distribution with an decreasing interval of v_d, when increasing d. The article presents mean, μ_{v_d} and 75 percentile, $p_{v_d}(75)$ for $d = 8, 10, 15, 20, 25, 40, 50, 60, 70, 80, 100$ and 150 nm.
In order to calculate the standard deviation of v_d, σ_{v_d}, the following relation was used:

$$p_{v_d}(75) = \mu_{v_d} + \sigma_{v_d}\lambda_{0.25},$$

where $\lambda_{0.25}$ is the 25%-quantile of the standard normal distribution, $N(0, 1)$. For $d < 15$ the random error was relatively large. In order to estimate the distribution function of v_d, a dataset with a population of $n = 10000$ from 1000 random numbers from each value of d from the normal distributions $N(\mu_{v_d}, \sigma_{v_d})$ was constructed in *Matlab* (see the *Matlab*-function *depvel.m* in section 8.3). Further, the random numbers were normalized for seasonal variation according to the previously mentioned method. A distribution was fit to the dataset, using the *Matlab* tool *dfittool*. The result showed that

$$v_d \sim N(500.8, 573.8).$$

This is an estimation of the distribution function of v_d based on data with $d \leq 150nm$. In the OMNIITOX BM algorithm, v_d is not limited by any value of d, but according to Grönholm et al. (2007) the interval of $N(\mu_{v_d}, \sigma_{v_d})$ decreases for increasing value of d, which means that $N(500.8, 573.8)$ covers values for v_d with $d > 150nm$.

4.3.2 Simulation

The output parameter $K_{a,fw,dry,eur}$ can be written as a function

$$Y = K_{a,fw,dry,eur}(I_1, I_2, \cdots, I_{15}),$$

where Y is the output and $I_1, I_2, \cdots, I_{15}$ are the input parameters of Table 4, with index i of I_i refering to the listindex of the table. I_1, I_7, I_9 and I_{10} are considered as continuous stochastic variables (see section 3.3), with the cumulative distribution functions $F_{I_1}(x), F_{I_7}(x), F_{I_9}(x)$ and $F_{I_{10}}(x)$ given in Table 6. The rest of the input parameters can be considered as single values equal to the default values of section 9.1. A simulation program called *simulation.m* (see 9.3) which follows a *Monte Carlo Simulation* method was implemented. The program runs the algorithm for the output parameter, Y, 10000 times with repetitive random number generation of I_1, I_7, I_9 and I_{10} according to section 3.3 and with the default values of the rest of the input parameters (see section 9.1).

The output data was later analyzed with the *Matlab* tool *dfittool* from the *Statistics toolbox*. With this tool, the output data was fitted to a distribution and the standard deviation, mean and 95%-confidence interval was determined. The result from this analysis was later used in the program *simplus.m* to simulate the contribution to the total uncertainty of OMNIITOX BM in calculation of the characterisation factors. The program executes the matrix multiplications

$$HDM = EM \cdot XM \cdot FM$$

and

$$EDM = EEM \cdot FM,$$

10000 times with $FM = -A_{sim1}^{-1}$ in the first simulation run and $FM = -A_{sim2}^{-1}$ in the second, where EM, XM and EEM are given from a default calculation of the characterisation factors of Toluene with the OMNIITOX web-tool. Every element in A_{sim1} except for $A_{sim1}(2,1)$ is equal to the corresponding element of the default A, where column 1 represents initial compartment air in Europe and row 2 represents final compartment freshwater in Europe. The element $A_{sim1}(2,1)$ is simulated as random numbers generated from the estimated distribution of $K_{a,fw,dry,eur}$. In the matrix A_{sim2} every element is randomly generated (see section 3.3) simular to $A_{sim1}(2,1)$, with the same distribution and relationship between standard deviation and mean as $K_{a,fw,dry,eur}$. For the output data of these simulations, the characterisation factors, the program presents some descriptive statistics.

4.4 Sensitivity analysis

The program *simulation.m* also measures the sensitivity of the input parameters with normalized correlation coefficients between the input parameters and the output parameter data. This is done with the built in Matlab function *corrcoeff.m* from the the *Statistics toolbox*. This function numerically executes the analytic expression

$$r_{O,I_i} = \frac{cov(O, I_i)}{\sigma_O \sigma_{I_i}}, i = 1 \cdots N$$

where r_{O,I_i} is the correlation coefficient between O and I, cov is the covariance, O is the stochastic variable of the output data, I_i is the stochastic variable of input parameter i, σ_O is the standard deviation of O, σ_{I_i} is the standard deviation of I_i and N is the number of input parameters. This function was also used to investigate the covariance between the input parameters. If $r_{O,I_i} > 0$ it means that O is increasing when increasing I_i. If $r_{O,I_i} < 0$ it means that O is decreasing when increasing I_i.

The sensitivity was measured through four different simulation runs of the program *simulation.m* with different specifications.

Sensitivity analysis 1 is based on the simulated data from the uncertainty analysis. The sensitivity is measured on the parameters of Table 6.

Sensitivity analysis 2 measure the sensitivity of all the nature specific input parameters distributed uniformally with an interval of the default values +− 5%.

Sensitivity analysis 3 measure the sensitivity of all the nature and chemical (Toluene) specific input parameters distributed uniformally with an interval of the default values +− 5%.

Sensitivity analysis 4 measure the sensitivity of all the nature and chemical (Toluene) specific plus the unspecified input parameters distributed uniformally with an interval of the default values +− 5%.

5 Results

5.1 Uncertainty analysis

Figure 3 shows the density of the output parameter $K_{a,fw,dry,eur}$ and four different distribution fits to the data. The red line represents the first fit which is a normal distribution fitted straight to the data at hand. The blue line represents a truncated normal distribution with the tails cut off at -0.05 and 0.05. The yellow line represents a logistic distribution fit and the brown line represents a t-location scale distribution fit. Further information about these distributions are available in section 9.2. Table 7 gives further information about the accuracy of the four fits. Figure 4 shows the results of the fits with their cumulative distribution functions.

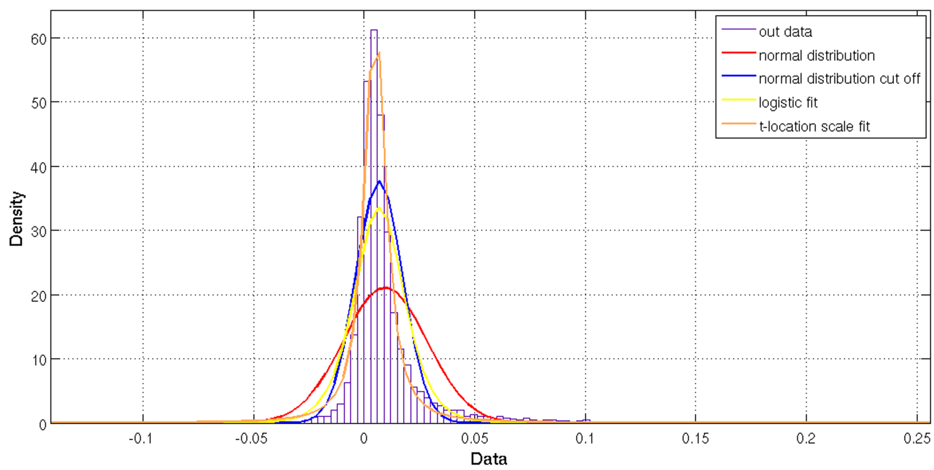

Figure 3: Distribution fit to output parameter, density function

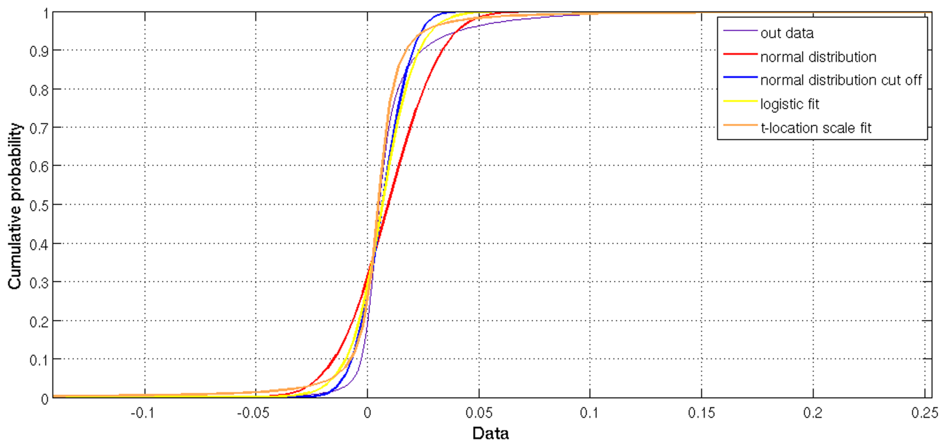

Figure 4: Distribution fit to output parameter, distribution function

Table 7: Distribution fit to output parameter

Distribution fit	Distribution specification	Log likelihood
Normal distribution	$N(0.00940, 0.01894)$	25478.1
Normal distribution cut-off	$N(0.00679, 0.01060)$	30020.7
Logistic	$\mu = 0.007$, $\sigma = 0.007$	28032.8
t-location scale	$\mu = 0.005$, $\sigma = 0.005$, $\nu = 1.42$	30385.5

The log likelihood value is a measure of how accurate the distribution fit is compared to the output data. A higher log likelihood value represents a better fit. Since the data of the output parameter is distributed with long tails and a skewness towards the negative values (the reason for this is unknown), the normal distribution fit is inaccurate. The best fit is the t-location scale distribution fit. However, the complexity level of this distribution and the logistic distribution is very high. In order to generate more manageable results and to simplify further work, the normal distribution cut-off fit was chosen for the output data.

The normal distribution cut-off fit gives a 95%-confidence interval of $[-0.0130, 0.0270]$. Table 8 shows some descriptive statistics of the characterisation factors for ecotoxicological damage and human damage (cancer effect only) when the matrix A_{sim1} was used instead of A. The element $A_{sim1}(2,1) = K_{a,fw,dry,eur}$ was randomly generated from the normal distribution cut-off fit.

Table 8: Uncertainty of characterisation factors contributed from one rate coefficient

Characterisation factor	mean	std	mean/std	Lower 95% c.i. bound	Upper 95% c.i. Bound
Eco, Air Europe	8,74E-004	2,77E-007	3,15E+003	8,74E-004	8,75E-004
Eco, Fresh water Europe	5,82E-001	1,93E-004	3,02E+003	5,82E-001	5,82E-001
Eco, Fresh water sediment Europe	5,42E-001	1,79E-004	3,02E+003	5,42E-001	5,42E-001
Eco, Sea Water Europe	9,26E-005	2,94E-008	3,15E+003	9,25E-005	9,27E-005
Eco, Sea Water sediment Europe	8,54E-005	2,71E-008	3,15E+003	8,54E-005	8,55E-005
Eco, Agricultural soil Europe	3,81E-003	1,25E-006	3,04E+003	3,81E-003	3,81E-003
Eco, Natural soil Europe	4,20E-003	1,38E-006	3,04E+003	4,20E-003	4,20E-003
Eco, Plantleaves Europe	8,74E-004	2,77E-007	3,15E+003	8,74E-004	8,75E-004
Eco, Plantstem Europe	1,60E-004	5,08E-008	3,15E+003	1,60E-004	1,60E-004
Eco, Air World	2,60E-004	9,39E-010	2,77E+005	2,60E-004	2,60E-004
Eco, Fresh water World	5,80E-001	3,51E-010	1,65E+009	5,80E-001	5,80E-001
Eco, Fresh water sediment World	5,40E-001	3,27E-010	1,65E+009	5,40E-001	5,40E-001
Eco, Sea Water World	2,76E-005	9,94E-011	2,77E+005	2,76E-005	2,76E-005
Eco, Sea Water Sediment World	2,54E-005	9,17E-011	2,77E+005	2,54E-005	2,54E-005
Eco, Agricultural soil World	8,89E-003	4,83E-010	1,84E+007	8,89E-003	8,89E-003
Eco, Natural soil World	9,98E-003	5,21E-010	1,91E+007	9,98E-003	9,98E-003
Eco, plantleaves World	2,60E-004	9,39E-010	2,77E+005	2,60E-004	2,60E-004
Eco, Plantstem World	4,78E-005	1,72E-010	2,77E+005	4,78E-005	4,78E-005
Human-cancer, Air Europe	9,86E-012	3,12E-015	3,15E+003	9,85E-012	9,86E-012
Human-cancer, Fresh water Europe	4,26E-009	2,17E-012	1,96E+003	4,25E-009	4,26E-009
Human-cancer, Fresh water sediment Europe	3,97E-009	2,02E-012	1,96E+003	3,96E-009	3,97E-009
Human-cancer, Sea Water Europe	2,37E-011	3,31E-016	7,16E+004	2,37E-011	2,37E-011
Human-cancer, Sea Water sediment Europe	2,19E-011	3,05E-016	7,16E+004	2,19E-011	2,19E-011
Human-cancer, Agricultural soil Europe	8,82E-008	1,41E-014	6,24E+006	8,82E-008	8,82E-008
Human-cancer, Natural soil Europe	3,27E-011	1,56E-014	2,10E+003	3,26E-011	3,27E-011
Human-cancer, Plantleaves Europe	1,09E-011	3,12E-015	3,48E+003	1,09E-011	1,09E-011
Human-cancer, Plantstem Europe	9,20E-007	5,73E-016	1,60E+009	9,20E-007	9,20E-007
Human-cancer, Air World	2,15E-012	1,06E-017	2,03E+005	2,15E-012	2,15E-012
Human-cancer, Fresh water World	3,10E-009	3,96E-018	7,82E+008	3,10E-009	3,10E-009
Human-cancer, Fresh water sediment World	2,88E-009	3,69E-018	7,82E+008	2,88E-009	2,88E-009
Human-cancer, Sea Water World	6,16E-011	1,12E-018	5,49E+007	6,16E-011	6,16E-011
Human-cancer, Sea Water Sediment World	5,68E-011	1,03E-018	5,49E+007	5,68E-011	5,68E-011
Human-cancer, Agricultural soil World	1,68E-008	5,45E-018	3,08E+009	1,68E-008	1,68E-008
Human-cancer, Natural soil World	5,37E-011	5,88E-018	9,13E+006	5,37E-011	5,37E-011
Human-cancer, plantleaves World	2,40E-012	1,06E-017	2,26E+005	2,40E-012	2,40E-012
Human-cancer, Plantstem World	1,53E-007	1,94E-018	7,88E+010	1,53E-007	1,53E-007

Results show that A_{sim1} caused insignificant uncertainty in the characterisation factors. Table 9 shows the same descriptive statistics of the characterisation factors when the matrix A_{sim2} was used instead of A where

$$\frac{std(K_{a,fw,dry,eur})}{mean(K_{a,fw,dry,eur})} = \frac{0.01060}{0.00679} = 1.561\ldots$$

Table 9: Uncertainty of characterisation factors contributed from all rate coefficients

Characterisation factor	**mean**	**std**	**mean/std**	**Lower 95% c.i. bound**	**Upper 95% c.i. Bound**
Eco, Air Europe	4,85E-004	1,78E-001	2,72E-003	-3,48E-001	3,49E-001
Eco, Fresh water Europe	-2,54E+000	2,56E+002	9,92E-003	-5,05E+002	5,00E+002
Eco, Fresh water sediment Europe	-8,25E+000	6,32E+002	1,31E-002	-1,25E+003	1,23E+003
Eco, Sea Water Europe	7,47E-004	6,47E-002	1,16E-002	-1,26E-001	1,28E-001
Eco, Sea Water sediment Europe	5,98E-004	9,99E-002	5,99E-003	-1,95E-001	1,96E-001
Eco, Agricultural soil Europe	-1,78E-002	1,98E+000	8,99E-003	-3,90E+000	3,87E+000
Eco, Natural soil Europe	-1,90E-001	1,31E+001	1,45E-002	-2,60E+001	2,56E+001
Eco, Plantleaves Europe	4,42E-003	4,21E-001	1,05E-002	-8,20E-001	8,29E-001
Eco, Plantstem Europe	2,52E-004	1,01E-001	2,48E-003	-1,98E-001	1,99E-001
Eco, Air World	7,81E-004	1,20E-001	6,53E-003	-2,33E-001	2,35E-001
Eco, Fresh water World	8,47E-002	2,32E+001	3,65E-003	-4,54E+001	4,55E+001
Eco, Fresh water sediment World	5,87E+000	4,99E+002	1,18E-002	-9,72E+002	9,84E+002
Eco, Sea Water World	-8,47E-004	1,15E-001	7,34E-003	-2,27E-001	2,25E-001
Eco, Sea Water Sediment World	-1,10E-003	1,35E-001	8,12E-003	-2,66E-001	2,64E-001
Eco, Agricultural soil World	6,72E-003	1,70E+000	3,96E-003	-3,32E+000	3,33E+000
Eco, Natural soil World	-8,87E-003	1,97E+000	4,49E-003	-3,88E+000	3,86E+000
Eco, plantleaves World	5,03E-004	4,91E-002	1,02E-002	-9,58E-002	9,68E-002
Eco, Plantstem World	4,59E-004	8,65E-002	5,30E-003	-1,69E-001	1,70E-001
Human-cancer, Air Europe	-4,32E-011	2,33E-009	1,85E-002	-4,61E-009	4,52E-009
Human-cancer, Fresh water Europe	-1,86E-008	1,87E-006	9,94E-003	-3,69E-006	3,66E-006
Human-cancer, Fresh water sediment Europe	-6,02E-008	4,62E-006	1,30E-002	-9,12E-006	9,00E-006
Human-cancer, Sea Water Europe	4,33E-011	3,07E-009	1,41E-002	-5,98E-009	6,06E-009
Human-cancer, Sea Water sediment Europe	2,81E-010	3,54E-008	7,94E-003	-6,90E-008	6,96E-008
Human-cancer, Agricultural soil Europe	9,45E-008	1,43E-005	6,59E-003	-2,80E-005	2,82E-005
Human-cancer, Natural soil Europe	-1,31E-009	9,63E-008	1,36E-002	-1,90E-007	1,87E-007
Human-cancer, Plantleaves Europe	-2,36E-011	5,26E-009	4,47E-003	-1,03E-008	1,03E-008
Human-cancer, Plantstem Europe	-5,52E-007	5,99E-005	9,22E-003	-1,18E-004	1,17E-004
Human-cancer, Air World	-2,29E-011	2,26E-009	1,01E-002	-4,45E-009	4,40E-009
Human-cancer, Fresh water World	4,41E-010	1,24E-007	3,56E-003	-2,42E-007	2,43E-007
Human-cancer, Fresh water sediment World	3,13E-008	2,66E-006	1,18E-002	-5,18E-006	5,24E-006
Human-cancer, Sea Water World	5,15E-011	3,04E-009	1,69E-002	-5,92E-009	6,02E-009
Human-cancer, Sea Water Sediment World	5,12E-011	1,63E-008	3,14E-003	-3,19E-008	3,20E-008
Human-cancer, Agricultural soil World	-1,22E-008	5,08E-006	2,40E-003	-9,97E-006	9,95E-006
Human-cancer, Natural soil World	-8,46E-011	1,12E-008	7,57E-003	-2,20E-008	2,18E-008
Human-cancer, plantleaves World	-8,15E-012	8,52E-010	9,56E-003	-1,68E-009	1,66E-009
Human-cancer, Plantstem World	-9,08E-008	1,35E-005	6,73E-003	-2,65E-005	2,64E-005

As we can see, the output data of the characterisation factors now show extremely high uncertainty. Negative values are generated and the standard deviation is around 100 to 10000 larger than the mean, giving a value of the $\frac{mean}{std}$ of the characterisation factors close to zero. Because of this highly unstable result, it was interesting to investigate the stability of the simulation further. In order to investigate the stability, the $\frac{std}{mean}$ of the rate coefficients was varied in the interval $0 < \frac{std}{mean} \leq 0.7$ and stability of the characterisation factors was measured with their standard deviation in *simplus.m*. 50 values are drawn from the interval of $\frac{std}{mean}$ and for each value the program runs the calculation of the characterisation factors 10000 times. The expected relationship between the $\frac{std}{mean}$ of the rate coefficients and the standard deviation of the characterisation factors was of exponential form, where the standard deviation of the characterisation factors at some point rapidly goes to infinity. This expected relationship is illustrated in Figure 5.

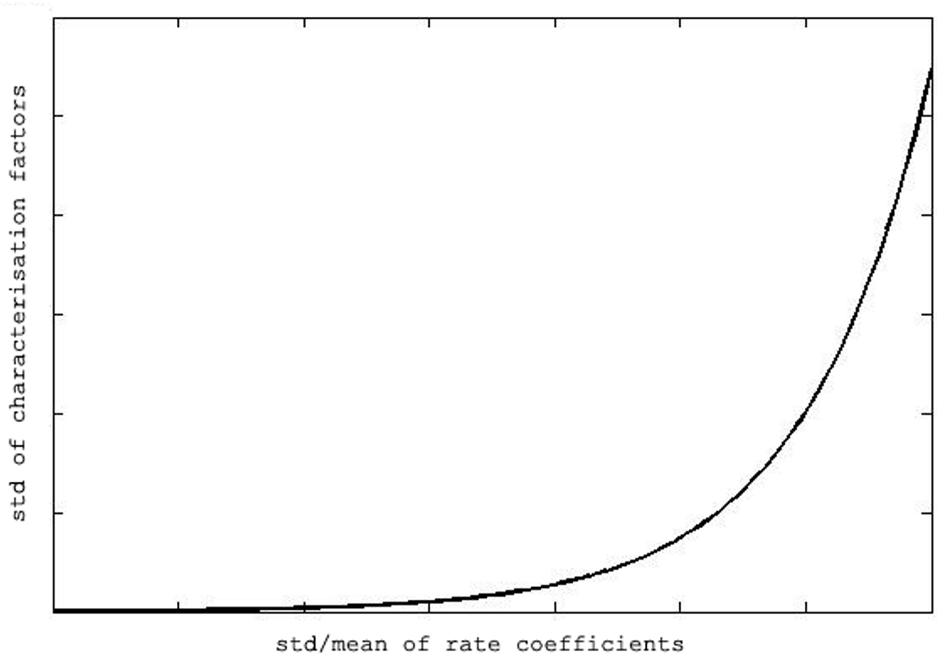

Figure 5: Expected relation between characterisation factors and rate coefficients

Figure 6 to 11 shows plots of standard deviation of the human- and ecotoxilogical characterisation factors in the compartments *air in Europe*, *fresh water in Europe*, *fresh water sediment in Europe* versus the $\frac{std}{mean}$ of the rate coefficients. The characterisation factors of the other compartments had similar relation to the rate coefficients.

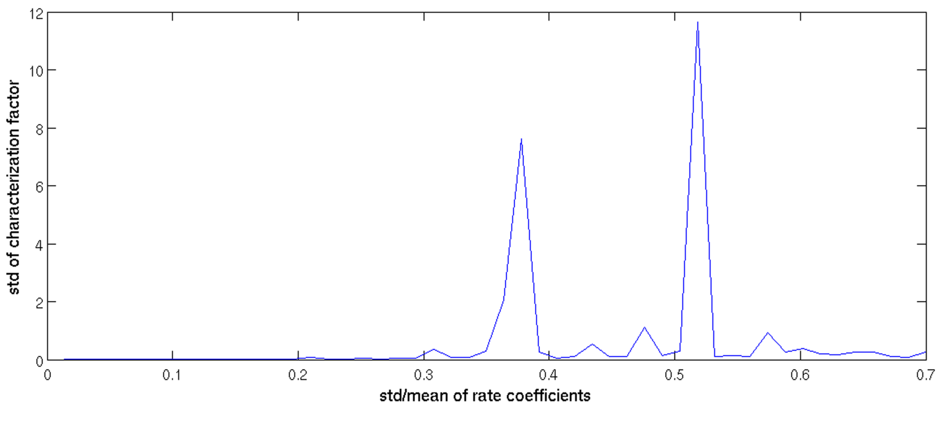

Figure 6: Stability of ecotoxicological damage factor of air in Europe

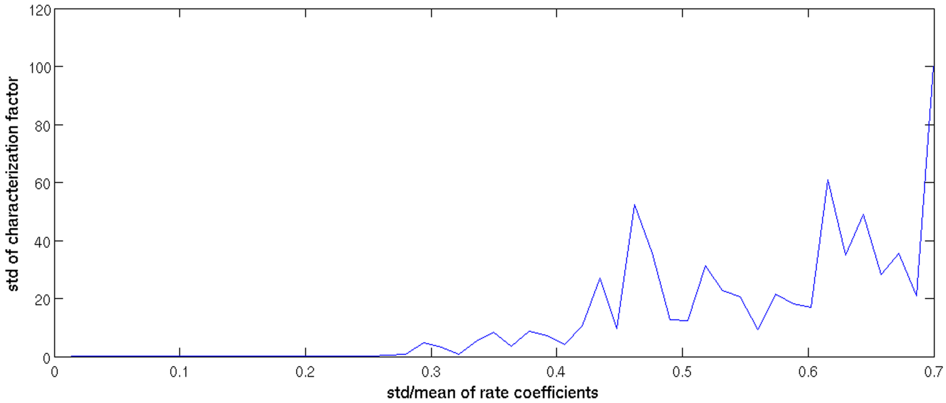

Figure 7: Stability of ecotoxicological damage factor of freshwater in Europe

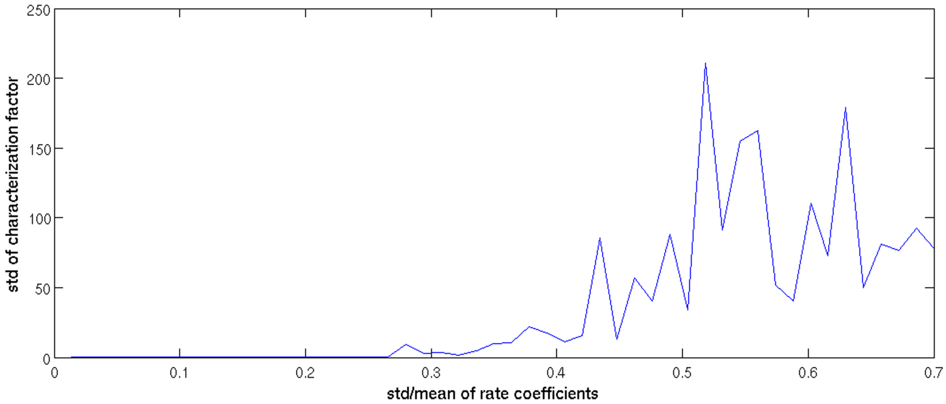

Figure 8: Stability of ecotoxicological damage factor of freshwater sediment in Europe

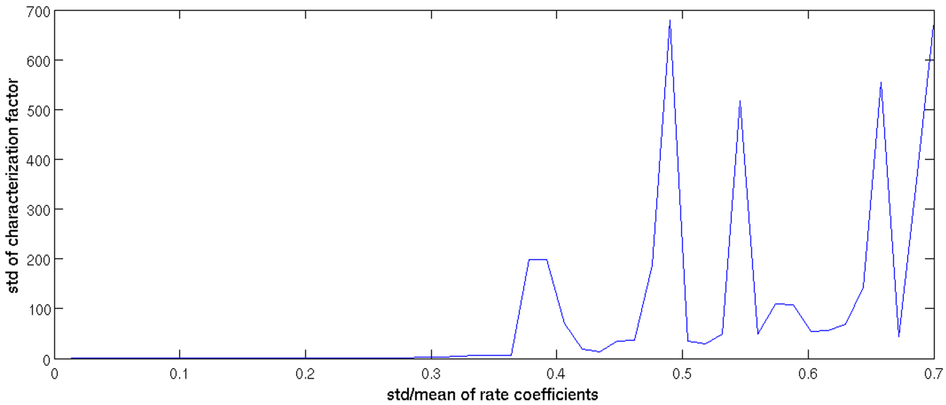

Figure 9: Stability of human damage factor of air in Europe

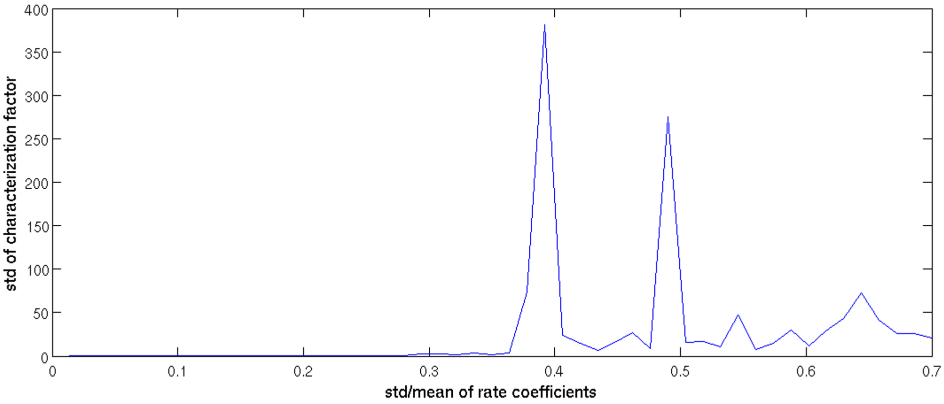

Figure 10: Stability of human damage factor of fresh water in Europe

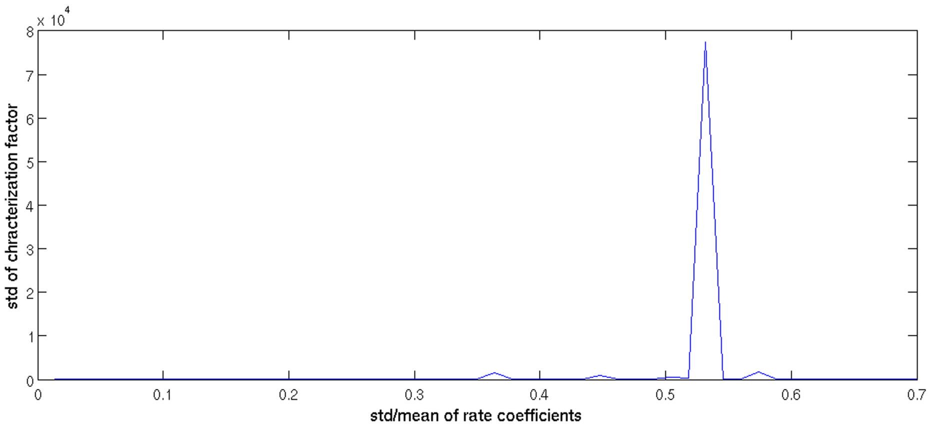

Figure 11: Stability of human damage factor of fresh water sediment in Europe

Clearly, the simulation did not generate the expected relationship between the characterisation factors and the rate coefficients. Instead the relationship was of some kind of oscillating nature. This will be discussed further in section 6.

5.2 Sensitivity analysis 1

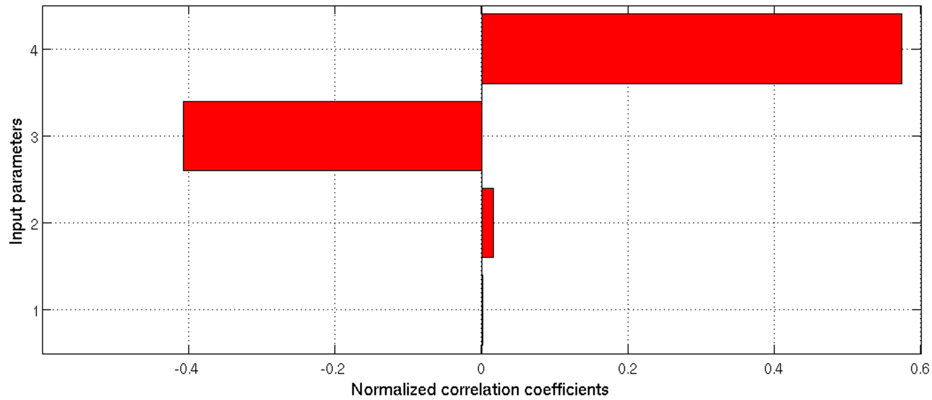

Figure 12: Sensitivity analysis 1

Figure 12 shows the normalized correlation coefficients between the output parameter and the input parameters with the indexes of the input parameter axis referring to

1. Diffusion coefficient for water in air
2. Specific surface area of aerosol particles
3. Mixing height of air
4. Particle dry deposition velocity in air

The covariance between the input parameters was close to zero.

5.3 Sensitivity analysis 2

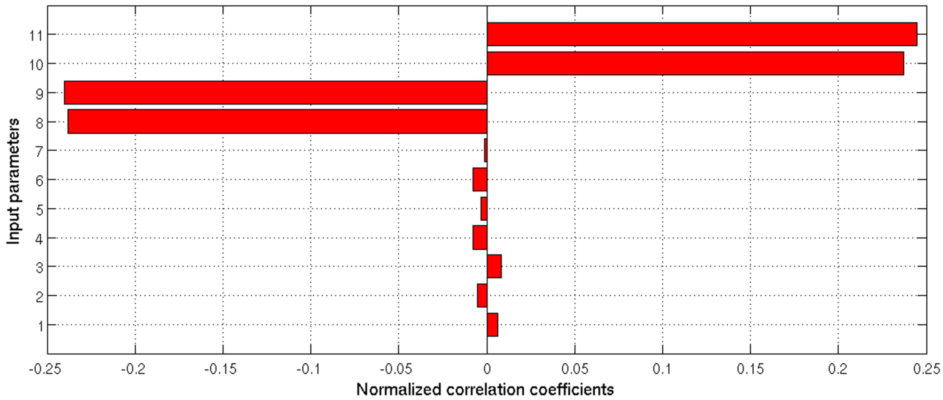

Figure 13: Sensitivity analysis 2

Figure 13 shows the normalized correlation coefficients between the output parameter and the input parameters with the indexes of the input parameter axis referring to

1. Diffusion coefficient for water in air
2. Mol weight water
3. Mean wind speed at 10 metres over land
4. Mean air temperature in Europe
5. Universal gas constant
6. Junge equation constant
7. Specific surface area of aerosol particles
8. Area of Europe
9. Mixing height of air
10. Particle dry deposition velocity in air
11. Surface area of fresh water compartment Europe

The covariance between the input parameters was close to zero.

5.4 Sensitivity analysis 3

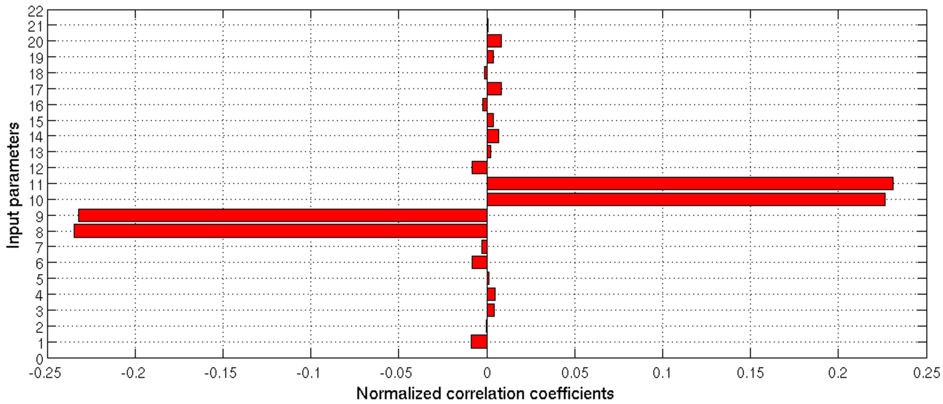

Figure 14: Sensitivity analysis 3

Figure 14 shows the normalized correlation coefficients between the output parameter and the input parameters with the indexes of the input parameter axis referring to

1. Diffusion coefficient for water in air
2. Mol weight water
3. Mean wind speed at 10 metres over land
4. Mean air temperature in Europe
5. Universal gas constant
6. Junge equation constant
7. Specific surface area of aerosol particles
8. Area of Europe
9. Mixing height of air
10. Particle dry deposition velocity in air
11. Surface area of fresh water compartment Europe
12. c_1
13. c_2
14. c_3
15. c_4
16. c_5
17. c_6
18. c_7
19. c_8
20. c_9
21. c_{10}

The covariance between the input parameters was close to zero.

5.5 Sensitivity analysis 4

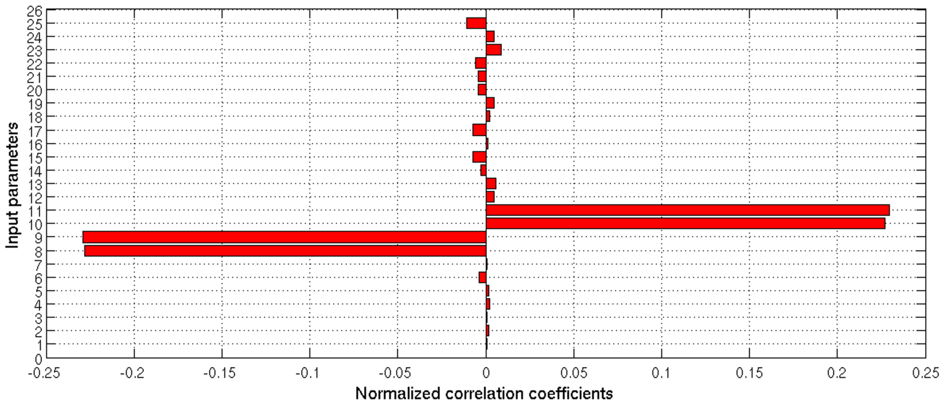

Figure 15: Sensitivity analysis 4

Figure 15 shows the normalized correlation coefficients between the output parameter and the input parameters with the indexes of the input parameter axis referring to

1. Diffusion coefficient for water in air
2. Mol weight water
3. Mean wind speed at 10 metres over land
4. Mean air temperature in Europe
5. Universal gas constant
6. Junge equation constant
7. Specific surface area of aerosol particles
8. Area of Europe
9. Mixing height of air
10. Particle dry deposition velocity in air
11. Surface area of fresh water compartment Europe
12. c_1
13. c_2
14. c_3
15. c_4
16. c_5
17. c_6
18. c_7
19. c_8
20. c_9

21. c_{10}
22. Molecular weight (Toluene)
23. Vapour pressure (Toluene)
24. Water solubility (Toluene)
25. Melting point (Toluene)

The covariance between the input parameters was close to zero.

5.6 Conclusion of the sensitivity analyses

The sensitivity analysis 1 to 4 show that it is four nature specific input parameters that are superior in sensitivity compared to all of the nature specific, chemical specific and unspecified input parameters. The most sensitive input parameters are

1. Area of Europe,
2. Mixing height of air,
3. Particle dry deposition velocity in air, and
4. Surface area of fresh water compartment Europe.

6 Discussion

It is clear that the level of uncertainty in the output parameter, $K_{a,fw,dry,eur}$ can be considered as high. In fact, so high that the uncertainty becomes a matter of model structure uncertainty (see section 3.1). An element $a_{i,j}$ of the rate coefficient matrix, A gives information about the flow of mass between two compartments depending on the row, i and column, j. The model is built so that $a_{i,j} \geq 0$ when $i \neq j$ and $a_{i,j} < 0$ when $i = j$, which represents the total flow from one compartment. The results of the uncertainty analysis show that a rate coefficient can have so high measurement uncertainty that it conflicts with these conditions. Negative values of the rate coefficient from air to fresh water in Europe are generated in OMNIITOX BM when randomly generating values of the parameters according to the distributions found in the literature. Thus, the negative values give information about the flow from fresh water to air in Europe which is already represented in another element in A. This causes misinformation in the calculations of the characterisation factors, which appears in the estimation of the total uncertainty of OMNIITOX BM. The *Rate coefficient air to fresh water Europe* is only one element of 62 elements in $A, \neq 0$. When randomly simulating only this element, the uncertainty of the characterisation factors is not significantly affected, see Table 8. When randomly simulating all the 62 rate coefficients similar to the distribution of $K_{a,fw,dry,eur}$, Table 9 shows an extremely high level of uncertainty of the characterisation factors. Negative values are generated and the standard deviation is around 100 to 10000 times bigger than the mean, giving a value of the ratio $\frac{mean}{std}$ close to zero. This result is not surprising since the standard deviations of the rate coefficients are about 160% of their mean, causing a very wide distribution in the simulation. Although Figure 6 to 11 show signs of instability in the characterisation factors in rather narrow distributions of the rate coefficients ($\frac{std}{mean} > 0.3$). The simulated data of the characterisation factors differs so much that the standard deviation peaks in periods of the ratio $\frac{std}{mean}$ of the rate coefficients. As the ratio $\frac{std}{mean}$ of the rate coefficients increases, these peaks become higher, hence higher rate of instability. What exactly causes these peaks is not clear. It can be a consequence of the negative values of the rate coefficients, but also the inversion method in *Matlab* when the operation $FM = -A^{-1}$ is executed. A method like this can be very numerically sensitive. When a matrix is not theoretically invertable the method approximates the inverse and may cause unstable results (Mathworks, 2009).

Of the four most sensitive parameters in the sensitivity analysis, there are two parameters that are considered as single values. *Area of Europe* has, when considered as an empirical quantity, neglible uncertainty compared to the other parameters. One can also argue that this is a model domain parameter, a boundary of the system, thus it inherits no uncertainty. *Surface area of fresh water compartment Europe* is a parameter that can be affected by seasonal change, rainfall and floods etc. In this master thesis this empirical parameter is considered to have neglible uncertainty, but it can be a good idea to investigate this in further studies. The other two input parameters of concern is not only the most sensitive parameters but also highly uncertain when it comes to measurement. *Particle dry deposition velocity in air* is the main reason for the model structure uncertainty since it can be measured as a negative value in upward particle fluxes leading to negative values of the rate coefficient. *Mixing height of air* is a parameter that needs to be investigated further. The uniform estimation of its distribution is an assumption based on lack of information. In reality this is a quite complex parameter that needs to be estimated through advanced meteorological modeling.

When interpreting the results of the uncertainty and sensitivity analysis of this master thesis, one should keep in mind the limitations in the methodology. This thesis only focuses on a small part of the OMNIITOX BM algorithm and measurement uncertainty in the nature specific input parameters with only one reference chemical. The estimations of the input parameter distributions in Table 6 are based on rather limited information. These estimations would have been more accurate given a complete dataset with a large number of observations of each input parameter. Further, when estimating the total uncertainty of the OMNIITOX BM, this thesis makes quite bold assumptions. The other 61 rate coefficients measurement uncertainties may have completely different distributions and magnitude than the rate coefficient that has been analyzed in this thesis.

However, the results should demonstrate an example of how large the parametric uncertainty of an intermediate parameter in the OMNIITOX BM algorithm can be and not as a solid statement of the quantitative uncertainty of OMNIITOX BM. The methodology should also be considered as an example of how one can estimate the quantitative uncertainty of the algorithm parameters, inspiring further work with more accurate results.

One can question if decisions can be made on such a uncertain model as OMNIITOX BM at all. Even if this thesis only is an example of how high the uncertainty can be, it indicates that the model does not possess a high reliability to base decisions on. It can with certainty be stated that further studies of the quantitative uncertainty needs to be done. This thesis has showed that the parametric uncertainty as well as the model structure uncertainty at this day can be very critical. It would be very useful to investigate the quantitative uncertainty in more general terms and further integrate this in the model.

Before going further with the quantitative uncertainty analysis of the OMNIITOX BM, a good idea would be to first make an extensive quantitative sensitivity analysis following the basics of this thesis methodology. When starting with this analysis one can determine which parameters that are the most important to investigate. Many of the parameters in the OMNIITOX BM, especially the nature specific input parameters involve a great deal of work to measure and estimate. Therefore a quantitative sensitivity analysis could be a good initial tool to make the uncertainty analysis cost effective.

If one wishes to integrate the uncertainties of the input parameters in the OMNIITOX BM algorithm, a number of changes in the implementation are needed to make sure that the values of the parameters do not conflict with the conditions of the algorithm. Since the OMNIITOX BM algorithm is normally only used for handling single values it will have to be modified to deal with random values that might cause unrealistic results. An example from this study would be the negative values of the rate coefficients and characterisation factors. Rules and conditions need to be established for handling these matters. Further, parametric uncertainty must be kept at a low level in order for the method to generate results that are numerically stable.

7 Conclusion

The quantitative uncertainty of the *Rate coefficient air to fresh water Europe* is remarkably high, with a 95%-confidence interval of $[-0.0130, 0.0270]$, $mean = 0.00679$ and $std = 0.01060$ if a normal distribution cut-off fit is chosen for the output data. A more exact but less informative representation would be to describe the quantitative uncertainty with a t-location scale distribution with location parameter $\mu = 0.005$, scale parameter $\sigma = 0.005$ and shape parameter $\nu = 1.42$. The input parameters that contributes the most to this uncertainty is *Mixing height of air* and *Particle dry deposition velocity in air*. When randomly generating numbers from the distribution function of *Rate coefficient air to fresh water Europe* in the calculation of characterisation factors, they were insignificantly affected. If the similar distribution was assumed for all rate coefficients as the analyzed intermediate parameter, the uncertainty of the characterisation factors became extremely high. The standard deviation of the characterisation factors show signs of instability when rather narrow distributions ($\frac{std}{mean} > 0.3$) of the rate coefficients were used. Small variations in the rate coefficients cause instability in the characterisation factors. This thesis has shown an example of how critical the uncertainty of OMNIITOX BM can be and that the model does not appear to constitute a reliable ground for decision making. Further studies of the uncertainty, in more general terms needs to be done and later integrated in the model. When integrating quantitative uncertainties in the parameters of OMNIITOX BM, the algorithm for calculating characterisation factors must be extended to be able to handle the parameters that conflict with the conditions of the model. For example, some parameters may be negative when assumed to be positive and the other way around. The parametric uncertainty can thus become a matter of model structure uncertainty. Further, the parametric uncertainty must be kept at a low enough level in order for the results to be numerically stable.

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9 Appendix

9.1 OMNIITOX default settings and values of parameters

At the OMNIITOX web site (OMNIITOX, 2008) under the links **Characterisation - Calculate characterisation factors - OMNIITOX base model** one can search for the chemical Toluene and further use the links **Select all- calculate - calculation result - View complete calculation of Ecotoxicological impact factor matrix / View complete calculation of Human damage factor matrix** and get a view of all default settings and parameter values. Below in Table 10 and 11 are the default values of the parameters most crucial for this thesis.

Table 10: Default values of input parameters

Input parameter	Default value
1. Diffusion coefficient for water in air	2.091 m^2/day
2. Mol weight water	18 $\frac{g}{mol}$
3. Mean wind speed at 10 metres over land	86400 m/day
4. Mean air temperature in Europe	281.9 K
5. Universal gas constant	8.315 $\frac{Pa \cdot m^3}{K \cdot mol}$
6. Junge equation constant	0.17 $Pa \cdot m$
7. Specific surface area of aerosol particles	$3.4 \cdot 10^{-4}$ m^{-1}
8. Area of Europe	$9.347 \cdot 10^{12}$ m^2
9. Mixing height of air	1000 m
10. Particle dry deposition velocity in air	130 m/day
11. Surface area of fresh water compartment Europe	$1.315 \cdot 10^{11}$ m^2
12. Molecular weight(Toluene)	92.14 $\frac{g}{mol}$
13. Vapour pressure(Toluene)	2880 Pa
14. Water solubility(Toluene)	0.526 $\frac{kg}{m^3}$
15. Melting point(Toluene)	178.3 K

Table 11: Default values of output parameters

Output parameter	Default value
1. Rate coefficient air to fresh water in Europe	$1.843 \cdot 10^{-3}$ $days^{-1}$
2. Rate coefficient air to fresh water dry period in Europe	$1.843 \cdot 10^{-3}$ $days^{-1}$

9.2 Distributions

The uniform distribution

Notation: $U(a,b)$

Density function: $f(x) = \frac{1}{b-a}$, $a \leq x \leq b$

Distribution function: $F(x) = x$, $a \leq x \leq b$

Expected value: $\frac{a+b}{2}$

Standard deviation: $\frac{a-b}{\sqrt{12}}$

The normal distribution

Notation: $N(\mu, \sigma)$

Density function: $f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)}{2\sigma^2}}$, $-\infty \leq x \leq \infty$

Expected value: μ

Standard deviation: σ

The logistic distribution

Density function: $f(x) = \frac{e^{\frac{x-\mu}{\sigma}}}{\sigma(1+e^{\frac{x-\mu}{\sigma}})^2}$

Location parameter: μ

Scale parameter: σ

The t-location scale distribution

Density function: $f(x) = \frac{\Gamma(\frac{\nu+1}{2})}{\sigma\sqrt{\nu\pi}\Gamma(\frac{\nu}{2})}(\frac{\nu+(\frac{x-\mu}{\sigma})^2}{\nu})^{-\frac{\nu+1}{2}}$

Location parameter: μ

Scale parameter: σ

Shape parameter: ν

9.3 Program code

simulation.m

```
function out = simulation


%***************SIMULATION SPECIFICATION*****************
NbrOfMeasures = 10000;
loopcount = 0;

%storage vectors:
nature1 = zeros(NbrOfMeasures, 1);
nature2=nature1;
nature3=nature1;
nature4=nature1;
nature5=nature1;
nature6=nature1;
nature7=nature1;
nature8=nature1;
nature9=nature1;
nature10=nature1;
nature11=nature1;
substance1=nature1;
substance2=nature1;
substance3=nature1;
substance4=nature1;
C1=nature1;
C2=nature1;
C3=nature1;
C4=nature1;
C5=nature1;
C6=nature1;
C7=nature1;
C8=nature1;
C9=nature1;
C10=nature1;
output=nature1;

while loopcount<NbrOfMeasures

%*****************INPUT*******************

%NATURE:

%1. Diffusion coefficient for water in air (m2/day):

DaH2O =1.8636+(2.1444-1.8636)*rand(1,1);             %2.091*(0.95+0.1*rand(1,1));
nature1(loopcount+1)=DaH2O;

%2. Mol weight water (g/mol):

mwH2O = 18; %*(0.95+0.1*rand(1,1));
nature2(loopcount+1)=mwH2O;

%3. Mean wind speed at 10 metres over land (m/day):

u10land = 86400; %*(0.95+0.1*rand(1,1));
nature3(loopcount+1)=u10land;

%4. Mean air temperature in Europe (K):

Taeur = 281.9; %*(0.95+0.1*rand(1,1));
nature4(loopcount+1)=Taeur;

%5. Universal gas constant (Pa*m3/(K*mol)):

R = 8.31451; %*(0.95+0.1*rand(1,1));
nature5(loopcount+1)=R;

%6. Junge equation constant (Pa*m):

Kjunge = 0.17; %*(0.95+0.1*rand(1,1));
nature6(loopcount+1)=Kjunge;

%7. Specific surface area of aerosol particles (1/m):

Ax =0.42*10^(-4)+(1.1*10^(-3)-0.42*10^(-4))*rand(1,1);         %3.5*10^(-4)*(0.95+0.1*rand(1,1));
nature7(loopcount+1)=Ax;

%8. Area of Europe (m2):

```

```
Aeur= 9.347*10^12; %*(0.95+0.1*rand(1,1));
nature8(loopcount+1)=Aeur;
%9. Mixing height of air (m):
ha = 100+2400*rand(1,1);                            %*(0.95+0.1*rand(1,1));
nature9(loopcount+1)=ha;
%10. Particle dry deposition velocity in air (m/day):
vadrydep =500.757+573.818*randn(1,1);   %130*(0.95+0.1*rand(1,1));
nature10(loopcount+1)=vadrydep;
%11. Surface area of fresh water compartment Europe (m2):
Afweur = 1.315*10^11;   %*(0.95+0.1*rand(1,1));
nature11(loopcount+1)=Afweur;
%-SUBSTANCE (Toluene):
%1. Molecular weight (g/mol):
mw = 92.14; %*(0.95+0.1*rand(1,1));
substance1(loopcount+1)=mw;
%2. Vapour pressure (Pa):
Pvap = 2880; %*(0.95+0.1*rand(1,1));
substance2(loopcount+1)=Pvap;
%3. Water solubility (kg/m3):
Solw = 0.526; %*(0.95+0.1*rand(1,1));
substance3(loopcount+1)=Solw;
%4. Melting point (K):
Tmelt = 178.3; %*(0.95+0.1*rand(1,1));
substance4(loopcount+1)=Tmelt;
%UNKNOWN PARAMETERS:
c1=6.79; %*(0.95+0.1*rand(1,1));
C1(loopcount+1)=c1;
c2= 864; %*(0.95+0.1*rand(1,1));
C2(loopcount+1)=c2;
c3=32; %*(0.95+0.1*rand(1,1));
C3(loopcount+1)=c3;
c4=0.285; %*(0.95+0.1*rand(1,1));
C4(loopcount+1)=c4;
c5=0.00004; %*(0.95+0.1*rand(1,1));
C5(loopcount+1)=c5;
c6=86400; %*(0.95+0.1*rand(1,1));
C6(loopcount+1)=c6;
c7=0.0004; %*(0.95+0.1*rand(1,1));
C7(loopcount+1)=c7;
c8=2/3; %*(0.95+0.1*rand(1,1));
C8(loopcount+1)=c8;
c9=0.2; %*(0.95+0.1*rand(1,1));
C9(loopcount+1)=c9;
c10=0.3; %*(0.95+0.1*rand(1,1));
C10(loopcount+1)=c10;
%*******************************************************
%OUTPUT:
%Rate coefficient air to fresh water dry deposition by particles in Europe:
Kafwdrypseur= kafwdrypseur(frxeur(Kjunge, Ax,
plseur(Taeur, Tmelt, Pvap, c1)), vadrydep, Afweur, vaeur(Aeur, ha));
%Rate coefficient air to fresh water dry deposition by gases in Europe:
```

```
Da = da(DaH2O, mwH2O, mw);
V  = vafwdiffeur(valand(DaH2O, Da, u10land, c2, c6, c8, c9, c10),
vfw(u10land, mw, c2, c3, c4, c5, c6, c7), hc(mw, Pvap, Solw), Taeur, R);
Kafwdrypgeur= kafwdrypgeur(V, frxeur(Kjunge, Ax, plseur(Taeur, Tmelt,
Pvap, c1)), Afweur, vaeur(Aeur, ha));
%Rate coefficient air to fresh water dry period in Europe:
Kafwdryeur = kafwdryeur(Kafwdrypgeur, Kafwdrypseur);
output(loopcount+1)=Kafwdryeur;
%*******************************************************
loopcount=loopcount+1;
end
%UNCERTAINTY ANALYSIS:
out=output;
%SENSITIVITY ANALYSIS:
C =[output nature1 nature7 nature9 nature10];
R=corrcoef(C);
corrc=R(1, 2:length(R(1,:)));
normc=corrc*(1/sum(abs(corrc)));
barh(normc,'r')
normc
end
```

simplus.m

```
function [R,S] = simplus

%**************SIMULATION SPECIFICATION*****************
NbrOfMeasures1 = 10000;
NbrOfMeasures2=50;
loopcount = 0;

%storage vectors:
eim1 = zeros(NbrOfMeasures1, 1);
eim2=eim1;
eim3=eim1;
eim4=eim1;
eim5=eim1;
eim6=eim1;
eim7=eim1;
eim8=eim1;
eim9=eim1;
eim10=eim1;
eim11=eim1;
eim12=eim1;
eim13=eim1;
eim14=eim1;
eim15=eim1;
eim16=eim1;
eim17=eim1;
eim18=eim1;
hdm1=eim1;
hdm2=eim1;
hdm3=eim1;
hdm4=eim1;
hdm5=eim1;
hdm6=eim1;
hdm7=eim1;
hdm8=eim1;
hdm9=eim1;
hdm10=eim1;
hdm11=eim1;
hdm12=eim1;
hdm13=eim1;
hdm14=eim1;
hdm15=eim1;
hdm16=eim1;
hdm17=eim1;
hdm18=eim1;
sigmamu=0.7/NbrOfMeasures2:(0.7/NbrOfMeasures2):0.7;
```

```
sigmatot1=zeros(NbrOfMeasures2,1);
sigmatot2=sigmatot1;
sigmatot3=sigmatot1;
sigmatot4=sigmatot1;
sigmatot5=sigmatot1;
sigmatot6=sigmatot1;

for k= 1:NbrOfMeasures2
    loopcount = 0;
    while loopcount<NbrOfMeasures1

        A= [-1.986*10^0 1.573*10^-2 0 3.584*10^-3 0 1.269*10^-2 1.269*10^-2 1.575*10^4 0 3.693*10^-3 0 0 0 0 0 0 0 0;
        1.843*10^-3 -4.614*10^-2 4.108*10^-2 0 0 1.445*10^-4 1.445*10^-4 0 0 0 7.369*10^-9 0 0 0 0 0 0 0;
        0 1.359*10^-4 -4.412*10^-2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
        3.529*10^-2 1.606*10^-5 0 -3.385*10^-2 3.743*10^-2 0 0 0 0 0 0 0 0 0 0 0 0 0;
        0 0 0 1.777*10^-5 -4.057*10^-2 0 0 0 0 0 0 0 0 0 0 0 0 0;
        3.232*10^-5 0 0 0 0 -2.508*10^-2 0 0 0 0 0 0 0 0 0 0 0 0;
        1.645*10^-5 0 0 0 0 0 -2.267*10^-2 0 0 0 0 0 0 0 0 0 0 0;
        7.007*10^-1 0 0 0 0 0 0 -1.575*10^4 3.429*10^-3 0 0 0 0 0 0 0 0 0;
        0 0 0 0 0 2.405*10^-3 0 4.834*10^-3 -1.869*10^-2 0 0 0 0 0 0 0 0 0;
        1.823*10^-1 0 0 0 0 0 0 0 0 -1.635*10^0 1.573*10^-2 0 3.583*10^-3 0 1.243*10^-2 1.243*10^-2 1.332*10^4 0;
        0 6.834*10^-6 0 0 0 0 0 0 0 4.827*10^-4 -4.625*10^-2 4.108*10^-2 0 0 3.838*10^-4 3.838*10^-4 0 0;
        0 0 0 0 0 0 0 0 0 0 1.359*10^-4 -4.412*10^-2 0 0 0 0 0 0;
        0 0 0 0 0 0 0 0 0 4.191*10^-3 1.371*10^-4 0 -3.385*10^-2 3.743*10^-2 0 0 0 0;
        0 0 0 0 0 0 0 0 0 0 0 0 1.777*10^-5 -4.057*10^-2 0 0 0 0;
        0 0 0 0 0 0 0 0 0 2.493*10^-5 0 0 0 0 -2.543*10^-2 0 0 0;
        0 0 0 0 0 0 0 0 0 1.405*10^-5 0 0 0 0 0 -2.265*10^-2 0 0;
        0 0 0 0 0 0 0 0 0 5.445*10^-1 0 0 0 0 0 0 -1.332*10^4 3.429*10^-3;
        0 0 0 0 0 0 0 0 0 0 0 0 0 0 2.785*10^-3 0 4.834*10^-3 -1.869*10^-2];

        EM= [8.257*10^-3 5.516*10^-3 8.257*10^-3 5.516*10^-3;
        0 4.568*10^-4 0 4.568*10^-4];

        XM = [6.351*10^-7 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
        3.927*10^-11 4.288*10^-7 0 1.677*10^-9 0 1.075*10^-12 0 2.574*10^-5 3.764*10^-5 0 0 0 0 0 0 0 0 0;
        0 0 0 0 0 0 0 0 0 1.786*10^-7 0 0 0 0 0 0 0 0;
        0 0 0 0 0 0 0 0 0 4.075*10^-12 3.126*10^-7 0 4.542*10^-9 0 1.035*10^-13 0 5.556*10^-6 6.261*10^-6];

        [rows, cols, vals]=find(A);
        r=(1+sigmamu(k)*randn(62,1));
        %r=(1+(0.010218/0.00698788)*randn(62,1));
        %r=(1+0.15*randn(62,1));
        vals=vals.*r;

        for i=1:62
            if rows(i)==cols(i)
                A(rows(i),cols(i))=(-1)*abs(vals(i));
            else
                A(rows(i),cols(i))=vals(i);
            end
        end

        %A(1,2)=0.00698788+0.010218*randn(1,1);
        EEM= [0 2.677*10^-2 0 0 0 0 0 0 0 0 2.677*10^-2 0 0 0 0 0 0 0];
        FM=inv(A)*(-1);
        EIM=EEM*FM;
        HDM=EM*XM*FM;

        eim1(loopcount+1)=EIM(1);
        eim2(loopcount+1)=EIM(2);
        eim3(loopcount+1)=EIM(3);
        eim4(loopcount+1)=EIM(4);
        eim5(loopcount+1)=EIM(5);
        eim6(loopcount+1)=EIM(6);
        eim7(loopcount+1)=EIM(7);
        eim8(loopcount+1)=EIM(8);
        eim9(loopcount+1)=EIM(9);
        eim10(loopcount+1)=EIM(10);
        eim11(loopcount+1)=EIM(11);
        eim12(loopcount+1)=EIM(12);
        eim13(loopcount+1)=EIM(13);
        eim14(loopcount+1)=EIM(14);
        eim15(loopcount+1)=EIM(15);
        eim16(loopcount+1)=EIM(16);
        eim17(loopcount+1)=EIM(17);
        eim18(loopcount+1)=EIM(18);
        hdm1(loopcount+1)=HDM(2,1);
        hdm2(loopcount+1)=HDM(2,2);
        hdm3(loopcount+1)=HDM(2,3);
        hdm4(loopcount+1)=HDM(2,4);
        hdm5(loopcount+1)=HDM(2,5);
```

```
        hdm6(loopcount+1)=HDM(2,6);
        hdm7(loopcount+1)=HDM(2,7);
        hdm8(loopcount+1)=HDM(2,8);
        hdm9(loopcount+1)=HDM(2,9);
        hdm10(loopcount+1)=HDM(2,10);
        hdm11(loopcount+1)=HDM(2,11);
        hdm12(loopcount+1)=HDM(2,12);
        hdm13(loopcount+1)=HDM(2,13);
        hdm14(loopcount+1)=HDM(2,14);
        hdm15(loopcount+1)=HDM(2,15);
        hdm16(loopcount+1)=HDM(2,16);
        hdm17(loopcount+1)=HDM(2,17);
        hdm18(loopcount+1)=HDM(2,18);
        loopcount=loopcount+1;
    end

    P=zeros(36, NbrOfMeasures1);
    P(1,:)=eim1;
    P(2,:)=eim2;
    P(3,:)=eim3;
    P(4,:)=eim4;
    P(5,:)=eim5;
    P(6,:)=eim6;
    P(7,:)=eim7;
    P(8,:)=eim8;
    P(9,:)=eim9;
    P(10,:)=eim10;
    P(11,:)=eim11;
    P(12,:)=eim12;
    P(13,:)=eim13;
    P(14,:)=eim14;
    P(15,:)=eim15;
    P(16,:)=eim16;
    P(17,:)=eim17;
    P(18,:)=eim18;
    P(19,:)=hdm1;
    P(20,:)=hdm2;
    P(21,:)=hdm3;
    P(22,:)=hdm4;
    P(23,:)=hdm5;
    P(24,:)=hdm6;
    P(25,:)=hdm7;
    P(26,:)=hdm8;
    P(27,:)=hdm9;
    P(28,:)=hdm10;
    P(29,:)=hdm11;
    P(30,:)=hdm12;
    P(31,:)=hdm13;
    P(32,:)=hdm14;
    P(33,:)=hdm15;
    P(34,:)=hdm16;
    P(35,:)=hdm17;
    P(36,:)=hdm18;
    Q=zeros(36,5);
    for i=1:36
        Q(i,1)=mean(P(i,:));
        Q(i,2)=std(P(i,:));
        Q(i,3)=abs(mean(P(i,:))/std(P(i,:)));
        Q(i,4)=Q(i,1)-Q(i,2)*1.96;
        Q(i,5)=Q(i,1)+Q(i,2)*1.96;
    end

    sigmatot1(k)=Q(1,2);
    sigmatot2(k)=Q(2,2);
    sigmatot3(k)=Q(3,2);
    sigmatot4(k)=Q(10,2);
    sigmatot5(k)=Q(11,2);
    sigmatot6(k)=Q(12,2);

end
figure;
plot(sigmamu,sigmatot1)
figure;
plot(sigmamu,sigmatot2)
figure;
plot(sigmamu,sigmatot3)
figure;
plot(sigmamu,sigmatot4)
figure;
plot(sigmamu,sigmatot5)
figure;
plot(sigmamu,sigmatot6)
```

```
R=Q;
S=P;
end
```

depvel.m

```
function vd = depvel
v=zeros(10000,1);
%Reconstructing season normalized dataset for particles 15-150 nm:
v(1:1000)=(1.49+1.43*randn(1000,1))*(0.7159/0.78);
v(1001:2000)=(1.18+1.52*randn(1000,1))*(0.7159/0.87);
v(2001:3000)=(1.23+1.26*randn(1000,1))*(0.7159/0.89);
v(3001:4000)=(0.94+0.87*randn(1000,1))*(0.7159/0.86);
v(4001:5000)=(0.74+0.83*randn(1000,1))*(0.7159/1.28);
v(5001:6000)=(0.62+0.72*randn(1000,1))*(0.7159/0.98);
v(6001:7000)=(0.66+0.7116*randn(1000,1))*(0.7159/1.06);
v(7001:8000)=(0.99+1.08*randn(1000,1))*(0.7159/1.66);
v(8001:9000)=(0.69+0.54*randn(1000,1))*(0.7159/0.95);
v(9001:10000)=(0.25+0.8747*randn(1000,1))*(0.7159/0.74);

%changing unit from cm/s to m/day:
vd=v*0.01*24*60*60;

end
```

vaeur.m

```
function V = vaeur(a, h)
V=a*h;
end
```

plseur.m

```
function Pls = plseur(Ta, Tm, Pvap, c1)
if Ta>Tm
    Pls=Pvap;
else
    Pls=Pvap/(2.71828^(c1*(1-Tm/Ta)));
end
end
```

frxeur.m

```
function frx = frxeur(Kjunge, Ax, Plseur)
frx=(Kjunge*Ax)/(Plseur+(Kjunge*Ax));
end
```

kafwdrypseur.m

```
function kafwdryps = kafwdrypseur(frxeur, Vadrydep, Afweur, Vaeur)
kafwdryps = (Afweur*Vadrydep*(1-frxeur))/Vaeur;
end
```

hc.m

```
function h = hc(mw, pvap, solw)
h=(mw*pvap)/(1000*solw);
end
```

vfw.m

```
function v = vfw(u10, mw, c2, c3, c4, c5, c6, c7)
v = c2*((c3/mw)^c4)*((c5*((u10)^2)/(c6^2))+c7);
end
```

valand.m

```
function v = valand(DaH2O, da, u10land, c2, c6, c8, c9, c10)
v = c2*((da/DaH2O)^c8)*(((c9*u10land)/c6)+c10);
end
```

vafwdiffeur.m

```
function v = vafwdiffeur(valand, vfw, Hph, Ta, R)
v= (vfw*R*Ta)/(Hph+1/valand);
end
```

kafwdrypgeur.m

```
function k = kafwdrypgeur(vafwdiffeur, frxeur, Afweur, Vaeur)
k = (Afweur*vafwdiffeur*(1-frxeur))/Vaeur;
end
```

kafwdryeur.m

```
function k = kafwdryeur(kafwdrypgeur, kafwdrypseur)
k = kafwdrypgeur + kafwdrypseur;
end
```