Front page for deliverables

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**Abbreviations**

\( \gamma \)-HCH / gHCH: Lindane; gamma-hexacyclocloxane

BaP: Benzo(a)pyrene

BbF: Benzo(b)fluoranthene

BkF: Benzo(k)fluoranthene

DBP: Di-n-butyl phthalate

DCB: 1,4-dichlorobenzene

DEHP: Di-(2ethylhexyl)phthalate

EDC: 1,2-dichloroethane

EDTA: Ethyelendiaminetetra acetic acid

HCB: Hexachlorobenzene

HHCB: 1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8-hexamethyl-cyclopenta-[g]-2-benzopyrane

HxCDD-1,2,3: 1,2,3,4,7,8 / 1,2,3,6,7,8 / 1,2,3,7,8,9-hexachloro-dibenzo-p-dioxin (respectively)

IP: Indeno(123cd)pyrene

K_{OC}: Organic carbon-water partition coefficient

K_{OW}: Octanol-water partition coefficient

LAS: Linear alkyl benzene sulfonates

MB: Model bias

OCDD: octachloro-dibenzo-p-dioxin

PAHs: Polycyclic aromatic hydrocarbons

PCDD/Fs: Polychlorinated-dibenzo-p-dioxins and furans

PeCDD: 1,2,3,7,8-pentachloro-dibenzo-p-dioxin

TCDD: 2,3,7,8-tetrachloro-dibenzo-p-dioxin

Robust ROS: Robust regression on order / robust probability plot method
Summary

The objective of this report was to generate an inventory of possible improvement options for existing models based on an empirical evaluation of model performance for a series of models developed on varying spatial scales. The main indicator of model performance considered in this report was the ability of the selected multimedia fate models to predict environmental concentrations of parent compounds that are in reasonable agreement with monitoring data. Based on emissions and monitoring data availability, the following substances were selected to be included in the evaluation exercise: BaP, BbF, BkF, IP, \( \gamma \)-HCH and HCB.

The model evaluation was limited to four spatially-explicit European-scale models (SimpleBox 3.0, BETR-Global, EVn-BETR, IMPACT 2002). The results of the evaluation exercise can be summarized as follows:

1. Model performance was best for predictions in the atmospheric compartment (e.g. often within a factor of 3) for all models. Improvements in model performance were noted for the more spatially-resolved models.

2. Model performance for all four models deteriorated in the freshwater, sediment and soil compartment and deviation from the central tendency of the monitoring data in the range of 1 – 3 orders of magnitude was often observed, particularly in the sediment and soil compartments. However, the performance of IMPACT 2002 in the freshwater compartment was much better than all other models, which suggests that some benefits can be gained by adopting a more spatially-resolved model.

In order to investigate possible causes for these results and assist the development of an inventory of improvement options for the existing models, a sensitivity and propagation of uncertainty analysis was conducted using EVn-BETR. Based on the results of this analysis along with theoretical considerations and the goals of the overall NOMIRACLE project, the following improvement options are suggested:

1. Expand the applicability of the models by updating the sorption algorithms (e.g. incorporate polyparameter linear free energy relationships) and allowing multi-species chemicals such as those that dissociate at environmental pHs to be simulated

2. Include the capability to perform dynamic (time-dependent) simulations in order to capture more of the spatial and temporal variability in emissions and other important parameters

3. Re-evaluate the parameterization of key processes such as air-surface exchange, intermedia transfer rates, advective flows between geographical areas and degradation half-lives.

4. Incorporate a multi-layered soil compartment as opposed to a single layer

5. Develop the capability to perform sensitivity / uncertainty analysis for all models in order to facilitate the interpretation of the results

These recommendations reflect the environmental behaviour of a limited set of compounds and therefore cannot be considered representative of all chemical classes. Future empirical model evaluations should include chemicals with a wider range of physical-chemical properties and mode of release. Effort should be focused on those substances for which reliable emission and monitoring data can be obtained.
1 Introduction

1.1 Background

According to European Union legislation, notified current-use and new substances are subject to assessment in order to determine the risk posed to human health and the environment. The European Union System for the Evaluation of Substances (EUSES), which was developed to address this need, relies on a regional distribution model based on the SimpleBox platform (Brandes et al., 1996) to generate predicted environmental concentrations (PECs) in environmental compartments (air, water, sediment etc.) which then serve as input to a human exposure model. The theoretical validity and performance of EUSES and its model components (the exposure model and regional distribution model) have been most thoroughly investigated by Jager (1998), Schwartz (2000), Berding (2000) and Matthies et al. (2004).

Key findings of these studies include the following:

1) EUSES and its model components are best suited for neutral organic compounds with a log $K_{ow}$ between $-1 – 7$ as many model algorithms are only valid in this range. For example, all sorption to solids is related to organic carbon and only the sorption algorithm for ‘predominantly hydrophobics’ is currently implemented (Jager, 1998).

2) For the substances considered, exposure module and environmental parameter uncertainty typically contributed more to overall output uncertainty than substance parameter uncertainty (Schwartz, 2000; Berding, 2000; Matthies et al. 2004). It was also noted that substance and environmental parameters contribute differently to output variance depending on individual substance properties and environmental compartment. These findings also depend on the estimated input uncertainty assigned to each parameter and also on the specific parameters varied in the analysis. For example, Fenner et al. (2003) concluded that substance parameter uncertainty exceeds environmental parameter uncertainty in a model evaluation exercise that omitted some of the environmental parameters included in Berding (2000) and Matthies et al. (2004).

3) Overall output uncertainty tends to be lower for air and water in comparison to more immobile compartments such as soil (Berding, 2000; Matthies et al., 2004)

4) Uncertainty in the mode of entry for substances emitted to more than one compartment does not seem to significantly influence the range of model output (Matthies et al., 2004).

5) Obtaining reliable emission estimates and representative monitoring data is problematic and deviations between predicted and measured concentrations may often be in the range of 1 to 4 orders of magnitude (Jager, 1998; Schwartz, 2000; Berding, 2000; Mathies et al., 2004). It is therefore difficult to distinguish between shortcomings related to model structure and process descriptions and issues related to poor emission estimates and monitoring data quality.

The potential influence of environmental parameters on model output is one factor that has encouraged the development of spatially-explicit models on a European continental scale that have the ability to represent some of the temporal and spatial variability present and reduce oversimplifications. Another important factor allowing such efforts is the increasing availability of spatially-resolved databases for landscape and climate parameters.

Model evaluations of spatially-explicit models tend to focus on comparisons to non-spatial versions. For example, Klepper & Den Hollander (1999) compared the results of the non-spatial version of SimpleBox 3.0 with spatially-explicit modules for air, soil and water based on the same model formulations. The authors reported that the average value of the spatially-explicit model for air and soil was close to the value calculated by the non-spatial version and the maximum value of the spatially-explicit version was within a factor of 10 in both media. For the water compartment, the non-spatial version underestimated the spatial average and was a factor of 100 – 1000 less than the maximum value of the spatially-explicit version.
A similar study was conducted by Pennington et al. (2005) that compared estimates of intake fraction and environmental concentrations generated by the spatially-explicit version of IMPACT 2002 with the results of the non-spatial version. The authors reported that the spatial and non-spatial model provide reasonably consistent estimates of intake fraction for substances with dispersed emissions to air (less than a factor of 2) and soil (less than a factor of 10) but not for chemicals emitted to water. In those cases, the nonspatial model deviated from the intake fraction calculated by the spatial version by up to 3 orders of magnitude. In comparison to monitoring data for 2,3,4,7,8-pentachloro-dibenzo-furan, both models underestimated the median value of the observations by 2 – 3 orders of magnitude depending on the environmental compartment and zone of the spatial model. However, the mean value of the spatially-resolved version was more consistent with observations than the output of the non-spatial version.

While it is clear that the spatial resolution of environmental fate models can have an important affect on model output and performance, further evaluation of spatially-explicit European scale models has been greatly hindered by 1) the lack of spatially-resolved emission estimates and 2) the lack of representative monitoring data distributed across Europe, similar to the problems encountered for the model evaluations of the performance of the regional distribution model in EUSES.

Recently, Armitage and Cousins (2005) compiled a database of European-wide monitoring data for a variety of substances including pesticides, semi-VOCs and persistent organic pollutants such as PCBs and PAHs. In combination with spatially-resolved emission estimates generated by EMEP and MSC-East (Shatalov et al., 2002; Shatalov et al., 2003), it is now possible to conduct a more thorough evaluation of a series spatially-explicit models for a limited set of substances.

1.2 Objectives of the Report

The objective of this report is to generate an inventory of possible improvement options for existing models based on an empirical evaluation of model performance for a series of models developed on varying spatial scales. The main indicator of model performance considered in this report is the ability of the selected multimedia fate models to predict environmental concentrations of parent compounds that are in reasonable agreement with monitoring data. When possible, a probabilistic approach was also employed to generate a range of model output and to determine model sensitivity and key uncertainties as another method to examine model performance and develop suggestions for model improvements.

2 Model Selection

The model evaluation was limited to four spatially-explicit European-scale models based on the model selection process described in detail by Hauck et al. (2006) for a separate but complementary NOMIRACLE report (D.2.4.2 Report on the indication of spatial detail). In brief, a list of multimedia fate models was compiled and the models were ranked in terms of spatial coverage, data requirements, availability of a steady-state version and manageability (e.g. computer requirements, user-friendliness). Based on this selection procedure, it was decided to include SimpleBox 3.0, BETR-Global, EVn-BETR and IMPACT 2002 in the model evaluation exercise. Literature references and a short description of the models are provided in the following sections although it is advisable to consult the original publications for more detailed information.

2.1 SimpleBox 3.0


SimpleBox 3.0 is the latest version of the SimpleBox platform. It is a nested multimedia fate model that includes a local, regional and continental scale as well as a global scale which represents the northern hemisphere as an arctic, moderate and tropic zone. The default settings of the continental scale component
are meant to represent the European region. The model generates steady-state predictions for each environmental compartment and is also capable of pseudo-dynamic simulations. For the purpose of the model evaluation, SimpleBox 3.0 represents the coarsest spatial resolution (i.e. non-spatial).

2.2 BETR-Global


BETR-Global is a global multimedia fate model that divides the earth into 288 linked model zones based on a 15° x 15° grid. Based on this geometry, Europe is represented by 12 zones (36 – 39, 60 – 68, 84 – 87) as shown below in Figure 2.2.1. The model generates predicted concentrations in various environmental compartments for each zone and is capable of both steady-state and dynamic simulations with a varying emission profile.

![Figure 2.2.1 BETR-Global Model Zones](image)

The model was first applied to describe the long-term fate of polychlorinated biphenyls and includes a very good description of advective flows in the atmospheric compartments. The parameterisation of the freshwater advective flows may not be as representative (MacLeod M, pers. comm.) and for these reasons, only predictions in the air and soil compartments were included in the model evaluation exercise.

2.3 EVn-BETR


EVn-BETR is a continental European-scale model that divides the area into 54 model zones using a 5° x 5° degree grid (see Figure 2.3.1). Fifty of the zones represent the main geographical area of Europe while 4 zones (51 - 54) are included as boundary regions representing the Arctic, Atlantic, Mediterranean and Eurasian regions of the globe. The model generates predicted concentrations in various environmental compartments for each zone and is capable of both steady-state and dynamic simulations with a varying emission profile. The model structure and process descriptions are very similar to BETR-Global due to their common origin.
2.4 IMPACT 2002


IMPACT 2002 is a continental-European scale model that divides the region into 135 irregular watershed areas (land zones) and a separate 156 air zones based on a 2.5° x 2.5° grid (see Figure 2.4.1), nested in non-spatial global model (Zone 0).
Further description of these four models and previous applications can be found in D.2.4.2 Report on the indication of spatial detail by Hauck et al. (2006).

It should be noted that the four multimedia fate models used in this model evaluation exercise were not normalized in an attempt to unify these tools in terms of model geometry, default parameter values, partition algorithms etc. even though a preliminary survey indicated that such differences do exist. For example, while the total surface areas of the freshwater compartment are similar in SimpleBox 3.0 and Evn-BETR, the volume of the freshwater compartment in SimpleBox 3.0 is nearly an order of magnitude smaller. In comparison to IMPACT 2002, the total volume of the freshwater compartment in SimpleBox 3.0 is approximately six times smaller. Another example is the algorithm selected to represent the relationship between \( K_{OW} \) and \( K_{OC} \). EVn-BETR and BETR-Global define this relationship as the following:

\[
K_{OC} = 0.41 K_{OW}
\]

In SimpleBox 3.0, this relationship is defined as:

\[
\log K_{OC} = 1.26 \log K_{OW}^{0.81}
\]

At a \( K_{OW} \) of 5, these equations yield nearly equivalent estimations of \( K_{OC} \) but diverge by a factor of up to five over the \( K_{OW} \) range 1 to 7. The implications of such differences will not be discussed until the results of the sensitivity and propagation of uncertainty analysis are presented (Section 4.7) since the purpose of that analysis is to identify the input parameters that influence model output the most.

## 3 Model Application

### 3.1 Chemicals

The selection of chemicals for the model evaluation exercise was limited by the availability of spatially-resolved emission estimates as well as representative monitoring data distributed over a reasonable geographical area. Together, these requirements present a significant constraint. Based on data availability, the following substances were included in the model evaluation exercise:

- Benzo(a)pyrene (CAS # 50-32-8)
- Benzo(b)fluoranthene (CAS # 205-99-2)
- Benzo(k)fluoranthene (CAS # 207-08-9)
- Indeno(123-cd)pyrene (CAS # 193-39-5)
- \( \gamma \)-HCH (CAS # 58-89-9)
- Hexachlorobenzene (CAS # 118-74-1)

The physico-chemical properties selected for these chemicals are shown in Table 3.1.1. Parameter values were based on several sources including Mackay D (2001), the SRC Interactive PhysProp Database (http://www.syrres.com/esc/physdemo.htm) and Gusev et al. (2005). Note that degradation half-lives for chemicals in the vegetation compartment were assumed to be similar to degradation half-lives in air (Cousins and Mackay, 2001; Prevedouros et al., 2004a; Foster et al., 2006).
Table 3.1.1. Basic Physicochemical Property Values Used for Model Evaluation Exercise

<table>
<thead>
<tr>
<th>Substance</th>
<th>B(a)P</th>
<th>B(b)F</th>
<th>B(k)F</th>
<th>IP</th>
<th>γ-HCH</th>
<th>HCB</th>
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<tr>
<td>MM (g/mol)</td>
<td>252.3</td>
<td>252.3</td>
<td>252.3</td>
<td>276.34</td>
<td>290.8</td>
<td>284.8</td>
</tr>
<tr>
<td>MP (deg C)</td>
<td>176.5</td>
<td>168</td>
<td>217</td>
<td>163.6</td>
<td>112.5</td>
<td>231.8</td>
</tr>
<tr>
<td>H (Pa-mg/mol)</td>
<td>4.60E-02</td>
<td>6.70E-02</td>
<td>5.90E-02</td>
<td>3.53E-02</td>
<td>5.20E-01</td>
<td>1.70E+02</td>
</tr>
<tr>
<td>VAP (Pa)</td>
<td>7.30E-07</td>
<td>6.70E-05</td>
<td>1.30E-07</td>
<td>1.67E-08</td>
<td>4.70E-03</td>
<td>2.40E-03</td>
</tr>
<tr>
<td>SOL (mg/l)</td>
<td>1.62E-03</td>
<td>1.50E-03</td>
<td>8.00E-04</td>
<td>1.90E-04</td>
<td>7.30E+00</td>
<td>6.20E-03</td>
</tr>
<tr>
<td>H (Pa-m3/mol)</td>
<td>4.60E-02</td>
<td>6.70E-02</td>
<td>5.90E-02</td>
<td>3.53E-02</td>
<td>5.20E-01</td>
<td>1.70E+02</td>
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<tr>
<td>VAP (Pa)</td>
<td>7.30E-07</td>
<td>6.70E-05</td>
<td>1.30E-07</td>
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<td>4.70E-03</td>
<td>2.40E-03</td>
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<tr>
<td>SOL (mg/l)</td>
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<td>1.50E-03</td>
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<td>1.90E-04</td>
<td>7.30E+00</td>
<td>6.20E-03</td>
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<td>logKow</td>
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<td>6.13</td>
<td>5.78</td>
<td>6.11</td>
<td>6.70</td>
<td>3.72</td>
</tr>
<tr>
<td>DEGair (h)</td>
<td>170</td>
<td>170</td>
<td>170</td>
<td>170</td>
<td>2030</td>
<td>14260</td>
</tr>
<tr>
<td>DEGwater (h)</td>
<td>1700</td>
<td>1700</td>
<td>1700</td>
<td>1700</td>
<td>1700</td>
<td>1700</td>
</tr>
<tr>
<td>DEGsoil (h)</td>
<td>17000</td>
<td>17000</td>
<td>17000</td>
<td>17000</td>
<td>17000</td>
<td>17000</td>
</tr>
<tr>
<td>DEGsed (h)</td>
<td>55000</td>
<td>55000</td>
<td>55000</td>
<td>55000</td>
<td>55000</td>
<td>55000</td>
</tr>
</tbody>
</table>

where MM = molecular mass ; MP = melting point; H = Henry Law constant; VAP = vapour pressure; SOL = aqueous solubility; Kow = octanol-water partition coefficient; DEG = degradation half-lives in respective media

It is important to recognize that while the selected chemicals span a significant range of physical-chemical properties, they are only representative of neutral organic compounds whereas the focus of the NOMIRACLE project is to develop methods and tools for various classes of compounds including modern biocides, pharmaceuticals and pesticides which tend to be more polar. However, given the fact that 1) the algorithms in the selected models are most valid theoretically for neutral compounds and 2) environmental parameters may have a more important influence on model uncertainty than substance parameters, the selected chemicals were considered acceptable for the purpose of the model evaluation exercise. The constraints imposed by the paucity of required data for other compound classes should also be realized.

3.2 Spatially-Resolved Emission Estimates

EMEP emission data (Shatalov et al., 2002; Shatalov et al., 2003, Rozovskaya et al. 2004, Shatalov et al., 2005) were obtained for the six chemicals listed in Table 3.1.1. These emission data, based on official data submitted to the UN ECE Secretariat by countries and available expert estimates, are available on a 50 km x 50 km grid and therefore had to be aggregated to match the various model grid zones using GIS software. Hauck et al. (2006) can be consulted for further details of this procedure and the spreadsheets containing the finalized emission data for the four selected models are available upon request (See Supporting Information). Note that a critical assumption of this evaluation exercise is that all substances are emitted 100% to the air compartment. The fact that these chemicals may be emitted to waterways via sewage treatment plants or applied to agricultural soils bound to sewage sludge solids has not been accounted for. However, since PAHs and HCB are released in industrialized countries mainly as a consequence of combustion and other thermal processes (Shatalov et al., 2005), the dominance of an atmospheric mode of entry is justifiable. The dominance of an atmospheric mode of entry for γ-HCH, an agricultural pesticide, is more questionable although consistent with Prevedouros et al. (2004a).

A summary of the emission totals for each chemical is provided in Table 3.2.1

Table 3.2.1. Total Emission Estimates Used

<table>
<thead>
<tr>
<th>Substance</th>
<th>Year</th>
<th>Total (tons / year)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaP</td>
<td>2003</td>
<td>309.86</td>
</tr>
<tr>
<td>BbF</td>
<td>2003</td>
<td>343.38</td>
</tr>
<tr>
<td>BkF</td>
<td>2003</td>
<td>186.78</td>
</tr>
<tr>
<td>IP</td>
<td>2003</td>
<td>291.11</td>
</tr>
<tr>
<td>γ-HCH</td>
<td>1995</td>
<td>803.38</td>
</tr>
<tr>
<td>HCB</td>
<td>1995</td>
<td>23.43</td>
</tr>
</tbody>
</table>
It is important to recognize that emission levels for all substances were higher in the past. For example, emission levels of PAHs were approximately 2 – 4 times higher in 1970 while emissions of γ-HCH and HCB were approximately 4 and 10 times higher respectively (Rozovskaya et al. 2004). This fact implies that using modern emission levels in a steady-state simulation automatically introduces a bias into the model exercise. However, since all of these fate models constitute linear systems, there is a roughly proportional relationship between emission levels and predicted concentrations. Therefore the maximum bias introduced to model predictions is the basically the same as the difference in emission levels i.e. 2 – 4 for PAHs, 4 and 10 for γ-HCH and HCB respectively. Furthermore, since emission levels have been declining relatively slowly over time and have also been relatively stable throughout the 1990s, it can be argued that the introduced bias is more limited. This potential bias will be most acute for immobile environmental compartments with limited degradation (e.g. soil, sediment) as advection and transformation often dominate loss processes in multimedia environmental fate models (Mackay, 2001).

This argument is not valid for γ-HCH, which was banned in the EU and phased out of use by 1998. For this reason, emission estimates from 1995 were used in the model evaluation exercise because the majority of monitoring data is also from that time period (see next section). Emission estimates from 1995 were also used for HCB because the decline in emissions between 1990 - 2002 has been only approximately 20% (Rozovskaya et al. 2004) and much of the available monitoring for this substance was also collected in the mid-1990s. In addition, updated spatially-resolved emissions estimates for 2003 are not currently available to the public.

### 3.3 Monitoring Data

Monitoring data for the six chemicals were taken from a European-wide monitoring database (Armitage and Cousins, 2005), which is available upon request. In brief, the majority of the monitoring data for the air compartment were taken from EMEP monitoring sites (http://www.emep.int), which were established as representative background locations. Freshwater and sediment measurements were based exclusively on the COMMPS database (http://europa.eu.int/com/environment/water/water-framework/preparation_priority_list.htm) which reportedly included a screening process to remove sampling locations that were obviously biased due to proximity to direct sources. Measurements of PAHs in soils were taken from an EMEP monitoring site in the Czech Republic and several studies available in the literature considered to have sampled at representative background locations (e.g. Aamot et al., 1996; Migaszewski et al., 2002; Bucheli et al., 2004). Monitoring data for HCB in soils included the EMEP site in the Czech Republic and all European background locations sampled by Meijer et al., (2003).

Measured concentrations in air, freshwater, sediment and soil were compiled into spreadsheets for each model based on the reported location of the monitoring site and the corresponding grid zones of each model. For the four PAHs and HCB, even though measurements were taken at various time periods between 1995 and 2003, all data was aggregated because emission estimates for these substances were relatively constant over that sampling period. For γ-HCH, the majority of the monitoring data for freshwater and sediment is from 1995 - 1996 which matches the time period of the emission estimates. Note that the model evaluation for this substance was only conducted for water and sediment compartments because representative and geographically distributed measurements in air and soil could not be located.

Summary statistics were calculated for each environmental media and model zone to allow data to be presented visually as box-plots representing the minimum, 25th-percentile, median, 75th-percentile and the maximum of the reported values. The ROS procedure (Helsel, 2005) was utilized to compute summary statistics as this method can handle datasets containing non-detects with multiple detection limits. Following the guidelines suggested by Helsel (2005), this procedure was only applied if there were more than 10 data points, at least 20% of which were measurements above the reported detection limits. If these two criteria were not fulfilled, the data was not included in the model evaluation exercise.

The complete set of compiled and summarized monitoring data for all four models is also available in electronic format upon request (see Supporting Information).
3.4 Indicator of Model Performance

To express the performance of each model in a quantitative way, the following measure known as model bias was adopted (Gobas et al. 1998; Arnot & Gobas, 2003). Overall model bias (MB) is calculated as:

\[
MB = 10^{\frac{\sum [\log (M_{pred} / M_{obs})]}{n}}
\]

where \(M_{pred}\) is the measurement predicted by the model, \(M_{obs}\) is the observed measurement and \(n\) is the number of comparisons. MB represents the factor by which the predictions tend to under- or overestimate the observations. For example, a MB of 5 indicates the predictions tend to overestimate observations by a factor of 5. Conversely, a MB of 0.2 indicates that the predictions tend to underestimate observations by a factor of 5. Note that this measure of model performance may be misleading in the sense that under- and overpredictions can cancel each other out and yield a very low MB. For example, if a model underpredicts by a factor of 100 for half of the comparisons and overpredicts by a factor of 100 for the other half, the MB equals one. One the other hand, a model that underpredicts by a factor of 2 for one-third of the comparisons and overpredicts by a factor of 4 for the remaining comparisons will have a MB of 2. For this reason, absolute model bias was also calculated. This measure is calculated as:

\[
|MB| = 10^{\frac{\sum |[\log (M_{pred} / M_{obs})]|}{n}}
\]

With this metric, under- and overpredictions will not cancel out yielding a measure of the average factor by which the model deviates from the observed value in either direction.

For the purposes of the model evaluation exercise, model bias was calculated for all chemicals in each environmental compartment as well as for individual chemicals in each compartment. The metrics chosen for comparison was the median concentration of the observed data and the concentration predicted by each model using the standard set of parameters (i.e. default settings).

3.5 Sensitivity and Propagation of Uncertainty Analysis

Sensitivity and propagation of uncertainty analysis was conducted if these procedures were possible given the model architecture and feasible in terms of computational effort. For SimpleBox 3.0, it is relatively easy to conduct this assessment through Monte Carlo simulations using the Crystal Ball software add-on but since this model does not include inter-regional flows between zones due to the coarse spatial resolution, it was deemed inappropriate for the purpose of this report. For EVn-BETR, the procedures necessary to allow this assessment are coded into the software. However, the process requires a great deal of computational effort as only 10 outputs can be monitored simultaneously for a given simulation, each of which takes in excess of 8 hours to complete on a typical computer system. The computational requirements are even more severe for BETR-Global given the increased number of model zones and for this reason the procedures were not implemented in this model. In the case of IMPACT 2002, sensitivity and propagation of uncertainty analysis cannot be implemented in the version used for this model evaluation due to the model architecture (e.g. output concentrations are generated in a separate worksheet which cannot be accessed before the model is run). Given these restrictions, sensitivity and uncertainty analysis was conducted using EVn-BETR for all chemicals in all environmental compartments in a limited number of representative zones.

MacLeod et al. (2002) described the theoretical background and assumptions inherent to an analytical approach for conducting a preliminary assessment of uncertainty in multimedia fate models which includes sensitivity analysis, analysis of propagation of variance and estimation of the contribution of individual input parameter uncertainties to the overall output parameter uncertainty. While a complete discussion of this technique is beyond the scope of this report, it is useful to briefly describe the input requirements.

The approach relies on the assumption that variability in all input parameters under consideration can be described by a log-normal distribution. While this may not be strictly true, it is still a reasonable and advantageous assumption in most cases (Slob, 1994) and greatly facilitates the analysis. The variance in an
input parameter is then represented by a confidence factor (CF), which equals the factor by which 95% of the parameter values are expected to deviate from the median value ($\mu$). For example, a CF of 5 indicates that 95% of the parameter values in the distribution are between $\mu / 5$ and $5\mu$. The CF is related to the standard deviation of the distribution ($\sigma$) by the following relationships:

$$\sigma = \frac{1}{2} \ln(CF) \quad \text{or} \quad CF = e^{2\sigma}$$

An important result of this formulation is that median output value of the uncertainty analysis is the same as the output value using standard settings. The default confidence factors for EVn-BETR, which are generally based on expert judgement rather than empirical data, were used and are listed in Appendix 1. These CF represent estimates of overall parameter uncertainty rather than spatial and/or temporal variability.

The input parameters varied and the corresponding confidence factors were also translated as best as possible to the SimpleBox 3.0 platform in order to generate model output ranges for the predicted concentrations. It should be noted however that the log-normal distribution in the version of Crystal Ball used requires that the mean parameter value be inserted rather than the median ($\mu$). However, median input values of a log-normal distribution can be converted to the mean by the following relationship:

$$\text{Mean} = e^{[\mu + (\sigma^2)/2]}$$

4 Results

The results of the simulations are presented in the following way. For SimpleBox 3.0, results are represented by box-plots that present the minimum, 25th-percentile, median, 75th-percentile and maximum value based on the default parameter values and the confidence factors used. For BETR-Global and IMPACT 2002, only the median estimate in each zone and compartment are presented. For EVn-BETR, the results are presented as the median value with the upper and lower 95% confidence intervals based on the set of results obtained for a limited number of model zones. These results suggested a typical overall output CF of approximately 3 in the air compartment, 5 – 7 in the freshwater compartment and 6 – 10 in the sediment and soil compartments. Results for all models are summarized in Section 4.5 followed by a comparison to other model evaluation exercises in Section 4.6. More detailed results of the sensitivity and uncertainty analysis and a discussion of the implications are presented in Section 4.7.

In terms of model performance, the following categories were defined:

- **Excellent**: Agreement within a factor of two
- **Good**: Agreement within a factor of five
- **Satisfactory**: Agreement within a factor of ten
- ** Unsatisfactory**: Agreement not within a factor of ten

In this model evaluation exercise, no distinction was made between over- and underprediction although it is recognized that bias in the positive direction (overprediction) is preferable in terms of risk assessment where a degree of conservatism is often assumed.

4.1 SimpleBox 3.0

The first set of comparisons using SimpleBox 3.0 are between the generic continental model output and all monitoring data collected for Europe. The purpose of this comparison is to assess the degree to which the non-spatial model corresponds to the spatially-averaged monitoring data.
4.1.1 Bulk Air

The overall and absolute average MB for all five chemicals was 2.6 indicating that the model performs quite well. Predictions typically overestimate the monitoring values.
4.1.2 Freshwater (total)

The overall average MB for freshwater was 0.66 meaning that observations are typically underestimated by a factor of 1.5. Combined with an absolute average MB of 2.90, it can be concluded that model predictions reflect European averages quite well. Note that the monitoring data for HCB contained too high a proportion of non-detects to be included in the comparison. Instead, minimum and maximum reported values are shown.
4.1.3 Bulk Sediment Solids

The overall average MB for predictions in the sediment compartment for all chemicals was 0.038, corresponding to average underpredictions of a factor of approximately 26. The absolute average MB corresponds to an average underprediction of a factor of approximately 29. Overall, the model performance is therefore unsatisfactory although it should be noted that the model performed much better for γ-HCH.
4.1.4 Bulk Soil Solids

The overall and absolute average MB for predictions in soil of all chemicals was 0.0028, which corresponds to a typical underprediction of a factor of approximately 360. Comparisons to IP and γ-HCH were not included due to lack of representative and geographically distributed data.

4.1.5 Summary

Overall, SimpleBox 3.0 performs remarkably well for predicting the central tendency of concentrations in the air and freshwater compartment. Model performance is unsatisfactory for sediment and soil with predicted values underestimating the observations on average by 1.5 and 2.5 orders of magnitude respectively.

Although the performance of SimpleBox 3.0 in air and water compartments is encouraging, the variability in concentrations between sites in Europe is not represented and areas at greater potential risk cannot be identified. The unsatisfactory model performance in the sediment and soil compartments is also of concern.

4.2 BETR-Global

The model evaluation exercise for BETR-Global includes comparisons to monitoring data compiled into each respective zone as well as to the predictions in the generic continental zone of SimpleBox 3.0 (i.e. no
attempt was made to re-parameterize the regional component of SimpleBox 3.0 to represent each model zone. For the sake of brevity, only illustrative examples of the model output are included in this section. Complete results for the model comparisons are presented in Appendix 2. Recall that only lower air and soil compartments are considered for this model.

4.2.1 Bulk Lower Air

For the PAHs, BETR-Global was able to capture some of the observed spatial variability in the monitoring data and consistently outperformed the non-spatial output generated by SimpleBox 3.0. The performance of BETR-Global is more mixed for HCB although the spatial model generally outperforms the non-spatial model. This result is reflected in the overall average MB for all chemicals of 1.45 and 2.92 for BETR-Global and SimpleBox 3.0 respectively. In terms of the absolute average MB, BETR-Global (MB = 1.92) again outperformed the non-spatial version (MB = 3.69).
4.2.2 Bulk Soil Solids

BaP

The overall and absolute average MB for BETR-Global and SimpleBox 3.0 was 0.0091 and 0.0066 respectively which corresponds to an average underprediction by factors of 110 and 150. Although a moderate gain in model performance is apparent, neither of the models predicts the central tendency of the monitoring data particularly well.

4.2.3 Summary

Both models are able to predict concentrations in the air compartment with a very satisfactory level of accuracy. The use of the more spatially-explicit model resulted in improved performance in the air compartment. Neither model can predict concentrations in the soil compartment within an order of magnitude. Note that differences in the performance of SimpleBox in this and all following sections is
different compared to Section 4.1. These differences are caused by the fact that the comparisons are being made to monitoring data based on the spatial resolution of the various models rather than the entire dataset.

4.3 EVn-BETR

The model evaluation exercise for EVn-BETR includes comparisons to monitoring data compiled into each respective zone as well as to the non-spatial output generated by SimpleBox 3.0. For the sake of brevity, only illustrative examples of the model output are included in this section. Complete results for the model comparisons are presented in Appendix 3.

4.3.1 Bulk Lower Air

BaP

The overall average MB for all chemicals in the lower air compartment was 1.01 and 3.38 for EVn-BETR and SimpleBox 3.0 respectively. EVn-BETR also performed better considering the absolute average MB ($M_B = 2.04$) in comparison to SimpleBox 3.0 ($M_B = 4.27$). In particular, EVn-BETR performed better for PAHs (absolute PAH MB = 1.81) in comparison to SimpleBox 3.0 (absolute PAH MB = 4.59).
4.3.2 Freshwater (total)

BaP

\[\text{Zone 16}\]

\[\text{Zone 24}\]

\[\gamma\text{-HCH}\]

\[\text{Zone 16}\]

\[\text{Zone 19}\]
The overall average MB for all chemicals in the freshwater compartment was 0.07 and 0.46 for EVn-BETR and SimpleBox 3.0 respectively which corresponds to underprediction by a factor of approximately 15 and 2 respectively. In terms of the absolute average MB, the average values were approximately 29 and 6. EVn-BETR performs particularly poorly for PAHs (absolute average MB PAH = 78) in comparison to SimpleBox 3.0 (absolute average MB = 5). On the other hand, EVn-BETR is able to accurately predict concentrations of γ-HCH in the freshwater compartment with an overall average MB of 1.89 for this substance in comparison to SimpleBox 3.0 (MB = 3.56). Neither model predicts concentrations of HCB in freshwater very well with observations being underpredicted by more than two orders of magnitude.

4.3.3 Bulk Sediment Solids

BaP
The overall average MB for all chemicals in the sediment compartment was approximately 0.07 and 0.05 for EVn-BETR and SimpleBox 3.0 respectively corresponding to an average underprediction by a factor of 14 and 20. The average absolute MB for both models was approximately 23. The overall average MB for PAHs was 0.034 and 0.046 for EVn-BETR and SimpleBox 3.0 respectively corresponding to an average underprediction by a factor of approximately 30 and 22. Model performance improved significantly for $\gamma$-HCH (EVn-BETR overall average MB = 5.4; SimpleBox 3.0 overall average MB = 1.05) but deteriorated significantly for HCB (EVn-BETR overall average MB = 0.051; SimpleBox 3.0 overall average MB = 0.0036).
### 4.3.4 Bulk Soil Solids

#### BaP

The overall and absolute average MB for all chemicals in the soil compartment was 0.013 and 0.0061 for EVn-BETR and SimpleBox 3.0 respectively which corresponds to average underprediction by a factor of approximately 75 and 160. For PAHs alone, the overall average MB corresponds to average underprediction by a factor of approximately 50 and 60 for EVn-BETR and SimpleBox 3.0 respectively. HCB is underpredicted by an average of more than 2 orders of magnitude by EVn-BETR and 3 orders of magnitude by SimpleBox 3.0.

#### Summary

EVn-BETR performs modestly better than SimpleBox 3.0 for predictions in the air compartment and is able to capture some of the spatial variability observed in the monitoring data. However, the ability of EVn-BETR to accurately predict concentrations in freshwater compartments was found to be notably inferior to SimpleBox.
In the two other environmental media considered, the overall model performance of EVn-BETR is similar or slightly improved compared to SimpleBox 3.0.

### 4.4 IMPACT 2002

The model evaluation exercise for IMPACT 2002 includes comparisons to monitoring data compiled into each respective zone as well as to the non-spatial output generated by SimpleBox 3.0. For the sake of brevity, only illustrative examples of the model output are included in this section. Complete results for the model comparisons are presented in Appendix 4.

#### 4.4.1 Bulk Lower Air

**BaP**

<table>
<thead>
<tr>
<th>Zone</th>
<th>1.0E-03</th>
<th>1.0E-02</th>
<th>1.0E-01</th>
<th>1.0E+00</th>
<th>1.0E+01</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zone 142</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Zone 156</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**HCB**

<table>
<thead>
<tr>
<th>Zone</th>
<th>1.0E+00</th>
<th>1.0E+01</th>
<th>1.0E+02</th>
<th>1.0E+03</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zone 140</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Zone 142</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The overall average MB for all chemicals in the lower air compartment was 1.78 and 2.59 for IMPACT 2002 and SimpleBox 3.0 respectively. On an absolute scale, the MB was 1.83 and 2.92. Although the performance improvements are once again quite modest, it is still apparent that the spatially-explicit model is able to capture some of the inherent spatial variability of the monitoring data.

### 4.4.2 Freshwater (total)

**BaP**

![BaP box plots](image)

**γ-HCH**

![γ-HCH box plots](image)
The overall average MB for all chemicals in the freshwater compartment was 2.71 and 1.61 for IMPACT 2002 and SimpleBox 3.0 respectively. In absolute terms, the MB was 4.7 and 5.7 for the two models respectively. The performance of IMPACT 2002 for PAHs (absolute MB = 3.6) and \( \gamma \)-HCH (absolute MB = 2.03) was actually superior to Simple Box 3.0 (absolute MB PAH = 5.15 ; absolute MB \( \gamma \)-HCH = 3) but much worse for HCB (IMPACT 2002 absolute MB = 1350 vs SimpleBox 3.0 absolute MB = 280). This result indicates that modest improvements for some chemicals can be realized in the freshwater compartment with a spatially-explicit model, in contrast to the results of the model evaluation for EVn-BETR. The fact that land zones in IMPACT 2002 are parameterised based on watershed basins may explain this improvement.

### 4.4.3 Bulk Sediment Solids

**BaP**
The overall average MB for all chemicals in the sediment compartment was 0.0095 and 0.0288 for IMPACT 2002 and SimpleBox 3.0 respectively which corresponds to average underprediction by a factor of approximately 105 and 35. The average overall model bias for PAHs was 0.016 and 0.033 for IMPACT 2002 and SimpleBox 3.0 respectively which corresponds to average underprediction by a factor of 65 and 30. Model performance was best for γ-HCH where both models were able to predict the central tendency of the observations within a factor of 5. The largest discrepancy was found for predictions of HCB where the model bias corresponded to underprediction by at least 2 orders of magnitude for both models.
4.4.4 Bulk Soil Solids

BaP

IP

HCB
The average overall MB for all chemicals in the soil compartment was 0.0018 and 0.0023 for IMPACT 2002 and SimpleBox 3.0 respectively which corresponds to average underprediction by a factor of 540 and 440. Both models show improved performance for PAHs alone (IMPACT 2002 underpredicts by factor of 85; SimpleBox 3.0 by a factor of 140). As in the sediment compartment, predictions for HCB show the largest deviation from the monitoring data.

4.4.5 Summary

IMPACT 2002 is able to capture some of the spatial variability in the monitoring data and performs particularly well in the air and water compartments although the non-spatial output from SimpleBox 3.0 is also very reasonable. Predictions in the sediment and soil compartments deviate substantially from the monitoring data for both models, particularly for HCB.

4.4.6 Comment on Assumed Emission Scenarios

As discussed earlier, emissions for all chemicals were assumed to occur 100% to the lower air compartment although other modes of entry are possible. For example, it is conceivable that these chemicals are emitted to freshwater from sewage treatment plants, which could have an influence on concentrations in the water column as well as in sediments even if sampled far from the sewage outfalls. While this could partly explain the performance of the models in these compartments, it has no influence on the (non-agricultural) soil compartment where predicted concentrations were also well below the median of the monitoring data.
4.5 Summary of Model Performance

Model performance for all models are presented below in Table 4.5.1. The values represent the order of magnitude and direction (underprediction is negative) of the deviation of predicted concentrations based on default settings from the median reported value.

<table>
<thead>
<tr>
<th>Substance</th>
<th>Air</th>
<th>Soil</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaP</td>
<td>0.17</td>
<td>0.26</td>
</tr>
<tr>
<td>BbF</td>
<td>0.64</td>
<td>1.02</td>
</tr>
<tr>
<td>BkF</td>
<td>0.06</td>
<td>0.32</td>
</tr>
<tr>
<td>IP</td>
<td>0.01</td>
<td>0.35</td>
</tr>
<tr>
<td>gHCH</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>HCB</td>
<td>0.001</td>
<td>0.47</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Substance</th>
<th>Air</th>
<th>Freshwater</th>
<th>Soil</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaP</td>
<td>0.20</td>
<td>0.45</td>
<td>-1.79</td>
</tr>
<tr>
<td>BbF</td>
<td>0.08</td>
<td>0.95</td>
<td>-2.31</td>
</tr>
<tr>
<td>BkF</td>
<td>-0.11</td>
<td>0.24</td>
<td>-1.71</td>
</tr>
<tr>
<td>IP</td>
<td>0.11</td>
<td>0.57</td>
<td>-1.61</td>
</tr>
<tr>
<td>gHCH</td>
<td>-</td>
<td>-</td>
<td>0.28</td>
</tr>
<tr>
<td>HCB</td>
<td>-0.43</td>
<td>0.47</td>
<td>-2.61</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Substance</th>
<th>Air</th>
<th>Freshwater</th>
<th>Sediment</th>
<th>Soil</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaP</td>
<td>0.32</td>
<td>0.49</td>
<td>-0.35</td>
<td>-0.27</td>
</tr>
<tr>
<td>BbF</td>
<td>0.32</td>
<td>0.72</td>
<td>-0.42</td>
<td>-1.19</td>
</tr>
<tr>
<td>BkF</td>
<td>0.08</td>
<td>0.04</td>
<td>-0.34</td>
<td>-0.19</td>
</tr>
<tr>
<td>IP</td>
<td>0.12</td>
<td>0.33</td>
<td>-0.31</td>
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</tr>
<tr>
<td>gHCH</td>
<td>-</td>
<td>-</td>
<td>0.01</td>
<td>0.45</td>
</tr>
<tr>
<td>HCB</td>
<td>0.46</td>
<td>0.49</td>
<td>-3.13</td>
<td>-2.44</td>
</tr>
</tbody>
</table>

Table 4.5.1 Summary of Model Evaluation Results
4.6 Comparison to Other Model Evaluation Exercises

The following list details some examples of other model evaluation exercises that have been conducted recently along with a brief description of the findings.


Jager (1998) reported preliminary results of a model comparison exercise using HAZCHEM (ECETOX, 1994) for simulations of acetonitril, acroleine, 1-4 DCB, naphthalene and tetrachloroethylene and obtained the following results. The values represent the approximate order of magnitude and direction (underprediction is negative) of the deviation of predicted results from the ‘typical’ reported value.

**Table 4.6.1 HAZCHEM Model Evaluation**

<table>
<thead>
<tr>
<th>Substance</th>
<th>Air</th>
<th>Water</th>
<th>Sediment</th>
<th>Soil</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetonitril</td>
<td>-1</td>
<td>-4</td>
<td>-3</td>
<td>-</td>
</tr>
<tr>
<td>Acroleine</td>
<td>-2</td>
<td>-4</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>1,4-DCB</td>
<td>-1</td>
<td>-2</td>
<td>-3</td>
<td>-</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>-1</td>
<td>-2</td>
<td>-2.5</td>
<td>-2.5</td>
</tr>
<tr>
<td>Tetrachloroethylene</td>
<td>-1</td>
<td>-2.5</td>
<td>-3</td>
<td>-</td>
</tr>
</tbody>
</table>

The author cautioned that monitoring data were unlikely to be representative (i.e. some sampling was conducted near known pollution sources) which would explain at least some of the observed discrepancies.

2) Berding (2000) – EUSES Regional Distribution Model (SimpleBox platform)

Berding (2000) used the regional distribution model incorporated into the EUSES package for simulations of a series of different substances with a range of physicochemical properties. When the model was adapted to represent the chemicals and region of interest (North Rhine-Westphalia) as realistically as possible, the following results were obtained. The values represent the approximate order of magnitude and direction (underprediction is negative) of the deviation of predicted results from the median reported value.

**Table 4.6.2 EUSES Regional Distribution Model Evaluation**

<table>
<thead>
<tr>
<th>Substance</th>
<th>Air</th>
<th>Water</th>
<th>Sediment</th>
<th>Soil</th>
</tr>
</thead>
<tbody>
<tr>
<td>TCDD</td>
<td>&lt; 1</td>
<td>-</td>
<td>-3</td>
<td>-3</td>
</tr>
<tr>
<td>PeCDD</td>
<td>&lt; -1</td>
<td>-</td>
<td>-2</td>
<td>-2</td>
</tr>
<tr>
<td>HxCDD-1</td>
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<td>-</td>
<td>-1.5</td>
<td>-2</td>
</tr>
<tr>
<td>HxCDD-2</td>
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<td>-</td>
<td>-2</td>
<td>-2</td>
</tr>
<tr>
<td>HxCDD-3</td>
<td>&lt; -1</td>
<td>-</td>
<td>-2</td>
<td>-2</td>
</tr>
<tr>
<td>HpCDD</td>
<td>-1</td>
<td>-</td>
<td>-2.5</td>
<td>-2</td>
</tr>
<tr>
<td>OCDD</td>
<td>-1.5</td>
<td>-</td>
<td>-2.5</td>
<td>-2</td>
</tr>
<tr>
<td>Benzene</td>
<td>1.5</td>
<td>1</td>
<td>&lt; 1</td>
<td>-</td>
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<td>DEHP</td>
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<td>1</td>
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<td>1.5</td>
<td>-</td>
<td>-1</td>
</tr>
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<td>1</td>
<td>-7</td>
</tr>
<tr>
<td>HHCB</td>
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<td>&lt; 1</td>
<td>1</td>
<td>-</td>
</tr>
<tr>
<td>LAS</td>
<td>-</td>
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</tbody>
</table>

It is also interesting to note that the default model parameter settings (i.e. not chemical or region-specific) actually predicted the monitored concentrations far better than the most realistic parameter set in water, sediments and soil (results not shown). The author suggested that a lack of representative monitoring data
was a major contributor to the observed discrepancies between predicted and monitored concentrations. The unreliability and uncertainty associated with emission estimates was also mentioned.

3) Struijs & Peijnenburg (2002) – SimpleBox 2.0

Struijs & Peijnenburg (2002) used SimpleBox 2.0 to simulate the fate of two phthalate esters (DEHP and DBP). Some of the results of this comparison study are presented below. The values represent the approximate order of magnitude and direction (underprediction is negative) of the deviation of predicted results from the median reported value.

Table 4.6.3 SimpleBox 2.0 Model Evaluation

<table>
<thead>
<tr>
<th>Substance</th>
<th>Air</th>
<th>Water</th>
<th>Sediment</th>
<th>Soil</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEHP</td>
<td>&lt; -1</td>
<td>&lt; -1</td>
<td>1</td>
<td>&lt; 1</td>
</tr>
<tr>
<td>DBP</td>
<td>-1</td>
<td>&lt; -1</td>
<td>&lt; 1</td>
<td>&lt; -2</td>
</tr>
</tbody>
</table>

4) Breivik & Wania (2002) – POPCycling-Baltic

Breivik & Wania (2002) evaluated the performance of POPCycling-Baltic using long-term emission and monitoring data for $\alpha$- and $\gamma$-HCH in the Baltic Region. The authors reported that predicted concentrations in air, water, marine sediment and pine needles were all within a factor of 10 of the observations.

5) Prevedouros et al. (2004a) – EVn-BETR

Prevedouros et al. (2004a) used EVn-BETR to simulate the fate of $\gamma$-HCH in continental Europe based on 1998 emission data. Reported concentrations of $\gamma$-HCH in the atmosphere could be predicted within a factor of 5 – 10. Comparisons in other environmental media were not reported.

6) Prevedouros et al. (2004b) – EVn-BETR

EVn-BETR was used to simulate the fate of PBDEs using historic emission estimates. Predicted concentrations of PBDE-47 and 99 in the lower air compartment were within a factor of 2 – 4 of monitoring data while predicted concentrations of PBDE-153 were within a factor of 11 – 15. A larger discrepancy was observed for concentrations of all congeners in the soil compartment.


Margni et al. (2004) simulated the fate of several PCDD/Fs using IMPACT 2002. For all congeners considered, the normalized spatial average of the predicted concentrations was within the minimum and maximum observed values in air, sediment, soil and vegetation. The authors reported that the best fits between predicted and monitored data were found in the sediment and air compartments.

8) Pennington et al. (2005) – IMPACT 2002

Pennington et al. (2005) simulated the fate of PeCDF and compared the predicted values to available monitoring data. Predicted air concentrations were most consistent with monitoring data followed by the sediment and soil compartments.

In the context of other model evaluation exercises, the results from this study can be considered typical. For example, the results for naphthalene reported by Jager (1998) and PCDDs reported by Berding (2000) are similar to the results for PAHs in this study i.e. model performance was best for predictions in the air compartment (within an order of magnitude) and least reliable in the sediment and soil compartments where underpredictions of 2 – 3 orders of magnitude were also reported. Results for $\gamma$-HCH are also similar to what has been reported by other authors. Unfortunately, the complexity of the models and inherent uncertainties
prevent further conclusions to be made. However, it would be useful to conduct further model evaluation exercises with the four models adopted for this study using chemicals with a wider range of physicochemical properties as soon as reliable spatially-resolved emission estimates become available.

4.7 Results of the Sensitivity and Propagation of Uncertainty Analysis

Example outputs of the sensitivity and propagation of uncertainty analysis produced by EVn-BETR are presented in Appendix 5. Note that the results vary depending on the compartment, physicochemical properties and to a lesser extent, the model zone of interest. Before proceeding with the discussion of the results, it is useful to recall that sensitivity refers to the proportional change in the output parameter related to the change in input parameter and that contribution to output variance is therefore a function of sensitivity and the magnitude of the confidence factor chosen for a given input parameter. Unless otherwise specified, parameters discussed in terms of contribution also ranked highly in terms of sensitivity.

4.7.1 Bulk Lower Air

The two parameters that contributed the most to the overall output variance for PAHs were direct emissions (to lower air) and advective flow rates (between lower air boxes). Degradation half-life, rain scavenging efficiency, aerosol deposition and rain rate also had a minor influence on the predicted concentrations in this compartment. Predicted concentrations were also found to be sensitive to the total surface area although this parameter was not assigned a CF and therefore had no influence on the overall output variance in these preliminary simulations. These results can be rationalized in terms of processes that represent sources and sinks of contaminants in this compartment. In this case, emissions are the most important source of contaminants and variation in emission rates will necessarily have an important influence. Advective air flows can be either a source or sink, depending on the direction, but it should be noted that advective loss terms (i.e. flow out of the model zone) had a greater influence than advective inflows from other model zones. Degradation and bulk deposition can also be important loss terms and thus it was not surprising to observe that input parameters related to these processes were identified as having an influence on the model predictions in the air compartment. The sensitivity of model output to the total surface area is also reasonable due to the fact that air-surface exchange rates between two compartments are directly related to the surface area.

Direct emissions and advective flow rates were also identified as having an important influence on overall output variance for γ-HCH although in this case variability in advective inflows contributed slightly more to overall variance than advective outflows. Other important parameters included enthalpy of vaporization (from water to air), aqueous solubility and vapour pressure indicating that different processes dominate the fate of this substance compared to PAHs. This finding is most likely due to the greater aqueous solubility and lower K_{OW} (two orders of magnitude) compared to the other substances modeled in this evaluation exercise.

The sensitivity and propagation of uncertainty analysis also identified advective air flows as the most important contributors to overall output uncertainty for HCB, at least in the model zones considered. Direct emissions also contributed significantly to the overall output CF. Model output for HCB was also found to be sensitive to enthalpy of vaporization (from water to air), aqueous solubility and vapour pressure. The relatively high vapour pressure and low water solubility likely explains the differences between the results for PAHs and for this substance.

4.7.2 Freshwater (total)

The most influential parameters on overall output CFs for PAHs in the freshwater compartment include the rain scavenging efficiency, sediment deposition rate, soil reaction half-life, volume fraction of particles in freshwater, direct emissions to lower air, soil solids run-off rate, rain rate, sediment resuspension, sediment reaction half-life, average freshwater sediment depth, K_{OW}, advective air flows, and freshwater half-life. These findings can also be rationalized in terms of sources and sinks of contaminants to the freshwater compartment. Since the emission scenarios adopted for the model evaluation exercise specify emissions to
lower air only, the processes which are related to transfer of contaminant from air to water and processes which remove chemical from this compartment should obviously impact the predicted results significantly. These parameters, divided into sources and sinks (direct, indirect) are shown below.

Table 4.7.2.1 Parameters Related to Sources and Sinks of PAHs in the Freshwater Compartment

<table>
<thead>
<tr>
<th>Sources</th>
<th>Sinks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rain scavenging efficiency</td>
<td>Sediment deposition rate</td>
</tr>
<tr>
<td>Direct emissions to lower air</td>
<td>Volume fraction of particles</td>
</tr>
<tr>
<td>Soil reaction half-life</td>
<td>Sediment reaction half-life</td>
</tr>
<tr>
<td>Soil solids run-off rate</td>
<td>Freshwater reaction half-life</td>
</tr>
<tr>
<td>Rain rate</td>
<td>Advective air outflows</td>
</tr>
<tr>
<td>Sediment resuspension</td>
<td></td>
</tr>
<tr>
<td>Advective air inflows</td>
<td></td>
</tr>
</tbody>
</table>

Rain scavenging efficiency and rain rate are two pathways for contaminants to be transferred from the air compartment to the freshwater compartment and it is reasonable to expect that these variation in these parameters along with direct emissions to lower air and advective air inflows would influence the overall output CF. It is interesting to note the apparent importance of exchange of contaminant from the soil compartment to the freshwater compartment, indicated by the influence of the soil reaction half-life (affects soil concentrations) and the soil solids run-off rate. Another related finding is that the sensitivity analysis for PAHs identified “% of soil covered by vegetation” as the most influential parameter in terms of sensitivity (but not contribution to overall output CF due to the narrow input CF selected for this variable). The vegetation compartment is important because of its role in intercepting contaminants from the air compartment and also depositing contaminants via litter fall. The decision to set degradation half-lives in the vegetation compartment equal to degradation half-lives in the air may therefore have a substantial influence on model outcomes.

The most important parameters in terms of contribution to overall output CF for γ-HCH include freshwater reaction half-life, soil reaction half-life, K<sub>OW</sub>, soil-water runoff, emissions to bulk lower air, advective air inflows and rain rate. It is interesting to note that parameters related to soil-freshwater exchange were also identified as influential in this analysis. In this case however, soil-water run-off rather than soil solids run-off rate is important, a finding that is related to the differences in key physicochemical properties between the more water-soluble γ-HCH compared to PAHs which tend to be particle-bound to a greater extent.

For HCB, the air-side air-freshwater mass transfer coefficient was shown to be another influential parameter in addition to sediment deposition, volume fraction of particles in freshwater, advective air flows, sediment resuspension, emission to air, sediment reaction half-life, freshwater half-life and K<sub>OW</sub>. The air-side air-freshwater mass transfer coefficient important for substances with higher vapour pressures because it is related to diffusive exchange between contaminant in the gaseous phase and freshwater.

4.7.3 Bulk Sediment Solids

The most influential parameters on overall output CFs for PAHs in the freshwater compartment include rain scavenging rate, sediment reaction half-life, average freshwater sediment depth, soil reaction half-life, emissions to bulk lower air, soil solids run-off, rain rate, sediment deposition, advective air flows, air reaction half-life and volume fraction of particles in freshwater. Because of the emission scenarios adopted for this study (to lower air only), concentrations in the sediment are determined by exchange from air to water and then water to sediment and it is therefore not surprising that the results of the sensitivity and propagation of uncertainty analysis are similar between the freshwater and sediment compartment. The sensitivity of model output to the % of soil covered by vegetation was also observed.

Similarly, the analysis for γ-HCH in the sediment compartment was closely related to the results for the freshwater compartment with parameters such as sediment deposition, freshwater reaction half-life, soil reaction half-life and soil-water run-off rate identified as influential parameters. The sediment reaction half-
life for HCB was also identified as important as was the average freshwater sediment depth, and air side air-freshwater mass transfer coefficient.

These results confirm the tight link between the freshwater and sediment compartments and the air compartment given the current assumptions regarding the emission scenarios and also indicate the importance of the soil compartment as an indirect source of contaminants to freshwater and freshwater sediments.

4.7.4 Bulk Soil Solids

The two most influential parameters for predictions of PAH concentrations in the soil compartment are the rain scavenging ratio (source) and the soil reaction half-life (sink). Rain rate (source), emissions to bulk lower air (indirect source), physical characteristics of the soil compartment such as average soil depth and density of soil solids, air reaction half-life and aerosol deposition (source) were also identified as being important. Once again, model output was most sensitive to the % of soil covered by vegetation. This result indicates that the interaction between air and vegetation and vegetation and soil might need to be considered in further detail in terms of the parameterization of variables related to process descriptions.

For γ-HCH, the analysis indicated that soil reaction half-life (sink), rain rate (source), emissions to bulk lower air and advective flows (indirect sources) as well as physical characteristics of the soil compartment like average soil depth were the most influential parameters. The results for HCB were similar to the results for PAHs with the soil reaction half-life (sink) and rain scavenging ratio (source) identified as influential parameters along with K_{OW}, rain rate (source), advective outflows, and average soil depth.

The importance of average soil depth for all chemicals considered is noteworthy since several publications have emerged over the past 10 years which have demonstrated that concentration profile with depth is not uniform for many substances, particularly for substances with physicochemical properties that favour the tendency to sorb to organic carbon (e.g. Cousins et al., 1999ab; McLachlan et al., 2002). For these substances, concentrations may be significantly greater in the top 5 cm, which is often the depth from which field samples are collected and homogenized. The assumption of a default soil depth of at least 10 cm by all models adopted for this evaluation exercise may therefore partially explain the deviation from monitoring data observed.

4.7.5 Model Sensitivity to Parameters Associated with Model Geometry

The sensitivity analysis indicated that in addition to parameters discussed in previous sections, model output is also sensitive to total surface area, % of surface covered by freshwater) and average lower air compartment height which suggests that differences in model geometry should be considered when comparing the model output among different models. However, this issue is complicated by the relationship between compartment volume and the residence times associated with advective flows and it is incorrect to automatically assume that decreasing a compartment volume will necessarily result in higher concentrations.

4.7.6 Conclusions

The patterns that emerge from the sensitivity and propagation of uncertainty analysis indicate the complex nature of the interactions between the compartments and various environmental processes included in this type of multimedia environmental fate model. However, the processes describing air-surface exchange, particularly those detailing deposition processes, were consistently identified as important both in terms of model sensitivity and contribution to output variance. The interaction between air, vegetation, and soil and the freshwater/sediment system was also identified as influential. In the soil and sediment compartments, the parameterization of the degradation half-life also appears to be particularly important. In addition, advective air flows were also seen to exert an influence on the model predictions in all compartments. These findings imply that future efforts to (re)parameterize similar multimedia fate models should focus on these processes. Finally, as expected, the importance of obtaining realistic emission estimates was highlighted by this analysis.
4.8 Illustrative Dynamic Simulation Using EVn-BETR

As discussed in a previous section, the maximum influence of the historic emission scenario is limited. However, the dynamic simulation mode with varying emission mode of EVn-BETR was utilized to more precisely investigate the potential effect of higher historic emissions on the predictions generated by the model. As an illustrative example, simulations were conducted from 1970 to 2000 for BaP. Summary results are presented below which include the median observed concentrations, the original steady-state (SS) solution and the dynamic solution for the year 1995 as well as the ratio of the latter two.

**Table 4.8.1 Steady-state and Dynamic Results for Bulk Lower Air**

<table>
<thead>
<tr>
<th>Zone</th>
<th>Observed</th>
<th>SS</th>
<th>Dynamic</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ng m-3</td>
<td>ng m-3</td>
<td>ng m-3</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.033</td>
<td>0.062</td>
<td>0.139</td>
<td>2.24</td>
</tr>
<tr>
<td>14</td>
<td>0.635</td>
<td>0.347</td>
<td>0.779</td>
<td>2.24</td>
</tr>
<tr>
<td>16</td>
<td>0.031</td>
<td>0.120</td>
<td>0.269</td>
<td>2.24</td>
</tr>
<tr>
<td>25</td>
<td>0.135</td>
<td>0.204</td>
<td>0.458</td>
<td>2.24</td>
</tr>
<tr>
<td>51</td>
<td>0.007</td>
<td>0.012</td>
<td>0.027</td>
<td>2.21</td>
</tr>
</tbody>
</table>

**Table 4.8.2 Steady-state and Dynamic Results for Freshwater (total)**

<table>
<thead>
<tr>
<th>Zone</th>
<th>Observed</th>
<th>SS</th>
<th>Dynamic</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ng m-3</td>
<td>ng m-3</td>
<td>ng m-3</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>3.58E-03</td>
<td>6.29E-05</td>
<td>1.59E-04</td>
<td>2.53</td>
</tr>
<tr>
<td>19</td>
<td>4.00E-03</td>
<td>2.51E-05</td>
<td>6.37E-05</td>
<td>2.53</td>
</tr>
<tr>
<td>24</td>
<td>1.45E-02</td>
<td>9.08E-05</td>
<td>2.27E-04</td>
<td>2.50</td>
</tr>
<tr>
<td>25</td>
<td>1.68E-03</td>
<td>1.75E-04</td>
<td>5.09E-04</td>
<td>2.91</td>
</tr>
</tbody>
</table>

**Table 4.8.3 Steady-state and Dynamic Results for Bulk Sediment Solids**

<table>
<thead>
<tr>
<th>Zone</th>
<th>Observed</th>
<th>SS</th>
<th>Dynamic</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ug kg-1</td>
<td>ug kg-1</td>
<td>ug kg-1</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>215.00</td>
<td>2.55</td>
<td>7.103</td>
<td>2.79</td>
</tr>
<tr>
<td>17</td>
<td>400.00</td>
<td>0.81</td>
<td>2.166</td>
<td>2.69</td>
</tr>
<tr>
<td>23</td>
<td>265.00</td>
<td>5.31</td>
<td>15.135</td>
<td>2.85</td>
</tr>
<tr>
<td>24</td>
<td>325.00</td>
<td>3.63</td>
<td>10.024</td>
<td>2.76</td>
</tr>
<tr>
<td>25</td>
<td>430.00</td>
<td>7.09</td>
<td>22.841</td>
<td>3.22</td>
</tr>
<tr>
<td>37</td>
<td>44.00</td>
<td>2.01</td>
<td>5.486</td>
<td>2.73</td>
</tr>
<tr>
<td>38</td>
<td>60.00</td>
<td>2.03</td>
<td>5.661</td>
<td>2.79</td>
</tr>
</tbody>
</table>

**Table 4.8.4 Steady-state and Dynamic Results for Bulk Soil Solids**

<table>
<thead>
<tr>
<th>Zone</th>
<th>Observed</th>
<th>SS</th>
<th>Dynamic</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ug kg-1</td>
<td>ug kg-1</td>
<td>ug kg-1</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>20</td>
<td>0.057</td>
<td>0.217</td>
<td>3.83</td>
</tr>
<tr>
<td>25</td>
<td>12</td>
<td>0.166</td>
<td>0.506</td>
<td>3.06</td>
</tr>
<tr>
<td>37</td>
<td>14</td>
<td>0.092</td>
<td>0.228</td>
<td>2.47</td>
</tr>
<tr>
<td>47</td>
<td>0.3</td>
<td>0.050</td>
<td>0.120</td>
<td>2.38</td>
</tr>
</tbody>
</table>

Although it is apparent that the incorporation of the historic emission scenario does lead to higher concentrations in all media for this substance, the resulting improvements in performance in freshwater, sediment and soil compartments, which were significantly underpredicted by the steady-state version of
EVn-BETR, comes at the expense of performance in the air compartment. Still, these initial results suggest that dynamic solutions with historic emission estimates can improve overall model performance, at least for some chemicals.

5 Inventory of Improvement Options

The following inventory of improvement options is based on theoretical considerations, the model evaluation exercise and the anticipated needs of the NOMIRACLE project in the future.

5.1 Expand Applicability of Models

The four multimedia fate models selected for this evaluation exercise are essentially limited to neutral organic compounds. However, there are both theoretical and practical reasons for expanding the applicability of these models, particularly in the context of the NOMIRACLE project.

5.1.1 Sorption Algorithms

Although K\textsubscript{OW} (and thus K\textsubscript{OC}) was not identified as an influential parameter for predicting concentrations in any compartment for the majority of the chemicals included in this report, there are several reasons why updating at least the K\textsubscript{OC}-K\textsubscript{OW} sorption algorithms is highly desirable. The two most important considerations are that 1) exposure models typically rely on an estimate of the freely-dissolved concentration in the water column and sediment pore-water to calculate concentrations in biota and 2) fate models typically assume that degradation of compounds can only occur if the chemical is in the freely-dissolved form. Given that K\textsubscript{OC} is the ratio between sorbed and freely-dissolved concentrations, there is a strong impetus to describe this relationship as accurately as possible.

Options

1) Include class-specific K\textsubscript{OC}-K\textsubscript{OW} relationships such as those reported by Sabljic (1995)

2) Include polyparameter linear free-energy relationships (PP-LFERs) for describing partitioning coefficients (e.g. Goss and Schwarzenbach, 2001; Breivik and Wania, 2003; Nguyen et al., 2005).

Feasibility

Incorporating new sorption algorithms into a multimedia fate model is relatively trivial. However, the two approaches are currently limited by the availability of compound class-specific K\textsubscript{OC}-K\textsubscript{OW} relationships (Option 1) and the molecular descriptors required to implement PP-LFERs for all environmental media (Option 2). Descriptions of the temperature-dependence of the partition coefficients generated by the PP-LFER approach may also be lacking for a broad range of substances. On the other hand, several partners within the NOMIRACLE consortium are specifically focused on generating data and techniques to facilitate the use of PP-LFERs (e.g. WP 2.1; http://nomiracle.jrc.it) and the possibilities to incorporate this new information into future modeling efforts will be greatly enhanced.

Benefits

The clearest benefit of implementing this option is that the models will be applicable to a greater range of compound classes on a theoretical basis. In particular, inclusion of PP-LFERs would represent a significant step forward.
5.1.2 Soot-carbon Inclusive Sorption Algorithms

The potential influence of soot-carbon on the distribution of certain compounds (generally planar) between the sorbed and freely-dissolved phase is well-established (e.g. Gustafsson et al., 1997; Naes et al., 1998; Kleineidam et al., 1999; Karapanagioti et al., 2000; Jonker et al., 2000; Schwarzenbach et al., 2003). Given that typical sediments and soils may contain 1 – 10% non-amorphous carbon (i.e. soot carbon, black carbon etc) according to Gustafsson and Gschwend (1998) and observed $K_{OC}$ may be up 2 – 3 orders of magnitude above the $K_{OC}$ based on conventional sorption algorithms as a result, this issue deserves further consideration, particularly in the context of a model evaluation exercise that included planar compounds (PAHs). Recall though that as stated in Section 5.1.1, predicted concentrations of majority of chemicals included in this study in soils and sediments were not highly sensitive to $K_{OW}$ (and thus $K_{OC}$) implying that including soot may have a limited influence on model output in that sense. The main concern is the influence of inaccurate freely-dissolved concentrations on predictions in biota generated by exposure models later in the risk assessment procedure.

Options

1) Incorporate a two-phase sorption isotherm (i.e standard $K_{OC}$-$K_{OW}$ relationship + soot-carbon component)

2) Meta-analysis of empirical $K_{OC}$-$K_{OW}$ relationships based on field studies (e.g. Jonker et al., 2000) to derive an estimate of the degree to which sorption to organic matter is typically enhanced by the presence of soot-carbon. Although not mechanistically-based, there may be data available for a wider range of substances

Feasibility

In the context of a risk assessment tool intended for application to potentially thousands of different chemicals, both options are hindered by the lack of data required to develop reliable estimates for a broad range of compounds. For example, the parameters required to implement a two-phase sorption isotherm are only available for a very narrow range of substances, which also happen to be the substances that field studies have generally focused on (e.g. PAHs). An initial survey of available literature would suggest that either approach is currently feasible for PAHs and PCDD/Fs and a few other substances (e.g. HCB)

Benefits

There are theoretical and empirical reasons to implement this type of approach for certain substances. The value to the NOMIRACLE project depends on what proportion of the substances of concern are affected by the presence of soot-carbon, which is difficult to assess a priori.

5.1.3 Multi-species Chemicals

Chemicals that dissociate to a significant degree at environmental pHs and those which are degraded to produce a significant quantity of metabolites of concern can not be simultaneously simulated with the models used in this study. However, approaches to address both of these possibilities are available and have been implemented in multimedia models with similar frameworks (e.g. Diamond et al., 1992; Fenner et al., 2000; Quartier and Müller-Herold, 2000; Gonzalez et al., 2001; Fenner et al., 2002; Cahill et al., 2003; Cahill and Mackay, 2003).

Feasibility

Dissociation need only be considered under certain circumstances. For example, it is not necessary to consider the dissociated form of an acidic compound if its pKa exceeds pH by 2 units or more due to the negligible presence of the ionic species (Mackay, 2001). Given the wide availability of pKa data, it is easy to screen for substances that require such treatment.
Simultaneous simulation of metabolites is only necessary if there is toxicological evidence to support inclusion of metabolites. If deemed necessary, the approach is straightforward to implement but could be limited by the availability of reliable degradation half-life data and conceivably the physico-chemical properties of the metabolite(s). The work of several NOMIRACLE partners (e.g. WP 2.3: http://nomiracle.jrc.it) on development of novel techniques to generate estimates of degradation rate constants will be extremely valuable in future efforts to improve parameterization of these processes.

Benefits

The main benefit of incorporating a multi-species approach is that it expands the applicability of the modelling tools. Since the approaches are already established in the scientific literature and may be required for pesticides and pharmaceuticals of interest to the NOMIRACLE project, implementing this option is considered a priority.

5.2 Include Capability to Perform Dynamic Simulations

As implied in Section 4.8, the capability to perform dynamic simulations using varying emission levels is likely to be beneficial if the substance of interest was emitted in substantially greater quantities in the past (i.e. current emissions are well below historic peak levels). Another relevant scenario that cannot be simulated by a steady-state model is the abrupt cessation of emissions typically associated with certain agricultural applications. For example, pesticides may only be applied over a brief period in spring or summer whereas the steady-state model assumes a constant emission rate.

Another consideration is that short-term or seasonal variations in temperature, rainfall and other climatic conditions can be incorporated into dynamic models. Such variability was recently shown by Lammel (2004) to produce predictions that can be substantially different from models that use time-averaged values.

Feasibility

Applying dynamic models on a continental European scale is hindered by challenges related to the intensified data requirements for parameterisation. To fully realize the potential of this approach, year-round climatic information would be required for each model zone (and compartment) as well as other information such as daily/seasonal advective flow rates and emission estimates. Another limitation is the impact on computational effort as the typical simulation time would be greatly lengthened, particularly as the spatial-resolution of the model is increased.

Benefits

The main benefit of implementing this option is the model simulations will be more representative of the temporal variation of the environmental medium under consideration as well as the emission profiles of certain substances such as pesticides, which are of great interest to the NOMIRACLE project. Furthermore, the influence of variable climate conditions on other processes (e.g. degradation) could be explored.

5.3 Re-evaluate Parameterisation of Key Processes

The following recommendations are based on model performance and on the sensitivity and propagation of uncertainty analysis conducted using EVn-BETR. As mentioned earlier, the interactions between environmental processes are complex and therefore alterations in certain parameters may not actually result in the anticipated changes to model predictions (e.g. increasing K_{OC} does not seem to influence soil and sediment concentrations for the PAHs simulated in this study). For this reason, a discussion of potential benefits has been omitted.

5.3.1 Air-surface exchange / Deposition
The transfer of chemicals from the atmosphere to other surfaces can occur via diffusion, rain dissolution, wet deposition and dry deposition (Mackay, 2001). While the processes can be described conceptually with relative ease, estimating or measuring the rate of these processes is problematic and models often rely on suggested typical values provided by Mackay (2001), which are arguably more illustrative than realistic. A further complication is that these transport processes are sensitive to temperature through the corresponding influence on partition coefficients (which alter the distribution of the chemical between phases) along with other parameters such as rain rate and aerosol deposition velocity. However, given that the results of the model evaluation exercise suggest that the flux of chemical from the atmosphere to all other compartments may be significantly underestimated, it seems advisable to reconsider the suitability of the parameter values adopted by all models for these processes.

Feasibility

Obtaining experimental evidence to support the parameterization of these processes is not feasible in the short-term. The use of evaluative models and consultation with experts is highly recommended as the effect of particular combinations of parameter values on air-surface exchange could be rapidly assessed for chemicals with a wide range of physicochemical properties.

5.3.2 Intermedia Transfer Between Air-Vegetation-Soil and Soil-Freshwater

The sensitivity and propagation of uncertainty analysis indicated the potential influence of parameters related to the transfer of contaminants from the atmosphere to vegetation and subsequent transfer to the soil compartment and the transfer of contaminants from the soil compartment to the freshwater compartment on predicted concentrations in these compartments. It is particularly noteworthy that both soil solid (for PAHs) and soil water run-off rates (for γ-HCH) ranked highly in their contribution to the overall output CF for concentrations in the freshwater and sediment compartments. However, due to the obvious linkages between these processes and compartments and the dependence on other processes (e.g. air-surface exchange in general), it is difficult to recommend a clear course of action. For example, increasing the exchange between soil and freshwater (e.g. by increasing erosion rates) may result in higher concentrations in the sediment compartment but will also result in lower concentrations in the soil compartment as a consequence. Regardless, the results of this model evaluation exercise do support many aspects of the modelling strategy proposed by Pistocchi (2005), particularly with regards to treatment of the soil compartment.

As for processes related to vegetation, the major issues and uncertainties associated with describing the fate of organic contaminants in this compartment was recently reviewed by Barber et al. (2004). The authors concluded that there is a definite need for greater mechanistic understanding of air-plant exchange and the relationships with physicochemical properties and other factors that influence these processes.

Feasibility

No assessment possible at this time.

5.3.3 Advection Rates (Air Flow)

Advection is one of the primary mechanisms by which a chemical is removed from an evaluative model environment (Mackay, 2001). In the context of a spatially-resolved model, advection can be seen as a mechanism of redistribution as well as removal. The results of the model evaluation and model sensitivity and propagation of uncertainty analysis seem to suggest that advection rates in the lower air compartments are overestimated and contaminants otherwise subject to deposition are being removed from the model zones too rapidly. Estimated air flows may therefore need to be adjusted. Another option could be to increase the mixing height of the air compartments resulting in a larger volume and thus a longer residence time (assuming advection rates are not changed).

Feasibility
To parameterise air flow rates, averaged values are typically calculated based on available wind velocity and trajectory data (e.g. Prevedouros et al., 2004a; Pennington et al., 2005). Consequently, daily/seasonal variation is not represented, which could also have an important influence on model predictions. However, this type of variability can only be captured by dynamic models, the application of which may not be practical for the risk assessment of thousands of chemicals.

5.3.4 Degradation Half-lives

The degradation of a substance in the environment is a highly variable process that depends on many factors including the intrinsic properties of the chemical, the compartment of interest and the environmental conditions (Mackay, 2001). Obtaining representative degradation half-lives is therefore difficult and selected parameter values are often highly uncertain. When degradation is identified as an important process controlling the environmental fate of a substance using the default values, the most conservative approach would be recalculate predicted concentrations assuming negligible degradation in all media (or at least the compartments which are most sensitive to the parameter value selected). Alternatively, the upper bounds of experimental values could be selected rather than the average value. As mentioned previously, the work of several NOMIRACLE partners (e.g. WP 2.3; http://nomiracle.jrc.it) on estimates of degradation rate constants will be extremely valuable in future modeling efforts.

5.3.5 Layered Soil Compartments

The four models selected for this empirical evaluation all have well-mixed soil compartments of at least 10 cm depth whereas the depth-dependence of soil concentrations has been described in the scientific literature (e.g. Cousins et al. 1999ab, McLachlan et al., 2002). Gusev et al. (2005) developed a regional fate model (MSCE-POP) which includes a soil compartment with seven sublayers which are 0.1, 0.3, 0.6, 1, 2, 5 and 11 cm thick respectively. This approach allows a more realistic comparison to be made between the depth of soil typically sampled in monitoring campaigns (i.e. 5 cm) and model output which is not averaged over an inappropriate total depth. Adopting a similar approach may thus lead to better agreement between measured and modeled concentrations however it should be noted that the evaluation of the performance of MSCE-POP (Shatalov et al., 2005) focused on measured concentrations in the atmosphere and precipitation rather than in the soil compartments so no conclusions can be drawn at this time.

Feasibility

Incorporation of a layered soil compartment can be accomplished relatively easily within typical multimedia fate model frameworks however there may be a significant cost in terms of computational effort when conducting simulations on a continental scale with additional layers in every model zone.

5.4 Include Sensitivity / Uncertainty Analysis

The process of interpreting and rationalizing model output is greatly facilitated by the results of model sensitivity and propagation of uncertainty analysis. Although computationally intense, the benefits of performing such simulations cannot be understated.

Options

1) Version compatible with Crystal Ball™

2) Built-in functionality
5.5 Limitations of the Evaluation Exercise / Future Work

The results of the empirical model evaluation are based on comparisons between available monitoring data in certain environmental compartments for a limited number of chemicals. As such, the recommendations cannot automatically be considered valid for all chemical classes and must be interpreted with caution. Furthermore, not all environmental processes of potential relevance have been considered here. For example, the ability of the models to predict the transfer of chemicals into vegetation from the atmosphere and soil has not been evaluated due to the lack of suitable monitoring data. These pathways may be of great importance for some chemicals in the context of a human risk assessment. It is also important to reiterate the fact that only emissions to the atmosphere were considered in this assessment.

Future efforts should focus on expanding the number of chemicals included in similar model evaluation exercises. The priority should be on the selection of chemicals with a wider range of physical-chemical properties and those that are representative of various chemical classes. There are obvious benefits of consulting the work of the NOMIRACLE partners mentioned in Section 5.3 and further communication between these groups is highly recommended. However, the need for more integrated monitoring programs is also evident. Empirical model evaluations cannot be conducted if monitoring data is sparse or non-representative. Therefore, chemicals selected for future empirical model evaluations must be selected judiciously and should take advantage of other programs (e.g. EMEP, PERFORCE) that may provide useful information and guidance.

Supporting Information

The spatially-resolved emission estimates for all chemicals and models as well as the model output and monitoring data have been compiled into excel spreadsheets and uploaded to the documents area of the WP 2.4 section of the NOMIRACLE project intranet (http://nomiracle.jrc.it/intranet) in the ITM folder. The files can be accessed immediately by all members of the NOMIRACLE consortium. Interested readers who are not involved in the project should contact the NOMIRACLE secretariat (nomiracle@dmu.dk).

Acknowledgments

Dennis Helsel and Steve Saiz are acknowledged for providing assistance related to calculations of summary statistics for censored data sets with multiple detection limits. Jasper Harbers is thanked for providing the spatially-resolved emission estimates and other valuable insights. Costas Prevedouros, Matt MacLeod, David Pennington and Ralph Rosenbaum are also acknowledged for providing information about the continental and global scale models selected for this evaluation exercise.

References


Armitage JM, Cousins IT (2005). M.2.4.2 European-wide Field Data Report About Selected Reference Compounds. EU Project 003956 : NOMIRACLE.


Appendices

1 Confidence factors for sensitivity and propagation of uncertainty analysis

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### 3. Environmental Characteristics in All Regions

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<tr>
<td>Volume Fraction Particles in fresh water</td>
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</tr>
<tr>
<td>Volume Fraction Fish in fresh water</td>
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</tr>
<tr>
<td>Volume Fraction Particles in coastal water</td>
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</tr>
<tr>
<td>Volume Fraction Fish in coastal water</td>
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<tr>
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<tr>
<td>Volume Fraction Water in soil</td>
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### 4. Inter-regional Flow Rates (Matrix G values)

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<td>Coastal water flow rate (m³/h)</td>
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### 2 Steady-state results for BETR-Global

| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 |
| 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 |
| 49 | 50 | 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 |
| 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 | 87 | 88 | 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 |
| 97 | 98 | 99 | 100 | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 | 119 | 120 |
| 121 | 122 | 123 | 124 | 125 | 126 | 127 | 128 | 129 | 130 | 131 | 132 | 133 | 134 | 135 | 136 | 137 | 138 | 139 | 140 | 141 | 142 | 143 | 144 |
| 145 | 146 | 147 | 148 | 149 | 150 | 151 | 152 | 153 | 154 | 155 | 156 | 157 | 158 | 159 | 160 | 161 | 162 | 163 | 164 | 165 | 166 | 167 | 168 |
| 169 | 170 | 171 | 172 | 173 | 174 | 175 | 176 | 177 | 178 | 179 | 180 | 181 | 182 | 183 | 184 | 185 | 186 | 187 | 188 | 189 | 190 | 191 | 192 |
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| 217 | 218 | 219 | 220 | 221 | 222 | 223 | 224 | 225 | 226 | 227 | 228 | 229 | 230 | 231 | 232 | 233 | 234 | 235 | 236 | 237 | 238 | 239 | 240 |
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| 265 | 266 | 267 | 268 | 269 | 270 | 271 | 272 | 273 | 274 | 275 | 276 | 277 | 278 | 279 | 280 | 281 | 282 | 283 | 284 | 285 | 286 | 287 | 288 |
Air

BaP

Zone 38

Zone 61

Zone 62
HCB

**Zone 37**

![Boxplot for Zone 37](image)

**Zone 38**

![Boxplot for Zone 38](image)

**Zone 61**

![Boxplot for Zone 61](image)

Soil

BaP

**Zone 37**

![Boxplot for Zone 37](image)

**Zone 61**

![Boxplot for Zone 61](image)
IP

Zone 61

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<tr>
<td>1.0E+00</td>
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<tr>
<td>1.0E+01</td>
</tr>
<tr>
<td>1.0E+02</td>
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<td>1.0E+03</td>
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Observed BETR-Global SimpleBox

Zone 37

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<td>1.0E+00</td>
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Observed BETR-Global SimpleBox

Zone 60

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Observed BETR-Global SimpleBox

Zone 61

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Observed BETR-Global SimpleBox

HCB
3 Steady-state results for EVn-BETR
Air

BaP

Zone 6

Zone 14

Zone 16

Zone 25

Zone 51
HCB

Zone 4

Zone 16

Zone 51

Water

BaP

Zone 16

Zone 19
BbF
BkF

Zone 25

Zone 16

Zone 19

Zone 24

Zone 25

Zone 24

Zone 25
IP

\[ \gamma \text{-HCH} \]

[Box plots for Zones 19, 24, 25, 16, and 17]
### HCB

#### Zone 37

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#### Zone 38

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#### Zone 16

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#### Zone 17

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Sediment

BaP
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Zone 38

Zone 16

Zone 17

Zone 23

Zone 24
\[ \gamma\text{-HCH} \]
HCB
Soil
BaP
BbF

Zone 37

Zone 47

Zone 25

Zone 37

Zone 47

Zone 47

Observed Evn-BETR SimpleBox

ug kg⁻¹

1.0E+02
1.0E+01
1.0E+00
1.0E-01
1.0E-02
1.0E-03

1.0E+02
1.0E+01
1.0E+00
1.0E-01
1.0E-02
1.0E-03

1.0E+02
1.0E+01
1.0E+00
1.0E-01
1.0E-02
1.0E-03

1.0E+02
1.0E+01
1.0E+00
1.0E-01
1.0E-02
1.0E-03

Zone 25

IP

Zone 37

Zone 47

IP
4 Steady-state results for IMPACT 2002

Model Zones : Air

Model Zones : Land (water, sediment, soil)
Air

BaP

Zone 95

Zone 142

Zone 156

BbF

Zone 95

Zone 142
HCB

Zone 140

Zone 142

Water

BaP

Zone 27

Zone 35
BaP

Zone 70

Zone 79

Zone 80

Zone 81

Zone 82

Zone 103

Observed
Model
SimpleBox

ug L⁻¹

1.0E-05
1.0E-04
1.0E-03
1.0E-02
1.0E-01
1.0E+00
Zone 27

Zone 35

Zone 66

Zone 70

Zone 79

Zone 80
BkF

Zone 70

Zone 79

Zone 80

Zone 81

Zone 82

Zone 103

Observed IMPACT SimpleBox

Observed IMPACT SimpleBox

Observed IMPACT SimpleBox

Observed IMPACT SimpleBox

ug L⁻¹

ug L⁻¹

ug L⁻¹

ug L⁻¹

1.0E+00
1.0E+00
1.0E+00
1.0E+00

1.0E-05
1.0E-05
1.0E-05
1.0E-05

1.0E-04
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1.0E-03

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1.0E-02

1.0E-01
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1.0E-01

1.0E-00
1.0E-00
1.0E-00
1.0E-00

1.0E+00
1.0E+00
1.0E+00
1.0E+00
g-HCH

Zone 27

Zone 79

Zone 103

Zone 3

Zone 6
g-HCH

**Zone 8**

![Box plot for Zone 8](image)

**Zone 10**

![Box plot for Zone 10](image)

**Zone 14**

![Box plot for Zone 14](image)

**Zone 15**

![Box plot for Zone 15](image)

**Zone 16**

![Box plot for Zone 16](image)

**Zone 22**

![Box plot for Zone 22](image)
g-HCH

Zone 59

Zone 60

Zone 62

Zone 64

Zone 65

Zone 66
g-HCH

[Box plots showing data for zones 67, 69, 70, 77, 79, and 80 with observed, IMPACT, and SimpleBox values for each zone in micrograms per liter (ug L^-1).]
g-HCH

Zone 81

Zone 82

Zone 102

Zone 103

Zone 104

Zone 105

Observed IMPACT SimpleBox
g-HCH

Zone 107

Zone 108

Zone 109

Zone 110

Zone 111

Zone 112
HCB

Zone 35

Zone 70

Zone 77

Zone 79

Zone 80

Zone 81
HCB

Sediment

BaP
IP

Zone 79

Observed IMPACT SimpleBox

Zone 27

Observed IMPACT SimpleBox

Zone 66

Observed IMPACT SimpleBox

Zone 67

Observed IMPACT SimpleBox

Zone 70

Observed IMPACT SimpleBox

g-HCH
Zone 71

Zone 79

Zone 80

Zone 81

Zone 82

Observed IMPACT SimpleBox
HCB

Zone 77

Zone 79

Zone 80

Zone 81

Zone 82

Observed  IMPACT  SimpleBox

Observed  IMPACT  SimpleBox

Observed  IMPACT  SimpleBox

Observed  IMPACT  SimpleBox

Observed  IMPACT  SimpleBox
Soil

BaP

Zone 20

Zone 79

Zone 113

BbF

Zone 20

Zone 79

Zone 113
BKF

Zone 20  
Zone 79  

IP

Zone 20  
Zone 79  

ug kg⁻¹

Observed  IMPACT  SimpleBox
HCB

Zone 79

Zone 102

Zone 104

Zone 113

Zone 114
### 5 Example outputs of sensitivity and propagation of uncertainty analysis

**Substance:** BaP  
**Region:** 4  
**Media:** Air  
**Overall Output CF:** 2.6

| Rank | Input Parameter | Region | Determination Region | Sensitivity ($S$) | | $|$ | Input | Confidence | Factor (CF) | Output | CF (due | Percent | to this | Contribution | Output | Variance |
|------|----------------|--------|----------------------|------------------|---------|---------|---------|-------------|---------|---------|----------|----------|-----------|----------|----------|
| 1    | Emissions to Bulk Lower Air (kg/y) | 4      | 1                    | 0.676262305      | 0.676262305 | 3       | 2.102127819 | 59.92904962 |
| 2    | Lower air flow rate (m$^3$/h)    | 4, 5   | 0.315650993          | 0.3157           | 3.00    | 1.41    | 13.06   |
| 3    | Lower air flow rate (m$^3$/h)    | 4, 51  | -0.223656221         | 0.2237           | 3.00    | 1.28    | 6.55    |
| 4    | Air Reaction half-life (h)       |        | 0.175220495          | 0.175220495      | 3       | 1.212275764 | 4.023248306 |
| 5    | rain scavenging ratio            | 4      | -0.07725184          | 0.07725184       | 10      | 1.194680677 | 3.435319714 |
| 6    | 4 aerosol deposition              | 4      | -0.155884647         | 0.155884647      | 3       | 1.168795465 | 3.184298085 |
| 7    | Lower air flow rate (m$^3$/h)    | 17, 4  | 0.107190385          | 0.1071           | 3.00    | 1.12    | 1.50    |
| 8    | 19 upper-lower air mixing MTC    | 4      | -0.049567918         | 0.049567918      | 10      | 1.120902707 | 1.414330335 |
| 9    | 3 rain rate                      | 4      | -0.090782207         | 0.090782207      | 3       | 1.104877477 | 1.079962065 |
| 10   | Lower air flow rate (m$^3$/h)    | 51, 4  | 0.089484883          | 0.0895           | 3.00    | 1.10    | 1.05    |
| 11   | Lower air flow rate (m$^3$/h)    | 3, 4   | 0.066032133          | 0.0680           | 3.00    | 1.08    | 0.57    |
| 12   | 4 aerosol deposition              | 51     | -0.064792091         | 0.064792091      | 3       | 1.073775978 | 0.55011882 |
| 13   | Lower air flow rate (m$^3$/h)    | 4, 3   | -0.059452828         | 0.0595           | 3.00    | 1.07    | 0.46    |
| 14   | Lower air flow rate (m$^3$/h)    | 5, 4   | 0.057157965          | 0.0572           | 3.00    | 1.06    | 0.43    |
| 15   | Lower air flow rate (m$^3$/h)    | 24, 17 | 0.040384619          | 0.0404           | 3.00    | 1.05    | 0.21    |

**Sorted by Sensitivity**

| Rank | Input Parameter | Region | Determination Region | Sensitivity ($S$) | | $|$ | Input | Confidence | Factor (CF) | Output | CF (due | Percent | to this | Contribution | Output | Variance |
|------|----------------|--------|----------------------|------------------|---------|---------|---------|-------------|---------|---------|----------|----------|-----------|----------|----------|
| 1    | Emissions to Bulk Lower Air (kg/y) | 4      | 1                    | 0.676262305      | 0.676262305 | 3       | 2.102127819 | 59.92904962 |
| 2    | Total Surface Area (km$^2$)       | 4      | -0.364302139         | 0.364302139      | 1       | 1       | 0        |
| 3    | Lower air flow rate (m$^3$/h)    | 4, 5   | -0.315650993         | 0.3157           | 3.00    | 1.41    | 13.06   |
| 4    | Lower air flow rate (m$^3$/h)    | 4, 51  | -0.223656221         | 0.2237           | 3.00    | 1.28    | 6.55    |
| 5    | Air Reaction half-life (h)       |        | 0.175220495          | 0.175220495      | 3       | 1.212275764 | 4.023248306 |
| 6    | 4 aerosol deposition              | 4      | -0.155884647         | 0.155884647      | 3       | 1.168795465 | 3.184298085 |
| 7    | Lower air flow rate (m$^3$/h)    | 17, 4  | 0.107190385          | 0.1071           | 3.00    | 1.12    | 1.50    |
| 8    | 19 upper-lower air mixing MTC    | 4      | -0.049567918         | 0.049567918      | 10      | 1.120902707 | 1.414330335 |
| 9    | 3 rain rate                      | 4      | -0.090782207         | 0.090782207      | 3       | 1.104877477 | 1.079962065 |
| 10   | Lower air flow rate (m$^3$/h)    | 51, 4  | 0.089484883          | 0.0895           | 3.00    | 1.10    | 1.05    |
| 11   | Lower air flow rate (m$^3$/h)    | 3, 4   | 0.066032133          | 0.0680           | 3.00    | 1.08    | 0.57    |
| 12   | 4 aerosol deposition              | 51     | -0.064792091         | 0.064792091      | 3       | 1.073775978 | 0.55011882 |
| 13   | Lower air flow rate (m$^3$/h)    | 4, 3   | -0.059452828         | 0.0595           | 3.00    | 1.07    | 0.46    |
| 14   | Lower air flow rate (m$^3$/h)    | 5, 4   | 0.057157965          | 0.0572           | 3.00    | 1.06    | 0.43    |
| 15   | Lower air flow rate (m$^3$/h)    | 24, 17 | 0.040384619          | 0.0404           | 3.00    | 1.05    | 0.21    |
| Rank | Input Parameter                  | Region | Sensitivity (S) | |S| | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|----------------------------------|--------|----------------|-----|--------------------------|-----------------------------------|------------------------------------------|
| 1    | Lower air flow rate (m³/h)      | 14     | 0.312075288    | 0.3121 | 3.00                      | 1.41                              | 15.99                                    |
| 2    | Lower air flow rate (m³/h)      | 7      | -0.293927504   | 0.2999 | 3.00                      | 1.38                              | 14.19                                    |
| 3    | Emissions to Bulk Lower Air (kg/y)| 14    | 0.2794501      | 0.2794501 | 3                         | 1.359350911                       | 12.82251995                             |
| 4    | Emissions to Bulk Lower Air (kg/y)| 7     | 0.275226129    | 0.275226129 | 3                         | 1.353057448                       | 12.43781717                             |
| 5    | Lower air flow rate (m³/h)      | 7      | -0.236528715   | 0.2365 | 3.00                      | 1.30                              | 9.19                                     |
| 6    | Air Reaction half-life (h)      |        | 0.186556462    | 0.186556462 | 3                         | 1.230167832                       | 5.837779488                             |
| 7    | Lower air flow rate (m³/h)      | 8      | 0.176416216    | 0.1764 | 3.00                      | 1.21                              | 5.11                                     |
| 8    | Lower air flow rate (m³/h)      | 6      | 0.149754256    | 0.1498 | 3.00                      | 1.18                              | 3.88                                     |
| 9    | 4 aerosol depositon             | 7      | -0.141731287   | 0.141731287 | 3                         | 1.168484645                       | 3.28634672                              |
| 10   | Lower air flow rate (m³/h)      | 7      | -0.121229044   | 0.1212 | 3.00                      | 1.14                              | 2.41                                     |
| 11   | Lower air flow rate (m³/h)      | 14     | -0.117430279   | 0.1174 | 3.00                      | 1.14                              | 2.26                                     |
| 12   | Emissions to Bulk Lower Air (kg/y)| 6     | 0.083161794    | 0.083161794 | 3                         | 1.096666188                       | 1.1365566435                            |
| 13   | Lower air flow rate (m³/h)      | 8      | -0.076362257   | 0.0764 | 3.00                      | 1.09                              | 0.96                                     |
| 14   | Emissions to Bulk Lower Air (kg/y)| 8      | 0.069923118    | 0.069923118 | 3                         | 1.079845956                       | 0.802798259                             |
| 15   | Emissions to Bulk Lower Air (kg/y)| 14    | -0.068916455   | 0.068916455 | 3                         | 1.078652379                       | 0.779849337                             |

Sorted by Sensitivity:
| Rank | Input Parameter                          | Region | Sensitivity (S)  | \(|S|\) | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|-----------------------------------------|--------|-----------------|-------|-----------------------------|-----------------------------------|----------------------------------------|
| 1    | Emissions to Bulk Lower Air (kg/y)      | 25     | 0.537811489     | 3     | 1.805515797                | 40.9769811                        |
| 2    | Lower air flow rate (m³/h)              | 25 26  | -0.292515362     | 3.00  | 1.38                        | 12.12                             |
| 3    | 4 aerosol deposition                    | 25 25  | -0.265236938     | 3     | 1.338298939                | 9.967278964                       |
| 4    | Lower air flow rate (m³/h)              | 26 25  | 0.212447062      | 3.00  | 1.26                        | 6.39                              |
| 5    | Emissions to Bulk Lower Air (kg/y)      | 24     | 0.182380666      | 3     | 1.22655103                 | 4.743719601                       |
| 6    | 19 upper-lower mixing MTC               | 25     | -0.085739787     | 10    | 1.218259443                | 4.575260972                       |
| 7    | Emissions to Bulk Lower Air (kg/y)      | 26     | 0.175838867      | 3     | 1.213099603                | 4.380647976                       |
| 8    | Air Reaction half-life (h)              |        | 0.173107619      | 3     | 1.209465054                | 4.245618519                       |
| 9    | Lower air flow rate (m³/h)              | 24 25  | 0.163614433      | 3.00  | 1.20                        | 3.79                              |
| 10   | Rain scavenging rate                    | 25     | -0.072880895     | 10    | 1.182717153                | 3.305814457                       |
| 11   | 3 rain rate                             | 25     | -0.06212724      | 3.00  | 1.099344792                | 1.053055698                       |
| 12   | Lower air flow rate (m³/h)              | 26 27  | -0.06439592      | 0.684 | 1.108                       | 0.66                              |
| 13   | Lower air flow rate (m³/h)              | 25 24  | -0.0840621       | 0.641 | 1.07                        | 0.58                              |
| 14   | 4 aerosol deposition                    | 24     | -0.05839725      | 3     | 1.066402132                | 0.485191477                       |
| 15   | 4 aerosol deposition                    | 26     | -0.053713631     | 3     | 1.060783311                | 0.408766697                       |

Sorted by Sensitivity

| Rank | Input Parameter                          | Region | Sensitivity (S)  | \(|S|\) | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|-----------------------------------------|--------|-----------------|-------|-----------------------------|-----------------------------------|----------------------------------------|
| 1    | Total Surface Area (km²)                | 25     | -0.567640483    | 1     | 1                           | 1                                 | 0                                      |
| 2    | Emissions to Bulk Lower Air (kg/y)      | 25     | 0.537811489     | 3     | 1.605515797                | 40.9769811                        |
| 3    | Lower air flow rate (m³/h)              | 25 26  | -0.292515362     | 3.00  | 1.38                        | 12.12                             |
| 4    | 4 aerosol deposition                    | 25 25  | -0.265236938     | 3     | 1.338298939                | 9.967278964                       |
| 5    | Lower air flow rate (m³/h)              | 26 25  | 0.212447062      | 3.00  | 1.26                        | 6.39                              |
| 6    | Emissions to Bulk Lower Air (kg/y)      | 24     | 0.182380666      | 3     | 1.22655103                 | 4.743719601                       |
| 7    | Emissions to Bulk Lower Air (kg/y)      | 26     | 0.175838867      | 3     | 1.213099603                | 4.380647976                       |
| 8    | Air Reaction half-life (h)              |        | 0.173107619      | 3     | 1.209465054                | 4.245618519                       |
| 9    | Lower air flow rate (m³/h)              | 24 25  | 0.163614433      | 3.00  | 1.20                        | 3.79                              |
| 10   | Total Surface Area (km²)                | 24     | -0.125657805     | 1     | 1                           | 0                                 | 0                                      |
| 11   | Total Surface Area (km²)                | 26     | -0.111619326     | 1     | 1                           | 0                                 | 0                                      |
| 12   | Average lower air compartment height    | 25     | -0.10388188      | 1.5   | 1.043020132                | 0.208260197                       |
| 13   | 3 rain rate                             | 25     | -0.06212724      | 3     | 1.099344792                | 1.053055698                       |
| 14   | 19 upper-lower mixing MTC               | 25     | 0.085739787      | 10    | 1.218259443                | 4.575260972                       |
| 15   | Property Temperature (C)               | 0.074925497 | 0.074925497 | 1     | 1                           | 0                                 | 0                                      |
| Rank | Input Parameter                                      | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------------------|--------|----------------|-------|-------------------------------|--------------------------------------|----------------------------------------|
| 1    | rain scavenging ratio                               | 25     | 0.370 823738   | 0.370 823738 | 10 | 2.348 679366 | 19.24652823 |                                       |
| 2    | 9 sediment deposition                               | 25     | -0.727 56665   | 0.727 56665  | 3  | 2.224 607119 | 16.88406875 |                                       |
| 3    | Soil Reaction half-life (h)                         | 25     | 0.497 503835   | 0.497 503835 | 3  | 1.727 30748  | 7.88196925  |                                       |
| 4    | Volume Fraction Particles in fresh water            | 25     | 0.481 477252   | 0.481 477252 | 3  | 1.697 160951 | 7.368289084 |                                       |
| 5    | Emissions to Bulk Lower Air (kg/y)                  | 25     | 0.470 363392   | 0.470 363392 | 3  | 1.676 56407  | 7.04931502  |                                       |
| 6    | 12 soil solids runoff                               | 25     | 0.424 563096   | 0.424 563096 | 3  | 1.626 133736 | 6.24582752  |                                       |
| 7    | 3 rain rate                                         | 25     | 0.424 470859   | 0.424 470859 | 3  | 1.594 131226 | 5.740774828 |                                       |
| 8    | 10 sediment resuspension                            | 25     | 0.422 467707   | 0.422 467707 | 3  | 1.560 228968 | 5.686716236 |                                       |
| 9    | Sediment Reaction half-life (h)                     | 25     | 0.361 76523    | 0.361 76523  | 3  | 1.488 011233 | 4.169442628 |                                       |
| 10   | Average fresh water sediment depth (cm)              | 26     | -0.336 112581  | 0.336 112581 | 3  | 1.446 659844 | 3.599517516 |                                       |
| 11   | Kow (not Log Kow)                                   | 25     | -0.265 903674  | 0.265 903674 | 3  | 1.393 310459 | 2.253265016 |                                       |
| 12   | Lower air flow rate (m3/h)                          | 25     | -0.245 624786  | 0.245 624786 | 3  | 1.31 1.92     |                                           |                                       |
| 13   | Fresh Water Reaction half-life (h)                  | 25     | 0.231 92156    | 0.231 92156  | 3  | 1.290 193073 | 1.713787618 |                                       |
| 14   | Emissions to Bulk Lower Air (kg/y)                  | 25     | 0.209 207029   | 0.209 207029 | 3  | 1.258 96639  | 1.394540186 |                                       |
| 15   | Air Reaction half-life (h)                          | 25     | 0.200 23003    | 0.200 23003  | 3  | 1.246 057937 | 1.277418427 |                                       |

Sorted by Sensitivity

| Rank | Input Parameter                                      | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------------------|--------|----------------|-------|-------------------------------|--------------------------------------|----------------------------------------|
| 1    | % Soil covered by vegetation                         | 25     | -0.937 85093   | 0.937 85093 | 1.10000000024 | 1.035003499 | 2.10927036 |                                       |
| 2    | Volume Fraction Sediment pore water                  | 25     | 0.785 604220   | 0.785 604220 | 1.10000000024 | 1.077 897809 | 0.147598983 |                                       |
| 3    | 9 sediment deposition                                | 25     | -0.727 85685   | 0.727 85685  | 3  | 2.224 067119 | 16.8840675 |                                       |
| 4    | Soil Reaction half-life (h)                          | 25     | 0.497 503835   | 0.497 503835 | 3  | 1.727 30748  | 7.88196925  |                                       |
| 5    | Total Surface Area (km2)                             | 25     | -0.495 18954   | 0.495 18954  | 3  | 1.727 30748  | 7.88196925  |                                       |
| 6    | Volume Fraction Particles in fresh water            | 25     | 0.481 477252   | 0.481 477252 | 3  | 1.697 160951 | 7.368289084 |                                       |
| 7    | % Surface covered by fresh water                     | 25     | -0.474 26571   | 0.474 26571  | 3  | 1.646 239222 | 0.53936794  |                                       |
| 8    | Emissions to Bulk Lower Air (kg/y)                  | 25     | 0.470 363392   | 0.470 363392 | 3  | 1.676 56407  | 7.04931502  |                                       |
| 9    | Average soil depth (cm)                              | 25     | -0.450 42039   | 0.450 42039  | 3  | 1.626 133736 | 6.24582752  |                                       |
| 10   | 12 soil solids runoff                                | 25     | 0.422 467707   | 0.422 467707 | 3  | 1.590 228968 | 5.686716236 |                                       |
| 11   | 3 rain rate                                         | 25     | 0.424 563096   | 0.424 563096 | 3  | 1.594 131226 | 5.740774828 |                                       |
| 12   | 10 sediment resuspension                             | 25     | 0.422 467707   | 0.422 467707 | 3  | 1.590 228968 | 5.686716236 |                                       |
| 13   | Sediment Reaction half-life (h)                     | 25     | 0.361 76523    | 0.361 76523  | 3  | 1.488 011233 | 4.169442628 |                                       |
| 14   | Average fresh water sediment depth (cm)              | 25     | -0.336 112581  | 0.336 112581 | 3  | 1.446 659844 | 3.599517516 |                                       |
| Rank | Input Parameter | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|----------------|--------|-----------------|-----|-----------------|-------------------------------|--------------------------------------|
| 1    | rain scavenging ratio | 25     | 0.370823738     | 0.370823738 | 10 | 2.348679396 | 20.30830042 |
| 2    | Sediment Reaction half-life (h) | 25     | 0.39049302      | 0.39049302 | 3  | 2.135260614 | 16.029303   |
| 3    | Average fresh water sediment depth (cm) | 25    | -0.66538129     | 0.66538129  | 3  | 2.077186973 | 14.88535525 |
| 4    | Soil Reaction half-life (h) | 25     | 0.497903835     | 0.497903835 | 3  | 1.72703748  | 8.3215666   |
| 5    | Emissions to Bulk Lower Air (kg/yr) | 25    | 0.670363922     | 0.670363922 | 3  | 1.676564078 | 7.438112678 |
| 6    | 12 soil solids runoff | 25     | 0.442630966     | 0.442630966 | 3  | 1.626133736 | 6.586856491 |
| 7    | 3 rain rate | 25     | 0.424470859     | 0.424470859 | 3  | 1.594131226 | 6.054775542 |
| 8    | 9 sediment deposition | 25     | 0.271311157     | 0.271311157 | 3  | 1.347250395 | 2.474750146 |
| 9    | Lower air flow rate (m3/h) | 25     | -0.245624786    | 0.245624786 | 3  | 1.31          | 2.03        |
| 10   | Fresh Water Reaction half-life (h) | 25     | 0.23192156      | 0.23192156  | 3  | 1.290193073 | 8.83323564 |
| 11   | Emissions to Bulk Lower Air (kg/yr) | 26    | 0.209079292     | 0.209079292 | 3  | 1.258966329 | 1.471473212 |
| 12   | Air Reaction half-life (h) | 25     | 0.20003003      | 0.20003003  | 3  | 1.246054703 | 1.34790079 |
| 13   | density of sediment solids (7,2) | 25    | -0.506142564    | 0.506142564 | 1.5| 1.227769017 | 1.173167016 |
| 14   | Emissions to Bulk Lower Air (kg/yr) | 24    | 0.185019799     | 0.185019799 | 3  | 1.225397185 | 1.150866409 |
| 15   | Volume Fraction Particles in fresh water | 25    | -0.179556317    | 0.179556317 | 3  | 1.218077459 | 1.04041232 |

Sorted by Sensitivity

| Rank | Input Parameter | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|----------------|--------|-----------------|-----|-----------------|-------------------------------|--------------------------------------|
| 1    | % Soil covered by vegetation | 25     | -0.937850093    | 0.937850093 | 1.100000024 | 1.093503499 | 0.225632399 |
| 2    | Sediment Reaction half-life (h) | 25     | 0.60049302      | 0.60049302 | 3  | 2.135260614 | 16.029303   |
| 3    | Average fresh water sediment depth (cm) | 25    | -0.66538129     | 0.66538129  | 3  | 2.077186973 | 14.88535525 |
| 4    | density of sediment solids (7,2) | 25    | -0.506142564    | 0.506142564 | 1.5| 1.227769017 | 1.173167016 |
| 5    | Soil Reaction half-life (h) | 25     | 0.497903835     | 0.497903835 | 3  | 1.72703748  | 8.3215666   |
| 6    | density of water (4,1) | 25     | -0.492010005    | 0.492010005 | 1.049999952 | 1.024295671 | 0.160851616 |
| 7    | Total Surface Area (km2) | 25     | -0.485169354    | 0.485169354 | 1  | 1           | 0          |
| 8    | % Surface covered by fresh water | 25     | -0.474266371    | 0.474266371 | 1.100000024 | 1.046239622 | 0.059115504 |
| 9    | Emissions to Bulk Lower Air (kg/yr) | 25    | 0.470363392     | 0.470363392 | 3  | 1.676564078 | 7.438112678 |
| 10   | Average soil depth (cm) | 25     | -0.45042039     | 0.45042039  | 1.5| 1.203800283 | 0.929163099 |
| 11   | 12 soil solids runoff | 25     | 0.442560969     | 0.442560969 | 3  | 1.626133736 | 6.58456491 |
| 12   | 3 rain rate | 25     | 0.424470859     | 0.424470859 | 3  | 1.594131226 | 6.054775542 |
| 13   | rain scavenging ratio | 25     | 0.370823738     | 0.370823738 | 10 | 2.348679396 | 20.30830042 |
| 14   | 9 sediment deposition | 25     | 0.271311157     | 0.271311157 | 3  | 1.347250395 | 2.474750146 |
| 15   | Volume Fraction Water in soil | 25     | 0.270486528     | 0.270486528 | 1.100000024 | 1.026115307 | 0.018513017 |
| Rank | Input Parameter                        | Region | Sensitivity (S) | |S| | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|---------------------------------------|--------|-----------------|-----|----------|-----------------------------|----------------------------------------|----------------------------------------|
| 1    | rain scavenging ratio                 | 25     | 0.629480956     | 0.629480956 | 10 | 4.260700001 | 43.05429729                         |                                        |
| 2    | Soil Reaction half-life (h)           | 25     | 0.989002564     | 0.989002564 | 3  | 2.965972526 | 24.19377718                         |                                        |
| 3    | 3 rain rate                           | 25     | 0.721690887     | 0.721690887 | 3  | 2.209703796 | 12.86283026                         |                                        |
| 4    | Emissions to Bulk Lower Air (kg/y)    | 25     | 0.48404778      | 0.48404778   | 3  | 1.7019609  | 5.795429961                         |                                        |
| 5    | Average soil depth (cm)               | 25     | -0.989002544    | 0.989002544  | 1.5| 1.493923882 | 3.302082737                         |                                        |
| 6    | density of soil solids (6,3)          | 25     | -0.799483884    | 0.799483884  | 1.5| 1.382872447 | 2.153507249                         |                                        |
| 7    | Lower air flow rate (m3/h)            | 25     | -0.206023532    | 0.2606       | 3.00| 1.33        | 1.63                                |                                        |
| 8    | Air Reaction half-life (h)            | 25     | 0.215856236     | 0.215856236  | 3  | 1.267621505 | 1.152493233                         |                                        |
| 9    | Emissions to Bulk Lower Air (kg/y)    | 24     | 0.203652605     | 0.203652605  | 3  | 1.25073847  | 1.025861613                         |                                        |
| 10   | Lower air flow rate (m3/h)            | 25     | 0.189263656     | 0.1893       | 3.00| 1.23        | 0.89                                |                                        |
| 11   | % Soil covered by vegetation          | 25     | -0.204233453    | 2.04233453   | 1.100000024 | 1.21489216 | 0.776519688                          |                                        |
| 12   | Emissions to Bulk Lower Air (kg/y)    | 26     | 0.172565785     | 0.172565785  | 3  | 1.208745315 | 0.73657712                          |                                        |
| 13   | Lower air flow rate (m3/h)            | 24     | 0.133894215     | 0.1331       | 3.00| 1.16        | 0.44                                |                                        |
| 14   | Upper air flow rate (m3/h)            | 25     | -0.123081242    | 0.1231       | 3.00| 1.14        | 0.37                                |                                        |
| 15   | 4 aerosol deposition                  | 25     | -0.088900118    | 0.089000118  | 3  | 1.103807287 | 0.199007627                         |                                        |

Sorted by Sensitivity

| Rank | Input Parameter                        | Region | Sensitivity (S) | |S| | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|---------------------------------------|--------|-----------------|-----|----------|-----------------------------|----------------------------------------|----------------------------------------|
| 1    | % Soil covered by vegetation          | 25     | -2.04233453     | 2.04233453 | 1.100000024 | 1.21489216 | 0.776519688                          |                                        |
| 2    | Average soil depth (cm)               | 25     | -0.989002544    | 0.989002544 | 1.5 | 1.493923882 | 3.302082737                         |                                        |
| 3    | Soil Reaction half-life (h)           | 25     | 0.989002564     | 0.989002564 | 3  | 2.965972526 | 24.19377718                         |                                        |
| 4    | density of soil solids (6,3)          | 25     | -0.799483884    | 0.799483884 | 1.5 | 1.382872447 | 2.153507249                         |                                        |
| 5    | 3 rain rate                           | 25     | 0.721690887     | 0.721690887 | 3  | 2.209703796 | 12.86283026                         |                                        |
| 6    | rain scavenging ratio                 | 25     | 0.629480956     | 0.629480956 | 10 | 4.260700001 | 43.05429729                         |                                        |
| 7    | Emissions to Bulk Lower Air (kg/y)    | 25     | 0.48404778      | 0.48404778   | 3  | 1.7019609  | 5.795429961                         |                                        |
| 8    | Total Surface Area (km2)              | 25     | -0.465566227    | 0.465566227  | 1  | 1          | 1.0                                  |                                        |
| 9    | Volume Fraction Air in soil           | 25     | 0.315774486     | 0.315774486  | 1.100000024 | 1.030554008 | 0.018563197                          |                                        |
| 10   | Volume Fraction Water in soil         | 25     | 0.23984501      | 0.23984501   | 1.100000024 | 1.0264536 | 0.013970936                          |                                        |
| 11   | Lower air flow rate (m3/h)            | 25     | -0.206023532    | 0.2606       | 3.00| 1.33        | 1.68                                |                                        |
| 12   | Air Reaction half-life (h)            | 25     | 0.215856236     | 0.215856236  | 3  | 1.267621505 | 1.152493233                         |                                        |
| 13   | Emissions to Bulk Lower Air (kg/y)    | 24     | 0.203652605     | 0.203652605  | 3  | 1.25073847  | 1.025861613                         |                                        |
| 14   | density of water (4,1)                | 25     | -0.199047783    | 0.199047783  | 1.049999952 | 1.00975885 | 0.001932853                         |                                        |
| 15   | Lower air flow rate (m3/h)            | 26     | 0.189263656     | 0.1893       | 3.00| 1.23        | 0.89                                |                                        |
**Substance:** BbF  
**Region:** 25  
**Media:** air  
**Overall Output CF:** 2.7

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<th>Input Parameter</th>
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<th>Sensitivity (S)</th>
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<th>Input Confidence Factor (CF)</th>
<th>Output CF (due to this parameter)</th>
<th>Percent Contribution to Output Variance</th>
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<td>Emissions to Bulk Lower Air (kg/ly)</td>
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**Sorted by Sensitivity**

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<th>Input Confidence Factor (CF)</th>
<th>Output CF (due to this parameter)</th>
<th>Percent Contribution to Output Variance</th>
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Substance: BbF  
Region: 25  
Media: freshwater  
Overall Output CF: 5.3

| Rank | Input Parameter | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|----------------|--------|----------------|----|----------------|-----------------------------|--------------------------------------|
| 1    | 9 sediment deposition | 25 | -0.635662115 | 0.635662115 | 3 | 2.010425138 | 17.4356706 |
| 2    | Emissions to Bulk Lower Air (kg/ly) | 25 | 0.467402621 | 0.467402621 | 3 | 1.671120339 | 9.426686649 |
| 3    | rain scavenging ratio | 25 | 0.197249236 | 0.197249236 | 10 | 1.574866411 | 7.374950807 |
| 4    | 10 sediment resuspension | 25 | 0.367588690 | 0.367588690 | 3 | 1.497560511 | 5.830693009 |
| 5    | Soil Reaction half-life (h) | 25 | 0.359602138 | 0.359602138 | 3 | 1.494004406 | 5.586161372 |
| 6    | 1 air side air-fresh water MTC | 25 | 0.331230925 | 0.331230925 | 3 | 1.438922205 | 4.734184825 |
| 7    | Volume Fraction Particles in fresh water | 25 | 0.322396881 | 0.322396881 | 3 | 1.425024741 | 4.480503585 |
| 8    | Sediment Reaction half-life (h) | 25 | 0.320030396 | 0.320030396 | 3 | 1.421324703 | 4.419452354 |
| 9    | 12 soil solids runoff | 25 | 0.304633027 | 0.304633027 | 3 | 1.397484153 | 4.004423203 |
| 10   | Vegetation Reaction half-life (h) | 25 | 0.297305411 | 0.297305411 | 3 | 1.386265666 | 3.814202017 |
| 11   | Average fresh water sediment depth (cm) | 25 | -0.294529449 | 0.294529449 | 3 | 1.382529372 | 3.74320596 |
| 12   | Fresh Water Reaction half-life (h) | 25 | 0.282403510 | 0.282403510 | 3 | 1.364423355 | 3.451983663 |
| 13   | Lower air flow rate (m/3h) | 25 | 0.265583243 | 0.265583243 | 3.00 | 1.34 | 3.04 |
| 14   | Kow (not Log Kow) | 25 | -0.264271103 | 0.264271103 | 3 | 1.336870562 | 3.013598235 |
| 15   | 3 rain rate | 25 | 0.253432514 | 0.253432514 | 3 | 1.3210463 | 2.77473062 |

Sorted by Sensitivity

| Rank | Input Parameter | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|----------------|--------|----------------|----|----------------|-----------------------------|--------------------------------------|
| 1    | Volume Fraction Sediment pore water | 25 | 0.687924663 | 0.687924663 | 1.100000024 | 1.067763462 | 0.150994253 |
| 2    | 9 sediment deposition | 25 | -0.635662115 | 0.635662115 | 3 | 2.010425138 | 17.4356706 |
| 3    | % Soil covered by vegetation | 25 | -0.555044655 | 0.555044655 | 1.100000024 | 1.054225702 | 1.00053309 |
| 4    | Total Surface Area (km2) | 25 | -0.472752528 | 0.472752528 | 1 | 1 | 0 |
| 5    | Emissions to Bulk Lower Air (kg/ly) | 25 | 0.467402621 | 0.467402621 | 3 | 1.671120339 | 9.426686649 |
| 6    | Enthalpy of vaporization (from water to air) (J/m³) | 25 | 0.451569894 | 0.451569894 | 1.200000048 | 1.058915904 | 0.242339865 |
| 7    | Property Temperature (°C) | 25 | 0.436775252 | 0.436775252 | 1 | 1 | 0 |
| 8    | 10 sediment resuspension | 25 | 0.367588690 | 0.367588690 | 3 | 1.497560511 | 5.830693009 |
| 9    | Soil Reaction half-life (h) | 25 | 0.359602138 | 0.359602138 | 3 | 1.494004406 | 5.586161372 |
| 10   | Volume Fraction Water in vegetation | 25 | 0.359465976 | 0.359465976 | 1.100000024 | 1.034854454 | 0.041965405 |
| 11   | % Surface covered by fresh water | 25 | -0.336456848 | 0.336456848 | 1.100000024 | 1.032568367 | 0.3676969 |
| 12   | 1 air side air-fresh water MTC | 25 | 0.331230925 | 0.331230925 | 3 | 1.438922205 | 4.734184825 |
| 13   | Volume Fraction Particles in fresh water | 25 | 0.322396881 | 0.322396881 | 3 | 1.425024741 | 4.480503585 |
| 14   | Sediment Reaction half-life (h) | 25 | 0.320030396 | 0.320030396 | 3 | 1.421324703 | 4.419452354 |
| 15   | Average soil depth (cm) | 25 | -0.316664115 | 0.316664115 | 1.5 | 1.137003451 | 0.589388664 |

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Substance : BbF  
Region : 25  
Media  : sediment  
Overall Output CF : 5.7  

| Rank | Input Parameter                          | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------|--------|----------------|---------|----------------------------|-------------------------------------|----------------------------------------|
| 1    | Sediment Reaction half-life (h)          | 25     | 0.647421568    | 0.647421568 | 3 | 2.036866477 | 16.65429524 |
| 2    | Average fresh water sediment depth (cm)  | 25     | -0.622449479   | 0.622449479 | 3 | 1.984153462 | 15.39429756 |
| 3    | Emissions to Bulk Lower Air (kgf/y)      | 25     | 0.487402621    | 0.487402621 | 3 | 1.671120359 | 8.68028449  |
| 4    | rain scavenging ratio                    | 25     | 0.197249236    | 0.197249236 | 10 | 1.574886411 | 6.790860836 |
| 5    | 9 sediment deposition                    | 25     | 0.362943871    | 0.362943871 | 3 | 1.489938132 | 5.233962487 |
| 6    | Soil Reaction half-life (h)              | 25     | 0.359982138    | 0.359982138 | 3 | 1.484004406 | 5.143741696 |
| 7    | 1 air side air-fresh water MTC           | 25     | 0.331230925    | 0.331230925 | 3 | 1.439322205 | 4.359266573 |
| 8    | 12 soil solids runoff                    | 25     | 0.304633027    | 0.304633027 | 3 | 1.397484153 | 3.687275971 |
| 9    | Vegetation Reaction half-life (h)        | 25     | 0.297309541    | 0.297309541 | 3 | 1.365285666 | 3.512120157 |
| 10   | Fresh Water Reaction half-life (h)       | 25     | 0.282840351    | 0.282840351 | 3 | 1.36442335 | 3.178589217 |
| 11   | Lower air flow rate (m³/h)               | 26     | -0.265583248   | 0.265583248 | 3.00 | 1.34 | 2.60 |
| 12   | 3 rain rate                              | 25     | 0.253432514    | 0.253432514 | 3 | 1.3210463 | 2.551974351 |
| 13   | Kow (not Log Kow)                        | 25     | 0.237170695    | 0.237170695 | 3 | 1.29765807 | 2.23490435 |
| 14   | Air Reaction half-life (h)               | 25     | 0.218798289    | 0.218798289 | 3 | 1.217725308 | 1.902127017 |
| 15   | 10 sediment resuspension                 | 25     | -0.210213145   | 0.210213145 | 3 | 1.259787108 | 1.75578532 |

Sorted by Sensitivity

| Rank | Parameter                          | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------|--------|----------------|---------|----------------------------|-------------------------------------|----------------------------------------|
| 1    | Property Temperature (C)           | 25     | 0.776015808    | 0.776015808 | 1 | 1 | 0 |
| 2    | Sediment Reaction half-life (h)    | 25     | 0.647421568    | 0.647421568 | 3 | 2.036866477 | 16.65429524 |
| 3    | Average fresh water sediment depth (cm) | 25     | -0.622449479   | 0.622449479 | 3 | 1.984153462 | 15.39429756 |
| 4    | % Soil covered by vegetation       | 25     | -0.555044655   | 0.555044655 | 1.100000024 | 1.054325702 | 0.09212922 |
| 5    | density of sediment solids (7.2)   | 25     | -0.504353338   | 0.504353338 | 1.5 | 1.226809661 | 1.37670725 |
| 6    | Total Surface Area (m²)            | 25     | -0.472752026   | 0.472752026 | 1 | 1 | 0 |
| 7    | Emissions to Bulk Lower Air (kgf/y) | 25     | 0.467402621    | 0.467402621 | 3 | 1.671120359 | 8.68028449 |
| 8    | Enthalpy of vaporization (from water to air) (J/mol) | 25     | 0.451596894    | 0.451596894 | 1.200000048 | 1.06815094 | 0.22314592 |
| 9    | density of water (4,1)             | 25     | -0.40326265    | 0.40326265 | 1.049999952 | 1.01970076 | 0.012743917 |
| 10   | Summer mean temperature (oC)       | 25     | -0.399643672   | 0.399643672 | 1.100000024 | 1.038824846 | 0.047726541 |
| 11   | 9 sediment deposition               | 25     | 0.362943871    | 0.362943871 | 3 | 1.489938132 | 5.233962487 |
| 12   | Soil Reaction half-life (h)        | 25     | 0.359982138    | 0.359982138 | 3 | 1.484004406 | 5.143741696 |
| 13   | Volume Fraction Water in vegetation | 25     | 0.359465976    | 0.359465976 | 1.100000024 | 1.034564435 | 0.03864178 |
| 14   | % Surface covered by fresh water   | 25     | -0.336465848   | 0.336465848 | 1.100000024 | 1.032588367 | 0.033855055 |
| 15   | 1 air side air-fresh water MTC      | 25     | 0.331230925    | 0.331230925 | 3 | 1.439922205 | 4.359266573 |
| Rank | Input Parameter                          | Region | Sensitivity (S) | | | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|-----------------------------------------|--------|----------------|---|----------------|-----------------------------------|----------------------------------------|
| 1    | Soil Reaction half-life (h)             |        | 0.986480327    | 0.998480327 | 3               | 2.9622722275                     | 28.20687533                         |
| 2    | rain scavenging ratio                   |        | 0.46107351     | 0.461107351 | 10              | 2.891394506                      | 26.96456373                         |
| 3    | 3 rain rate                             | 25     | 0.539332879    | 0.593532879 | 3               | 1.202128476                      | 10.18060841                         |
| 4    | Emissions to Bulk Lower Air (kg/yr)     | 25     | 0.47090319     | 0.47090319  | 3               | 1.697162522                      | 6.628438421                         |
| 5    | Vegetation Reaction half-life (h)       |        | 0.372168778    | 0.372168778 | 3               | 1.505114828                      | 3.998766325                         |
| 6    | Average soil depth (cm)                 | 25     | -0.989455056   | 0.998455056 | 1.5             | 1.493600281                      | 3.849900579                         |
| 7    | Kow (not Log Kow)                       |        | 0.32448784     | 0.32448784  | 3               | 1.428300203                      | 3.03901165                          |
| 8    | density of soil solids (6,3)            | 25     | -0.798932526   | 0.798932526 | 1.5             | 1.382564862                      | 2.51005165                          |
| 9    | Lower air flow rate (m/3hr)             | 25     | -0.261764881   | 0.2618      | 3.00            | 1.36                             | 0.29                                 |
| 10   | Volume Fraction Particles in lower air  | 25     | 0.206797087    | 0.206797087 | 3               | 1.340585634                      | 2.05499064                          |
| 11   | Air Reaction half-life (h)              | 25     | 0.249496157    | 0.249496157 | 3               | 1.308771361                      | 1.73216626                          |
| 12   | Lower air flow rate (m/3hr)             | 26     | 0.196372048    | 0.1964      | 3.00            | 1.24                             | 0.11                                 |
| 13   | Emissions to Bulk Lower Air (kg/yr)     | 24     | 0.185847476    | 0.185847476 | 3               | 1.230569093                      | 1.02960512                          |
| 14   | Enthalpy of vaporization (from water to air) (J/mol) | 25 | 1.025915575 | 1.025915575  | 1.2000000084 | 1.205634277 | 0.836871729 |
| 15   | Emissions to Bulk Lower Air (kg/yr)     | 26     | 0.160059408    | 0.160059408 | 3               | 1.204098005                      | 0.82513886                          |

Sorted by Sensitivity:

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Overall Output CF : 7.7
| Rank | Input Parameter                              | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|---------------------------------------------|--------|----------------|-----|----------------|-------------------------------------|----------------------------------------|
| 1    | Emissions to Bulk Lower Air (kg/y)          | 25     | 0.552421358    | 0.552421358 | 3    | 1.834729194      | 41.74874308                            |
| 2    | Lower air flow rate (m3/h)                 | 25     | -0.298322557   | 0.2983   | 3.00 | 1.39             | 12.18                                 |
| 3    | 4 aerosol deposition                       | 25     | -0.280556094   | 0.280556094 | 3    | 1.361003605      | 10.7816978                             |
| 4    | Lower air flow rate (m3/h)                 | 26     | 0.217133076    | 0.2171   | 3.00 | 1.27             | 8.45                                  |
| 5    | 19 upper-lower air mixing MTC              | 25     | -0.086657834   | 0.086657834 | 10   | 1.226472564      | 4.72366607                            |
| 6    | Emissions to Bulk Lower Air (kg/y)         | 26     | 0.180576882    | 0.180576882 | 3    | 1.219430543      | 4.460944106                            |
| 7    | Air Reaction half-life (h)                 |        | 0.174652645    | 0.174652645 | 3    | 1.211518724      | 4.17304257                            |
| 8    | Emissions to Bulk Lower Air (kg/y)         | 24     | 0.170514106    | 0.170514106 | 3    | 1.206028372      | 3.977618329                            |
| 9    | rain scavenging ratio                      | 25     | -0.076539554   | 0.076539554 | 10   | 1.19272289       | 3.520601007                           |
| 10   | Lower air flow rate (m3/h)                 | 24     | 0.150979453    | 0.1510   | 3.00 | 1.18             | 3.12                                  |
| 11   | 3 rain rate                                | 25     | -0.080316129   | 0.080316129 | 3    | 1.092246175      | 0.882486403                           |
| 12   | Lower air flow rate (m3/h)                 | 26     | -0.071193072   | 0.0712   | 3.00 | 1.08             | 0.69                                  |
| 13   | Lower air flow rate (m3/h)                 | 25     | -0.064893374   | 0.0649   | 3.00 | 1.07             | 0.58                                  |
| 14   | 4 aerosol deposition                       | 24     | -0.056090026   | 0.056090026 | 3    | 1.065869832      | 0.461642337                           |
| 15   | 4 aerosol deposition                       | 26     | -0.057902399   | 0.057902399 | 3    | 1.065679141      | 0.458664991                           |

Sorted by Sensitivity

| Rank | Input Parameter                              | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|---------------------------------------------|--------|----------------|-----|----------------|-------------------------------------|----------------------------------------|
| 1    | Total Surface Area (km2)                    | 25     | -0.560198496   | 0.560198496 | 1    | 1                  | 0                                     |
| 2    | Emissions to Bulk Lower Air (kg/y)          | 25     | 0.552421358    | 0.552421358 | 3    | 1.834729194      | 41.74874308                            |
| 3    | Lower air flow rate (m3/h)                 | 26     | -0.298322557   | 0.2983   | 3.00 | 1.39             | 12.18                                 |
| 4    | 4 aerosol deposition                       | 25     | -0.280556094   | 0.280556094 | 3    | 1.361003605      | 10.7816978                             |
| 5    | Lower air flow rate (m3/h)                 | 25     | 0.217133076    | 0.2171   | 3.00 | 1.27             | 8.45                                  |
| 6    | Emissions to Bulk Lower Air (kg/y)         | 26     | 0.180576882    | 0.180576882 | 3    | 1.219430543      | 4.460944106                            |
| 7    | Air Reaction half-life (h)                 |        | 0.174652645    | 0.174652645 | 3    | 1.211518724      | 4.17304257                            |
| 8    | Emissions to Bulk Lower Air (kg/y)         | 24     | 0.170514106    | 0.170514106 | 3    | 1.206028372      | 3.977618329                            |
| 9    | rain scavenging ratio                      | 25     | -0.076539554   | 0.076539554 | 10   | 1.19272289       | 3.520601007                           |
| 10   | Lower air flow rate (m3/h)                 | 24     | 0.150979453    | 0.1510   | 3.00 | 1.18             | 3.12                                  |
| 11   | 3 rain rate                                | 25     | -0.080316129   | 0.080316129 | 3    | 1.092246175      | 0.882486403                           |
| 12   | Lower air flow rate (m3/h)                 | 26     | -0.071193072   | 0.0712   | 3.00 | 1.08             | 0.69                                  |
| 13   | Lower air flow rate (m3/h)                 | 25     | -0.064893374   | 0.0649   | 3.00 | 1.07             | 0.58                                  |
| 14   | 4 aerosol deposition                       | 24     | -0.056090026   | 0.056090026 | 3    | 1.065869832      | 0.461642337                           |
| 15   | 4 aerosol deposition                       | 26     | -0.057902399   | 0.057902399 | 3    | 1.065679141      | 0.458664991                           |
Substance : IP  
Region : 25  
Media : freshwater  
Overall Output CF : 7.7

| Rank | Input Parameter                          | Region | Sensitivity (S) | | S | | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------|--------|----------------|----|----|-----------------------------|-------------------------------------|----------------------------------------|
| 1    | rain scavenging ratio                    | 25     | 0.397389686    | 0.397389686 | 10 | 2.496384002 | 20.08511905                          |
| 2    | 9 sediment deposition                     | 25     | -0.77563003    | 0.77563003  | 3  | 2.346222384 | 17.41870227                          |
| 3    | Volume Fraction Particles in fresh water | 25     | 0.659670044    | 0.659670044 | 3  | 2.064156394 | 12.5947018                           |
| 4    | Emissions to Bulk Lower Air (kg/y)       | 25     | 0.489924265    | 0.489924265 | 3  | 1.712983896 | 6.946594567                          |
| 5    | Soil Reaction half-life (h)              |        | 0.477419668    | 0.477419668 | 3  | 1.689612334 | 6.593272685                          |
| 6    | 10 sediment resuspension                 | 25     | 0.451092636    | 0.451092636 | 3  | 1.641443296 | 5.891559001                          |
| 7    | 12 soil solids runoff                    | 25     | 0.437747399    | 0.437747399 | 3  | 1.617564217 | 5.548134459                          |
| 8    | 3 rain rate                              | 25     | 0.41311099     | 0.41311099  | 3  | 1.574358396 | 4.941176448                          |
| 9    | Sediment Reaction half-life (h)          |        | 0.379878998    | 0.379878998 | 3  | 1.517918116 | 4.176306856                          |
| 10   | Average fresh water sediment depth (cm)  |        | -0.357381688   | 0.357381688 | 3  | 1.480861354 | 3.697966888                          |
| 11   | Lower air flow rate (m3/h)               | 25     | -0.265527259   | 0.265527259 | 3  | 1.32         | 1.89                                 |
| 12   | Emissions to Bulk Lower Air (kg/y)       | 26     | 0.208669458    | 0.208669458 | 3  | 1.257652428 | 1.260713871                          |
| 13   | Air Reaction half-life (h)               |        | 0.202750473    | 0.202750473 | 3  | 1.249500662 | 1.192072019                          |
| 14   | Fresh Water Reaction half-life (h)       |        | 0.189185913    | 0.189185913 | 3  | 1.231018615 | 1.036371865                          |
| 15   | Lower air flow rate (m3/h)               | 26     | 0.186002463    | 0.186002463 | 3  | 1.23         | 1.00                                 |

Sorted by Sensitivity

1. % Soil covered by vegetation  
2. Volume Fraction Sediment pore water  
3. 9 sediment deposition  
4. Volume Fraction Particles in fresh water  
5. Emissions to Bulk Lower Air (kg/y)  
6. Total Surface Area (km²)  
7. Soil Reaction half-life (h)  
8. % Surface covered by fresh water  
9. 10 sediment resuspension  
10. Average soil depth (cm)  
11. 12 soil solids runoff  
12. 3 rain rate  
13. rain scavenging ratio  
14. Sediment Reaction half-life (h)  
15. Average fresh water sediment depth (cm)
| Rank | Input Parameter | Region | Sensitivity (S) | | | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|-----------------|--------|----------------|---|-----------------|-----------------------------------|--------------------------------------|
| 1    | rain scavenging ratio | 25 | 0.367389666 | 0.307380666 | 10 | 2.49634002 | 22.666811568 |
| 2    | Sediment Reaction half-life (h) | 25 | 0.706401659 | 0.706401659 | 3 | 2.18076668 | 16.4438802 |
| 3    | Average fresh water sediment depth (cm) | 25 | -0.687477152 | 0.687477152 | 3 | 2.128187859 | 15.44299025 |
| 4    | Emissions to Bulk Lower Air (kg/ly) | 25 | 0.458924265 | 0.49624265 | 3 | 1.712683396 | 7.842282246 |
| 5    | Soil Reaction half-life (h) | 25 | 0.477419668 | 0.477419668 | 3 | 1.89612334 | 7.447350671 |
| 6    | 12 soil solids runoff | 25 | 0.437747939 | 0.437747939 | 3 | 1.671554217 | 6.26127935 |
| 7    | 3 rain rate | 25 | 0.41311009 | 0.41311009 | 3 | 1.574358396 | 5.76304303 |
| 8    | Lower air flow rate (m3h) | 25 26 | -0.255527259 | 0.2555 | 3.00 | 1.32 | 2.13 |
| 9    | 9 sediment deposition | 25 | 0.24201489 | 0.24201489 | 3 | 1.279034519 | 1.639715983 |
| 10   | Emissions to Bulk Lower Air (kg/ly) | 26 | 0.20866458 | 0.20866458 | 3 | 1.257652428 | 1.422763234 |
| 11   | Air Reaction half-life (h) | 25 | 0.202750473 | 0.202750473 | 3 | 1.249500862 | 1.343193588 |
| 12   | Volume Fraction Particles in fresh water | 25 | -0.190661544 | 0.190661544 | 3 | 1.233268646 | 1.192087944 |
| 13   | Fresh Water Reaction half-life (h) | 25 | 0.189155913 | 0.189155913 | 3 | 1.231018615 | 1.194705661 |
| 14   | density of sediment solids (7.2) | 25 | -0.506842147 | 0.506842147 | 1.5 | 1.228147339 | 1.143347833 |
| 15   | Lower air flow rate (m3h) | 26 25 | 0.186002453 | 0.1860 | 3.00 | 1.23 | 1.13 |

| Rank | Input Parameter | Region | Sensitivity (S) | | | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|-----------------|--------|----------------|---|-----------------|-----------------------------------|--------------------------------------|
| 1    | % Soil covered by vegetation | 25 | -0.993784115 | 0.993784115 | 1.100000024 | 1.099384502 | 0.242878365 |
| 2    | Sediment Reaction half-life (h) | 25 | 0.706401659 | 0.706401659 | 3 | 2.18076668 | 16.4438802 |
| 3    | Average fresh water sediment depth (cm) | 25 | -0.687477152 | 0.687477152 | 3 | 2.128187859 | 15.44299025 |
| 4    | density of sediment solids (7.2) | 25 | -0.506842147 | 0.506842147 | 1.5 | 1.228147339 | 1.143347833 |
| 5    | density of water (4.1) | 25 | -0.49286439 | 0.49286439 | 1.04999952 | 1.02434447 | 0.015662448 |
| 6    | Emissions to Bulk Lower Air (kg/ly) | 25 | 0.49024265 | 0.49024265 | 3 | 1.712683396 | 7.842282246 |
| 7    | Total Surface Area (km2) | 25 | -0.473835596 | 0.473835596 | 1 | 1 | 0 |
| 8    | Soil Reaction half-life (h) | 25 | 0.477419668 | 0.477419668 | 3 | 1.89612334 | 7.447350671 |
| 9    | % Surface covered by fresh water | 25 | -0.460289026 | 0.460289026 | 1.100000024 | 1.04846767 | 0.05103389 |
| 10   | Average soil depth (cm) | 25 | -0.436312213 | 0.436312213 | 1.5 | 1.195217893 | 0.8692932 |
| 11   | 12 soil solids runoff | 25 | 0.457374399 | 0.457374399 | 3 | 1.67554217 | 6.25127935 |
| 12   | 3 rain rate | 25 | 0.41311009 | 0.41311009 | 3 | 1.574358396 | 5.76304303 |
| 13   | rain scavenging ratio | 25 | 0.397380666 | 0.397380666 | 10 | 2.49634002 | 22.666811568 |
| 14   | Volume Fraction Water in soil | 25 | 0.26411022 | 0.26411022 | 1.100000024 | 1.025491868 | 0.017154365 |
| 15   | Lower air flow rate (m3h) | 26 25 | -0.255527259 | 0.2555 | 3.00 | 1.32 | 2.13 |
| Rank | Input Parameter                                      | Region   | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------------------|----------|-----------------|----|-----------------------------|----------------------------------------|----------------------------------------|
| 1    | rain scavenging ratio                               | 25       | 0.69060367      | 0.69060367 | 10                           | 4.904594056                          | 47.50248515                           |
| 2    | Soil Reaction half-life (h)                         | 25       | 0.989219375     | 0.989219375 | 3                             | 2.9646784                            | 22.18717667                           |
| 3    | 3 rain rate                                         | 25       | 0.718266251     | 0.718266251 | 3                             | 2.201405742                          | 11.69735781                           |
| 4    | Emissions to Bulk Lower Air (kg/y)                  | 25       | 0.499443962     | 0.499443962 | 3                             | 1.726245369                          | 5.599273959                           |
| 5    | Average soil depth (cm)                             | 25       | -0.990200871    | 0.990200871 | 1.5                           | 1.494065665                          | 3.028224782                           |
| 6    | density of soil solids (6,3)                        | 25       | -0.799705213    | 0.799705213 | 1.5                           | 1.382996554                          | 1.97512587                           |
| 7    | Lower air flow rate (m^3/h)                         | 25       | -0.265401765    | 0.2654      | 3.00                          | 1.34                                | 1.60                                  |
| 8    | Air Reaction half-life (h)                          | 25       | 0.219839138     | 0.219839138 | 3                             | 1.273180345                          | 1.095788655                           |
| 9    | % Soil covered by vegetation                        | 25       | -2.23802151     | 2.23802151  | 1.1000000024                  | 1.237763897                          | 0.854742376                           |
| 10   | Lower air flow rate (m^3/h)                         | 26       | 0.19316409      | 0.1932      | 3.00                          | 1.24                                | 0.85                                  |
| 11   | Emissions to Bulk Lower Air (kg/y)                  | 24       | 0.192364238     | 0.192364238 | 3                             | 1.235324534                          | 0.839006887                           |
| 12   | Emissions to Bulk Lower Air (kg/y)                  | 26       | 0.178246693     | 0.178246693 | 3                             | 1.261361285                          | 0.720369615                           |
| 13   | Upper air flow rate (m^3/h)                         | 25       | -0.123971806    | 0.1294      | 3.00                          | 1.15                                | 0.38                                  |
| 14   | Lower air flow rate (m^3/h)                         | 24       | 0.121365507     | 0.1214      | 3.00                          | 1.14                                | 0.33                                  |
| 15   | 19 upper-lower air mixing MTC                       | 25       | 0.042679585     | 0.042679585 | 10                            | 1.103264351                          | 0.184126077                           |

Sorted by Sensitivity

| Rank | Input Parameter                                      | Region   | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------------------|----------|-----------------|----|-----------------------------|----------------------------------------|----------------------------------------|
| 1    | % Soil covered by vegetation                        | 25       | -2.23802151     | 2.23802151  | 1.1000000024                  | 1.237763897                          | 0.854742376                           |
| 2    | Average soil depth (cm)                              | 25       | -0.990200871    | 0.990200871 | 1.5                           | 1.494065665                          | 3.028224782                           |
| 3    | Soil Reaction half-life (h)                          | 25       | 0.989219375     | 0.989219375 | 3                             | 2.9646784                            | 22.18717667                           |
| 4    | density of soil solids (6,3)                         | 25       | -0.799705213    | 0.799705213 | 1.5                           | 1.382996554                          | 1.97512587                           |
| 5    | 3 rain rate                                         | 25       | 0.718266251     | 0.718266251 | 3                             | 2.201405742                          | 11.69735781                           |
| 6    | rain scavenging ratio                               | 25       | 0.69060367      | 0.69060367 | 3                             | 1.564498662                          | 22.18717667                           |
| 7    | Emissions to Bulk Lower Air (kg/y)                  | 25       | 0.499443962     | 0.499443962 | 3                             | 1.726245369                          | 5.599273959                           |
| 8    | Total Surface Area (km^2)                           | 25       | -0.51055685     | 0.51055685  | 1                             | 1.00                                | 1.00                                  |
| 9    | Volume Fraction Air in soil                         | 25       | 0.315862105     | 0.315862105 | 1.1000000024                  | 1.030562515                          | 0.017025574                           |
| 10   | Volume Fraction Water in soil                       | 25       | 0.274076441     | 0.274076441 | 1.1000000024                  | 1.064666455                          | 0.012818879                           |
| 11   | Lower air flow rate (m^3/h)                         | 25       | -0.265401765    | 0.2654      | 3.00                          | 1.34                                | 1.60                                  |
| 12   | Air Reaction half-life (h)                          | 25       | 0.219839138     | 0.219839138 | 3                             | 1.273180345                          | 1.095788655                           |
| 13   | density of water (4,1)                               | 25       | -0.199015349    | 0.199015349 | 1.049999852                   | 1.009801618                          | 0.001787245                           |
| 14   | Lower air flow rate (m^3/h)                         | 25       | 0.192364238     | 0.192364238 | 3                             | 1.235324534                          | 0.839006887                           |
| Rank | Input Parameter                                      | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|-----------------------------------------------------|--------|----------------|---|----------------|-------------------------------------|----------------------------------------|
| 1    | Emissions to Bulk Lower Air (kg/y)                  | 54     | 0.682347257    | 0.682347257 | 3              | 2.116227626 | 30.68975214 |
| 2    | Lower air flow rate (m³/h)                          | 54     | 0.644636922    | 0.6446       | 3.00           | 2.03                  | 27.37          |
| 3    | Lower air flow rate (m³/h)                          | 30     | 0.479213313    | 0.4792       | 3.00           | 1.69                  | 15.13          |
| 4    | Enthalpy of vaporization (from water to air) (J/mol) |        | -1.338095654   | 1.338095654  | 1.2000000048   | 1.276298723 | 3.248244708   |
| 5    | Aqueous solubility (g/m³)                           |        | -0.593217239   | 0.593217239  | 1.5            | 1.271921681 | 3.157408938   |
| 6    | Vapor pressure (Pa)                                 |        | 0.592096698    | 0.592096698  | 1.5            | 1.271343922 | 3.14546166   |
| 7    | 19 upper-lower air mixing MTC                       | 54     | -0.10145601    | 0.1015       | 10.00          | 1.26                  | 2.98           |
| 8    | Lower air flow rate (m³/h)                          | 29     | 0.187324262    | 0.1873       | 3.00           | 1.23                  | 2.31           |
| 9    | Kow (not Log Kow)                                   | 29     | -0.17484153    | 0.17484153   | 3              | 1.211771155 | 2.01605564   |
| 10   | 3 rain rate                                         | 30     | 0.142035134    | 0.142035134  | 3              | 1.168874781 | 1.3285249    |
| 11   | Lower air flow rate (m³/h)                          | 30     | -0.136228746   | 0.1369       | 3.00           | 1.16                  | 1.24           |
| 12   | Lower air flow rate (m³/h)                          | 54     | -0.102744321   | 0.1027       | 3.00           | 1.12                  | 0.70           |
| 13   | Vegetation Reaction halftime (h)                    |        | 0.098349103    | 0.098349103  | 3              | 1.115325338 | 0.65041909   |
| 14   | Lower air flow rate (m³/h)                          | 30     | -0.090252571   | 0.0903       | 3.00           | 1.10                  | 0.54           |
| 15   | Volume Frac (Pseudo)Octanol in vegetation flesh     | 54     | -0.080158744   | 0.080158744  | 3              | 1.092067335 | 0.423240296 |

Sorted by Sensitivity

| Rank | Input Parameter                                      | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|-----------------------------------------------------|--------|----------------|---|----------------|-------------------------------------|----------------------------------------|
| 1    | Property Temperature (C)                            |        | -1.995366596   | 1.995366596 | 1              | 1                                  | 1                                     |
| 2    | Enthalpy of vaporization (from water to air) (J/mol)|        | -1.338095654   | 1.338095654  | 1.2000000048   | 1.276298723 | 3.248244708   |
| 3    | Emissions to Bulk Lower Air (kg/y)                  | 54     | 0.682347257    | 0.682347257 | 3              | 2.116227626 | 30.68975214 |
| 4    | Lower air flow rate (m³/h)                          | 54     | 0.644636922    | 0.6446       | 3.00           | 2.03                  | 27.37          |
| 5    | Aqueous solubility (g/m³)                           |        | -0.593217239   | 0.593217239  | 1.5            | 1.271921681 | 3.157408938   |
| 6    | Molar Mass (g/mol)                                  |        | 0.592165529    | 0.592165529  | 1              | 1                                  | 0                                     |
| 7    | Vapor pressure (Pa)                                 |        | 0.592096698    | 0.592096698  | 1.5            | 1.271343922 | 3.14546166   |
| 8    | Lower air flow rate (m³/h)                          | 30     | -0.479213313   | 0.4792       | 3.00           | 1.69                  | 15.13          |
| 9    | Total Surface Area (km²)                            | 54     | -0.270105846   | 0.270105846  | 1              | 1                                  | 0                                     |
| 10   | Volume Fraction Water in vegetation                | 54     | 0.265162258    | 0.265162258  | 1.100000024    | 1.025594739 | 0.034857707 |
| 11   | Summer mean temperature (°C)                        | 30     | 0.25239919     | 0.25239919   | 1.100000024    | 1.024625283 | 0.03297575   |
| 12   | Total Surface Area (km²)                            | 30     | -0.218414265   | 0.218414265  | 1              | 1                                  | 0                                     |
| 13   | Summer mean temperature (°C)                        | 54     | 0.206976549    | 0.206976549  | 1.100000024    | 1.019835296 | 0.021053761 |
| 14   | Lower air flow rate (m³/h)                          | 30     | 0.18574262     | 0.1873       | 3.00           | 1.23                  | 2.31           |
| 15   | Kow (not Log Kow)                                   | 54     | -0.17484153    | 0.17484153   | 3              | 1.211771155 | 2.01605564   |
| Rank | Input Parameter                          | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|----------------------------------------|--------|----------------|---|-----------------|----------------------------------|----------------------------------------|
| 1    | Fresh Water Reaction half-life (h)     |        | 0.850621804    | 0.850621804 | 3               | 2.545949251                       | 18.63948427                           |
| 2    | Soil Reaction half-life (h)            |        | 0.834442556    | 0.834442556 | 3               | 2.501113935                       | 17.93745123                           |
| 3    | Kow (not Log Kow)                     |        | -0.758202088   | 0.758202088 | 3               | 2.300155789                       | 14.80941262                           |
| 4    | 11 soil water runoff                  | 25     | 0.63551506      | 0.63551506  | 3               | 2.010100367                       | 10.40429274                          |
| 5    | Emissions to Bulk Lower Air (kg/y)     | 24     | 0.55350491      | 0.55350491  | 3               | 1.836914563                       | 7.802304368                          |
| 6    | Lower air flow rate (m³/h)            | 24, 25 | 0.531773915     | 0.5318      | 3.00            | 1.79                              | 7.28                                  |
| 7    | 3 rain rate                           | 25     | 0.505447406     | 0.505447406 | 3               | 1.742447405                       | 6.581317081                          |
| 8    | Average fresh water depth (m)         | 25     | -0.77535535     | 0.77535535  | 1.5             | 1.369409385                       | 2.10950479                           |
| 9    | Lower air flow rate (m³/h)            | 25, 26 | -0.275041604    | 0.2750      | 3.00            | 1.35                              | 1.95                                  |
| 10   | Average soil depth (cm)               | 25     | -0.734877296    | 0.734877296 | 1.5             | 1.34711747                       | 1.884997318                          |
| 11   | Emissions to Bulk Lower Air (kg/y)     | 23     | 0.230638279     | 0.230638279 | 3               | 1.283375403                       | 1.370325206                          |
| 12   | Fraction OC Soil solids               | 25     | -0.596671705    | 0.596671705 | 1.5             | 1.273704467                       | 1.249251349                          |
| 13   | density of soil solids (6,3)          | 25     | -0.596642921    | 0.596642921 | 1.5             | 1.273688901                       | 1.24913002                           |
| 14   | 3 rain rate                           | 24     | -0.206811258    | 0.206811258 | 3               | 1.259230102                       | 1.134014081                          |
| 15   | Fresh water flow rate (m³/h)          | 25, 16 | -0.206889457    | 0.2009      | 3.00            | 1.25                              | 1.04                                  |

Sorted by Sensitivity

| Rank | Input Parameter                          | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|----------------------------------------|--------|----------------|---|-----------------|----------------------------------|----------------------------------------|
| 1    | Fresh Water Reaction half-life (h)     |        | 0.850621804    | 0.850621804 | 3               | 2.545949251                       | 18.63948427                           |
| 2    | Soil Reaction half-life (h)            |        | 0.834442556    | 0.834442556 | 3               | 2.501113935                       | 17.93745123                           |
| 3    | Kow (not Log Kow)                     |        | -0.758202088   | 0.758202088 | 3               | 2.300155789                       | 14.80941262                           |
| 4    | 11 soil water runoff                  |        | 0.63551506      | 0.63551506  | 3               | 2.010100367                       | 10.40429274                          |
| 5    | Emissions to Bulk Lower Air (kg/y)     |        | 0.55350491      | 0.55350491  | 3               | 1.836914563                       | 7.802304368                          |
| 6    | Lower air flow rate (m³/h)            |        | 0.531773915     | 0.5318      | 3.00            | 1.79                              | 7.28                                  |
| 7    | 3 rain rate                           |        | 0.505447406     | 0.505447406 | 3               | 1.742447405                       | 6.581317081                          |
| 8    | Average fresh water depth (m)         |        | -0.77535535     | 0.77535535  | 1.5             | 1.369409385                       | 2.10950479                           |
| 9    | Lower air flow rate (m³/h)            |        | -0.275041604    | 0.2750      | 3.00            | 1.35                              | 1.95                                  |
| 10   | Average soil depth (cm)               |        | -0.734877296    | 0.734877296 | 1.5             | 1.34711747                       | 1.884997318                          |
| 11   | Emissions to Bulk Lower Air (kg/y)     |        | 0.230638279     | 0.230638279 | 3               | 1.283375403                       | 1.370325206                          |
| 12   | Fraction OC Soil solids               |        | -0.596671705    | 0.596671705 | 1.5             | 1.273704467                       | 1.249251349                          |
| 13   | density of soil solids (6,3)          |        | -0.596642921    | 0.596642921 | 1.5             | 1.273688901                       | 1.24913002                           |
| 14   | 3 rain rate                           |        | -0.206811258    | 0.206811258 | 3               | 1.259230102                       | 1.134014081                          |
| 15   | Fresh water flow rate (m³/h)          |        | -0.206889457    | 0.2009      | 3.00            | 1.25                              | 1.04                                  |
### Table of Sensitivity Analysis

| Rank | Input Parameter                          | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------|--------|----------------|---|-----------------------------|------------------------------------|----------------------------------------|
| 1    | 9 sediment deposition                    | 25     | 0.875336288     | 0.875336288 | 3                           | 2.616022941                         | 15.48124539                           |
| 2    | Fresh Water Reaction half-life (h)       |        | 0.850621804     | 0.850621804 | 3                           | 2.545949251                         | 14.61938321                           |
| 3    | Soil Reaction half-life (h)              |        | 0.834449256     | 0.834449256 | 3                           | 2.501113935                         | 14.06876229                           |
| 4    | 11 soil water runoff                     | 25     | 0.63551506      | 0.63551506  | 3                           | 2.010100367                         | 8.1603                                |
| 5    | Kow (not Log Kow)                        |        | 0.583662445     | 0.583662445 | 3                           | 1.836914563                         | 6.88302789                            |
| 6    | Emissions to Bulk Lower Air (kg/y)       | 24     | 0.55350491      | 0.55350491  | 3                           | 1.836914563                         | 6.1901188                             |
| 7    | Lower air flow rate (m3/h)               | 24     | 0.531773915     | 0.531773915 | 3.00                        | 1.79                                | 5.71                                  |
| 8    | 3 rain rate                              | 25     | 0.505447406     | 0.505447406 | 3                           | 1.742447495                         | 5.16188081                            |
| 9    | 8 sediment-water diffusion MTC           | 25     | -0.349498751    | -0.349498751| 3                           | 1.458092036                         | 2.4680121                             |
| 10   | Fraction OC Particles in fresh water     | 25     | 0.867196519     | 0.867196519 | 1.5                         | 1.421364783                         | 2.69703569                            |
| 11   | density of water particles (4,2)         | 25     | 0.867146512     | 0.867146512 | 1.5                         | 1.421336021                         | 2.06945351                            |
| 12   | 10 sediment resuspension                 | 25     | -0.305967538    | 0.305967538 | 3                           | 1.399534523                         | 1.89150168                            |
| 13   | Average fresh water depth (m)            | 25     | -0.77535535     | 0.77535535  | 1.5                         | 1.369409385                         | 1.65453917                            |
| 14   | Lower air flow rate (m3/h)               | 25     | -0.275041604    | 0.275041604 | 3.00                        | 1.45                                | 1.35                                  |
| 15   | Average soil depth (cm)                  | 25     | -0.734877296    | 0.734877296 | 1.5                         | 1.34711747                         | 1.486290692                           |

### Sorted by Sensitivity

| Rank | Input Parameter                          | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------|--------|----------------|---|-----------------------------|------------------------------------|----------------------------------------|
| 1    | Volume Fraction Sediment pore water      | 25     | -1.183016915    | 1.183016915 | 1.100000024 | 1.119356088 | 0.212827531                     |
| 2    | Property Temperature (C)                 |        | 0.929664761     | 0.929664761 | 1.00           | 0.929664761 | 0.212827531                     |
| 3    | 9 sediment deposition                    | 25     | 0.875336288     | 0.875336288 | 3                           | 2.616022941                         | 15.48124539                           |
| 4    | Fraction OC Particles in fresh water     | 25     | 0.867196519     | 0.867196519 | 1.5                         | 1.421364783                         | 2.69703569                            |
| 5    | density of water particles (4,2)         | 25     | 0.867146512     | 0.867146512 | 1.5                         | 1.421336021                         | 2.06945351                            |
| 6    | Fresh Water Reaction half-life (h)       |        | 0.834449256     | 0.834449256 | 3                           | 2.051113935                         | 14.06876229                           |
| 7    | Soil Reaction half-life (h)              |        | 0.834449256     | 0.834449256 | 3                           | 2.051113935                         | 14.06876229                           |
| 8    | Average fresh water depth (m)            | 25     | -0.77535535     | 0.77535535  | 1.5                         | 1.369409385                         | 1.65453917                            |
| 9    | Average soil depth (cm)                  | 25     | -0.734877296    | 0.734877296 | 1.5                         | 1.34711747                         | 1.486290692                           |
| 10   | Summer mean temperature (oC)             | 25     | -0.7295118      | 0.7295118   | 1.100000024 | 1.072004131 | 0.08093186                      |
| 11   | % Surface covered by fresh water         | 25     | -0.720282368    | 0.720282368 | 1.100000024 | 1.071061643 | 0.07889564                      |
| 12   | 11 soil water runoff                     | 25     | 0.63551506      | 0.63551506  | 3                           | 2.010100367                         | 8.1603                                |
| 13   | Fraction OC Soil solids                  | 25     | -0.596671705    | 0.596671705 | 1.5                         | 1.273704467                         | 0.97981705                           |
| 14   | density of soil solids (6,3)             | 25     | -0.596642921    | 0.596642921 | 1.5                         | 1.273704467                         | 0.97981705                           |
| 15   | Kow (not Log Kow)                        |        | 0.583662445     | 0.583662445 | 3                           | 1.836914563                         | 6.88302789                            |
| Rank | Input Parameter                                      | Region Distribution Region | Sensitivity (S)   | | | | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------------------|----------------------------|-------------------|---|---|-----------------------------|----------------------------------------|----------------------------------------|
| 1    | Soil Reaction half-life (h)                         |                            | 0.912865546       | 0.912865546       | 3  | 2.726106282                | 34.82110679                            |                                         |
| 2    | 3 rain rate                                         | 25                         | 0.604710088       | 0.604710088       | 3  | 1.943211338                | 15.28033607                            |                                         |
| 3    | Emissions to Bulk Lower Air (kg/ly)                 | 24                         | 0.574096896       | 0.574096896       | 3  | 1.875893333                | 13.77247695                            |                                         |
| 4    | Lower air flow rate (m3/h)                          | 24 25                      | 0.556186479       | 0.556186479       | 3.00| 1.85                      |                                         |                                         |
| 5    | Lower air flow rate (m3/h)                          | 25 26                      | -0.34444435       | 0.34444435        | 3.00| 1.46                      |                                         |                                         |
| 6    | Average soil depth (cm)                             | 25                         | -0.901339355      | 0.901339355       | 1.5| 1.441179188                | 4.62416371                             |                                         |
| 7    | density of soil solids (6.3)                        | 25                         | -0.710073983      | 0.710073983       | 1.5| 1.333333333                | 2.86988077                             |                                         |
| 8    | Emissions to Bulk Lower Air (kg/ly)                 | 23                         | 0.236713055       | 0.236713055       | 3  | 1.29700255                 | 2.34143282                             |                                         |
| 9    | 3 rain rate                                         | 24                         | -0.217488904      | 0.217488904       | 3  | 1.26897236                 |                                         |                                         |
| 10   | Lower air flow rate (m3/h)                          | 23 24                      | 0.193676688       | 0.193676688       | 3.00| 1.24                      |                                         |                                         |
| 11   | Entropy of evaporation (from water to air) (J/mol)  |                            | 0.534528374       | 0.534528374       | 1.200000048 | 1.00236301 | 0.32826894               |                                         |
| 12   | 19 upper-lower air mixing MTC                       | 24                         | -0.041595814      | 0.041595814       | 10 | 1.00514613                 | 3.17599785                             |                                         |
| 13   | Lower air flow rate (m3/h)                          | 24 17                      | -0.059989154      | 0.059989154       | 3.00| 1.10                      |                                         |                                         |
| 14   | Upper air flow rate (m3/h)                          | 25 26                      | -0.078744475      | 0.078744475       | 3.00| 1.09                      |                                         |                                         |
| 15   | 19 upper-lower air mixing MTC                       | 25                         | -0.03576586       | 0.03576586        | 10 | 1.08584006                 | 2.34160295                             |                                         |

Sorted by Sensitivity

| Rank | Input Parameter                                      | Region Distribution Region | Sensitivity (S)   | | | | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------------------|----------------------------|-------------------|---|---|-----------------------------|----------------------------------------|----------------------------------------|
| 1    | Soil Reaction half-life (h)                         |                            | 0.912865546       | 0.912865546       | 3  | 2.726106282                | 34.82110679                            |                                         |
| 2    | Average soil depth (cm)                             | 25                         | 0.901339355       | 0.901339355       | 1.5| 1.441179188                | 4.62416371                             |                                         |
| 3    | density of soil solids (6.3)                        | 25                         | -0.710073983      | 0.710073983       | 1.5| 1.333333333                | 2.86988077                             |                                         |
| 4    | Emissions to Bulk Lower Air (kg/ly)                 | 24                         | 0.236713055       | 0.236713055       | 3  | 1.29700255                 | 2.34143282                             |                                         |
| 5    | 3 rain rate                                         | 24                         | -0.217488904      | 0.217488904       | 3  | 1.26897236                 |                                         |                                         |
| 6    | Lower air flow rate (m3/h)                          | 23 24                      | 0.193676688       | 0.193676688       | 3.00| 1.24                      |                                         |                                         |
| 7    | Entropy of evaporation (from water to air) (J/mol)  |                            | 0.534528374       | 0.534528374       | 1.200000048 | 1.00236301 | 0.32826894               |                                         |
| 8    | 19 upper-lower air mixing MTC                       | 24                         | -0.041595814      | 0.041595814       | 10 | 1.00514613                 | 3.17599785                             |                                         |
| 9    | Lower air flow rate (m3/h)                          | 24 17                      | -0.059989154      | 0.059989154       | 3.00| 1.10                      |                                         |                                         |
| 10   | Upper air flow rate (m3/h)                          | 25 26                      | -0.078744475      | 0.078744475       | 3.00| 1.09                      |                                         |                                         |
| 11   | 19 upper-lower air mixing MTC                       | 25                         | -0.03576586       | 0.03576586        | 10 | 1.08584006                 | 2.34160295                             |                                         |

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### Substance: HCB
### Region: 10
### Media: air
### Overall Output CF: 2.7

| Rank | Input Parameter                                      | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|-------------------------------------------------------|--------|----------------|---|-----------------------------|-----------------------------------|------------------------------------------|
| 1    | Lower air flow rate (m$^3$/h)                         | 10     | $-0.493285657$ | 0.4933 | 3.00                         | 1.72                              | 30.06                                    |
| 2    | Lower air flow rate (m$^3$/h)                         | 54     | 0.415873557     | 0.4159 | 3.00                         | 1.58                              | 21.87                                    |
| 3    | Emissions to Bulk Lower Air (kg/hy)                   | 54     | 0.297472757     | 0.297472757 | 3                 | 1.38646857                         | 10.29006648                             |
| 4    | Lower air flow rate (m$^3$/h)                         | 10     | 0.27508639      | 0.2751 | 3.00                         | 1.35                              | 9.35                                     |
| 5    | 19 upper-lower air mixing MTC                         | 54     | -0.084972712    | 0.0850 | 10.00                        | 1.22                              | 3.92                                     |
| 6    | Lower air flow rate (m$^3$/h)                         | 9      | 0.161589025     | 0.1616 | 3.00                         | 1.19                              | 3.23                                     |
| 7    | Upper air flow rate (m$^3$/h)                         | 54     | -0.15833083     | 0.1583 | 3.00                         | 1.19                              | 3.10                                     |
| 8    | Lower air flow rate (m$^3$/h)                         | 10     | -0.141133241    | 0.1411 | 3.00                         | 1.17                              | 2.46                                     |
| 9    | Lower air flow rate (m$^3$/h)                         | 54     | 0.109030585     | 0.1090 | 3.00                         | 1.13                              | 1.47                                     |
| 10   | Lower air flow rate (m$^3$/h)                         | 54     | -0.08943038     | 0.0894 | 3.00                         | 1.10                              | 0.99                                     |
| 11   | Lower air flow rate (m$^3$/h)                         | 10     | -0.08832067     | 0.0883 | 3.00                         | 1.10                              | 0.96                                     |
| 12   | Lower air flow rate (m$^3$/h)                         | 54     | -0.06640768     | 0.0664 | 3.00                         | 1.10                              | 0.92                                     |
| 13   | Enthalpy of vaporization (from water to air) (J/m$^3$) | 54     | -0.512782988    | 0.512782988 | 1                 | 2000000048                         | 1.098002238                             | 0.894715731                             |
| 14   | Lower air flow rate (m$^3$/h)                         | 10     | -0.07620276     | 0.0782 | 3.00                         | 1.09                              | 0.76                                     |
| 15   | Aqueous solubility (g/m$^3$)                          | 54     | -0.204228651    | 0.204228651 | 1.5                | 1.08633277                         | 0.7018962651                            |

| Rank | Input Parameter                                      | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|-------------------------------------------------------|--------|----------------|---|-----------------------------|-----------------------------------|------------------------------------------|
| 1    | Property Temperature (°C)                             | 54     | 0.689614926    | 0.689614926 | 1                 | 1.098002238                         | 0.894715731                             |
| 2    | Enthalpy of vaporization (from water to air) (J/m$^3$) | 54     | -0.512782988    | 0.512782988 | 1                 | 2000000048                         | 1.098002238                             | 0.894715731                             |
| 3    | Lower air flow rate (m$^3$/h)                         | 10     | 0.403285657     | 0.4033 | 3.00                         | 1.72                              | 30.06                                    |
| 4    | Lower air flow rate (m$^3$/h)                         | 54     | 0.415873557     | 0.4159 | 3.00                         | 1.58                              | 21.87                                    |
| 5    | Emissions to Bulk Lower Air (kg/hy)                   | 54     | 0.297472757     | 0.297472757 | 3                 | 1.38646857                         | 10.29006648                             |
| 6    | Lower air flow rate (m$^3$/h)                         | 10     | 0.27508639      | 0.2751 | 3.00                         | 1.35                              | 9.35                                     |
| 7    | Molar Mass (g/mol)                                    | 54     | 0.204257963     | 0.204257963 | 1                 | 1.098002238                         | 0.894715731                             |
| 8    | Aqueous solubility (g/m$^3$)                          | 54     | -0.204228651    | 0.204228651 | 1.5                | 1.08633277                         | 0.7018962651                            |
| 9    | Vapor pressure (Pa)                                   | 54     | 0.204190604     | 0.204190604 | 1.5                | 1.0863616011                        | 0.701634789                             |
| 10   | Lower air flow rate (m$^3$/h)                         | 9      | 0.161589025     | 0.1616 | 3.00                         | 1.19                              | 3.23                                     |
| 11   | Upper air flow rate (m$^3$/h)                         | 54     | -0.15833083     | 0.1583 | 3.00                         | 1.19                              | 3.10                                     |
| 12   | Lower air flow rate (m$^3$/h)                         | 54     | -0.141133241    | 0.1411 | 3.00                         | 1.17                              | 2.46                                     |
| 13   | Lower air flow rate (m$^3$/h)                         | 10     | 0.109030585     | 0.1090 | 3.00                         | 1.13                              | 1.47                                     |
| 14   | Total Surface Area (km$^2$)                           | 54     | 0.108125771     | 0.108125771 | 1                 | 1.098002238                         | 0.894715731                             |
| 15   | Total Surface Area (km$^2$)                           | 54     | -0.101551878    | 0.101551878 | 1                 | 1.098002238                         | 0.894715731                             |
| Rank | Input Parameter                                      | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------------------|--------|----------------|-----|-----------------------------|--------------------------------------|-----------------------------------------|
| 1    | 9 sediment deposition                                | 10     | -0.630573506   | 0.630573506 | 3                           | 1.990217398                         | 19.42920343                            |
| 2    | 1 air side air-fresh water MTC                       | 10     | 0.506157714    | 0.506157714 | 3                           | 1.743807751                         | 12.51864396                            |
| 3    | Lower air flow rate (m3/h)                           | 54     | 0.374132408    | 0.374132408 | 3                           | 1.65                                | 10.07                                  |
| 4    | Lower air flow rate (m3/h)                           | 10     | 0.374132408    | 0.374132408 | 3                           | 1.65                                | 10.07                                  |
| 5    | Volume Fraction Particles in fresh water            | 10     | 0.36678319     | 0.368708319 | 3                           | 1.499403692                         | 6.64290403                             |
| 6    | 10 sediment resuspension                             | 10     | 0.36480776     | 0.36480776  | 3                           | 1.492992191                         | 6.502999241                            |
| 7    | Emissions to Bulk Lower Air (kg/y)                   | 54     | 0.304649641    | 0.304649641 | 3                           | 1.397505857                         | 4.535079581                            |
| 8    | Sediment Reaction half-life (h)                      | 10     | 0.303836387    | 0.303836387 | 3                           | 1.39621613                          | 4.510920067                            |
| 9    | Average fresh water sediment depth (cm)              | 10     | -0.290244686   | 0.290244686 | 3                           | 1.378290662                         | 4.167587476                            |
| 10   | Fresh Water Reaction half-life (h)                   | 54     | 0.260756254    | 0.260756254 | 3                           | 1.331718248                         | 3.32242328                             |
| 11   | Lower air flow rate (m3/h)                           | 54     | 0.253320911    | 0.253320911 | 3                           | 1.32                                | 3.14                                   |
| 12   | Kow (not Log Kow)                                    | 10     | -0.202280826   | 0.202280826 | 3                           | 1.248856336                         | 1.999378444                            |
| 13   | 19 upper-lower air mixing MTC                        | 54     | -0.083579099   | 0.083579099 | 10.00                      | 1.21                                | 1.50                                   |
| 14   | 2 water side air-fresh water MTC                     | 54     | 0.172285754    | 0.172285754 | 3                           | 1.208373507                         | 1.450383437                            |
| 15   | Upper air flow rate (m3/h)                           | 54     | -0.166944796   | 0.166944796 | 3                           | 1.20                                | 1.38                                   |

Sorted by Sensitivity

| Rank | Input Parameter                                      | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------------------|--------|----------------|-----|-----------------------------|--------------------------------------|-----------------------------------------|
| 1    | Enthalpy of vaporization (from water to air) (J/mol) | 10     | 0.810935861    | 0.810935861 | 1.2000000048 | 1.159340307                          | 0.855005629                            |
| 2    | Volume Fraction Sediment pore water                  | 10     | 0.692125011    | 0.692125011 | 1.100000026 | 1.067713493                          | 0.717121482                            |
| 3    | 9 sediment deposition                                | 10     | -0.630573506   | 0.630573506 | 3                           | 1.999217398                         | 19.42920343                            |
| 4    | Property Temperature (C)                             | 10     | 0.608001615    | 0.608001615 | 3                           | 1.999217398                         | 19.42920343                            |
| 5    | 1 air side air-fresh water MTC                       | 10     | 0.506157714    | 0.506157714 | 3                           | 1.743807751                         | 12.51864396                            |
| 6    | Lower air flow rate (m3/h)                           | 10     | -0.454042221   | 0.454042221 | 3                           | 1.65                                | 10.07                                  |
| 7    | Summer mean temperature (oC)                         | 10     | -0.401067329   | 0.401067329 | 1.000000004 | 1.039656457                          | 0.059156457                            |
| 8    | Lower air flow rate (m3/h)                           | 54     | 0.374132408    | 0.374132408 | 3                           | 1.51                                | 6.84                                   |
| 9    | Volume Fraction Particles in fresh water            | 10     | 0.368708319    | 0.368708319 | 3                           | 1.499403692                         | 6.64290403                             |
| 10   | 10 sediment resuspension                             | 10     | 0.36480776     | 0.36480776  | 3                           | 1.492992191                         | 6.502999241                            |
| 11   | Emissions to Bulk Lower Air (kg/y)                   | 54     | 0.304649641    | 0.304649641 | 3                           | 1.397505857                         | 4.535079581                            |
| 12   | Sediment Reaction half-life (h)                      | 10     | 0.303836387    | 0.303836387 | 3                           | 1.39621613                          | 4.510920067                            |
| 13   | Winter mean temperature (oC)                         | 10     | 0.297829063    | 0.297829063 | 1.000000004 | 1.028799952                          | 0.032835728                            |
| 14   | Average fresh water sediment depth (cm)              | 10     | -0.290244686   | 0.290244686 | 3                           | 1.378290662                         | 4.167587476                            |
| 15   | Fraction OC Particles in fresh water                 | 10     | -0.261552518   | 0.261552518 | 1.5                         | 1.111877936                         | 0.455324948                            |
| Rank | Input Parameter                                      | Region | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|------------------------------------------------------|--------|----------------|---|--------------------------|--------------------------------------|------------------------------------------|
| 1    | Average fresh water sediment depth (cm)              | 12     | -0.6021664     | 0.6021664 | 3                        | 1.952856043                         | 16.41052279                             |
| 2    | Sediment Reaction halftime (h)                      | 12     | 0.60912547     | 0.60912547 | 3                        | 1.952854626                         | 16.41451118                             |
| 3    | Lower air flow rate (m3/h)                          | 12     | -0.488277257   | 0.4883    | 3.00                     | 1.71                                | 10.55                                   |
| 4    | 1 air side air fresh water MTC                      | 12     | 0.42032319     | 0.42032319 | 3                        | 1.56683804                          | 7.816013804                             |
| 5    | 9 sediment deposition                                | 12     | 0.391473003    | 0.391473003| 3                        | 1.537377466                         | 6.770914777                            |
| 6    | Kow (not Log Kow)                                   | 12     | 0.367484547    | 0.367484547| 3                        | 1.497381172                         | 5.974433565                            |
| 7    | Fresh Water Reaction halftime (h)                   | 12     | 0.248602237    | 0.248602237| 3                        | 1.314054602                         | 2.734188671                            |
| 8    | Lower air flow rate (m3/h)                          | 12     | 0.231751779    | 0.2318    | 3.00                     | 1.29                                | 2.38                                    |
| 9    | 10 sediment resuspension                            | 12     | -0.226742438   | 0.226742438| 3                        | 1.262372917                         | 2.274491035                            |
| 10   | 2 water side air fresh water MTC                     | 12     | 0.19479339     | 0.19479339 | 3                        | 1.238625643                         | 1.678676599                            |
| 11   | Lower air flow rate (m3/h)                          | 12     | 0.19206673     | 0.1921    | 3.00                     | 1.23                                | 1.63                                    |
| 12   | rain scavenging ratio                               | 12     | 0.091322974    | 0.091322974| 10                       | 1.234022203                         | 1.620769163                            |
| 13   | Lower air flow rate (m3/h)                          | 12     | -0.189071194   | 0.1891    | 3.00                     | 1.23                                | 1.58                                    |
| 14   | density of sediment solids (7,2)                    | 12     | -0.504150852   | 0.504150852| 1.5                      | 1.226807884                         | 1.531643475                            |
| 15   | Enthalpy of vaporization (from water to air) (J/mol)| 12     | 1.103998301    | 1.103998301| 1.200000048              | 1.222970497                         | 1.465356685                            |

Sorted by Sensitivity

| Rank | Property Temperature (C)                           | Sensitivity (S) | | S | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|-----------------------------------------------------|----------------|---|--------------------------|--------------------------------------|------------------------------------------|
| 1    | Property Temperature (C)                           | 1.42491778     | 1 | 1                        |                                      |                                         |
| 2    | Enthalpy of vaporization (from water to air) (J/mol)| 1.103998301    | 1 | 1                        |                                      |                                         |
| 3    | Summer mean temperature (C)                         | -0.718324665   | 0.718324665 | 1.100000024 | 0.071914819 | 0.172528899 |                          |
| 4    | Average fresh water sediment depth (cm)             | -0.60921664    | 0.60921664 | 3                        | 1.952855643 | 16.41052279 |                          |
| 5    | Sediment Reaction halftime (h)                      | 0.60912547     | 0.60912547 | 3                        | 1.952854626 | 16.41451118 |                          |
| 6    | Molar Mass (g/mol)                                  | -0.372676126   | 0.372676126 | 1                        | 1         | 1             |                          |
| 7    | Molar Mass (g/mol)                                  | -0.372585046   | 0.372585046 | 1.5                      | 1.63078345 | 0.836541543 |                          |
| 8    | Molar Mass (g/mol)                                  | 0.37294383     | 0.37294383 | 1.5                      | 1.62941282 | 0.83526386 |                          |
| 9    | Molar Mass (g/mol)                                  | 0.367484547    | 0.367484547 | 3                        | 1.497381172 | 5.974433565 |                          |
| 10   | Molar Mass (g/mol)                                  | 0.360674429    | 0.360674429 | 1.100000024 | 1.034973635 | 0.043315086 |                          |
Substance: HCB  
Region: 25  
Media: soil  
Overall Output CF: 8.6

| Rank | Input Parameter | Region | Sensitivity (S) | |S| | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|-----------------|--------|----------------|-----|-----|-----------------------------|----------------------------------|------------------------------------------|
| 1    | Soil Reaction half-life (h) | 10     | 0.988801554 | 0.988801554 | 3 | 2.963317856 | 25.50060345 |
| 2    | rain scavenging ratio | 3     | 0.432704709 | 0.432704709 | 10 | 2.70834951 | 21.45151122 |
| 3    | Kow (not Log Kow) | 8     | 0.72786019 | 0.72786019 | 3 | 2.224305656 | 13.81084461 |
| 4    | 3 rain rate | 5     | 0.502402716 | 0.502402716 | 3 | 1.73662886 | 6.53186123 |
| 5    | Lower air flow rate (m3/h) | 10 | -0.3705385 | -0.3705385 | 3.00 | 1.50 | 3.57 |
| 6    | Average soil depth (cm) | 7     | -0.989587481 | 0.989587481 | 1.5 | 1.49368048 | 3.47903675 |
| 7    | Enthalpy of vaporization (from water to air) (J/mol) | 7     | 2.159097415 | 2.159097415 | 1.200000048 | 1.482381754 | 3.34805433 |
| 8    | Volume Fraction PseudoOctanol in vegetation flesh | 10 | 0.352883065 | 0.352883065 | 3 | 1.47562091 | 3.24750478 |
| 9    | Lower air flow rate (m3/h) | 54 | 0.296968622 | 0.296968622 | 3.00 | 1.39 | 2.30 |
| 10   | Emissions to Bulk Lower Air (kg/ly) | 54 | 0.29572644 | 0.29572644 | 3 | 1.383876614 | 2.280932789 |
| 11   | Volume Fraction Particles in upper air | 10 | 0.268172141 | 0.268172141 | 3 | 1.34261231 | 1.875463231 |
| 12   | Vapor pressure (Pa) | 10 | -0.657337384 | 0.657337384 | 1.5 | 1.305740944 | 1.537891194 |
| 13   | Aqueous solubility (g/l) | 10 | 0.657500555 | 0.657500555 | 1.5 | 1.35536372 | 1.53963157 |
| 14   | Upper air flow rate (m3/h) | 54 | 0.214472164 | 0.214472164 | 3.00 | 1.27 | 1.20 |
| 15   | Lower air flow rate (m3/h) | 10 | -0.205168621 | 0.205168621 | 3.00 | 1.26 | 1.10 |

Sorted by Sensitivity

| Rank | Input Parameter | Region | Sensitivity (S) | |S| | Input Confidence Factor (CF) | Output CF (due to this parameter) | Percent Contribution to Output Variance |
|------|-----------------|--------|----------------|-----|-----|-----------------------------|----------------------------------|------------------------------------------|
| 1    | Property Temperature (C) | 20 | 2.569990711 | 2.569990711 | 1 | 1 | 0 |
| 2    | Enthalpy of vaporization (from water to air) (J/mol) | 10 | 2.159097415 | 2.159097415 | 1.200000048 | 1.482381754 | 3.34805433 |
| 3    | Volume Fraction Water in vegetation | 10 | -1.177638428 | 1.177638428 | 1.100000024 | 1.118728495 | 0.2723627 |
| 4    | Summer mean temperature (oC) | 10 | -1.126876714 | 1.126876714 | 1.100000024 | 1.113828657 | 0.24927278 |
| 5    | Average soil depth (cm) | 10 | -0.989587481 | 0.989587481 | 1.5 | 1.49368048 | 3.47903675 |
| 6    | Soil Reaction half-life (h) | 10 | 0.988801554 | 0.988801554 | 3 | 2.963317856 | 25.50060345 |
| 7    | Winter mean temperature (oC) | 10 | 0.836054757 | 0.836054757 | 1.100000024 | 1.083022834 | 0.137458333 |
| 8    | Kow (not Log Kow) | 10 | 0.72786019 | 0.72786019 | 3 | 2.224305656 | 13.81084461 |
| 9    | Molar Mass (g/mol) | 10 | -0.658106847 | 0.658106847 | 1 | 1 | 0 |
| 10   | Vapor pressure (Pa) | 10 | -0.657337384 | 0.657337384 | 1.5 | 1.305740944 | 1.537891194 |
| 11   | Aqueous solubility (g/l) | 10 | 0.657500555 | 0.657500555 | 1.5 | 1.35536372 | 1.53963157 |
| 12   | % Soil covered by vegetation | 10 | -0.552290191 | 0.552290191 | 1.100000024 | 1.054089489 | 0.058876542 |
| 13   | Enthalpy of solution (from octanol to water) (J/mol) | 10 | 0.502402716 | 0.502402716 | 1.200000048 | 1.09092635 | 0.151916896 |
| 14   | 3 rain rate | 10 | 0.502402716 | 0.502402716 | 3 | 1.73662886 | 6.53186123 |
| 15   | rain scavenging ratio | 10 | 0.432704709 | 0.432704709 | 10 | 2.70834951 | 21.45151122 |