4FUN

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Deliverable 2.4 : SWOT analysis of different exposure models

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PU	Public	PU
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

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1 Introduction

The 2-FUN model was developed under the sixth Framework Program of the European Union (contract n° FP6-2005-GLOBAL-4-036976) within the project “Full-chain and uncertainty approaches for assessing health risks in future environmental scenarios”. 2-FUN aimed to provide decision-makers with state of the art tools to analyse the current and future trends in environmental conditions and pressures that may lead to health problems. Its main objective was to support the evaluation and ranking of management options through a range of functionalities able to generate outputs of high concern for health risk assessment: building of long-term environmental and socio-economic scenarios, exposure assessment, provision of uncertainty margins, and identification of sensitive pathways and risks. The 2-FUN multimedia modelling tool allows the user to assemble a model for a specific scenario, to enter input data and parameter values for selected contaminants and finally to run deterministic (best or worst-case estimate) or probabilistic (Monte Carlo) simulations.

This 2-FUN model is however only a prototype software containing a library of models for exposure assessment, coupling environmental multimedia and pharmacokinetic models. The objective of the 4-FUN project is to further improve and standardise the 2-FUN model and guarantee its long-term technical and economic viability.

During the consortium meeting of 3-5th of February in Barcelona, a consensus was found for the name of the 2-FUN model: MERLIN-Expo. The name of this model will be used throughout this document.

1.1 Objective

The main objective of Work Package 2 (WP2) is to identify strengths and weaknesses of the 2-FUN model and other exposure models using a SWOT (Strengths-Weaknesses-Opportunities-Threats) analysis. SWOT analysis (alternatively SWOT Matrix) is a structured planning method used to evaluate the Strengths, Weaknesses, Opportunities, and Threats involved in a project or in a business venture. This identification will be used as an input for the design of the final integrated MERLIN-Expo model (WP3), for marketing and further extensions after the 4FUN project.

1.2 Exposure models

To put the MERLIN-Expo model into perspective and to identify its strengths and weaknesses, a comparison was made between the MERLIN-Expo model and existing exposure models. An overview of currently available exposure models was presented in Deliverable 2.1: List of exposure models to be included in the SWOT analysis. This overview consisted of environmental concentration, human intake, dietary exposure, consumer exposure and aggregate or multimedia models. In total 97 models were identified, from which 60 models were multimedia models.

Note that the term “model” will be used in its broadest sense to describe “tool”, “software package” as well as the more narrow definition of “mathematical model”.

2 Methodology

Several quantitative (Multi-Criteria Decision Analysis, Weight of Evidence,…) and qualitative (expert judgment) methods are available to conduct a SWOT analysis. The SWOT analysis in this project will include a number of them to ensure robust conclusions. Several criteria and frameworks will be used to assess scope and functionality of the exposure models. These are further outlined in the sections below.

2.1 List of criteria/questions

In order to perform an objective and reproducible SWOT (Strengths, Weaknesses, Opportunities and Threats) analysis of the MERLIN-Expo model and currently existing exposure models, a comprehensive list of criteria was set up to structure the assessment of the characteristics of the exposure models.

Relevant aspects, features, functionalities related to an exposure model were identified and translated into a set of evaluation criteria, which in turn were written as yes/no/not applicable-questions. Experts within the consortium evaluated these questions. These criteria were the result of a systematic review of the characteristics of exposure models and models available in the literature, the requirements of regulatory frameworks (REACH, biocides, plant protection products) and the incorporation of expert judgement about relevant aspects for environmental exposure modelling. This resulted in a total of 128 criteria/questions, which are presented in Deliverable 2.2.

The obtained questions are organized based on a hierarchical structure, which relates the different aspects of exposure models in a clear and solid fashion. The constructed hierarchical structure that was used consists of four (4) Lines of Evidence, thirty six (36) categories, forty two (42) sub-categories, and hundred twenty eight (128) criteria/questions.

In a first instance, the hierarchical structure was analysed by an expert panel to assess the importance and relevance of each criterium as well as dependencies between criteria. In a second step, the list of criteria/questions will be used for the comparative assessment of exposure models.

2.2 Step 1 - Analysis of the hierarchical structure

The identified questions are analysed according to the MCDA-based (Multi-Criteria Decision Analysis) Weight of Evidence approach. MCDA includes a wide variety of methods for the evaluation and ranking, or selection, of different alternatives that consider all the aspects of a decision problem involving many actors. The methodology incorporates the use of MCDA methods and specifically is based on the use of Multi-Attribute Value Theory (MAVT), combined with fuzzy logic as well as basic elements of group decision theory (Isigonis et al., 2012)

The pillars, upon which the WoE methodology is developed, are:

1. the creation of a hierarchical evaluation structure;
2. the collection of the knowledge and input of an expert panel;
3. the analysis of the hierarchical structure;

4. the assessment of exposure model elements on the basis of the hierarchical structure;
5. the automatic calculation of a final graded score based on pillars 1, 2, 3 and 4.

The analysis of the hierarchical structure is performed with the help of 5 experts (from AEIFORIA, ENVIRESEARCH, VITO, UNICATT and EDF) from the consortium, which were invited to assess the complete structure through the use of a dedicated online questionnaire. The online questionnaire was designed for collecting the opinions and insights of experts on three basic elements:

- Identification of the relations between criteria;
- Identification of the relative importance of each criterion:
- Identification of the possible inherent uncertainty:
    - in the form of unreported information
    - in the form of disputable information/conditions
    - in the form of lack of knowledge of the experts.

These elements were translated into the following questions:

1. Does an optimum (i.e. green answer), or conversely, worst (i.e. red answer) evaluation of one of the following criteria make all/some of the other criteria within the same category irrelevant?
2. Rank the importance of each criterion by assigning each of them to the appropriate category (Not relevant - Slightly important - Moderately important - Highly important - Prerequisite).
3. Supposing a criterion is applicable for the type of human exposure model under assessment but not reported in the paper/manual or not specified by the person evaluating the model's quality, which action would you take? Each criterion should be assigned, based on your judgment for its effects on model evaluation, in Substituted by optimum – No idea on how to substitute – Substituted by worst
4. Evaluate if the Optimum/Worst answer is disputable (i.e. highly depend on the model assessor) or consensus-based (i.e. based on largely recognized assumptions/desired conditions). Each criterion should be assigned in Disputable – Non-disputable.

The five experts that participated in the online questionnaire indicated that some questions were very difficult and ambiguous. E.g. the relevance questions are highly dependent on the scenario/framework of consideration and therefore there is no straightforward answer possible to these questions. For other questions, the wording was too ambiguous or too subjective. Therefore some of the expert answers were highly dependent on the interpretation of the criteria that could be read in more than one way. Therefore an alternative criteria setup was developed for the non-relevance criteria. The new set of criteria were split between general criteria which are not framework specific and relevance criteria which are highly framework specific. The general criteria are presented in Appendix A and the relevance criteria are presented in Appendix B. The new set of criteria consisted of 155 criteria/questions in total.

The general criteria were analysed again according to the methodology described above by three experts from EDF and ARCHE. The relevance criteria were not analysed using the online questionnaire, as these criteria were too framework specific. In order to be able to include these criteria in the overall assessment, expert judgement was used in order to score the criteria on their importance in a certain framework. The following frameworks where the use of exposure models is relevant were identified (based on results of break-out sessions on the consortium meeting in Milan):

- REACH Regulation (No. 1354/2007)
- Plant Protection Products Regulation (No. 1107/2009)
- Biocide Regulation (No. 528/2012)
- Environmental Oriented Directives (e.g. Water Framework Directive (2000/60/EC))
- Food Oriented Regulations/Directives (e.g. Food Contact Materials (No. 1935/2004)
- Site specific assessment (e.g. local contaminations)
- Sustainability (assessment was conducted for hazard-based approaches such as e.g. in Cradle to Cradle; note that the relevancy of the criteria for risk-based approaches such as LCA with USEtox or GLOBOX would perform better)

Every criterion was scored from 1 (not relevant) to 5 (prerequisite) for their importance in a certain framework. The scoring of all relevance criteria is presented in Table 1.

Table 1: Scoring to importance of criteria according to different frameworks

Question	REACH	PPP	Biocide	Environ. compartment Oriented Directives	Food oriented Directives	Site specific assessment	Sustain-ability
Does the model cover exposure to worker (PPP: worker + operator, REACH: consumer, industrial and professional use)?	5	5	5	1	1	1	3
Does the model cover exposure via the general population (PPP: resident + consumer), reach: indirect via environment)?	4	5	4	3	5	4	3
Does the model cover exposure to subpopulations (adults, children, etc.)	1	5	1	1	3	4	1
Does the model calculate concentrations in ground water?	4	5	4	4	2	4	4
Does the model calculate concentrations in surface water?	5	5	5	4	2	4	4
Does the model calculate concentrations in sediment?	5	5	5	4	2	4	2
Does the model calculate concentrations in marine water?	5	1	3	4	2	4	2
Does the model calculate concentrations in soil?	5	5	5	4	2	4	2
Does the model calculate concentrations in pore water?	4	5	4	3	2	4	1
Does the modelcalculate concentrations in air?	4	4	4	1	2	4	2
Does the model calculate concentrations in the human body?	2	1	2	1	3	3	1
Does the model calculate concentration in organs?	2	1	2	1	3	3	1
Does the model calculate concentrations in milk?	1	1	1	1	3	3	1
Does the model calculate concentations in blood?	2	1	2	1	3	3	1
Does the model calculate concentrations in fish?	5	5	5	1	3	4	1
Does the model calculate concentrations in leafy crops?	4	4	4	1	3	4	1
Does the model calculate concentrations in root crops?	4	4	4	1	3	4	1
Does the model calculate concentrations in livestock?	4	1	4	1	3	3	1
Does the model calculate concentrations in eggs?	1	1	1	1	3	3	1

Does the model calculate concentrations in dairy products?	4	1	4	1	3	3	1
Does the model calculate concentrations in earthworms?	5	5	5	2	1	3	1
Does the model cover exposure by oral intake of food and drinks?	5	5	5	2	5	4	3
Does the model cover exposure by oral intake of soil or dust ingestion?	1	1	1	1	2	4	1
Does the model cover exposure through inhalation?	5	5	5	1	1	4	2
Does the model cover exposure by dermal absorption?	5	5	5	1	1	3	2
Does the model cover the run-off process?	5	5	5	4	2	4	2
Does the model cover leaching of substances in soil?	5	5	5	4	2	4	2
Does the model cover the volatilization process from water?	5	3	5	4	2	4	1
Does the model cover the volatilization process from vegetation?	3	5	3	3	2	4	1
Does the model cover the volatilization process from soil?	5	5	5	4	2	4	1
Does the model cover wet and dry deposition to soil?	5	3	5	4	2	4	1
Does the model cover wet and dry deposition to water?	4	3	4	4	2	4	1
Does the model cover wet and dry deposition to vegetation?	3	3	3	3	2	4	1
Does the model cover adsorption/desorption processes?	5	5	5	4	2	4	1
Does the model cover linear/non-linear sorption?	1	5	1	4	2	4	1
Does the model cover sediment burial?	4	4	4	3	2	4	1
Does the model cover sedimentation/resuspension?	4	4	4	3	2	4	1
Does the model cover biotic and abiotic degradation?	5	5	5	4	2	4	2
Does the model cover degradation in the air compartment?	5	5	5	4	2	4	1
Does the model cover degradation in the water compartment?	5	5	5	4	2	4	2
Does the model cover degradation in the sediment compartment?	5	5	5	4	2	4	2
Does the model cover degradation in the soil compartment?	5	5	5	4	2	4	2
Does the model cover bioconcentration of substances?	5	5	5	2	2	4	2
Does the model cover excretion and degradation by animals	1	5	1	1	2	4	1
Does the model cover the food processing step of raw material?	1	5	1	1	4	4	2
Does the model cover the vegetal transpiration process?	1	4	1	2	2	3	1
Does the model cover transport of the substance by plant death?	1	1	1	2	1	3	1
Does the model cover an editable transport factor of the substance at harvest of the vegetation (e.g. only roots, complete plant, etc.)?	1	5	1	1	3	4	2
Does the model take crop interception into consideration?	1	5	1	2	2	4	1
Does the model take irrigation into consideration?	1	5	1	2	2	4	1
Does the model cover internal absorption of substances in the human body?	2	1	2	1	3	4	1

Does the model cover distribution of substances in the human body?	2	1	2	1	3	4	1
Does the model cover biotransformation in the human body?	2	1	2	1	3	4	1
Does the model cover excretion from the human body?	2	1	2	1	3	4	1
Does the model describe bioavailability of a substance in the human body? (= passage of a substance from the site of absorption into the blood of the general circulation)	2	1	2	1	3	4	1
Does the model describe the linear and non-linear saturation process in the human body?	2	1	2	1	3	4	1
Does the model describe accumulation in the human body (i.e. the extent of accumulation reflects the relation between the body-burden compared with the steady-state condition)?	2	1	2	1	3	4	1
Does the model cover acute exposure?	5	5	5	1	4	4	1
Does the model cover chronic exposure	5	5	5	1	4	4	1
Is the model based on a dynamic approach?	1	3	1	2	2	4	1
Does the model cover exposure at the local scale (e.g.1km2)?	5	5	5	3	1	4	1
Does the model provide spatially explicit outputs (e.g. Spatial distribution of contaminant concentration in an area/region)?	2	2	1	5	1	3	1
Does the model cover exposure at a regional scale (e.g. The Netherlands)?	5	2	1	3	3	2	1
Does the model cover the formation of metabolites?	1	5	1	1	4	3	1
Is the model focused on organics in general?	5	5	5	5	5	5	4
Does the model cover inorganic chemicals?	5	5	5	5	5	5	4
Does the model cover metals?	5	5	5	5	5	5	4
Can the model perform cumulative exposure assessment of multiple chemicals?	2	3	2	3	4	4	1
Can background concentrations (environmental and human compartments) be taken into account ?	3	2	2	3	1	4	1
Does the model cover point source release?	5	1	5	4	1	4	1
Does the model cover diffuse release?	1	5	1	4	1	4	1
Does the model cover exposure to the bystander?	1	5	1	1	1	1	1
Does the model cover exposure to the surface water and air via spray drift?	1	5	1	1	1	1	1

From Table 1, it can be concluded that if a model scores ‘yes’ on the majority of the criteria, it is expected to be a model that is highly suitable to be used in a site-specific assessment. Site-specific assessments are in general characterised by more flexibility in the exposure assessment (flexibility that is required for the site-specifics of the assessment) and can be used in a variety of circumstances, which leads to a fairly high score on all criteria. Concerning the assessment carried out in the framework of the REACH/Biocide/PPP

regulations, it is clear that if a model scores high on the majority of the proposed criteria it is expected to be fairly compliant to what is required in the regulation. As for the REACH/Biocide/PPP regulation, internal concentrations are not taken into account yet, the criteria related to the pharmacokinetic modelling therefore receive a low score, which results in a lower amount of red blocks in the importancy scoring compared to the site specific assessment.

For the environmental compartment oriented directives and food oriented directives, the number of important relevance criteria is much smaller as the assessment in these directives is generally focused on a single or smaller amount of compartments and media compared to other regulations that covers a broad range of compartments and where e.g. the exposure of man via the environment is assessed.

Finally, it can be concluded that the criteria proposed are not very suitable for the assessment of models used for sustainability assessment. Models used for sustainability assessment are not always as detailed as the models used for exposure assessment in the proposed regulations.

Subsequently, the scoring of the criteria on importance (question 2) per framework was combined with the answer of the five experts on question 1, 3 and 4 in order to be able to continue with the MCDA Weight of Evidence approach.

The output of the questionnaire and scoring of relevance criteria was collected, stored and further used for the creation of a knowledge base. This knowledge base allows to clarify and quantify the relations among the evaluation criteria, and further among the rest of the elements of the hierarchical structure, and is subsequently used at the final stage of the assessment process for the analysis of a given human exposure model.

2.3 Step 2: Comparative assessment of exposure models using the MCDA Weight of Evidence approach

In the assessment process, evaluators were asked to assess the given exposure models according to the proposed criteria/questions. These evaluations will be analysed according to the MCDA methodology and specific aggregation techniques. The result is an index obtained for each exposure model under assessment. This index is an indicator of its reliability/performance and can be used for the comparison of models through a standardised unit of measure.

By assessing the strengths and limitations of publicly available exposure models and modelling systems in regard to the needs defined for development of the MERLIN-Expo model, the features of the various models are determined that may be further incorporated into the model.

3 Exposure models

Based on the list of models described in Deliverable 2.1 and based on the expertise of partners in the consortium, the following exposure models were selected to include in our comparative assessment:

- CalTOX
- ESCAPE
- EUSES
- FUZZY model
- GLOBOX
- GREAT-ER
- MACRO
- MERLIN-Expo
- MODULERS
- PBPK
- PEARL
- STEPS1-2
- TOXSWA
- USEtox

A short introduction to each model is presented below.

3.1 CalTOX

3.1.1 Model purpose

CalTOX is a software model, which was designed to help to assess human health risk levels due to contaminated sites and define remediation soil levels. It was developed for the California Environmental Protection Agency (Cal-EPA). The software can also be used at a regional scale, with continuous emissions in soil, air and water.

3.1.2 Model context

It consists of:

- A transportation and transformation model enabling to calculate the concentrations in the environmental media (air, surface soil, root zone soil, vadose soil, surface water, superficial sediment, leaf of plant, cuticle plant, groundwater).
- An exposure model enabling to calculate the concentrations in the exposure media and the exposure to humans from the environmental concentrations.

The exposure routes available are inhalation, ingestion and dermal contact. Inhalation concerns gases and particles in outdoor and indoor air. The pathways included for dermal uptake are linked to dermal contact with surface soil and ground or surface water during bathing and swimming. Oral intake can result from 1) ingestion of groundwater or surface water as drinking water, 2) ingestion of plants contaminated by transfer from air, surface soil, root-zone soil and irrigation water, 3) ingestion of meat, dairy products and eggs contaminated by inhalation of air and ingestion of water, plants and surface soil by the animal, 4) ingestion of fish contaminated by surface water, 5) ingestion of surface water during recreational activities and 6) incidental ingestion of soil.

Reference toxicological values are used to calculate the carcinogenic and non-carcinogenic risks, as well the soil concentration risks.

The database contains values for 349 chemicals (organic and inorganic). The scenarios defined by CalTOX can include only one age class, in addition to the infants.

3.1.3 Model type

CalTOX is a multimedia exposure model, performing analytical computation. It is an Excel file using Visual Basic macros. It was developed in Excel 2000.

CalTOX includes an eight-compartimental dynamic fugacity model to calculate environmental concentrations. The root-zone, vadose soil and groundwater concentrations are calculated relative to time, whereas the concentrations in the other media are assumed to be at quasi steady state with the root-zone soil and vadose soil compartments.

CalTOX is intended for applications from months to years.

It is a zero dimension model, but off-site concentrations due to air and groundwater transfers can be computed too. The user's guide also indicates that the software should not be used for landscapes in which water occupies more than 10% of the land surface area.

CalTOX was designed to perform sensitivity and uncertainty analysis easily, by using the software Crystal Ball version 4.0 and the predefined distribution provided for each parameter.

3.1.4 Information links

CalTOX was developed by the Lawrence Berkeley National Laboratory (LBNL) and is available at the following email address http://eetd.lbl.gov/ied/era.

3.2 ESCAPE

3.2.1 Model purpose

A software called ESCAPE (Estimation of Soil Concentration After PEsticide applications) was developed that can be used to calculate actual as well as time weighted average concentrations in soil for the parent compound and additional metabolites. In addition to SFO kinetics (single first order) the software is able to consider hockey stick – kinetics (HS), FOMC- kinetics (first order multi compartment) and DFOP- kinetics (double first order in parallel). ESCAPE can handle singular and multiple applications over a simulation period of 10 years. The user may also enter irregular application pattern within a year. ESCAPE considers different soil depths and performs corrections of actual rates dependent on the current crop interception automatically. Visualisation of results is carried out graphically (diagram showing the simulated concentrations vs. time) and tabularly based on time intervals as defined by EU or national regulations.

In the new version 2.0 of ESCAPE in addition to traditional total contents also pore water concentrations can be calculated. Furthermore, degradation rates can be corrected based on actual soil moisture and temperature data. Finally, realistic worst case scenarios based on specific information on soil cores and climate data sets containing daily weather series can be used for the calculations.

3.2.2 Model context

Within the registration of pesticides time dependent concentrations in soil have to be calculated for all active ingredients and their main metabolites. Traditionally these estimations are performed considering first order degradation kinetics as described in the FOCUS-document Soil persistence models and EU registration finalised in 1997. Calculated actual (PECact) and time weighted average concentrations (PECTWA) are used for

comparisons with respective results of eco-toxicity tests as the base for the risk assessment of these substances in soil.

As first order degradation means that the half life of a compound is only a function of the rate constant and therefore constant over time and independent on the actual soil concentration, this kinetics has many advantages especially when complicated application pattern with different application amounts, rates or times have to be considered.

However, in the final report of the FOCUS working group on degradation kinetics which came out recently (FOCUS 2006) additional degradation kinetics were described, which are often more suitable to describe the fate of pesticides in soil than the traditional methodology based on single first order degradation (FOCUS nomenclature: SFO: Single First Order). Additional recommended kinetics are e.g. HS: hockey stick, DFOP: double first order in parallel, or FOMC: first order multi compartment.

For single applications FOCUS Degradation Kinetics published algorithms allowing the calculation of time dependent concentrations in soil for parent and metabolite compounds. Unfortunately, for complicated application pattern with irregular application timing and rates currently no bug-free and user-friendly is available that can be used to calculated actual and average concentrations in soil. Additionally, models to estimate plateau concentrations are currently not available. The commonly used leaching models (PELMO, PEARL) are also not appropriate, as long as they consider first order degradation in soil only. The main difficulty is the non-existence of simple mathematical solutions for the concentration dependency for more complicated application pattern. However, consideration of non-kinetic sorption modules in these models could be an alternative.

In contrast to simple first order kinetics the strategy of handling residues from earlier applications has to be defined clearly when using more complicated degradation kinetics. To consider also soil concentrations based on different weather conditions the degradation rates can be corrected based on temperature and soil moisture.

This version of ESCAPE is finally able to consider pore water concentrations as e.g. recommended by EFSA.

3.2.3 Model type

ESCAPE considers in total 4 different degradation kinetics SFO: (Single First Order), HS (Hockey Stick), DFOP: (Double First Order in Parallel) and FOMC: First Order Multi Compartment). All models are available for parent compounds. However, the identification of a suitable model for the description of the formation and degradation of metabolites are much more complex. As the description of the concentration curve of a single metabolite depends on a correct description of the degradation of the parent substance and of the degradation of the metabolite itself. Due to the parallel formation of metabolites only two of the four available models can be used also for metabolites namely the SFO and the DFOP kinetics. The other models are not conceptually correct for a metabolite that is gradually formed over a period of time (FOCUS 2006).

3.2.4 Information link

The ESCAPE software can be downloaded via the following link: http://server.ime.fraunhofer.de/download/permanent/mk/ESCAPE/

3.3 EUSES

3.3.1 Model purpose

The European Union System for the Evaluation of Substances (EUSES) is a decision-support instrument which enables government authorities, research institutes and chemical companies to carry out rapid and efficient assessments of the general risks posed by chemical substances. EUSES is intended mainly for initial and refined risk assessments rather than for comprehensive assessments. Besides the release estimation, only a few data on substance properties are needed to calculate PECs at Tier 1. The output of EUSES is a quantitative comparison per substance of the results of the effects and the exposure assessment. The system can be used to carry out tiered risk assessments of increasing complexity on the basis of increasing data requirements.

The model was developed to perform risk assessment of substances under the REACH Regulation (EC 1907/2006) and the Biocidal Product Directive (BPD) (98/8/EC) (Replaced by the Biodical Product Regulation (BPR) (EC 528/2012).

3.3.2 Model context

EUSES 2.0 is designed to support decision-making by risk managers in government agencies, scientific institutes and industry in the evaluation of new and existing chemical substances. It can be used for organic and inorganic chemicals but appears to be less suitable for the assessment of chemicals outside the neutral organic compounds. The human population considered in EUSES is man exposed via environment, non-professional users of biocides, consumers and workers. The following media are considered in the EUSES model: atmosphere, surface water (fresh and marine water), sediment (fresh and marine environment), soil (natural, agricultural and industrial soil) and two terrestrial compartments (natural and agricultural soil).

3.3.3 Model type

EUSES is a steady state, simulation, deterministic, distributed and analytical model. In line with most assessment procedures EUSES can be used to carry out tiered risk assessments of increasing complexity, requiring additional data. Using OECD terminology, EUSES can specifically be used in the initial, or screening, and intermediate, or refined, stages of assessment. With EUSES, substances can be assessed for their potential risks to man and the environment. On the basis of this screening, it can be decided if more data need to be generated and if a more refined (i.e. intermediate) assessment is necessary. When dealing with (large) numbers of chemicals, this screening can be used to set priorities for data gathering or refined assessments. EUSES can also be applied for intermediate or refined assessments by allowing the replacement of default values, estimated parameter values, or intermediate results by more accurately estimated values or by measured data. EUSES is not specifically designed for site-specific assessments, but adjustment of parameters may allow for insight into specific local or regional situations.

3.3.4 Information link

The EUSES software can be downloaded via the following link: http://ihcp.jrc.ec.europa.eu/our_activities/public-health/risk_assessment_of_Biocides/euses/euses

3.4 "Fuzzy logic"-model

3.4.1 Model purpose

The "Fuzzy logic" model is a new methodology to assess the risk of water effluents, from Waste Water Treatment Plants, based on fuzzy logic, a well-known theory to deal with uncertainty and vagueness, especially in the environmental field where data are often not fully available. The "Fuzzy logic" name is referring to the model and not specifically to the mathematical theory. The results obtained using the fuzzy model, could be used to characterize and compare the different wastewater treatment plants according to their associated risk as well as prioritizing the compounds according to their relative risk. The model was developed to answer to the requirements of two main regulations, Directive 2008/105/EC, concerning the Environmental quality standards in the field of water policy, and the Regulation No 166/2006, concerning the establishment of a European Pollutant Release and Transfer Register.

3.4.2 Model context

The "Fuzzy logic"-model was developed to assess the risk of water effluents. It can be used for both organic and inorganic chemicals. The main variables taken into consideration are: human toxicity, environmental toxicity, persistence, bioconcentration, exposure, toxicity, hazard and risk. First of all, to determine the risk it is necessary to know all the variable values. From the environmental toxicity and human toxicity, the output toxicity is obtained. Then, the output hazard is obtained with inputs toxicity, persistence and bioconcentration. Finally, with hazard and exposure it is possible to determine the risk. Different fuzzy sets can be considered for the input parameters: negligible, low, medium, high and very high. Using this model, cumulative risk assessment of multiple chemicals can be performed.

3.4.3 Model type

The "Fuzzy logic"-model can be used to achieve a relative risk based prioritization of chemicals. In the Fuzzy logic theory, the expert's judgment strongly influences the risk ranking values. Fuzzy logic is not specifically designed for site-specific assessments, but adjustment of parameters may allow for insight into specific local situations. Furthermore, the default values for forcing variables and parameters can be easily modified if more accurately estimated values are available.

3.4.4 Information link

The "Fuzzy logic" model is not freely available.

3.5 GLOBOX

3.5.1 Model purpose

Multimedia environmental models are widely used for toxicity characterisation in LCA. The spatial scope of the fate and intake model is generally linked to the magnitude of the region for which it is to be applied. Product life cycles, however, usually include processes from all over the world. Therefore there was a need to expand the spatial scope of regional models for use in LCA. GLOBOX was developed, as LCA requires region-specific characterisation factors (CFs) for releases of any toxic chemical at any location in the world. GLOBOX is is a spatially differentiated multimedia fate, exposure and effect model. It is used for the calculation of spatially differentiated LCA characterisation factors on a global scale. It is

largely based on the European Union model EUSES version 2.0 (current version is 2.1.2), but can be considered as an extended and more refined elaboration of this model.

3.5.2 Model context

Although the GLOBOX model has been primarily developed for the calculation of LCA toxicity characterisation factors, it is basically a multimedia model for fate, exposure and effect modelling, with a much broader range of application than just LCA.

The chemicals considered in GLOBOX are organic chemicals and metals. Compared to EUSES, on which GLOBOX is based, metal-specific equations in water are introduced. Intake routes, which are considered, are air, drinking water, leaf crops, root crops, meat, dairy, freshwater fish, sea fish. The following emission/distribution compartments are considered in the GLOBOX model: Air, rivers, freshwater lakes, freshwater lake sediments, salt lakes, slat lake sediments, natural, agricultural and urban soil, groundwater, seawater and sea water sediments.

3.5.3 Model type

Globox is a steady-state and a spatially distributed model. The GLOBOX package contains a substance data collection for 3402 substances. The GLOBOX parameter sets are gathered in GLOBACK and contain the spatially differentiated parameters for the GLOBOX model. The parameters have a global coverage but are differentiated on a number of different levels.

3.5.4 Information link

http://www.cml.leiden.edu/software/software-globox.html

3.6 GREAT-ER

3.6.1 Purpose

The GREAT-ER model (Geo-referenced Regional environmental Exposure Assessment Model for European Rivers) is a model for environmental risk assessment and management of chemicals in river basins. The GREAT-ER model is designed as an advanced environmental exposure model for chemicals in river basins, for use e.g. in the European chemicals risk assessment process (REACH), and in the EU Water Framework Directive (WFD). The model is implemented as part of a software system that combines a GIS (Geographic Information System) with fate models to produce a simple and clear visualization of predicted chemical concentrations and water quality along a river.

3.6.2 Model concept

The determination whether a substance presents a risk to organisms in the environment is based on the comparison of a predicted environmental concentration (PEC) with a predicted no effect concentration (PNEC) to organisms in ecosystems (ECETOC, 1993). Such assessment can be performed for different compartments (e.g. air, water and soil) and on different spatial scales (local, regional). The current version of GREAT-ER desktop comes with a model system covering four sub-models: emission, sewer, treatment plant and river. There are up to three complexity modes for each of these sub-models. In its lowest complexity mode, the fate processes are comparable to EUSES. The main-added value of GREAT-ER is that the exposure assessment is geo-referenced, i.e. an assessment is conducted on site-specific as well as river basin scale. For application within European Union chemical legislation, this is further captured in a number of European Commission documents (EEC, 1993, 1994a), and implemented in the European Union System for the Evaluation of Substances EUSES (Vermeire et al., 1997).

3.6.3 Model type

GREAT-ER is a steady-state model. Apart from deterministic simulations, the GREAT-ER model can also perform a stochastic or probabilistic Monte Carlo simulation. This results in statistical distributions of predicted concentrations, which can be used for risk assessment. Some of the other features are: comfortable scenario management, direct work with model results in ArcGIS, considerably possibilities to analyse simulation results, build up complex scenarios easily and possibility to compare and evaluate scenarios and measures.

3.6.4 Information link

www.great-er.org

3.7 MACRO

3.7.1 Model purpose

MACRO is a one-dimensional non-steady state model of water flow and solute transport in structured or macroporous field soils (Larsbo and Jarvis, 2003).

The primary objectives behind the development of MACRO were: to synthesize current understanding of flow and transport processes in structured soils, and to develop an easy-to-use physically-based simulation model that could be used as a management tool to evaluate the impacts of macropore flow on water flow and solute transport both to surface and ground-waters (Larsbo and Jarvis, 2003).

3.7.2 Model context

The concern over the diffuse pollution threat to surface and groundwater posed by the use of agrochemicals has been recently increasing. The soil unsaturated zone acts as a critical buffer to solute transport and determines the risk of contamination of receiving water bodies by diffuse pollutants. MACRO considers preferential flow to describe the irregular wetting of soils and the non-uniform patterns of solute displacement (Larsbo and Jarvis, 2003).

MACRO version 5.2 was adapted to enable higher-tier simulations for pesticide risk assessments in the EU pesticide registration process (MACRO in FOCUS 5.5.3). It includes FOOTPRINT pedotransfer functions.

3.7.3 Model type

MACRO is a mechanistic model of water flow and solute transport in structured or macroporous field soils. A complete water balance is considered in the model, including treatments of precipitation (rain, snowpack, and irrigation), variably-saturated water flow, losses to primary and secondary field drainage systems, evapotranspiration, and root water uptake. The model includes descriptions of processes such as canopy interception and wash off, convective-dispersive solute transport with ‘two-site’ (kinetic and instantaneous) sorption, first-order degradation controlled by soil moisture and temperature conditions and plant uptake.

The model is run in two flow domains: a high-conductivity/low porosity macropore domain is coupled to a low conductivity/high porosity domain, representing the soil matrix. Mass exchange between the domains is calculated with approximate, physically-based, first-order expressions.

Version 5.0 of MACRO can be used to simulate non-reactive tracers (e.g. bromide), tritium, and pesticides, including a single metabolite (Larsbo and Jarvis, 2003).

3.7.4 Information link

Relevant documents and the download of the model can be done using the following link: http://www.slu.se/en/collaborative-centres-and-projects/centre-for-chemical-pesticides-ckb1/areas-of-operation-within-ckb/models/macro-52

3.8 MERLIN-Expo

3.8.1 Model purpose

Integration of exposure assessment over the full chain

The MERLIN-Expo software is a decision-support instrument that integrates on the same platform a library of both multimedia and PBPK (including metabolites formation) models, allowing to cover the complete exposure assessment chain (from concentrations in water, air and/or soil to internal dose to target organs and eventually pathology risks). The model thus allows lifetime risk for different human populations (e.g. general population, children at different ages, pregnant women) including exposure through multiple pathways.

Uncertainty/Sensitivity analysis

The MERLIN-Expo model contains a set of functionalities for uncertainty/sensitivity analysis that are in line with the tiered approach recommended by WHO (i.e. One-At-a-Time (OAT) methods for screening sensitivity analysis and variance-based methods for quantitative sensitivity analysis). The availability of such options for uncertainty and sensitivity analysis should facilitate the incorporation of such issues in future decision making.

Flexibility in the scenario building

All the models included in the MERLIN-Expo model are implemented on the same platform (*i.e.* Ecolego® - see www.facilia.se) in order to facilitate integrated full-chain assessments for combined exposures. One of the main characteristics of Ecolego is the use of Interaction Matrices to create and visualise models, similar to what is written ‘on the paper’ when building the conceptual models (‘easy-to-understand’ criteria). A large model can be cleanly separated into independent modules that represent a certain part of the model and that can be easily coupled (‘easy-to-use’ and ‘flexible’ criteria). Finally, two products were actually developed by the 2-FUN project: a software for the research community (where end-users can modify the models themselves, i.e. the set of equations), and a software for ‘non-experts’ (where only scenario building, i.e. components assemblage and scenario parameters selection, have to be updated).

Standardisation

The MERLIN-Expo model followed a process to satisfy requirements in term of Quality Assurance and Standardisation, especially on: (i) conceptual and numerical verification of the model; (ii) benchmarking with other models based on generic scenarios; (iii) standard documentation and; (iv) demonstration.

3.8.2 Model context

MERLIN-Expo is designed: (i) to support decision-making by risk managers in the evaluation of new and existing chemical substances; (ii) to support site analysis for reconstruction of past exposure patterns; (iii) to conduct scientific studies in exposure assessment, especially through uncertainty and sensitivity analysis. It can be used for organic and inorganic

chemicals. For organic chemicals, its applicability domain depends on the availability of reliable QSAR or read-across models able to parameterize the model(s). The human population considered in MERLIN-Expo is man (including several sub-populations like children and pregnant women) exposed via environment. The following models are considered in the MERLIN-Expo library: atmosphere, rivers, lakes, soil (natural, agricultural and industrial soil), vegetables (tubers, leaf vegetables, root vegetables, fruits, cereals, grass), animal food (beef meat, milk), aquatic food-web (phytoplankton, zooplankton, fish).

3.8.3 Model type

MERLIN-Expo is based on a library of dynamic models that can be flexibly coupled. All the uncertain parameters are informed by Probability Density Functions allowing further uncertainty/sensitivity analysis. MERLIN-Expo can be used to carry out tiered risk assessments of increasing complexity (initial, or screening, intermediate, or refined stages of assessment). Environmental and Human exposures can be assessed. End-users can use default best estimates and default PDFs proposed in the model, but can also change these values according to their own scenario.

3.8.4 Information link

The MERLIN-Expo software can be downloaded via the following link:

http://software.4funproject.eu/

3.9 MODULERS

3.9.1 Model purpose

MODUL'ERS is software dedicated to the human health risk assessment performed in the framework of the French regulation for the management of contaminated sites and the chemical emissions of the registered facilities. It has been supported by the French ministry in charge of Environment and is mainly intended to be used by consultants and companies. It was developed to improve the practices in the risk assessment studies. In accordance to the principles defined in the French guidance's for risk assessment, it was designed and developed to adapt to various site conditions and deepening levels of studies, to provide a transparent approach and to be helpful in conducting uncertainties analysis.

MODUL'ERS establishes the link between the definition of the site conceptual model and the step of exposure calculation, enabling the user to build a specific model for one's case study.

The end-points of MODUL'ERS are the non carcinogenic and carcinogenic levels of risks for humans, provided with various levels of aggregation (per chemical, per target organs, per route,…). However, all the intermediate results are visible.

3.9.2 Model context

MODUL'ERS is designed to assess exposure concentrations, exposure levels and chronic risk levels for organic and inorganic chemicals.
MODUL'ERS contains a library of twelve modules. Eleven of them are dedicated to the calculation of concentrations and exposure levels, relative to a medium, as a function of time. In each module, one or several mathematical approaches are proposed to calculate the concentrations. For example, the concentrations in animal tissues can be estimated with measurement data, or by a calculation at steady-state, using a bioconcentration factor, a biotransfer coefficient, or with a dynamic approach. The concentrations attributable to the studied source (contaminated soil or facility's emissions) and the total concentrations, by

adding the background concentrations, can be yielded. Exposure levels are estimated for every age class defined by the user (up to ten classes) and for an individual profile, whose exposure parameters change with one's age. A twelfth module is used to calculate the chronic exposure levels. In addition to these modules, eight variations of the module for plants and five variations of the module for terrestrial animals are given. Each of them is parameterized with a set of values relative to a type of plant (root vegetables, leafy vegetables, fruit vegetables, fruits, tubers, forage, silage and grains) or animal (cows, steers, pigs, hens and chickens).
The user has to build his model by downloading modules from the library, connecting them and selecting the transfer processes that he or she wants to include. The numerous options available enable to create a customized application.

The set of equations, input data and intermediate results are easily accessible and the changes made by the user to preset values for the input data are highlighted on the screen and in the editable report.

3.9.3 Model type

MODUL'ERS is a modelling and simulation platform, performing numerical computations.

Depending on the modules, the media concentrations can be calculated at steady state, with a dynamic approach or both.

It can compute deterministic, multiple (several runs in a same simulation, each run corresponding to a subset of different values of parameters) or probabilistic simulations. MODUL'ERS is not a real spatialized model but it can also be run in a batch way to decline a scenario in many different points of an area, varying the source terms in each point.

3.9.4 Information links

MODUL'ERS was developed by INERIS (French National Institute for Industrial Environment and Risks). The software is delivered with its whole documentation in the course of a training period of 2 days. Information is available at the following email address: modulers@ineris.fr

3.10 PBPK

3.10.1 Model purpose

In order to provide a proof of concept on how combining in vitro and in silico methods to predict target organ effects on humans under repeated dose exposure, a PBK model to predict route to route extrapolation and IVIV extrapolations was built.

3.10.2 Model context

The model was built as part of a PhD research within the COSMOS cluster part of the SEURAT 1 consortium where alternatives to animal testing are exploited. The PBK/D models mainly users are the scientific community and the risk assessors. It can be used for a wide range of chemicals: Coumarin, Hydroquinone, Caffeine, Nicotine, Isopropanol Ethanol, Estragole, Quercetin, Styrene, Methyl iodide.

3.10.3 Model type

PBK/D model is a steady-state/dynamic model developed by Monika Gajeswka and Andrew Worth and Alicia Paini as advisors from the Joint Research Center from Ispra, Italy.

3.10.4 Information link

More information could be found at the following links:

http://www.seurat-1.eu/

http://www.cosmostox.eu/home/welcome/

http://www.sciencedirect.com/science/article/pii/S0378427414001350

3.11 PEARL

3.11.1 Model purpose

PEARL (Pesticide Emission Assessment at the Regional and Local scale) is used to evaluate the leaching of pesticides to groundwater, drainage of pesticides to surface waters and persistence of pesticides in topsoil. Primary aim is to support European and Dutch pesticide registration for first and higher tier assessments. Higher tier assessments include the interpretation of lysimeter studies for pesticide registration. For assessment of pesticide leaching in the EU evaluation process, PEARL was designed to include all the information relative to the standard ground water scenarios developed by the FOCUS (Forum for the Co-ordination of Pesticide Fate Models and their Use).

The model was developed to calculate the concentrations of plant protection products in groundwater in the EU review process according to Council Directive 91/414/EEC.

3.11.2 Model context

PEARL calculates the leaching of pesticides at 1 m depth, but also allows evaluation of leaching at greater depths. As PEARL is able to describe fluctuating groundwater tables and can use information on transformation rates in subsoil, effects of these processes can be studied as well. The PEARL User Interface was developed as a user-friendly environment for running the ground water FOCUS scenarios. The interface is an integrated environment for data storage and data retrieval, model control and viewing of output data.

3.11.3 Model type

PEARL is a one-dimensional numerical model of pesticide behaviour in the soil-plant system, which has been developed by two Dutch institutes (Alterra and RIVM) in close co-operation.

Water flow in soil is described by Richard’s equation including a range of possible lower boundary conditions (for instance groundwater levels that fluctuate in response to the rainfall input). Soil evaporation and plant transpiration are calculated via multiplying a reference evapotranspiration rate with soil and crop factors. Heat flow in soil is described with Fourier’s law. The thermal properties are a function of porosity and water content and are therefore a function of time and soil depth. PEARL is based on: the convection/dispersion equation including diffusion in the gas phase with a temperature dependent Henry coefficient, a two-site Freundlich sorption model (one equilibrium site and one kinetic site), a transformation rate that depends on water content, temperature and depth in soil, a passive plant uptake rate. The model includes formation and behaviour of transformation products and describes also lateral pesticide discharge to drains. PEARL does not simulate preferential flow. Volatilisation from the soil surface is calculated assuming a laminar air layer at the soil surface. PEARL uses an explicit finite difference scheme that excludes numerical dispersion (the dispersion length was set to 5 cm).

3.11.4 Information link

The PEARL software can be downloaded via the following link: http://www.pearl.pesticidemodels.eu/home.htm

3.12 STEPS 1-2

3.12.1 Model purpose

STEPS1-2 in FOCUS is a stand-alone Surface water Tool for Exposure Predictions -Steps 1 & 2 for the derivation of PEC values in water and sediment based upon the chosen scenario. The model requires a minimum of input values (molecular weight, water solubility, $DT50_{soil}$, Koc, $DT50_{sediment/water}$, number of applications, application interval and application rate) and is designed to evaluate both active substances and metabolites.

STEPS1-2 in FOCUS is a true windows development that was programmed using Microsoft© Visual Basic and runs under Microsoft©Windows 95/98/NT/2000.

STEPS1-2 in FOCUS developer: Michael Klein (klein@ime.fhg.de)

3.12.2 Model context

The major objective of FOCUS is to implement a harmonised approach for European Tier 1 and Tier 2 risk assessments according to Council Directive 91/414/EEC. The process implementation and the scenario definitions for STEPS 1-2 in FOCUS were defined by the FOCUS Working Group on Surface Water Scenarios.

3.12.3 Model type

At Step 1 inputs of spray drift, run-off, erosion and/or drainage are evaluated as a single loading to the water body and "worst-case" surface water and sediment concentrations are calculated. The loading to surface water is based upon the number of applications multiplied by the maximum single use rate unless 3 x DT50 in sediment/water systems (combined water + sediment) is less than the time between individual applications. In such a case the maximum individual application rate is used to derive the maximum PEC as there is no potential for accumulation in the sediment/water system. For first order kinetics the value of 3 * DT50 is comparable to the DT90 value.

At Step 2 inputs of spray drift, run-off, erosion and/or drainage are evaluated as a series of individual loadings comprising drift events (number, interval between applications and rates of application as defined in Step 1) followed by a loading representing a run-off, erosion and/or drainage event four days after the final application. This assumption is similar to that developed by the United States EPA in their GENEEC model (Parker, 1995). Degradation is assumed to follow first-order kinetics in soil, surface water and sediment and the registrant also has the option of using different degradation rates in surface water and sediment.

3.12.4 Information link

The STEP1-2 software can be downloaded via the following link: http://focus.jrc.ec.europa.eu/sw/index.html

3.13 TOXSWA

3.13.1 Model purpose

TOXSWA (TOXic substances in Surface Waters) calculates predicted environmental concentrations in surface water to support the pesticide registration procedures in the Netherlands since 1999 for first and higher tier assessments. Higher tier assessments include the interpretation of field studies for pesticide registration as well as the interpretation of water-sediment studies to determine transformation rates in water and in sediment.

Since 2003 TOXSWA is used for pesticide exposure assessment in the EU evaluation process. FOCUS-TOXSWA 1.1.1 was developed in view of the FOCUS (Forum for the Co-ordination of Pesticide Fate Models and their Use) Surface Water Scenarios.

3.13.2 Model context

TOXSWA describes the behaviour of pesticides in a water body at the edge-of-field scale, i.e. a ditch, pond or stream adjacent to a single field. It calculates pesticide concentrations in the water layer in horizontal direction only and in the sediment layer in both horizontal and vertical directions. It calculates exposure in water and in sediment at the downstream end of a ditch, stream or pond neighbouring a treated field in the FOCUS Surface Water Scenarios.

3.13.3 Model type

TOXSWA was developed by Alterra, a Dutch institute. It is a pseudo-dimensional model, describing pesticide behaviour in a water layer and its underlying sediment at the edge-of-field scale.

TOXSWA considers four processes: transport, transformation, sorption and volatilisation. In the water layer, pesticides are transported by advection and dispersion, while in the sediment, diffusion is included as well. The transformation rate covers the combined effects of hydrolysis, photolysis and biodegradation and it is a function of temperature. It does not simulate formation of metabolites. Sorption to suspended solids and to sediment is described by the Freundlich equation. Sorption to macrophytes is described by a linear sorption isotherm. Pesticides are transported across the water-sediment interface by diffusion and by advection. FOCUS-TOXSWA handles transient hydrology and pesticide fluxes resulting from surface runoff, erosion and drainage as well as instantaneous entries via spray drift deposition.

In order to simulate the flow dynamics in an edge-of-field water body in a realistic way, the field-scale system is defined as the downstream part of a small catchment basin. Water flow is described with the aid of a simple water balance, accounting for all major incoming and outgoing water fluxes. The water level is a function of time, but assumed to be constant in the water body system considered. Water levels are calculated either by assuming uniform flow conditions (Chézy-Manning equation), or by assuming a backwater curve in front of a weir.

TOXSWA uses an explicit finite-difference scheme to solve the water balance and mass conservation equations. Distances between the nodes in the water and sediment layers are in the order of magnitude of metres and millimetres, respectively.

3.13.4 Information link

The TOXSWA software can be downloaded via the following link: http://www.pesticidemodels.eu/toxswa/download

3.14 USEtox

3.14.1 Introduction/objectives

USEtox™ is used for characterising human and ecotoxicological impacts in the framework of the LCIA (Life Cycle Impact Assessment) and the CRA (Comparative Risk Assessment). USEtox calculates characterisation factors for human toxicity and freshwater ecotoxicity. The human toxicity to a chemical is evaluated by estimating the intake fraction, which is derived from the environmental fate and human exposure, and the human effect factor, which is estimated from the dose-response and the chemical severity. The fresh water ecotoxicity is evaluated by estimating the fate factor and the ecotox effect factor derived from the concentration–response and the fraction of species potentially affected. USEtox™ is implemented in Microsoft Excel® and applied for 3000+ organic chemicals and 20+ metal species.

3.14.2 Context

In 2005, a comprehensive comparison of the models used for the toxicity characterisation for the LCIA was initiated by the United Nations Environment Program (UNEP) – Society for Environmental Toxicology and Chemistry (SETAC) Life Cycle Initiative. The main objectives of this effort were:

- To identify specific sources of differences between the models' results and structures;
- To detect the indispensable model components;
- To build a scientific consensus model from the models.

This effort led to the development of USEtox™, a scientific consensus model that contains only the most influential model elements.

3.14.3 Chemical considered

Organic chemicals and metal species

3.14.4 Model type

- Spatial scale: Global and continental scales are considered
- Environmental media:
    1. Continental scale: Rural air, urban air, agricultural soil, natural soil, freshwater, and coastal marine water
    2. Global scale: Rural air, agricultural soil, natural soil, freshwater, and ocean
- Calculation method: The fate model part of USEtox™ calculates the residence time of a chemical, based on the quantification of all these environmental processes. This is done, by solving the mass balance under steady state conditions with the help of linear algebra calculation rules. In this context, steady state means that concentrations do not change over time in the compartments considered, when there is a constant emission rate.
- Transparency :

The formulas to calculate the fate factor (environmental fate) are not presented in the user manual. Users are allowed to see those formulas only on the excel sheet but they are not shown in a user-friendly manner.

- Other remarks :

USEtox™ returns 'characterization factors' as final outputs. For Non LCA practitioners, the definition may not be as straightforward as exposure concentration in humans. However, the user manual can help users understand it.

3.14.5 Information link

http://www.usetox.org

4 Comparative assessment

The comparative assessment of exposure models was performed in two ways: via the results of the MCDA Weight of Evidence approach and via expert judgement.

4.1 MCDA Weight of Evidence approach

As mentioned in 2.2, the relevance criteria/questions were highly dependent on the framework/scenario of the experts. Therefore, the criteria were split into two hierarchies: relevance criteria/questions (hierarchy 1) and general criteria/questions (hierarchy 2). The importance of the relevance/criteria questions was scored for a certain type of framework (Regulations, directives, etc.).

The questionnaire was filled in for 14 exposure models and processed using the knowledge database obtained from Step 1 of the MCDA approach. The MCDA methodology is using hierarchical aggregations. The scores are analysed for each expert separately before they are aggregated to the overall scores. This resulted in a:

- General score for each model/framework (both hierarchies)
- Score for each model/framework for hierarchy 1
- Score for each model for hierarchy 2
- Score for each model/framework/category for hierarchy 2
- Score for each model/framework/subcategory for hierarchy 2
- Score for each model/category for hierarchy 1
- Score for each model/subcategory for hierarchy 2

The scores range between 0-1, the higher the number the better this model scores in a certain framework, in the general model aspects, in a certain category or in a certain subcategory.

4.1.1 Hierarchy 1: Relevance/framework specific criteria

A score was assigned to each model per framework (Figure 1). The following remarks/conclusions can be made from the graphs:

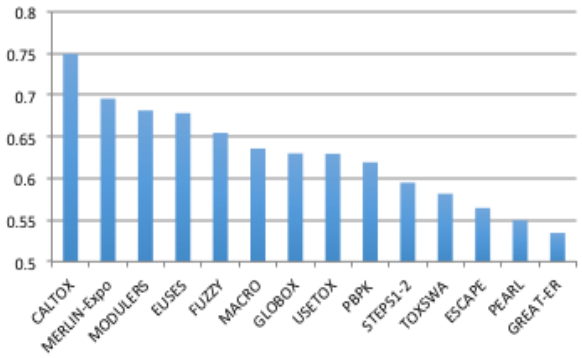
- The scores are for most frameworks between 0.5 and 0.85, which suggests that the variance between the models is small. As determination of a confidential interval is not possible with this methodology, it is very difficult to assess whether models are significantly different or not.
- The Fuzzy Model, which was scored ‘Not applicable’ or ‘No’ to a lot of the relevance questions leads to high scores in some frameworks. This gives a potential wrong interpretation that these models perform well in these frameworks. Therefore the scores of this model are not taken into account and are not further discussed. This is similar to the scores of the PBPK model, which only focus on the transport and degradation of chemicals inside the human body. It therefore does not cover a lot of the questions from the questionnaire.
- The multimedia models such as MERLIN-Expo, CalTOX, EUSES and MODULERS in general have the highest scores for all the frameworks. These multimedia models cover mostly a lot of media and contain a lot of different processes, etc., which explains the higher scores of these models. Slightly lower scores can be found for the LCA multimedia models GLOBOX and USEtox. These models are generally less detailed than the before mentioned models. Lastly in the order, we can find for the

majority of frameworks that the models which or mainly focused on one or more compartments score lower (e.g. Macro, Pearl, Toxswa, etc.).

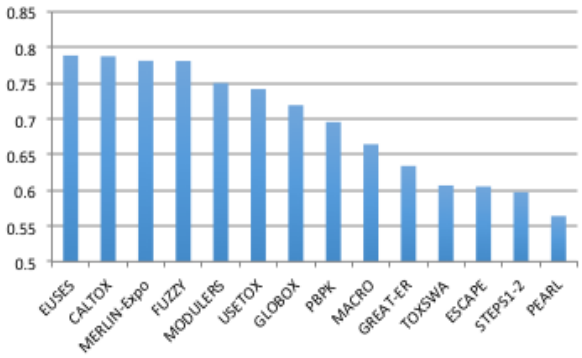
- The scores for MERLIN-Expo are quite good in all considered frameworks, which indicate that MERLIN-Expo is a flexible model that can be used in different frameworks.
- EUSES scores highest in the REACH framework, which follows the recommendations to use EUSES as a model for exposure assessment under REACH.
- It can be derived from the results that the models, which are at the moment recommended for use in the PPP regulation, do not score very well for this regulation. This is an illogical observation since the PPP models were specifically designed for the PPP regulation. This is caused by the fact that these models are not multimedia models and therefore receive a lower score on several criteria. It does not mean they are not applicable/suitable for this regulation.
- The scores for the sustainability framework are higher compared to the other frameworks. This is also in contrast to what was expected as most of the criteria/questions for this framework were not very applicable and therefore received a low importancy score. In contrast, the site specific assessment is a framework which is not strictly bound to any EU regulation and which can have a very broad range of application and is therefore quite applicable to all criteria (i.e. it received a fairly high score on importance for most of the criteria). Nevertheless, scores are lower than the other frameworks.

Hence from the conclusions/remarks made above it can be concluded that some of the MCDA weight of evidence approach outcomes were found to be insufficiently suitable for the comparative assessment of models. Other outcomes are in line with what would be expected.

A.



B.



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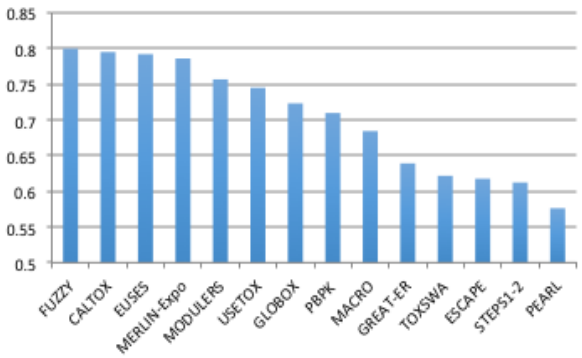

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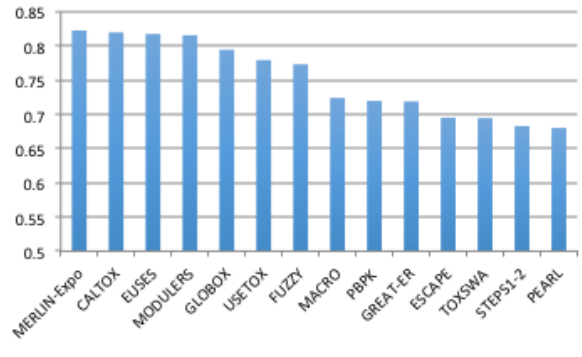

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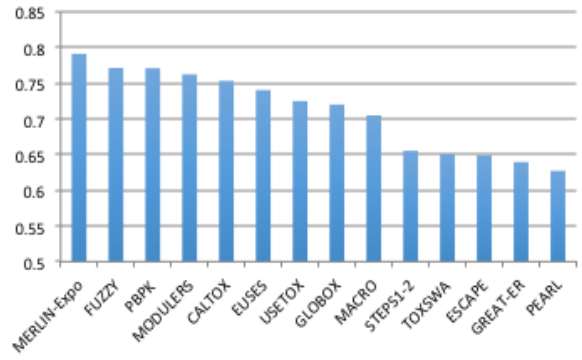
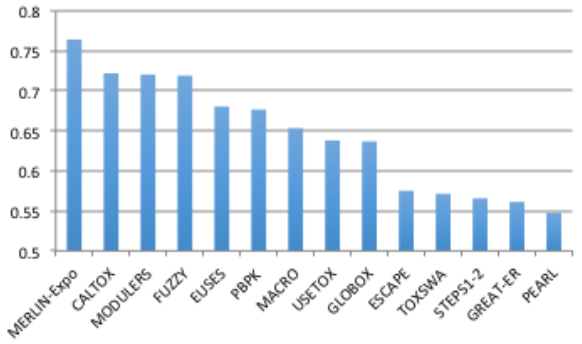


F.



G.

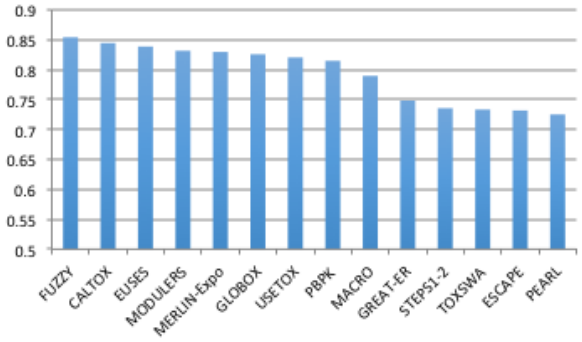


Figure 1: An overview of the scores of the 14 exposure models per framework (A. PPP Regulation, B. REACH regulation, C. Biocidal Product Regulation, D. Environmental Oriented Directives, E. Food Oriented Directives, F. Site Specific Assessment, G. Sustainability).

What concerns the MERLIN-Expo model, based on the responses of the questionnaire the following aspects could be considered to be included (not in order of importance):

- Exposure to worker (perhaps also bystander for PPPs)
- Concentrations in ground water, marine water, eggs and earthworms
- Dermal absorption
- Non-linear sorption
- Sediment burial
- Influence of food processing
- Bioavailability in the human body
- Saturation process in the human body
- Spatially explicit outputs
- Formation of metabolites
- Inclusion of spray drift (specifically for PPPs)

4.1.2 Hierarchy 2: General model criteria

The general model criteria are criteria, which are related to user-friendliness, documentation, uncertainty-, sensitivity-analysis, validation, etc. and are not directly related to a certain framework. This is in contrast to the criteria in hierarchy 1, where the scoring of the criteria was highly dependent on the type of framework.

From Figure 2 the following conclusions can be drawn:

- The scores of the different models vary between 0.7 and 0.9; hence this suggests variation between the models is low. It is not clear whether there are statistically differences between models.
- Pearl is the model, which scores 'yes' on 60 out of 82 criteria. Pearl is a model which has an obligatory use in the framework of the Plant Protection Product Regulation and is therefore regularly updated and continuously supported. The model has a clear defined use; is spatially and temporally clearly defined; the model structure, equations, media, processes, variables, etc. are clearly defined in publications and manuals; is well validated. Pearl is also very user-friendly with a clear user interface, helpdesk, free availability, etc.
- USEtox scores 'yes' on only 33 out of 82 criteria. USEtox is mainly based on USES, which was also the framework EUSES is built upon. EUSES also scores quit low, which is logic if they are based on the same model. USEtox and calTOX are both spreadsheets models, which might decrease the user-friendliness of the models.
- The MERLIN-Expo model scores high compared to the other exposure models. What could still be considered to be improved or added based on the criteria is:
    - Justification on worst-case assumption of certain default parameters
    - No comparison of results is yet performed for reference scenarios using other models (will be dealt with in WP4)
    - Comparison of the model results with monitoring data is currently lacking (will be dealt with in WP5)
    - Calculated intermediate results can not be overwritten with e.g. measured data
    - Test examples are not yet available (will be dealt with in WP3)
    - Metabolite formation is not included in the current version of the model

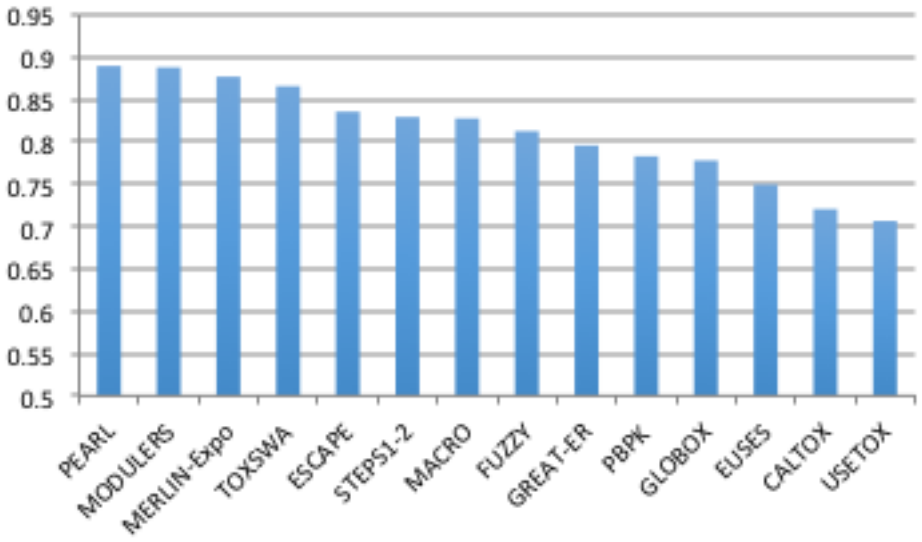


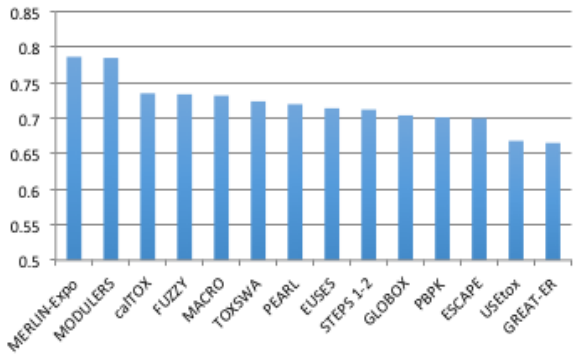
Figure 2: An overview of the scores of the 14 exposure models for hierarchy 2: general model criteria.

4.1.3 Combination of hierarchy 1- 2

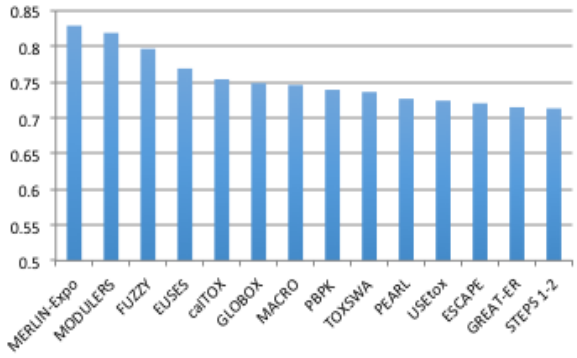
Figure 3 presents the scores of the 14 exposure models for the 7 different frameworks when hierarchy 1 (framework specific criteria) and hierarchy 2 (general model criteria) are combined. From these graphs, it could be concluded that:

- The range of the scores of the different models is even smaller compared to the ranges of scores of hierarchy 1. This is probably caused by the smaller variation in scores between models in hierarchy 2. As it is not possible to determine whether one model is significantly different from another, it is difficult to draw absolute conclusions.
- MERLIN-Expo and MODULERS, which are both based on the ECOLEGO software, received the highest score in all frameworks. These models score high in hierarchy 1 and hierarchy 2.
- EUSES and calTOX which scored fairly high in hierarchy 1, score in most framework more average. This is caused by the fact that these models score lower on the general model criteria.
- PEARL, which for most frameworks scored low, increases in the ranking due to its high score in hierarchy 1.

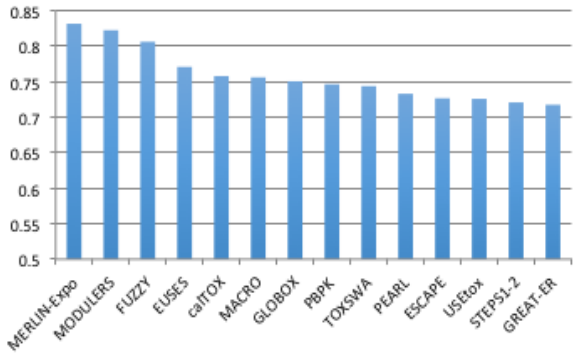
A.



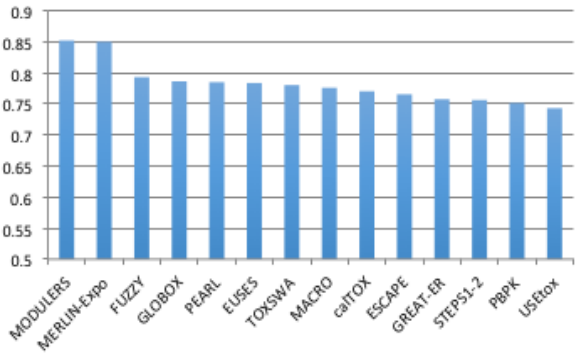
B.



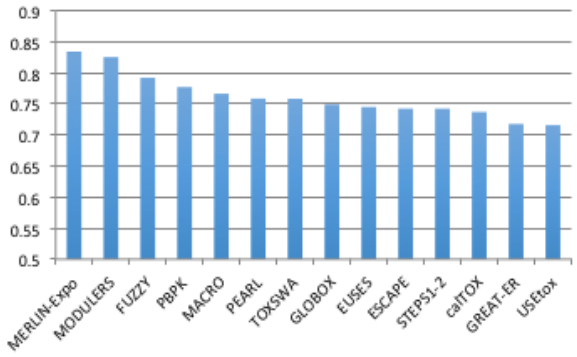
C.



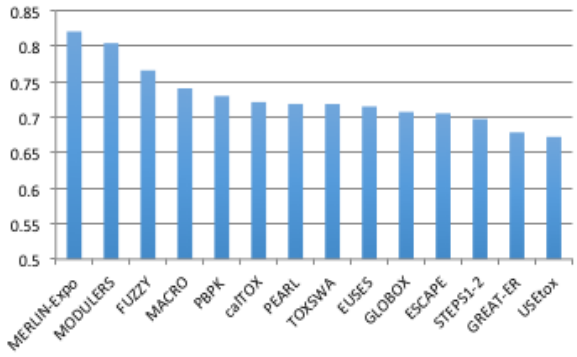
D.



E.



F.



G.

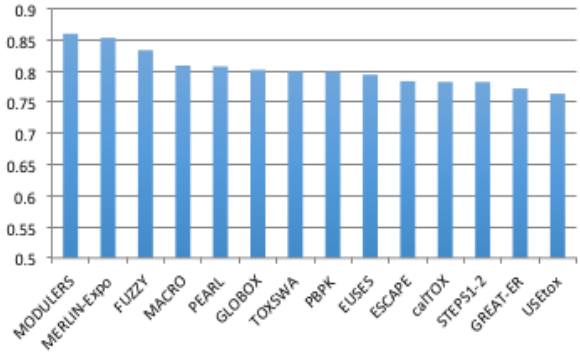


Figure 3: An overview of the scores of the 14 exposure models per framework (A. PPP Regulation, B. REACH regulation, C. Biocidal Product Regulation, D. Environmental Oriented Directives, E. Food Oriented Directives, F. Site Specific Assessment, G. Sustainability).

4.1.4 Conclusion

The results of the MCDA approach cannot be used on its own (without additional expert judgement) for the comparative assessment of the selected exposure models, because in general:

- The range of scores of the different models was fairly small and determination of a confidential interval is not possible with this methodology, hence it is very difficult to determine whether results for the models are significantly different or not
- Inconsistent results were observed for models not covering a lot of the criteria (e.g. the fuzzy model received a high score for certain frameworks) or models, which are specifically designed for certain frameworks.

4.2 Expert judgement

4.2.1 Quantitative analysis based on the importance scoring of hierarchy 1

In Step 1: analysis of the hierarchical structure the relevance criteria were scored based on their importance in a certain framework. This scoring was used to calculate a score for each exposure model depending on the framework. Based on their 'yes' answer to the relevance criteria a score was obtained as follows:

- All 'yes' criteria got a score of 1, all 'no' criteria 0
- These scores were multiplied with the scoring presented in Table 1 per criteria
- All scores were summed

This resulted in a final score per framework (see Table 2).

Table 2: Total score of the selected exposure models per framework based on only the relevance criteria

	Reach	PPP	Biocide	Environmental oriented Directives	Food oriented directives	Site specific impact assessment	Sustainability
MERLIN-Expo	199	206	194	142	146	**221**	84
CalTOX	178	**201**	174	134	115	184	79
EUSES	**197**	190	190	135	111	177	79
GLOBOX	**167**	161	160	124	99	156	69
MODULERS	166	**184**	164	126	117	182	76
USEtox	**164**	153	157	110	93	145	61
Fuzzy model	**40**	**40**	39	31	29	39	19
GREAT-ER	**72**	67	67	59	42	64	30
PBPK	66	67	66	36	71	**89**	34
PEARL	61	**87**	60	61	37	74	26
STEPS1-2	82	**101**	82	61	50	81	34
TOXSWA	65	**77**	65	54	39	65	27
MACRO	62	**85**	62	59	40	71	29
ESCAPE	52	**66**	51	45	35	60	21

In general, based on Table 2, it can be concluded that the multimedia models obtained a much higher score compared to the other models, which are more focused on one or more compartments. What concerns the frameworks, it can be concluded that the selected models are least applicable to assess sustainability. Exposure assessment in e.g. Cradle2Cradle assessment is less detailed and therefore requires less complex models. The food and environmental oriented frameworks cover less compartments/media than REACH, PPP, Biocides and site-specific assessments, therefore the selected exposure models have lower scores for these types of frameworks.

More specifically for each model:

- **MERLIN-Expo** has the highest overall score and appears to be ideal for use in **site-specific assessment**. The MERLIN-Expo model, which is a multimedia model containing a lot of processes and media, contains an environmental exposure model AND a model able to calculate internal concentrations of chemicals in the human body (PBPK model). The extensive environmental exposure model and the presence of a pharmacokinetic model leads to a higher score compared to the other models, which in general do not contain a PBPK model. As site-specific assessments are less restricted to regulations and can be very variable depending on national, regional or local requirements, a lot of the relevance criteria might potentially be important. Hence, the combination of both makes the MERLIN-Expo model highly suitable for site-specific assessment.
- The **CalTOX** model has a high score for use in the **PPP** regulation as it covers some processes which are important in this regulation such as: it covers exposure to subpopulations, concentrations in pore water, volatilization from vegetation, linear/non-linear sorption, the vegetal transpiration process, crop interception, irrigation, wide dispersive use and exposure to bystanders. Nonetheless, CalTOX is not completely compliant with the PPP regulation. For example, CalTOX does not cover point source releases, the formation of metabolites, etc. Moreover, for some compartments, the models to be used are predefined. E.g. to determine the concentration in ground water, PEARL or PELMO should be used.
- **EUSES** obtained the highest score for **REACH**, which is expected, as the model is, recommend for use in the REACH regulation. Similar scores were obtained for the PPP and Biocide Regulation.
- **GLOBOX**, which is more or less based on EUSES, also appears mostly suitable for **REACH**, however it does not contain some essential aspects necessary for REACH: no worker/general population exposure, no concentrations in earthworms, no local scale, etc. A lot of the background processes available are in compliance with REACH, however the outcome are characterisation factors and not exposure concentrations which makes this model not applicable for the REACH regulation.
- **MODULERS** received the highest score for the **PPP** regulation and for **site-specific assessment.** MODULERS contains some PPP specific aspects such as, linear/non-linear sorption, excretion/degradation by animals, food processing, irrigation and wide dispersive release.
- **USEtox,** which was also based on EUSES, obtained the highest score for the REACH regulation. Similar to GLOBOX, the outcome are characterization factors which is useful in LCA frameworks but not useful in REACH.
- **Fuzzy model** has a low score in all frameworks and will not be taken further into account.
- **GREAT-ER** is recommended as a higher-tier model for the fate of chemicals in surface water in the REACH regulation. This explains the highest score of this model for this framework. However, as its use is limited to exposure to water, the score is fairly low compared to the multimedia models. Therefore this model will not further be included in the comparative assessment.
- **PBPK** is a pharmacokinetic model and is therefore focused on determining the internal concentrations in the human body. This model scored highest on the site-specific assessment as this type of assessment might take internal concentrations

into consideration, which is currently not the case yet for e.g. REACH, PPP and biocides. This model will not further be included in the comparative assessment.

- **MACRO, PEARL, STEPS1-2, TOXSWA, ESCAPE** obtained the highest score for the PPP regulation. All these models are recommended by the authorities for use in the environmental exposure assessment of plant protection products. As they are not multimedia models and therefore less suitable for comparison, these models will not be further discussed.

4.3 Advantages and disadvantages of the selected multimedia models

A literature search on the multimedia models listed above was performed in order to document the advantages and disadvantages.

CalTOX	
ADVANTAGES	**DISADVANTAGES**
• Multiple exposure routes and pathways can be evaluated • Applicable for a wide range of chemicals • Re-suspension of soil particles from soil to air • Advanced modelling of soil (three vertical layers) • It incorporates ageing of chemicals • It allows dynamic modelling in soil layers • Oral ingestion via several routes: 1) ingestion of groundwater or surface water as drinking water, 2) ingestion of plants contaminated by transfer from air, surface soil, root-zone soil and irrigation water, 3) ingestion of meat, dairy products and eggs contaminated by inhalation of air and ingestion of water, plants and surface soil by the animal, 4) ingestion of fish contaminated by surface water, 5) ingestion of surface water during recreational activities and 6) incidental ingestion of soil. • Free • Accessibility to all equations and intermediate results • Easy export/import of data/results • Weighted average of human intake at conditions with and without rainfall • Able to simulate time varying source concentrations • Can be used to generate a distribution	• Marine environment and coastal zone not included for fate modelling • Only evaluates exposures for adults and nursing infants in contact with the local environment • It assumes a closed system at continental scale for all organic chemicals and a removal via surface water to the ocean for metals. • No purification of drinking water is introduced • Only for low concentrations. • Default parameters are set for Californian residents • No facility for performing cumulative assessments for multiple chemicals • Limited treatment of dietary exposures in terms of concentration levels in food as eaten and consumption patterns • Unable to perform acute and intermediate duration exposure assessments. • Limited range of pollutants • Only one spatial scale • One generic soil compartment (no industrial, natural and agricultural soil) • Does not account for temperature and pH dependency of some substance properties • Not a fully dynamic model since emission incidents cannot be introduced other than at the initial stage. • No dynamic modelling in air, surface

of possible exposure levels and health risks • All input parameter values can be distributions • It includes parameter sensitivity analysis and uncertainty importance ranking, it also includes Monte Carlo Uncertainty analysis using Crystal Ball • Many parameters can be estimated using other parameters (QSARs) • Ability to adapt all parameter values •	water and sediments • No initial pool of contaminants possible in sediments • Only two classes of age: infant/adult • Not applicable for ionic organic chemicals • Not applicable for time periods less than one month • Limited in the extent of the environmental settings (not for landscapes in which water occupies more than 10% of the land surface area and for small areas/sites) • No control of the range of values introduced by the user • No user-friendly GUI, excel based • Fixed units • Limited output of risk values, only risk assessment for humans

(RISKCYCLE, 2011; Sonneman *et al*., 2005; Huijbregts *et al*., 2005; Maddalena *et al*.; 1995; Bonnard, 2006)

EUSES	
ADVANTAGES	**DISADVANTAGES**
• It has the ability to deal with a variety of substances. • Initially requires relatively few input parameters • Stable • A lot of media considered • Uncertainty analysis available • Considers a variety of different exposure sources – occupational, consumer and environmental • Able to function at various levels of the risk assessment framework • Can evaluate multiple exposure pathways and aggregate these results • Operates at a variety of spatial scales • Implemented step-by-step input • Control of range of data introduced by the user • Possibility of introducing the data in different units • Great amount of different output data • Great amount of European default data	• It is a conservative approach using reasonable worst case assumptions and default values • It is not designed to perform site-specific exposure assessments • Only steady-state simulations • The chemical applicability of the system has been found to be limited • EUSES links the overall uptake to probable health endpoints through exposure/response relations without taking into account the toxicokinetics/toxicodynamis and the related internal dose • It includes no method for incorporating variability and uncertainty into exposure assessments • High complexity • Low modularity • Incomplete documentation • It is possible to input physically impossible data • Does not provide minimal network

• Wide range of time and spatial scales • Implemented life-cycle steps for individual assessments • Contains the model SimpleTreat: a model to predict the distribution and elimination of chemicals by sewage treatment plants • Recommended by ECHA for exposure assessment in the REACH regulation and the Biocide regulation	support • Does not exercise the options offered by the Windows operating system • No combined assessment of substances • Difficulties in the operation of certain substances • Includes no method for incorporating variability and uncertainty into exposure assessments • Data exchange/export is difficult and does not work automatically • No graphical visualization of the results • No sensibility/uncertainty analysis

(Schwartz *et al*., 1998; www.tags.cperi.certh.gr, RISKCYCLE, 2011; Sonneman *et al*., 2005)

GLOBOX	
ADVANTAGES	**DISADVANTAGES**
• Spatial differentiation (separate countries and oceans) • Metal specific processes in freshwater and marine environments handled • Inclusion of spatially differing parameters in the model equations (e.g. temperature dependency of degradation) • Developed for LCA, but it is a multimedia model for fate, exposure and effect modelling. One possible application is the analysis of distribution and exposure patterns, resulting from the emission profile of a certain chemical in a certain region • Spatial differentiation of fate parameters AND intake parameters • Temperature dependency of environmental degradation rates • Number of aquatic environmental compartments is larger than in most multimedia models (rivers, freshwater lakes, salt lakes and groundwater)	• Regions distinguished are very different in size and are characterised by a wide variation in environmental parameters • The modelling of export and import of food for determining the intake by humans requires data and assumptions that may introduce additional uncertainty • Steady-state model which is sufficient for LCA CFs, however they are more difficult to validate, since it requires well documented steady state situations • Differentiation at the level of countries and seas has advantages with respect to data availability

(RISKCYCLE, 2011; Sleeswijk & Heijungs, 2010)

MODULERS	
ADVANTAGES	**DISADVANTAGES**
• Flexibility: choice between measurement data or using a modeling approach for media concentrations and external doses • Selection of the transfer processes to take into account by the user • Several models for the same mechanism can be provided to assess the uncertainties due to models • The choices can be different among chemicals studied • Ability to define the number of age classes to define the human receptor (up to 10 class ages) • Reconstruction of the exposure dose during the exposure period using the change of the value of the exposure parameters with age • References and information on the predefined values of the parameters provided inside the software • Access to all the equations, parameters and intermediate results by hyperlinks • Tests stopping the simulation if the user forgot to assign significant values to the input data • Models to assess indoor air concentration due to soil contamination • Ability to perform multi-simulation, changing the value of one or several parameters • Export to Excel and import of data from Excel	• Devoted to the risk assessment for a local source due to contaminated sites or emissions of facilities • Language: French • No calculation of the internal doses • Simple approach for surface water • Some calculations assuming a source at steady-state • No lateral transfer of chemical • No GIS integrated

(Bonnard, personal communication, 2014)

USETOX	
ADVANTAGES	**DISADVANTAGES**
• Contains a database of over 3000 organic chemicals • Intermittent wet atmospheric deposition • Parsimonious and transparent model • Forms the basis of the recommendations from UNEP-SETAC's Life Cycle Initiative	• Quality of the data • No spatial differentiation • Insufficient accuracy of the environmental behaviour of metals and ionizing compounds • Exposure and effect modelling is insufficient for the marine and terrestrial

• Model uncertainty was partly quantified • Regular trainings are provided • Helpdesk and user-forum available	compartment • There is uncertainty and variability related to input parameters • Assumption of homogenous compartments results in uncertainty • The vegetation model does not include degradation • It does not account for speciation of metals and other important specific processes for metals, metal compounds and certain types of organic chemicals • The following exposure routes are not available: indoor air and dermal exposure • No user-friendly GUI, excel based • Documentation not yet available

(Rosenbaum et al., 2008, 2011)

5 SWOT analysis of the MERLIN-Expo model

A SWOT analysis is a structured planning method used to evaluate strengths, weaknesses, opportunities, and threats. It involves specifying the objective and identifying the internal and external factors that are favourable and unfavourable to achieve that objective.

Based on the MCDA weight of evidence approach and the literature review combined with expert expert judgement on selected multimedia models a SWOT analysis is performed on the MERLIN-Expo MERLIN-Expo model. An overview of the strengths, weaknesses, opportunities and threats is presented presented in Table 3 and

Table 4, for respectively, relevance/framework dependent aspects of models (cfr. Hierarchy 1) and for general model aspects (cfr. Hierarchy 2).

All identified points that arose from the MCDA analysis and the literature review were categorized into strengths and weaknesses. Threats and opportunities were determined based on respectively strengths and weaknesses, if applicable. Strengths and weaknesses are on their turn divided in general aspects and detailed aspects.

The following remarks should be made to the tables:

Based on the answers to the questionnaire (Appendix C), a comparison of the 'yes' answers was answers was performed between the MERLIN-Expo model and the other multimedia exposure models to exposure models to identify the strengths and added value of the MERLIN-EXPO model. A criterion where model. A criterion where only the MERLIN-Expo model (or maximum one other model scored 'yes'), was scored 'yes'), was considered as a strength and was included in Table 3 and

Table 4. Similarly, based on the 'no' answers, the weaknesses/shortcomings of the model were compared with the other multimedia exposure models (Appendix D). A criteria where the MERLIN-Expo model scored 'no' (with maximum one extra model also scoring 'no'), was considered to be a weakness and was also reported in Table 3 and

- Table 4. Hence, there are more strengths than listed in the summary, however not to make the list to extensive, the added value and the weaknesses compared to the other models were highlighted.
- The general strengths listed below could serve as a basis to market the MERLIN-Expo model as this highlights the added value.
- The weaknesses/opportunities can be considered as actions, which can be implemented, if desirable and feasible.

Table 3: SWOT analysis of the MERLIN-Expo model with a focus on relevance/framework dependent aspects and processes of models

Strengths		Threats	Weaknesses		Opportunities
General	**Detailed**		**General**	**Detailed**	
Covers internal absorption, distribution of substances, biotransformation, accumulation and excretion in/from the human body and determines concentrations in the human body, organs and blood (PBPK model)		Not all regulations require this		Saturation process in the human body is missing	Implementing the saturation process in the human body
				Bioavailability in the human body is missing	Implement bioavailability in the human body
Applicable for a wide range of chemicals		Not all regulations require this		No speciation and bioavailability processes for metals included	Implement speciation and bioavailability processes for metals
It covers the majority of the processes, media, exposure routes and human populations	Covers excretion and degradation by animals	Not all regulations require this	Not all processes, media, exposure routes and human populations are covered	No calculations in ground water	Implementing a ground water model
	All ages can be evaluated	Not all regulations require this		No non-linear sorption	Implementing non-linear sorption
	Discriminates between background and anthropogenic concentrations	Not all regulations require this		No sediment burial	Implementing sediment burial
	Covers an editable transport factor of the substance at harvest of the vegetation	Not all regulations require this		No dermal exposure	Implementing dermal exposure
	Performs cumulative (i.e. parallel) exposure assessment of multiple chemicals	Not all regulations require this		No ageing of chemicals in soil	Implementing ageing of chemicals in soil
				No concentrations in eggs	Implement calculation of concentrations in eggs
				Marine environment and coastal zone not included for fate modelling	Implementing a marine compartment

				No concentrations in earthworms	Implementing equations to calculate earthworm concentrations for secondary poisoning
				No Influence of food processing	Food processing could be included before ingestion
				No formation of metabolites	Implementing metabolite formation cfr. MACRO, PEARL
				No purification of drinking water	Add a purification step before ingestion of surface water
				Inclusion of spray drift	Inclusion of a drift calculator based on Ganzelmeier
				No ingestion of surface water during recreational activities	Insert ingestion of surface water during recreational activities
				No weighted average of human intake at conditions with and without rainfall	Insert weighted average of human intake at conditions with and without rainfall
				Does not contain a model for elimination of chemicals by sewage treatment plants and sludge application on soil	A model for the elimination of chemical by sewage treatment plants can be inserted, e.g. SIMPLETREAT
				No lateral transfer of chemicals	Inclusion of the advection process
				Does not consider occupational and consumer exposure	Implementing an occupational and consumer exposure model
				No indoor air exposure	Implementing an indoor air compartment
				One generic soil compartment	Differentiate between industrial, agricultural and natural soil, cfr. EUSES

Table 4: SWOT analysis of the MERLIN-Expo model with a focus on general model aspects

Strengths		Threats	Weaknesses		Opportunities
General	**Detailed**		**General**	**Detailed**	
QSARs are available to estimate certain parameters		Unreliable results because QSAR predictions can be highly uncertain and/or not applicable			
User-friendly model	User-friendly GUI		Helpdesk and user forum are not available yet		Setting up a helpdesk and user forum
	Easy import/export of data/results			Test examples are not yet available	Include test examples (will be dealt with in WP3)
	Control of out of range of values introduced by the user		Only exposure, no risk assessment		Hazard assessment should be added to calculate risks
	Implemented step-by-step input				
	Graphical visualization of the results				
Complete documentation for novice and expert	Extrapolation rules are indicated		Default parameters	Justification of certain default parameters	Include justification in documentation
	Number and origin of the data used to estimate parameter values from empirical data is clearly indicated		Substance database	Limited quality control of the substance data	Perform quality control or only keep QC data
	Applicability domain of QSARs or read-across is well indicated			Limited range of pollutants in the database	Expand the database
	Number and origin of the data used for QSARs or read-across is well indicated			Requires a relatively large amount of input parameters if the substance is not in the database	Expand the database

	Model assumptions using the Bayesian approach to estimate parameter values are clearly indicated				
	Number and origin of the data allowing calculating the posterior distribution of parameter values estimated using a Bayesian approach are clearly indicated				
	Type (conservative, mean, mode or best-estimate) of default value is clearly indicated				
	The database used for generating probability density functions of parameters are clearly identified				
Regular trainings are provided		No continuation after termination of the project, low attendance			
Models were verified	Implementation of equations was verified		Validation	No comparison of results for reference scenarios using other models	Will be dealt with in WP4: benchmarking
	Numerical solutions were verified by comparing the results with analytical results or with other number solvers			Comparison of the model results with monitoring data is lacking	Will be dealt with in WP5: case studies
Modular and flexible model	All parameter values can be adopted	Misuse by users, potentially lower acceptability by regulators as it less standardized		Intermediate results can not be overwritten	Insert functionality were intermediate results can be overwritten by e.g. measured data
	No fixed units		Undefined scope	Not recommended or authorized for use in any	Advocacy

				regulation yet	
	Ability to perform multi-simulations changing the values of one or several parameters			Not fully compliant with the REACH, PPP, Biocide regulation	Make equations/parameters compliant to one of the regulations
	Equations and intermediate results are highly accessible				
	Able to simulate dynamic scenarios	Not all regulations require this	Spatially explicit outputs		Consider implementation of spatially explicit GIS based models

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7 Appendices

7.1 Appendix A: Hierarchical structure of the assessment methodology based on LoE, Categories, Criteria and Questions: general criteria

LoE	Category	Sub-category	Question
Contextual knowledge	Model purpose	Model goal	Are the outputs that the end-user is able to calculate clearly defined? (e.g. units, unambiguous definition, etc)
			Are the potential decision(s) that can be taken from the model outputs clearly defined? (e.g. screening level assessment, priority setting, labeling, higher exposure tier, etc)
			Are the regulatory framework(s) that the model could be useful for clearly defined? (e.g. REACH, Water Framework Directive, Biocide directive, etc)
	Model applicability	Spatial and temporal issues	Is the spatial applicability domain clearly defined? (e.g. area and/or volume(s) dimensions, near-field vs global scale, spatial boundaries, minimum spatial resolution)
			Is the temporal applicability domain clearly defined? (e.g. minimum temporal resolution, capability to account for daily/monthly/seasonal variability, etc)
			Is the capability to simulate dynamic scenarios (e.g. intermittent emissions, accidental emissions) explicitly indicated?
		Chemicals	Are the chemicals (or family of chemicals) for which the model is applicable (and inversely non applicable) clearly defined?
			If the model is partially applicable for some chemicals, are the applied extrapolation rules indicated? (e.g. read-across, extrapolation from neutral organics to ionic organics, etc)
Conceptual knowledge	Model structure	Media	Are the media that are included in the model clearly defined?
		Emissions and losses	Are the emissions that can be used as input data in the model clearly defined, e.g. point and/or diffuse sources to surface waters, atmosphere, soils, etc?

			Are the chemical losses from the system that are governed by transport processes (e.g. advection, diffusion) clearly defined?
			Are the chemical losses from the system that are governed by chemical processes (e.g. degradation) clearly defined?
		Exchange processes	Are the chemical exchanges between media clearly defined?
			Are potential chemical exchanges with other coupled models clearly defined?
	Variables	Forcing variables	Are the meteorological forcing variables (e.g. rain, wind speed, temperature, etc) that are necessary for the simulation clearly defined (e.g. time and spatial resolution, units, etc)?
			Are the agronomical and anthropogenic forcing variables (e.g. harvest period, spatial distribution of crops, time and spatial patterns, etc) that are necessary for the simulation clearly?
			Are the other forcing variables that are necessary for the simulation clearly defined?
	Parameters	State variables	Are the state variables that are calculated by the model clearly defined (e.g. unambiguous definition, units, etc)?
			For a given state variable, are the other components of the model that are necessary for its calculation (e.g. parameters, forcing variables, other state variables) clearly and comprehensively defined?
		Parameters	Are the parameters that are necessary for model calculation clearly defined (e.g. unambiguous definition, units, etc)?
			Are the scenario-specific parameters that must be updated by the end user for each case study clearly identified and distinguished from generic parameters? (e.g. e.g. river depth, land use coverage, vegetables production in the investigated region, etc)
Process knowledge	Scientific background	Process relevance	For each process included in the model, is its relevance justified from the scientific background?

			Does the documentation include a list of processes that are not included in the model, with a justification of their exclusion?
		Alternative and limits	For the model selected for representing a given process, is its applicability domain clearly defined? (e.g. chemicals, spatial and time issues, etc)
			If relevant, are the alternative models available in the literature for representing a given process presented and critically evaluated?
		Model typology	For each process included in the model, is it indicated (with justification) if this latter is based on mechanistic considerations or empirical relationships (e.g empirically fitted multilinear relationship between a state variable and parameters)?
			For each process represented in the model, is it indicated (with justification) if this latter is based on steady-state or dynamic assumptions?
	Model equations	Equations	Are model equations clearly and comprehensively documented?
Numerical knowledge	Initial conditions	Initial conditions	Are the default values proposed for the initial conditions (e.g. concentrations in media at time zero) clearly defined?
			Can the initial values be modified by the end-user for each new simulation?
	Forcing variables	Forcing variables	Are the default values proposed for the forcing variables (e.g. atmospheric conditions) clearly defined?
			Can the values for forcing variables be modified by the end-user for each new simulation?
	Parameter values source	Calibration	If parameter values were estimated from calibration using empirical data, are the number and origin of the data clearly indicated? (e.g. name and accessibility of the databases, literature references, etc)
			If the parameter values were estimated from calibration using empirical data, is the uncertainty margin indicated? (e.g. probability density function, mean and standard deviation, quartiles, etc)
		QSAR or read-across	If QSAR or read-across are used for deriving parameter values, do they clearly

			indicate for each chemical if it satisfies the applicability domain?
			If QSAR or read-across are used for deriving parameter values, are the number and origin of the data indicated?
			If QSAR or read-across are used for deriving parameter values, is the goodness of fit (or other indicator of correlation performance) indicated?
		Expert judgment and elicitation	If expert judgment is used for deriving parameter values, is the identity of the expert (or group of experts) clearly indicated?
			If expert judgment is used for deriving parameter values, is the expert(s) justification clearly reminded?
		Bayesian approach	If parameter values were estimated from a Bayesian approach, are the model assumptions (e.g. prior knowledge) clearly indicated?
			If parameter values were estimated from a Bayesian approach, are the number and origin of the data allowing calculating the posterior distribution clearly indicated? (e.g. name and accessibility of the databases, literature references, etc)
	Parameter values typology	Default values	If a default value is proposed for each parameter, is it clearly indicated if it corresponds to a conservative value (i.e. for worst-case scenario), mean, mode or best-estimate?
			If the default value proposed for each parameter is indicated as being a conservative value (i.e. for worst-case scenario), is it justified that it is actually conservative?
		Probabilistic values	If probabilistic density functions are proposed for all/some parameters, is the database used for generating them clearly identified?
			If probabilistic density functions are proposed for all/some parameters, is the statistical method used for generating them clearly described?
Validation process	Implementation verification	Mathematical verification	Was the correct implementation of equations verified, e.g. against implementation on other models?

			If the model requires numerical solutions, was the numerical scheme verified by comparing simulation results against results obtained analytically and with other numerical solvers?
	Benchmarking	Benchmarking	Were the simulation results obtained for reference scenarios compared with results obtained for these scenarios using other models?
			When results obtained on reference scenarios differ from those obtained with other models, are these differences justified?
	Validation agains actual data	(Bio)monitoring validation	Was the model compared to monitoring data collected on abiotic media (e.g. surface waters, air, soil)?
			Was the model compared to monitoring data collected on biological environmental media (e.g. plants, milk, fish, etc)?
			Was the model compared to biomonitoring data collected on human material (e.g. blood, urine, hair)?
			Were the differences between deterministic simulation results and actual monitoring data acceptable and/or explainable?
			Were actual monitoring data included in the uncertainty margin given by probabilistic simulation?
User friendliness	Numerical treatment	Model inputs	Is it possible and easy to change the default values for the forcing variables and parameters?
			Can calculated intermediate results be overwritten e.g. by measured data?
		Model outputs	Is it possible to export the output e.g. to Excel, Word, pdf?
			Is it possible to present the outputs in a graphical form?
			Is it possible to present the outputs in a tabular form?
			Does the user have access to intermediate results (e.g. exposure estimate for individual exposure routes)?
	Checking	Checking	Does the model provide alert messages in case of irrelevant or poorly

			plausible values for parameters? (e.g. in case of unit mistake)
			Does the model provide error messages in case of impossible simulation and are these messages clear?
			Is it possible to contact a support (e.g. model developer)?
	Running a simulation	Simulation time	Does the model take shorter than 15 minutes to run a simulation under deterministic conditions (e.g. without uncertainty analysis)?
			Does the model take shorter than 8 hours to run a simulation under probabilistic conditions (i.e. for conducting an uncertainty analysis)?
		Simulation repetition	Is it easy to re-run a previous case study? Will the user be able to refine the same results (conservation of previous versions)?
	Training	Training	Is a user-manual available?
			Are test examples available and easily accessible (e.g. in the user manual, on line, etc)?
			Is a helpdesk/demonstrator available?
	General	General	Is the model freely available?
			Is the model able to communicate with other software (e.g. input from excel)
Scenario relevance	General purpose	Chemicals	Does the model cover the chemical(s) you want to study?
			Can the model perform cumulative exposure assessment for the multiple chemicals you want to study?
			If the chemical you want to study is naturally present, can the model discriminate background and anthropogenic concentrations?
			Does the model cover the formation of metabolites that can be formed from the chemical(s) you want to study?
Uncertainty / sensitivity	Uncertainty	Uncertainty process	Does the model allow to define each parameter by the widely used distributions (e.g. (log-)normal, (log-)uniform, discrete, Student, etc)

			Does the model allow generating random samples for each uncertain parameter by the widely used methods (e.g. Monte Carlo, Latin Hypercube)?
			Does the model allow to define correlations between parameters and to rank sample values for respecting such correlations?
			Does the model provide statistical summaries for the probabilistically generated outputs (e.g. mean, percentiles, etc)?
		Sensitivity process	Does the model cover screening methods to conduct sensitivity analysis (e.g. Morris design, etc)?
			Does the model cover regression methods to conduct sensitivity analysis?
			Does the model cover variance-based methods to conduct sensitivity analysis (e.g. EFAST, Sobol, etc

7.2 Appendix B: Hierarchical structure of the assessment methodology based on LoE, Categories, Criteria and Questions: relevance criteria

Category	Sub-category	Question
Exposure population	Exposure to worker	Does the model cover exposure to worker (PPP: worker + operator, REACH: consumer, industrial and professional use)?
	Exposure via the general population	Does the model cover exposure via the general population (PPP: resident + consumer), reach: indirect via environment)?
	Exposure to subpopulations	Does the model cover exposure to subpopulations (adults, children, etc.)?
Compartments	Ground water	Does the model calculate concentrations in ground water?
	Surface watter	Does the model calculate concentrations in surface water?
	Sediment	Does the model calculate concentrations in sediment?
	Marine water	Does the model calculate concentrations in marine water?
	Soil	Does the model calculate concentrations in soil?
	Pore water	Does the model calculate concentrations in pore water?
	Air	Does the model calculate concentrations in air?
	Human body	Does the model calculate concentrations in the human body?

	Organs	Does the model calculate concentrations in organs?
	Milk	Does the model calculate concentrations in milk?
	Blood	Does the model calculate concentrations in blood?
	Fish	Does the model calculate concentrations in fish?
	Leafy crops	Does the model calculate concentrations in leafy crops?
	Root crops	Does the model calculate concentrations in root crops?
	Livestock	Does the model calculate concentrations in livestock?
	Eggs	Does the model calculate concentrations in eggs?
	Dairy products	Does the model calculate concentrations in dairy products?
	Earthworms	Does the model calculate concentrations in earthworms?
Exposure routes	Oral intake of food and drinks	Does the model cover exposure by oral intake of food and drinks?
	Oral intake of soil or dust ingestion	Does the model cover exposure by oral intake of soil or dust ingestion?
	Inhalation	Does the model cover exposure through inhalation?
	Dermal absorption	Does the model cover exposure by dermal absorption?

Environmental processes	Run-off process	Does the model cover the run-off process?
	Leaching of substances in soil	Does the model cover leaching of substances in soil?
	Volatilization process from water	Does the model cover the volatilization process from water?
	Volatilization process from vegetation	Does the model cover the volatilization process from vegetation?
	Volatilization process from soil	Does the model cover the volatilization process from soil?
	Wet and dry deposition to soil	Does the model cover wet and dry deposition to soil?
	Wet and dry deposition to water	Does the model cover wet and dry deposition to water?
	Wet and dry deposition to vegetation	Does the model cover wet and dry deposition to vegetation?
	Adsorption/desorption processes	Does the model cover adsorption/desorption processes?
	Linear/non-linear sorption	Does the model cover linear/non-linear sorption?
	Sediment burial	Does the model cover sediment burial?
	Sedimentation/resuspension	Does the model cover sedimentation/resuspension?
	Biotic and abiotic degradation	Does the model cover biotic and abiotic degradation?

	Degradation in the air compartment	Does the model cover degradation in the air compartment?
	Degradation in the water compartment	Does the model cover degradation in the water compartment?
	Degradation in the sediment compartment	Does the model cover degradation in the sediment compartment?
	Degradation in the soil compartment	Does the model cover degradation in the soil compartment?
	Bioconcentration of substances	Does the model cover bioconcentration of substances?
	Excretion and degradation by animals	Does the model cover excretion and degradation by animals?
	Food processing step of raw material	Does the model cover the food processing step of raw material?
	Vegetal transpiration process	Does the model cover the vegetal transpiration process?
	Transport of the substance by plant death	Does the model cover transport of the substance by plant death?
	Editable transport factor	Does the model cover an editable transport factor of the substance at harvest of the vegetation (e.g. only roots, complete plant, etc.)?
	Crop interception	Does the model take crop interception into consideration?
	Irrigation	Does the model take irrigation into consideration?
Human processes	Internal absorption of substances	Does the model cover internal absorption of substances in the human body?

	Distribution of substances	Does the model cover distribution of substances in the human body?
	Biotransformation	Does the model cover biotransformation in the human body?
	Excretion	Does the model cover excretion from the human body?
	Bioavailability of a substance	Does the model describe bioavailability of a substance in the human body?(= passage of a substance from the site of absorption into the blood of the general circulation)
	Linear and non-linear saturation process	Does the model describe the linear and non-linear saturation process in the human body?
	Accumulation	Does the model describe accumulation in the human body (i.e. the extent of accumulation reflects the relation between the body-burden compared with the steady-state condition)?
Time	Acute exposure	Does the model cover acute exposure?
	Chronic exposure	Does the model cover chronic exposure?
	Dynamic approach	Is the model based on a dynamic approach?
Spatial resolution	Exposure at the local scale	Does the model cover exposure at the local scale (e.g.1km2)?
	Spatially explicit outputs	Does the model provide spatially explicit outputs (e.g. Spatial distribution of contaminant concentration in an area/region)?
	Exposure at a regional scale	Does the model cover exposure at a regional scale (e.g. The Netherlands)?
Metabolites	Formation	Does the model cover the formation of metabolites?

Chemical substance	Organics	Is the model focused on organics in general?
	Inorganic chemicals	Does the model cover inorganic chemicals?
	Metals	Does the model cover metals?
	Cumulative exposure assessment	Can the model perform cumulative exposure assessment of multiple chemicals?
	Background concentrations	Can background concentrations (environmental and human compartments) be taken into account?
Releases	Point source release	Does the model cover point source release?
	Disperive release	Does the model cover wide disperive release?
Plant protection products	Exposure to the bystander	Does the model cover exposure to the bystander (for plant protection products)?
	Exposure to the surface water and air	Does the model cover exposure to the surface water and air via spray drift (for plant protection products

7.3 ppendix C: Overview of the positive responses of the multimedia models (yellow: Merlin-Expo only and/or one additional model fulfilling these criteria)

			MERLIN-Expo	CalTOX	EUSES	GLOBOX	MODULERS	USEtox
Category	Criterion	Question	YES	YES	YES	YES	YES	YES
Relevance criteria - Framework related								
Exposure population	Exposure to worker	Does the model cover exposure to worker (PPP: worker + operator, REACH: consumer, industrial and professional use)?			x			
	Exposure via the general population	Does the model cover exposure via the general population (PPP: resident + consumer), reach: indirect via environment)?	x	x	x		x	x
	Exposure to subpopulations	Does the model cover exposure to subpopulations (adults, children, etc.)?	x	x			x	
Compartments	Ground water	Does the model calculate concentrations in ground water?		x	x	x	x	
	Surface watter	Does the model calculate concentrations in surface water?	x	x	x	x	x	x
	Sediment	Does the model calculate concentrations in sediment?	x	x	x	x	x	
	Marine water	Does the model calculate concentrations in marine water?			x	x		x
	Soil	Does the model calculate concentrations in soil?	x	x	x	x	x	x
	Pore water	Does the model calculate concentrations in pore water?	x	x	x		x	
	Air	Does the model calculate concentrations in air?	x	x	x	x	x	x
	Human body	Does the model calculate concentrations in the human body?	x			x		
	Organs	Does the model calculate concentrations in organs?	x					
	Milk	Does the model calculate concentrations in milk?	x	x		x	x	
	Blood	Does the model calculate concentrations in blood?	x					
	Fish	Does the model calculate concentrations in fish?	x	x	x	x	x	x
	Leafy crops	Does the model calculate concentrations in leafy crops?	x	x	x	x	x	x
	Root crops	Does the model calculate concentrations in root crops?	x	x	x	x	x	x
	Livestock	Does the model calculate concentrations in livestock?	x	x	x	x	x	x
	Eggs	Does the model calculate concentrations in eggs?		x			x	
	Dairy products	Does the model calculate concentrations in dairy products?	x		x	x	x	x
	Earthworms	Does the model calculate concentrations in earthworms?			x			

Exposure routes	Oral intake of food and drinks	Does the model cover exposure by oral intake of food and drinks?	x	x	x	x	x	x
	Oral intake of soil or dust ingestion	Does the model cover exposure by oral intake of soil or dust ingestion?	x	x			x	
	Inhalation	Does the model cover exposure through inhalation?	x	x	x	x	x	x
	Dermal absorption	Does the model cover exposure by dermal absorption?		x				
Environmental processes	Run-off process	Does the model cover the run-off process?	x	x	x	x	x	x
	Leaching of substances in soil	Does the model cover leaching of substances in soil?	x	x	x	x	x	x
	Volatilization process from water	Does the model cover the volatilization process from water?	x	x	x	x	x	x
	Volatilization process from vegetation	Does the model cover the volatilization process from vegetation?	x	x	x			
	Volatilization process from soil	Does the model cover the volatilization process from soil?	x	x	x	x		x
	Wet and dry deposition to soil	Does the model cover wet and dry deposition to soil?	x	x	x	x	x	x
	Wet and dry deposition to water	Does the model cover wet and dry deposition to water?	x	x	x	x	x	x
	Wet and dry deposition to vegetation	Does the model cover wet and dry deposition to vegetation?	x	x	x	x	x	x
	Adsorption/desorption processes	Does the model cover adsorption/desorption processes?	x		x	x		x
	Linear/non-linear sorption	Does the model cover linear/non-linear sorption?		x		x	x	x
	Sediment burial	Does the model cover sediment burial?		x	x	x		x
	Sedimentation/resuspension	Does the model cover sedimentation/resuspension?	x	x	x	x	x	x
	Biotic and abiotic degradation	Does the model cover biotic and abiotic degradation?	x	x	x	x	x	x
	Degradation in the air compartment	Does the model cover degradation in the air compartment?	x	x	x	x		x

	Degradation in the water compartment	Does the model cover degradation in the water compartment?	x	x	x	x	x	x
	Degradation in the sediment compartment	Does the model cover degradation in the sediment compartment?	x	x	x	x		x
	Degradation in the soil compartment	Does the model cover degradation in the soil compartment?		x		x	x	x
	Bioconcentration of substances	Does the model cover bioconcentration of substances?	x	x	x	x	x	x
	Excretion and degradation by animals	Does the model cover excretion and degradation by animals?	x				x	
	Food processing step of raw material	Does the model cover the food processing step of raw material?			x		x	
	Vegetal transpiration process	Does the model cover the vegetal transpiration process?	x	x	x			x
	Transport of the substance by plant death	Does the model cover transport of the substance by plant death?	x	x	x			
	Editable transport factor	Does the model cover an editable transport factor of the substance at harvest of the vegetation (e.g. only roots, complete plant, etc.)?	x					
	Crop interception	Does the model take crop interception into consideration?	x	x			x	
	Irrigation	Does the model take irrigation into consideration?	x	x		x	x	
Human processes	Internal absorption of substances	Does the model cover internal absorption of substances in the human body?	x					
	Distribution of substances	Does the model cover distribution of substances in the human body?	x					
	Biotransformation	Does the model cover biotransformation in the human body?	x					
	Excretion	Does the model cover excretion from the human body?	x					
	Bioavailability of a substance	Does the model describe bioavailability of a substance in the human body?(= passage of a substance from the site of absorption into the blood of the general circulation)						
	Linear and non-linear saturation process	Does the model describe the linear and non-linear saturation process in the human body?						

	Accumulation	Does the model describe accumulation in the human body (i.e. the extent of accumulation reflects the relation between the body-burden compared with the steady-state condition)?	x					
Time	Acute exposure	Does the model cover acute exposure?	x		x		x	x
	Chronic exposure	Does the model cover chronic exposure?	x	x	x	x	x	x
	Dynamic approach	Is the model based on a dynamic approach?	x	x			x	
Spatial resolution	Exposure at the local scale	Does the model cover exposure at the local scale (e.g.1km2)?	x	x	x		x	x
	Spatially explicit outputs	Does the model provide spatially explicit outputs (e.g. Spatial distribution of contaminant concentration in an area/region)?				x	x	
	Exposure at a regional scale	Does the model cover exposure at a regional scale (e.g. The Netherlands)?	x	x	x	x		x
Metabolites	Formation	Does the model cover the formation of metabolites?						
Chemical substance	Organics	Is the model focused on organics in general?	x	x	x	x	x	
	Inorganic chemicals	Does the model cover inorganic chemicals?	x	x	x	x	x	x
	Metals	Does the model cover metals?	x	x	x	x	x	x
	Cumulative exposure assessment	Can the model perform cumulative exposure assessment of multiple chemicals?	x				x	
	Background concentrations	Can background concentrations (environmental and human compartments) be taken into account?	x		x		x	x
Releases	Point source release	Does the model cover point source release?	x		x		x	
	Disperive release	Does the model cover wide disperive release?	x	x	x	x	x	
Plant protection products	Exposure to the bystander	Does the model cover exposure to the bystander (for plant protection products)?		x				
	Exposure to the surface water and air	Does the model cover exposure to the surface water and air via spray drift (for plant protection products						
Other criteria								
Model purpose	Model outputs	Are the outputs that the end-user is able to calculate clearly defined? (e.g. units, unambiguous definition, etc)	x	x	x	x	x	x
	Potential decision(s)	Are the potential decision(s) that can be taken from the model outputs clearly defined? (e.g. screening level assessment, priority setting, labeling, higher exposure tier, etc)	x	x	x	x	x	x

	Regulatory framework(s)	Are the regulatory framework(s) that the model could be useful for clearly defined? (e.g. REACH, Water Framework Directive, Biocide directive, etc)	x	x	x		x	
Model applicability	Spatial scale and resolution	Is the spatial applicability domain clearly defined? (e.g. area and/or volume(s) dimensions, near-field vs global scale, spatial boundaries, minimum spatial resolution)	x	x	x	x	x	x
	Temporal scale and resolution	Is the temporal applicability domain clearly defined? (e.g. minimum temporal resolution, capability to account for daily/monthly/seasonal variability, etc)	x	x			x	
	Dynamic context	Is the capability to simulate dynamic scenarios (e.g. intermittent emissions, accidental emissions) explicitly indicated?	x				x	
	Chemical applicability domain	Are the chemicals (or family of chemicals) for which the model is applicable (and inversely non applicable) clearly defined?	x		x	x	x	x
	Extrapolations	If the model is partially applicable for some chemicals, are the applied extrapolation rules indicated? (e.g. read-across, extrapolation from neutral organics to ionic organics, etc)	x					
Model structure	Model media	Are the media that are included in the model clearly defined?	x	x	x	x	x	x
	Emissions	Are the emissions that can be used as input data in the model clearly defined, e.g. point and/or diffuse sources to surface waters, atmosphere, soils, etc?	x		x	x	x	x
	Transport loss	Are the chemical losses from the system that are governed by transport processes (e.g. advection, diffusion) clearly defined?	x	x	x	x	x	x
	Chemical loss	Are the chemical losses from the system that are governed by chemical processes (e.g. degradation) clearly defined?	x	x	x	x	x	x
	Exchanges between media	Are the chemical exchanges between media clearly defined?	x		x	x	x	x
	Exchanges with other models	Are potential chemical exchanges with other coupled models clearly defined?	x		x			x
Variables	Meteorological forcing variables	Are the meteorological forcing variables (e.g. rain, wind speed, temperature, etc) that are necessary for the simulation clearly defined (e.g. time and spatial resolution, units, etc)?	x	x	x	x	x	x
	Agronomical and anthropogenic forcing variables	Are the agronomical and anthropogenic forcing variables (e.g. harvest period, spatial distribution of crops, time and spatial patterns, etc) that are necessary for the simulation clearly?	x	x			x	
	Other forcing variables	Are the other forcing variables that are necessary for the simulation clearly defined?	x	x	x	x	x	
Parameters	Definitions	Are the state variables that are calculated by the model clearly defined (e.g. unambiguous definition, units, etc)?	x	x	x	x	x	x
	Relations with the other model components	For a given state variable, are the other components of the model that are necessary for its calculation (e.g. parameters, forcing variables, other state variables) clearly and comprehensively defined?	x		x	x	x	
	Definitions	Are the parameters that are necessary for model calculation clearly defined (e.g. unambiguous definition, units, etc)?	x	x	x	x	x	x

	Scenario-specific parameters	Are the scenario-specific parameters that must be updated by the end user for each case study clearly identified and distinguished from generic parameters? (e.g. e.g. river depth, land use coverage, vegetables production in the investigated region, etc)	x		x	x	x	x
Scientific background	Process relevance	For each process included in the model, is its relevance justified from the scientific background?	x	x		x	x	x
	Process non-relevance	Does the documentation include a list of processes that are not included in the model, with a justification of their exclusion?	x				x	
	Applicability domain	For the model selected for representing a given process, is its applicability domain clearly defined? (e.g. chemicals, spatial and time issues, etc)	x	x			x	
	Alternative models	If relevant, are the alternative models available in the literature for representing a given process presented and critically evaluated?	x					
	Mechanistic vs empirical model	For each process included in the model, is it indicated (with justification) if this latter is based on mechanistic considerations or empirical relationships (e.g empirically fitted multilinear relationship between a state variable and parameters)?	x	x	x			
	Steady state vs dynamic model	For each process represented in the model, is it indicated (with justification) if this latter is based on steady-state or dynamic assumptions?	x	x		x	x	x
Model equations	Equations	Are model equations clearly and comprehensively documented?	x		x	x	x	
Initial conditions	Default initial values	Are the default values proposed for the initial conditions (e.g. concentrations in media at time zero) clearly defined?	x	x		x	x	
	Scenario-specific initial values	Can the initial values be modified by the end-user for each new simulation?	x	x	x	x	x	
Forcing variables	Default values	Are the default values proposed for the forcing variables (e.g. atmospheric conditions) clearly defined?	x	x	x	x	x	x
	Scenario-specific values	Can the values for forcing variables be modified by the end-user for each new simulation?	x	x	x	x	x	x
Parameter values source	Database	If parameter values were estimated from calibration using empirical data, are the number and origin of the data clearly indicated? (e.g. name and accessibility of the databases, literature references, etc)	x				x	
	Uncertainty margin	If the parameter values were estimated from calibration using empirical data, is the uncertainty margin indicated? (e.g. probability density function, mean and standard deviation, quartiles, etc)	x	x			x	
	Applicability domain	If QSAR or read-across are used for deriving parameter values, do they clearly indicate for each chemical if it satisfies the applicability domain?	x				x	
	Data for QSAR	If QSAR or read-across are used for deriving parameter values, are the number and origin of the data indicated?	x				x	
	Goodness of fit	If QSAR or read-across are used for deriving parameter values, is the goodness of fit (or other indicator of correlation performance) indicated?	x	x			x	
	Expert(s) identification	If expert judgment is used for deriving parameter values, is the identity of the expert (or group of experts) clearly indicated?	x			x	x	

	Expert(s) justification	If expert judgment is used for deriving parameter values, is the expert(s) justification clearly reminded?	x			x	x	
	Model assumption	If parameter values were estimated from a Bayesian approach, are the model assumptions (e.g. prior knowledge) clearly indicated?	x					
	Database	If parameter values were estimated from a Bayesian approach, are the number and origin of the data allowing calculating the posterior distribution clearly indicated? (e.g. name and accessibility of the databases, literature references, etc)	x					
Parameter values typology	Default value type	If a default value is proposed for each parameter, is it clearly indicated if it corresponds to a conservative value (i.e. for worst-case scenario), mean, mode or best-estimate?	x				x	
	Conservative value	If the default value proposed for each parameter is indicated as being a conservative value (i.e. for worst-case scenario), is it justified that it is actually conservative?					x	
	Database for probabilistic values generation	If probabilistic density functions are proposed for all/some parameters, is the database used for generating them clearly identified?	x				x	
	Statistical method for probabilistic values generation	If probabilistic density functions are proposed for all/some parameters, is the statistical method used for generating them clearly described?	x	x			x	
Implementation verification	Mathematical consistency	Was the correct implementation of equations verified, e.g. against implementation on other models?	x				x	
	Numerical accuracy	If the model requires numerical solutions, was the numerical scheme verified by comparing simulation results against results obtained analytically and with other numerical solvers?	x				x	
Benchmarking	Benchmarking with other models	Were the simulation results obtained for reference scenarios compared with results obtained for these scenarios using other models?					x	
	Benchmarking interpretation	When results obtained on reference scenarios differ from those obtained with other models, are these differences justified?						
Validation agains actual data	Validation against data in abiotic media	Was the model compared to monitoring data collected on abiotic media (e.g. surface waters, air, soil)?						
	Validation against data in biological environmental media	Was the model compared to monitoring data collected on biological environmental media (e.g. plants, milk, fish, etc)?						
	Validation against data in human media	Was the model compared to biomonitoring data collected on human material (e.g. blood, urine, hair)?						
	Validation deterministic results	Were the differences between deterministic simulation results and actual monitoring data acceptable and/or explainable?						

	Validation probabilistic results	Were actual monitoring data included in the uncertainty margin given by probabilistic simulation?						
Numerical treatment	Modification capability	Is it possible and easy to change the default values for the forcing variables and parameters?	x	x	x	x	x	x
	Overwritting intermediate results	Can calculated intermediate results be overwritten e.g. by measured data?		x	x	x	x	
	Results export	Is it possible to export the output e.g. to Excel, Word, pdf?	x		x	x	x	x
	Graphs	Is it possible to present the outputs in a graphical form?	x				x	x
	Tables	Is it possible to present the outputs in a tabular form?	x			x	x	x
	Intermediate results	Does the user have access to intermediate results (e.g. exposure estimate for individual exposure routes)?	x	x	x	x	x	x
Checking	Parameters checking	Does the model provide alert messages in case of irrelevant or poorly plausible values for parameters? (e.g. in case of unit mistake)	x		x		x	
	Error messages	Does the model provide error messages in case of impossible simulation and are these messages clear?	x	x	x		x	
	Support	Is it possible to contact a support (e.g. model developer)?	x	x	x	x	x	x
Running a simulation	Calculation time under deterministic simulation	Does the model take shorter than 15 minutes to run a simulation under deterministic conditions (e.g. without uncertainty analysis)?	x	x	x	x	x	x
	Calculation time under uncertainty simulation	Does the model take shorter than 8 hours to run a simulation under probabilistic conditions (i.e. for conducting an uncertainty analysis)?	x	x			x	
	Re-running case study	Is it easy to re-run a previous case study? Will the user be able to refine the same results (conservation of previous versions)?	x	x	x	x	x	x
Training	User-Manual	Is a user-manual available?	x	x	x	x	x	x
	Test examples	Are test examples available and easily accessible (e.g. in the user manual, on line, etc)?				x	x	x
	Helpdesk/Demonstrator	Is a helpdesk/demonstrator available?	x		x		x	x
General	Availability	Is the model freely available?	x	x	x	x	x	x
	Communication	Is the model able to communicate with other software (e.g. input from excel)	x			x	x	x
General purpose	Chemical applicability domain	Does the model cover the chemical(s) you want to study?	x	x		x	x	x
	Cumulative exposure assessment	Can the model perform cumulative exposure assessment for the multiple chemicals you want to study?	x				x	x
	Background	If the chemical you want to study is naturally present, can the model discriminate background and anthropogenic	x				x	

	concentrations	concentrations?						
	Metabolites	Does the model cover the formation of metabolites that can be formed from the chemical(s) you want to study?						
Uncertainty	Probability density functions	Does the model allow to define each parameter by the widely used distributions (e.g. (log-)normal, (log-)uniform, discrete, Student, etc)	x	x			x	
	Random sampling	Does the model allow generating random samples for each uncertain parameter by the widely used methods (e.g. Monte Carlo, Latin Hypercube)?	x	x			x	
	Correlations	Does the model allow to define correlations between parameters and to rank sample values for respecting such correlations?	x	x			x	
	Statistical treatment	Does the model provide statistical summaries for the probabilistically generated outputs (e.g. mean, percentiles, etc)?	x	x			x	
	Screening methods	Does the model cover screening methods to conduct sensitivity analysis (e.g. Morris design, etc)?	x	x			x	
	Regression methods	Does the model cover regression methods to conduct sensitivity analysis?	x	x			x	
	Variance-based methods	Does the model cover variance-based methods to conduct sensitivity analysis (e.g. EFAST, Sobol, etc	x				x	

7.4 Appendix D: Overview of the negative responses of the multimedia models (yellow: Merlin-Expo only and/or one additional model not fulfilling these criteria)

			MERLIN-Expo	CalTOX	EUSES	GLOBOX	MODULERS	USEtox
Category	Criterion	Question	NO	NO	NO	NO	NO	NO
Relevance criteria - Framework related								
Exposure population	Exposure to worker	Does the model cover exposure to worker (PPP: worker + operator, REACH: consumer, industrial and professional use)?	x	x		x	x	x
	Exposure via the general population	Does the model cover exposure via the general population (PPP: resident + consumer), reach: indirect via environment)?				x		
	Exposure to subpopulations	Does the model cover exposure to subpopulations (adults, children, etc.)?			x	x		x
Compartments	Ground water	Does the model calculate concentrations in ground water?	x					x
	Surface watter	Does the model calculate concentrations in surface water?						
	Sediment	Does the model calculate concentrations in sediment?						x
	Marine water	Does the model calculate concentrations in marine water?	x	x			x	
	Soil	Does the model calculate concentrations in soil?						
	Pore water	Does the model calculate concentrations in pore water?				x		
	Air	Does the model calculate concentrations in air?						
	Human body	Does the model calculate concentrations in the human body?		x	x		x	x
	Organs	Does the model calculate concentrations in organs?		x	x	x	x	x
	Milk	Does the model calculate concentrations in milk?			x			x
	Blood	Does the model calculate concentrations in blood?		x	x	x	x	x
	Fish	Does the model calculate concentrations in fish?						
	Leafy crops	Does the model calculate concentrations in leafy crops?						
	Root crops	Does the model calculate concentrations in root crops?						
	Livestock	Does the model calculate concentrations in livestock?						
	Eggs	Does the model calculate concentrations in eggs?	x		x			x
	Dairy products	Does the model calculate concentrations in dairy products?		x				

	Earthworms	Does the model calculate concentrations in earthworms?	x	x		x	x	x
Exposure routes	Oral intake of food and drinks	Does the model cover exposure by oral intake of food and drinks?						
	Oral intake of soil or dust ingestion	Does the model cover exposure by oral intake of soil or dust ingestion?			x	x		x
	Inhalation	Does the model cover exposure through inhalation?						
	Dermal absorption	Does the model cover exposure by dermal absorption?	x		x	x	x	x
Environmental processes	Run-off process	Does the model cover the run-off process?						
	Leaching of substances in soil	Does the model cover leaching of substances in soil?						
	Volatilization process from water	Does the model cover the volatilization process from water?						
	Volatilization process from vegetation	Does the model cover the volatilization process from vegetation?				x	x	x
	Volatilization process from soil	Does the model cover the volatilization process from soil?					x	
	Wet and dry deposition to soil	Does the model cover wet and dry deposition to soil?						
	Wet and dry deposition to water	Does the model cover wet and dry deposition to water?						
	Wet and dry deposition to vegetation	Does the model cover wet and dry deposition to vegetation?						
	Adsorption/desorption processes	Does the model cover adsorption/desorption processes?		x			x	
	Linear/non-linear sorption	Does the model cover linear/non-linear sorption?	x		x			
	Sediment burial	Does the model cover sediment burial?	x				x	
	Sedimentation/resuspension	Does the model cover sedimentation/resuspension?						
	Biotic and abiotic degradation	Does the model cover biotic and abiotic degradation?						
	Degradation in the air compartment	Does the model cover degradation in the air compartment?					x	
	Degradation in the water compartment	Does the model cover degradation in the water compartment?						

	Degradation in the sediment compartment	Does the model cover degradation in the sediment compartment?					x	
	Degradation in the soil compartment	Does the model cover degradation in the soil compartment?						
	Bioconcentration of substances	Does the model cover bioconcentration of substances?						
	Excretion and degradation by animals	Does the model cover excretion and degradation by animals?		x	x	x		x
	Food processing step of raw material	Does the model cover the food processing step of raw material?	x	x		x		x
	Vegetal transpiration process	Does the model cover the vegetal transpiration process?				x	x	
	Transport of the substance by plant death	Does the model cover transport of the substance by plant death?				x	x	x
	Editable transport factor	Does the model cover an editable transport factor of the substance at harvest of the vegetation (e.g. only roots, complete plant, etc.)?			x	x		x
	Crop interception	Does the model take crop interception into consideration?			x			x
	Irrigation	Does the model take irrigation into consideration?			x			x
Human processes	Internal absorption of substances	Does the model cover internal absorption of substances in the human body?		x	x	x	x	x
	Distribution of substances	Does the model cover distribution of substances in the human body?		x	x	x	x	x
	Biotransformation	Does the model cover biotransformation in the human body?		x	x	x	x	x
	Excretion	Does the model cover excretion from the human body?		x	x	x	x	x
	Bioavailability of a substance	Does the model describe bioavailability of a substance in the human body?(= passage of a substance from the site of absorption into the blood of the general circulation)	x	x	x	x	x	x
	Linear and non-linear saturation process	Does the model describe the linear and non-linear saturation process in the human body?	x	x	x	x	x	x
	Accumulation	Does the model describe accumulation in the human body (i.e. the extent of accumulation reflects the relation between the body-burden compared with the steady-state condition)?		x	x	x	x	x
Time	Acute exposure	Does the model cover acute exposure?		x		x		
	Chronic exposure	Does the model cover chronic exposure?						
	Dynamic approach	Is the model based on a dynamic approach?			x	x		x
Spatial resolution	Exposure at the local scale	Does the model cover exposure at the local scale (e.g.1km2)?				x		

	Spatially explicit outputs	Does the model provide spatially explicit outputs (e.g. Spatial distribution of contaminant concentration in an area/region)?	x	x	x			x
	Exposure at a regional scale	Does the model cover exposure at a regional scale (e.g. The Netherlands)?						
Metabolites	Formation	Does the model cover the formation of metabolites?	x	x	x	x	x	x
Chemical substance	Organics	Is the model focused on organics in general?						x
	Inorganic chemicals	Does the model cover inorganic chemicals?						
	Metals	Does the model cover metals?						
	Cumulative exposure assessment	Can the model perform cumulative exposure assessment of multiple chemicals?			x	x		x
	Background concentrations	Can background concentrations (environmental and human compartments) be taken into account?		x		x		
Releases	Point source release	Does the model cover point source release?				x		
	Disperive release	Does the model cover wide disperive release?						
Plant protection products	Exposure to the bystander	Does the model cover exposure to the bystander (for plant protection products)?	x		x	x	x	x
	Exposure to the surface water and air	Does the model cover exposure to the surface water and air via spray drift (for plant protection products	x		x	x	x	x
Other criteria								
Model purpose	Model outputs	Are the outputs that the end-user is able to calculate clearly defined? (e.g. units, unambiguous definition, etc)						
	Potential decision(s)	Are the potential decision(s) that can be taken from the model outputs clearly defined? (e.g. screening level assessment, priority setting, labeling, higher exposure tier, etc)						
	Regulatory framework(s)	Are the regulatory framework(s) that the model could be useful for clearly defined? (e.g. REACH, Water Framework Directive, Biocide directive, etc)						
Model applicability	Spatial scale and resolution	Is the spatial applicability domain clearly defined? (e.g. area and/or volume(s) dimensions, near-field vs global scale, spatial boundaries, minimum spatial resolution)						
	Temporal scale and resolution	Is the temporal applicability domain clearly defined? (e.g. minimum temporal resolution, capability to account for daily/monthly/seasonal variability, etc)						
	Dynamic context	Is the capability to simulate dynamic scenarios (e.g. intermittent emissions, accidental emissions) explicitly indicated?			x			x

	Chemical applicability domain	Are the chemicals (or family of chemicals) for which the model is applicable (and inversely non applicable) clearly defined?		x				
	Extrapolations	If the model is partially applicable for some chemicals, are the applied extrapolation rules indicated? (e.g. read-across, extrapolation from neutral organics to ionic organics, etc)		x	x		x	x
Model structure	Model media	Are the media that are included in the model clearly defined?		x				
	Emissions	Are the emissions that can be used as input data in the model clearly defined, e.g. point and/or diffuse sources to surface waters, atmosphere, soils, etc?		x				
	Transport loss	Are the chemical losses from the system that are governed by transport processes (e.g. advection, diffusion) clearly defined?						
	Chemical loss	Are the chemical losses from the system that are governed by chemical processes (e.g. degradation) clearly defined?						
	Exchanges between media	Are the chemical exchanges between media clearly defined?		x				
	Exchanges with other models	Are potential chemical exchanges with other coupled models clearly defined?						
Variables	Meteorological forcing variables	Are the meteorological forcing variables (e.g. rain, wind speed, temperature, etc) that are necessary for the simulation clearly defined (e.g. time and spatial resolution, units, etc)?						
	Agronomical and anthropogenic forcing variables	Are the agronomical and anthropogenic forcing variables (e.g. harvest period, spatial distribution of crops, time and spatial patterns, etc) that are necessary for the simulation clearly?						
	Other forcing variables	Are the other forcing variables that are necessary for the simulation clearly defined?						x
Parameters	Definitions	Are the state variables that are calculated by the model clearly defined (e.g. unambiguous definition, units, etc)?						
	Relations with the other model components	For a given state variable, are the other components of the model that are necessary for its calculation (e.g. parameters, forcing variables, other state variables) clearly and comprehensively defined?		x				
	Definitions	Are the parameters that are necessary for model calculation clearly defined (e.g. unambiguous definition, units, etc)?						
	Scenario-specific parameters	Are the scenario-specific parameters that must be updated by the end user for each case study clearly identified and distinguished from generic parameters? (e.g. e.g. river depth, land use coverage, vegetables production in the investigated region, etc)		x				
Scientific background	Process relevance	For each process included in the model, is its relevance justified from the scientific background?			x			
	Process non-relevance	Does the documentation include a list of processes that are not included in the model, with a justification of their exclusion?		x	x	x		x
	Applicability domain	For the model selected for representing a given process, is its applicability domain clearly defined? (e.g. chemicals, spatial and time issues, etc)			x			x
	Alternative models	If relevant, are the alternative models available in the literature for representing a given process presented and critically evaluated?		x	x	x	x	x

	Mechanistic vs empirical model	For each process included in the model, is it indicated (with justification) if this latter is based on mechanistic considerations or empirical relationships (e.g empirically fitted multilinear relationship between a state variable and parameters)?				x		x
	Steady state vs dynamic model	For each process represented in the model, is it indicated (with justification) if this latter is based on steady-state or dynamic assumptions?						
Model equations	Equations	Are model equations clearly and comprehensively documented?		x				x
Initial conditions	Default initial values	Are the default values proposed for the initial conditions (e.g. concentrations in media at time zero) clearly defined?						x
	Scenario-specific initial values	Can the initial values be modified by the end-user for each new simulation?						
Forcing variables	Default values	Are the default values proposed for the forcing variables (e.g. atmospheric conditions) clearly defined?						
	Scenario-specific values	Can the values for forcing variables be modified by the end-user for each new simulation?						
Parameter values source	Database	If parameter values were estimated from calibration using empirical data, are the number and origin of the data clearly indicated? (e.g. name and accessibility of the databases, literature references, etc)		x	x	x		
	Uncertainty margin	If the parameter values were estimated from calibration using empirical data, is the uncertainty margin indicated? (e.g. probability density function, mean and standard deviation, quartiles, etc)			x	x		
	Applicability domain	If QSAR or read-across are used for deriving parameter values, do they clearly indicate for each chemical if it satisfies the applicability domain?		x	x	x		
	Data for QSAR	If QSAR or read-across are used for deriving parameter values, are the number and origin of the data indicated?		x	x	x		
	Goodness of fit	If QSAR or read-across are used for deriving parameter values, is the goodness of fit (or other indicator of correlation performance) indicated?			x	x		
	Expert(s) identification	If expert judgment is used for deriving parameter values, is the identity of the expert (or group of experts) clearly indicated?		x	x			
	Expert(s) justification	If expert judgment is used for deriving parameter values, is the expert(s) justification clearly reminded?		x	x			
	Model assumption	If parameter values were estimated from a Bayesian approach, are the model assumptions (e.g. prior knowledge) clearly indicated?						
	Database	If parameter values were estimated from a Bayesian approach, are the number and origin of the data allowing calculating the posterior distribution clearly indicated? (e.g. name and accessibility of the databases, literature references, etc)						
Parameter values typology	Default value type	If a default value is proposed for each parameter, is it clearly indicated if it corresponds to a conservative value (i.e. for worst-case scenario), mean, mode or best-estimate?		x	x	x		x
	Conservative value	If the default value proposed for each parameter is indicated as being a conservative value (i.e. for worst-case scenario), is it justified that it is actually conservative?		x	x			
	Database for probabilistic values generation	If probabilistic density functions are proposed for all/some parameters, is the database used for generating them clearly identified?		x				

	Statistical method for probabilistic values generation	If probabilistic density functions are proposed for all/some parameters, is the statistical method used for generating them clearly described?						
Implementation verification	Mathematical consistency	Was the correct implementation of equations verified, e.g. against implementation on other tools?			x	x		
	Numerical accuracy	If the model requires numerical solutions, was the numerical scheme verified by comparing simulation results against results obtained analytically and with other numerical solvers?				x		
Benchmarking	Benchmarking with other models	Were the simulation results obtained for reference scenarios compared with results obtained for these scenarios using other models?	x			x		x
	Benchmarking interpretation	When results obtained on reference scenarios differ from those obtained with other models, are these differences justified?						x
Validation agains actual data	Validation against data in abiotic media	Was the model compared to monitoring data collected on abiotic media (e.g. surface waters, air, soil)?	x			x	x	
	Validation against data in biological environmental media	Was the model compared to monitoring data collected on biological environmental media (e.g. plants, milk, fish, etc)?	x			x	x	
	Validation against data in human media	Was the model compared to biomonitoring data collected on human material (e.g. blood, urine, hair)?	x		x			
	Validation deterministic results	Were the differences between deterministic simulation results and actual monitoring data acceptable and/or explainable?						
	Validation probabilistic results	Were actual monitoring data included in the uncertainty margin given by probabilistic simulation?						
Numerical treatment	Modification capability	Is it possible and easy to change the default values for the forcing variables and parameters?						
	Overwritting intermediate results	Can calculated intermediate results be overwritten e.g. by measured data?	x					x
	Results export	Is it possible to export the output e.g. to Excel, Word, pdf?						
	Graphs	Is it possible to present the outputs in a graphical form?			x	x		
	Tables	Is it possible to present the outputs in a tabular form?			x			
	Intermediate results	Does the user have access to intermediate results (e.g. exposure estimate for individual exposure routes)?						
Checking	Parameters checking	Does the model provide alert messages in case of irrelevant or poorly plausible values for parameters? (e.g. in case of unit mistake)		x		x		x
	Error messages	Does the model provide error messages in case of impossible simulation and are these messages clear?				x		x

	Support	Is it possible to contact a support (e.g. model developer)?						
Running a simulation	Calculation time under deterministic simulation	Does the model take shorter than 15 minutes to run a simulation under deterministic conditions (e.g. without uncertainty analysis)?						
	Calculation time under uncertainty simulation	Does the model take shorter than 8 hours to run a simulation under probabilistic conditions (i.e. for conducting an uncertainty analysis)?						
	Re-running case study	Is it easy to re-run a previous case study? Will the user be able to refine the same results (conservation of previous versions)?						
Training	User-Manual	Is a user-manual available?						
	Test examples	Are test examples available and easily accessible (e.g. in the user manual, on line, etc)?	**x**	**x**	**x**			
	Helpdesk/Demonstrator	Is a helpdesk/demonstrator available?		**x**		**x**		
General	Availability	Is the model freely available?						
	Communication	Is the model able to communicate with other software (e.g. input from excel)		**x**	**x**			
General purpose	Chemical applicability domain	Does the model cover the chemical(s) you want to study?						
	Cumulative exposure assessment	Can the model perform cumulative exposure assessment for the multiple chemicals you want to study?			**x**	**x**		
	Background concentrations	If the chemical you want to study is naturally present, can the model discriminate background and anthropogenic concentrations?			**x**	**x**		**x**
	Metabolites	Does the model cover the formation of metabolites that can be formed from the chemical(s) you want to study?	**x**	**x**	**x**	**x**	**x**	**x**
Uncertainty	Probability density functions	Does the model allow to define each parameter by the widely used distributions (e.g. (log-)normal, (log-)uniform, discrete, Student, etc)			**x**	**x**		**x**
	Random sampling	Does the model allow generating random samples for each uncertain parameter by the widely used methods (e.g. Monte Carlo, Latin Hypercube)?			**x**	**x**		**x**
	Correlations	Does the model allow to define correlations between parameters and to rank sample values for respecting such correlations?			**x**	**x**		**x**
	Statistical treatment	Does the model provide statistical summaries for the probabilistically generated outputs (e.g. mean, percentiles, etc)?			**x**	**x**		**x**
	Screening methods	Does the model cover screening methods to conduct sensitivity analysis (e.g. Morris design, etc)?			**x**	**x**		**x**
	Regression methods	Does the model cover regression methods to conduct sensitivity analysis?			**x**	**x**		**x**
	Variance-based methods	Does the model cover variance-based methods to conduct sensitivity analysis (e.g. EFAST, Sobol, etc		**x**	**x**	**x**		**x**