SWOT Analysis of the MERLIN-Expo Tool and Its Relevance in Legislative Frameworks

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Abstract The MERLIN-Expo tool was evaluated using a SWOT analysis, which was based on expert judgement and literature review. A list of criteria was set up containing the major model characteristics, which were divided in general model criteria and relevance model criteria. Relevance model criteria were defined as criteria, which are highly depending on the regulatory framework the model is used in. From the analysis presented above, it appeared that certain regulatory chemical frameworks (e.g. REACH, biocides) are stricter towards their requirements compared to others (e.g. site-specific/local regulatory frameworks). Based on expert judgement, the MERLIN-Expo tool was evaluated using the general and relevance criteria. MERLIN-Expo has many advanced functionalities (such as uncertainty

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analysis, modular approach, dynamic model, combines environmental fate with pharmacokinetics) and models (many fate processes and environmental compartments, different human populations). At the same time, the threat is that current (regulatory) applicability frameworks do not always require these advanced assessment functionalities. The MERLIN-Expo tool appeared to be most suitable for the site-specific assessment as this is the most flexible framework. Based on this analysis, weaknesses of the MERLIN-Expo tool for its use in a certain regulatory framework could also be identified. These weaknesses are at the same time further development opportunities for MERLIN-Expo. On general model characteristics, MERLIN-Expo was identified as a highly documented (both for novice and expert level), transparent, user-friendly tool with regular trainings. Its main treat now is to ensure continuing support and mechanisms for future developmental work and updates.

Keywords Exposure models • MERLIN-Expo • Multimedia models • Regulatory framework • SWOT analysis

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1 Introduction

Chemicals play a major role in modern society, contributing to our well-being and comfort and providing a number of economic benefits. However, many chemicals also pose risks to human health and the environment. Regulatory frameworks are in place in order for chemicals to be used properly, safely and in an environmentally-friendly and healthy manner. Regulatory frameworks exist on an international (focus here is the European level) and national level and/or for specific groups of chemicals such as biocides, agrochemicals, pharmaceuticals and cosmetics. These regulations can require a risk assessment for hazardous substances in order to ensure the safety of the environment and human health indirect via the environment. A risk assessment is a systematic approach to assess potential risks associated with exposure to known or potentially toxic agents.

To accurately evaluate the risk from a chemical, it is necessary to estimate the likely exposure to humans and the environment. Assessment of exposure

concentrations can be done by measurements or by estimation such as model-based computation. Several model-based computation tools are available for this purpose.

MERLIN-Expo has been developed within the 2-FUN project "Full-chain and uncertainty approaches for assessing health risks in future environmental scenarios" and 4FUN project. The MERLIN-Expo tool aims 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 is 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 scenarios, exposure assessment, provision of uncertainty margins and identification of sensitive pathways and risks. The MERLIN-Expo multimedia modelling tool allows the user to assemble several models for a specific scenario, to enter input data and parameter values for selected contaminants, to run deterministic (best- or worst-case estimate) or probabilistic (Monte Carlo) simulations and finally to perform sensitivity analysis.

The main objective of this chapter is to identify the strengths and weaknesses of existing exposure tools (aiming at predicting environmental and human (via the environment) exposure), more in particular the MERLIN-Expo tool (see below) using a SWOT analysis. A SWOT analysis is a structured planning method used to evaluate the Strengths, Weaknesses, Opportunities and Threats.

Reviews of exposure tools have been conducted in the past, but resulting analyses generally remain subjective and qualitative because they are not based on a set of transparent and structured criteria. To overcome this drawback and to facilitate thus an objective and reproducible SWOT evaluation, a comprehensive list of criteria was set up to structure the characteristics of exposure tools. In addition, the applicability of exposure tools towards a certain regulatory framework was assessed based on expert judgement.

2 Methodology

The following frameworks where the use of exposure models is relevant were identified:

- REACH Regulation (No. 1354/2007)
- Plant Protection Products Regulation (No. 1107/2009)
- Biocide Regulation (No. 528/2012)
- Environmental compartment-oriented directives (e.g. Water Framework Directive (WFD, 2000/60/EC))
- Food-oriented regulations/directives (e.g. Food Contact Materials (No. 1935/2004)
- Site-specific assessment (e.g. local contaminations)
- Sustainability assessments (SWOT assessment was conducted for hazard-based approaches such as 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)

In this section, the definition of criteria, their importance following regulatory frameworks and exposure models to be assessed, is further outlined. These are the elements for the subsequent comparative assessment and SWOT analysis.

2.1 Assessment Criteria

In order to perform an objective and reproducible SWOT 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 exposure models. Relevant aspects, features and functionalities related to an exposure model were identified and translated into a set of evaluation criteria.

The criteria were in first instance the result of a systematic review of the characteristics of exposure models and models available in the literature (EU FP7 Riskcycle [1], EU FP7 Browse [2–4]; EPA [5]; [1, 6–19]).

Secondly, the requirements of certain chemical regulatory frameworks in which MERLIN-Expo can be used to predict environmental and human (indirect via the environment) exposure were taken into account: REACH (EC 1907/2006), Plant protection products (EC 1107/2009), Biocides (EC 528/2012) were covered. These chemical regulatory frameworks were selected as they are relevant at the EU level in the context of chemical substances management and they deal with different classes of chemicals, which have the potential to cause indirect exposure to humans via the environment. Local/regional regulations are also applicable in the evaluation of chemicals; however, the specificities of these regulations are quite variable and are therefore not taken into account in the assessment criteria.

Finally, expert judgement on relevant aspects for environmental exposure modelling was used to improve the list of criteria. This resulted in a total of 155 criteria. The criteria can be distinguished between general criteria (see Table 1 organised in several lines of evidence) and relevance criteria (Table 2).

- General criteria: general model characteristics not related to a certain (regulatory) applicability framework
- Relevance criteria: specific model characteristics of which the importance is highly dependent on the (regulatory) applicability framework in which the exposure tools are used

In order to support the evaluation of exposure models by selected experts, all the obtained criteria were transformed into the form of yes/no questions. A set of experts was asked to use the resulting questionnaire as a guideline to evaluate each exposure model considered in the comparative assessment, as will be detailed below.

Table 1 Hierarchical structure of the assessment methodology based on lines of evidence, categories, subcategories and questions: general criteria

Line of evidence	Category	Subcategory	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 decisions that can be taken from the model outputs clearly defined? (e.g. screening level assessment, priority setting, labelling, higher exposure tier, etc.)
			Are the regulatory frameworks 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

(continued)

Table 1 (continued)

Line of evidence	Category	Subcategory	Question
			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?
		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?

(continued)

Table 1 (continued)

Line of evidence	Category	Subcategory	Question
	Parameters	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. 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?

(continued)

Table 1 (continued)

Line of evidence	Category	Subcategory	Question
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?
		**Quantitative structure–activity relationship* models (QSAR models)	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 judgement and elicitation	If expert judgement is used for deriving parameter values, is the identity of the expert (or group of experts) clearly indicated?
			If expert judgement is used for deriving parameter values, is the expert(s) justification clearly reminded?

(continued)

Table 1 (continued)

Line of evidence	Category	Subcategory	Question
		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?

(continued)

Table 1 (continued)

Line of evidence	Category	Subcategory	Question
	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 against 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)?

(continued)

Table 1 (continued)

Line of evidence	Category	Subcategory	Question
	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 min to run a simulation under deterministic conditions (e.g. without uncertainty analysis)?
			Does the model take shorter than 8 h 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 reproduce 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, online, 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?

(continued)

Table 1 (continued)

Line of evidence	Category	Subcategory	Question
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.)

2.2 *Relevance Criteria Importance for Regulatory Frameworks*

In order to evaluate exposure models towards their compatibility in a certain (regulatory) applicability framework, the relevance criteria were scored on their importance in a certain framework as introduced in Sect. 2. All other criteria were considered to be equally important in all frameworks. The scoring was done based on expert judgement. 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 3.

From Table 3, it can be concluded that for site-specific assessment, the majority of the criteria are important (fairly high importance on all criteria). This can be explained because 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.

Table 2 Hierarchical structure of the assessment methodology based on categories, subcategories and questions: relevance criteria

Category	Subcategory	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 groundwater?
	Surface water	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?

(continued)

Table 2 (continued)

Category	Subcategory	Question
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.)?

(continued)

Table 2 (continued)

Category	Subcategory	Question
	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. 1 km^2)?
	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?
	Dispersive release	Does the model cover wide dispersive 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)

Table 3 Scoring to importance of relevance criteria according to different frameworks of the assessment methodology based on categories, subcategories and questions: relevance criteria

Question	REACH	PPP	Biocide	Environ. compartment oriented directives	Food oriented directives	Site specific assessment	Sustainability
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 groundwater?	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 model calculate 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 concentrations 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

(continued)

Table 3 (continued)

Question	REACH	PPP	Biocide	Environ. compartment oriented directives	Food oriented directives	Site specific assessment	Sustainability
Does the model cover wet and dry deposition to surface waters?	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

(continued)

Table 3 (continued)

Question	REACH	PPP	Biocide	Environ. compartment oriented directives	Food oriented directives	Site specific assessment	Sustainability
Does the model cover exposure at the local scale (e.g. 1 km^2)?	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

As for the REACH/Biocide/PPP chemical regulation, internal (human) concentrations are not taken into account yet; the criteria related to the pharmacokinetic modelling therefore receive a low importance score.

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 cover a broad range of compartments and where e.g. the exposure of man via the environment is assessed.

Finally, it can be concluded that several criteria proposed are not very important for the sustainability assessment. Models used for sustainability assessment are not always as detailed as the models used for exposure assessment in the proposed regulations. For example, a model used to evaluate pesticide leaching will contain detailed processes on the fate of pesticides in the soil, while sustainability models are more hazard based or consider exposure in broad categories and will therefore not require and contain such detailed processes.

2.3 Exposure Models

To identify the strengths and weaknesses of the MERLIN-Expo model, a comparison was made between the MERLIN-Expo model and existing exposure models. Based on a literature review, 97 exposure models were identified, which could be divided into the following categories: environmental concentration, human intake, dietary exposure, consumer exposure and aggregate or multimedia models. Sixty of the identified models were multimedia models. Based on this list and the expertise of the expert panel, the following exposure models were selected to be included in the comparative assessment: CalTOX, ESCAPE, EUSES, GLOBOX, GREAT-ER, MACRO, MERLIN-Expo, MODULERS, PBPK model, PEARL, STEPS 1–2, TOXSWA and USEtoxs. More information on these models can be found below.

2.3.1 CalTOX

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 [20]. 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.

2.3.2 ESCAPE

ESCAPE (Estimation of Soil Concentrations After PEsticide applications) is able to calculate the fate of the parent compound and up to two metabolites. ESCAPE

calculates initial, time-related and TW (time-weighted average concentrations) in the soil. It is able to calculate plateau concentrations (background concentrations after many years of pesticide application) (http://www.ime.fraunhofer.de/en/business_areas_AE/Fate_Effects_Agrochem/Exposure_modeling.html).

2.3.3 EUSES

The EUSES (European Union System for the Evaluation of Substances) 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 [21]. 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 (Predicted Environmental Concentrations) at Tier 1. The output of EUSES is a quantitative comparison per substance of the results of the effects and the exposure assessments respectively. The system can be used to carry out tiered risk assessments of increasing complexity on the basis of increasing data requirements.

2.3.4 GLOBOX

GLOBOX 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 [22].

2.3.5 GREATER-ER

The GREAT-ER model (Geo-referenced Regional environmental Exposure Assessment Tool for European Rivers) is a model for environmental risk assessment and management of chemicals in river basins (www.great-er.org) 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. 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 visualisation of predicted chemical concentrations and water quality along a river.

2.3.6 MACRO

MACRO is a one-dimensional non-steady state model of water flow and solute transport in structured or macroporous field soils [23]. The primary objectives behind the development of MACRO were to synthesise 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 groundwaters.

2.3.7 MERLIN-Expo

The MERLIN-Expo software [24] is a decision-support instrument that integrates on the same platform a library of both multimedia and PBPK (physiologically based pharmacokinetics) (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.

2.3.8 MODULERS

MODULERS is a 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.

2.3.9 PBPK

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 PBPK model to predict route to route extrapolation and IVIV (in vitro–in vivo) extrapolations was built by the JRC (Joint Research Center).

2.3.10 PEARL

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 [25]. 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 groundwater 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.

2.3.11 STEPS 1–2

STEPS 1–2 in FOCUS is a stand-alone Surface water Tool for Exposure Predictions – Steps 1 and 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 (http://www.ime.fraunhofer.de/en/business_areas_AE/Fate_Effects_Agrochem/Exposure_modeling.html).

2.3.12 TOXSWA

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 (http://www.pesticidemodels.eu/toxswa). 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.

2.3.13 USEtox

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) (www.usetox.org). 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 Comparative Assessment

Several quantitative (e.g. MCDA (Multi-Criteria Decision Analysis), Weight of Evidence) and qualitative (expert judgement) methods can be used to support a SWOT analysis (e.g. [26, 27]). The main purpose of the MCDA methodology is to rank different models in a relative way. The MCDA methodology appeared very useful to structure the SWOT analysis and could be used in a semi-quantitative matter (see Deliverable 2.4 (2014) of the 4FUN project). Further considerations will here be obtained through a qualitative evaluation of individual models based on expert judgement.

In general, multimedia models receive good scoring for a lot of the general criteria. As far as the relevance criteria are concerned (following applicability frameworks), it can be concluded that the assessed exposure models are least applicable to assess sustainability. The assessed exposure models are less applicable to the food and environmental oriented frameworks because the frameworks cover less compartments/media than REACH, PPP, Biocides and site-specific assessments.

The following observations can be made more specifically for each model:

- *MERLIN-Expo* is assumed to be highly suitable 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 lead 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. Moreover, given a comprehensive description of many environmental processes, MERLIN-Expo is a versatile and flexible tool for several applications.
- In theory, the *CalTOX* model would fit 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. Moreover, for some compartments, the models to be used are predefined. For example, to determine the concentration in groundwater, PEARL or PELMO should be used.

- *EUSES* is highly suitable for *REACH and biocides* as the model covers a large amount of the relevance criteria which are important for REACH and biocides. It is also the recommended model for use in the REACH regulation and the Biocidal Product Regulation.
- *GLOBOX*, which is more or less based on EUSES, will be mostly suitable for *REACH*; however, it does not contain some essential aspects necessary for REACH: no worker/general population exposure, no concentrations in earthworms, or no local scale. 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* contains some PPP specific aspects such as linear sorption, excretion/degradation by animals, food processing, irrigation and wide dispersive release. Moreover it would also be applicable for site-specific assessments, and it is a fairly versatile model.
- *USEtox*, which was also based on EUSES, could be used in the exposure assessment for substances under the REACH regulation. However, similar to GLOBOX, the outcomes are characterisation factors which are useful in LCA (Life Cycle Analysis) frameworks but not useful in REACH.
- *GREAT-ER* is recommended as a higher-tier model for the fate of chemicals in surface water in the REACH regulation. Therefore the model is suitable to cover exposure assessment of surface water for this framework. However, as its use is limited to exposure to water, the 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 can be useful for 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. However, since it does not include any environmental aspect, this model will not further be included in the comparative assessment.
- *MACRO*, *PEARL*, *STEPS 1–2*, *TOXSWA*, *ESCAPE*. 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.

Table 4 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 bioaccumulation, excretion and degradation by animals	Not all regulations require this	Not all processes, media, exposure routes and human populations are covered	No calculations in groundwater	Implementing a groundwater 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

(continued)

Table 4 (continued)

Strengths		Threats	Weaknesses		Opportunities
General	Detailed		General	Detailed	
	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

Table 5 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
	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 visualisation of the results				
Complete documentation for novice and expert	Extrapolation rules are indicated				
	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
	Number and origin of the data used to estimate parameter values from empirical data is clearly indicated			Limited range of pollutants in the database	Expand the database

	Applicability domain of 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
	Number and origin of the data used for QSARs or read-across is well indicated				
	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			

(continued)

Table 5 (continued)

Strengths		Threats	Weaknesses		Opportunities
General	Detailed		General	Detailed	
Models were verified	Implementation of equations was verified. Benchmarking with other exposure models was done		Validation		
	Numerical solutions were verified by comparing the results with analytical results or with other number solvers. Model results were compared with monitoring data				
Modular and flexible model	All parameter values can be adopted	Misuse by users, potentially lower acceptability by regulators as it less standardised		Intermediate results cannot be overwritten	Insert functionality were intermediate results can be overwritten by e.g. measured data
	No fixed units		Undefined scope	Not recommended or authorised for use in any regulation yet	Advocacy
	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

4 SWOT Analysis of the MERLIN-Expo Model

A SWOT analysis involves specifying the objective and identifying the internal and external factors that are favourable and unfavourable to achieve that objective. The objective here is to assess exposure tools aiming at predicting environmental and human (via the environment) exposure. The comparative assessment above is the basis for the SWOT analysis (with particular focus on MERLIN-Expo). An overview of the strengths, weaknesses, opportunities and threats is presented in Tables 4 and 5, for, respectively, relevance/framework dependent aspects of models and for general model aspects.

All identified points were categorised 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. Not all identified missing aspects should receive the same importance. For example, concentrations in eggs, soil ingestion, ingestion of meat contaminated via soil ingestion, ingestion of water during recreational activities are of less importance than the inclusion of a groundwater and a marine compartment. Hence, the implementation of each opportunity should be decided on a case-by-case basis.

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.

5 Conclusion

MERLIN-Expo has many advanced functionalities (such as uncertainty analysis, modular approach, dynamic model, combines environmental fate with pharmacokinetics) and models (many fate processes and environmental compartments, different human populations). At the same time, the threat is that current (regulatory) applicability frameworks do not always require these advanced assessment functionalities. The MERLIN-Expo tool appeared to be most suitable for the site-specific assessment as this is the most flexible framework. Based on this analysis, weaknesses of the MERLIN-Expo tool for its use in a certain regulatory framework could also be identified. These weaknesses are at the same time further development opportunities for MERLIN-Expo. On general model characteristics, MERLIN-Expo was identified as a highly documented (both for novice and expert level), transparent, user-friendly tool with regular trainings. Its main threat now is to ensure continuing support and mechanisms for future developmental work and updates.

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