4FUN

"The FUture of FUlly integrated human exposure assessment of chemicals: Ensuring the long-term viability and technology transfer of the EU-FUNded 2-FUN tools as standardised solution"

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Deliverable D4.2: Report of the verification of models

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Revision	

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Dissemination Level		
PU	Public	x
PP	Restricted to other programme participants (including the Commission Services)	
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1 Introduction

The overall objective of the 4FUN project is to further improve the 2-FUN tool (developed during the EU-FP6 funded 2-FUN project) as a standardised solution for integrated assessment of human exposure to chemicals.

In response, the 4FUN project developed the MERLIN-Expo software which contains a library of models for exposure assessment coupling environmental multimedia and pharmacokinetic (PBPK) models. All models within the tool are implemented on the same platform (Ecolego [1]) to facilitate integrated full-chain assessments for combined exposures.

Within the context of Work Package 4 and in conjunction with European Committee for Standardisation (CEN) a standard framework for model documentation has been developed with the aim of ensuring the rigorous formulation of exposure models, comparability between the different exposure models and transparency and ease of understanding for the users of the tool.

According to the objectives of Task 4.2 “Verification and benchmarking process”, a verification process was performed by auditing the implementation of the Multimedia and PBPK models in MERLIN-Expo tool against the standard documentation describing the models (Deliverable D4.4).

This report aims to describe how the verification process was conducted.

1.1 Models of the MERLIN-Expo library

A summarize of the models that are/will be developed for the final library of models available in the MERLIN-Expo tool can be found in the report “Updated 2-FUN library of models” (Deliverable 3.1).

In MERLIN-Expo the models are accessible from the Library windows in the Model screen [2] (Figure 1).

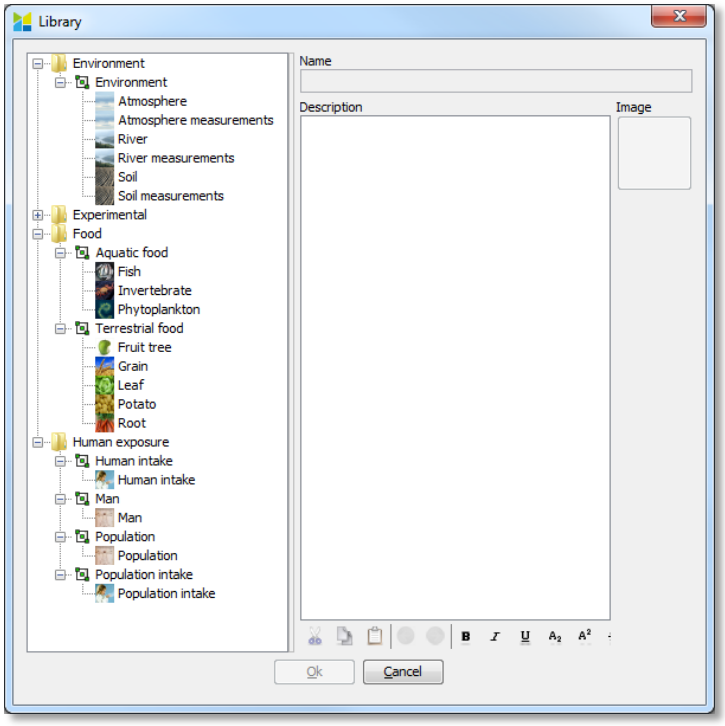


Figure 1 - Model library window in MERLIN-Expo tool

2 Verification

The validation is an essential part of model development; this includes testing, verification and benchmarking of the models.

Verification is the task of determining if the implementation of a model has been done correctly with good input and structure.

2.1 Verification procedure

The correct implementation of the multimedia and PBPK models in MERLIN-Expo has been verified by auditing the implementation against the standard documentation developed in Task 4.3 (Deliverable D4.4).

The verification procedure carried out to verify the models in MERLIN-Expo includes the following actions:

- Verification that the mathematical description of the model (Level 4 “Mathematical information” in the documentation) corresponds to the equations in the Ecolego model.

- Verification that the default parameter values in the documentation (Level 3 “Numerical information”) matches the values in the Ecolego model.

- Verification that the name, unit and full name are correct for all blocks in the Ecolego model. These are given in chapter 3 “Model components”. The name is written as abbreviation in the tables of chapter 3. The full name is the name as given in tables of chapter 3. The unit is written together with the abbreviation.

- Verification that the description is correct for all blocks in the Ecolego model, except for transfers and compartments for which there are no descriptions in the documentation. Descriptions are given in the tables of chapter 3, in the column Purpose. Additional description of parameters is given in chapter 5.

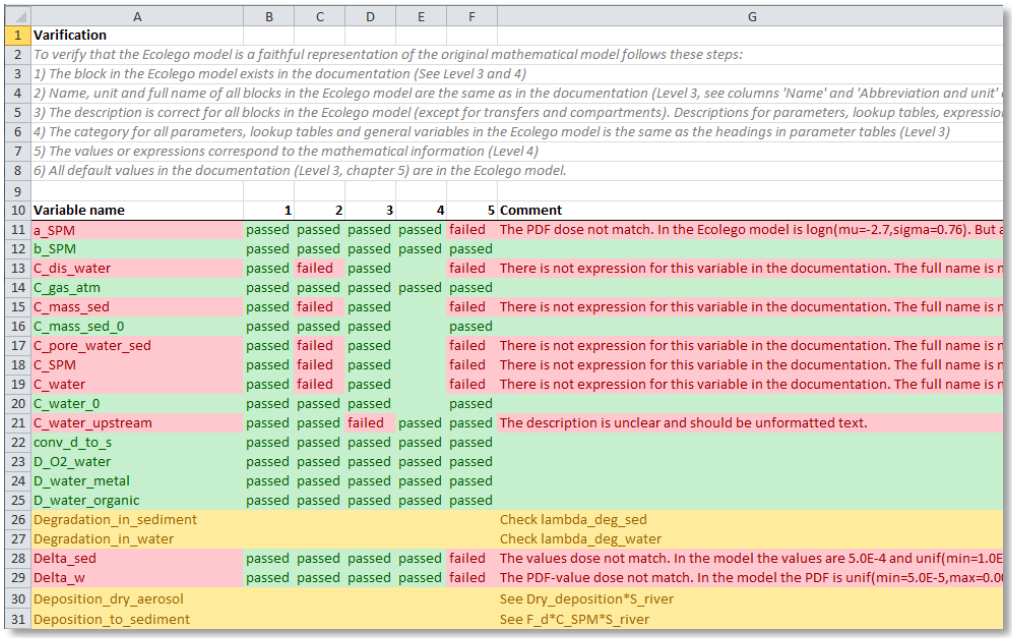
- Verification that the category is correct for all parameters, lookup tables and general variables. The category is given by the headings in chapter 5 e.g.: “Site specific”, “Partition between phases”, etc…

- Simple sanity check to assure that the models can be run with the default values and pdf’s, with simple inputs:
  - That no error messages appear for deterministic or probabilistic simulations.
  - That the model can be run deterministically or probabilistically without errors with default input data.

- All errors have to be listed in a verification log (Figure 2) and any modification to the Ecolego model should appear registered in a changelog (Figure 3) attached to the Ecolego project (under Documents node in the Ecolego project).

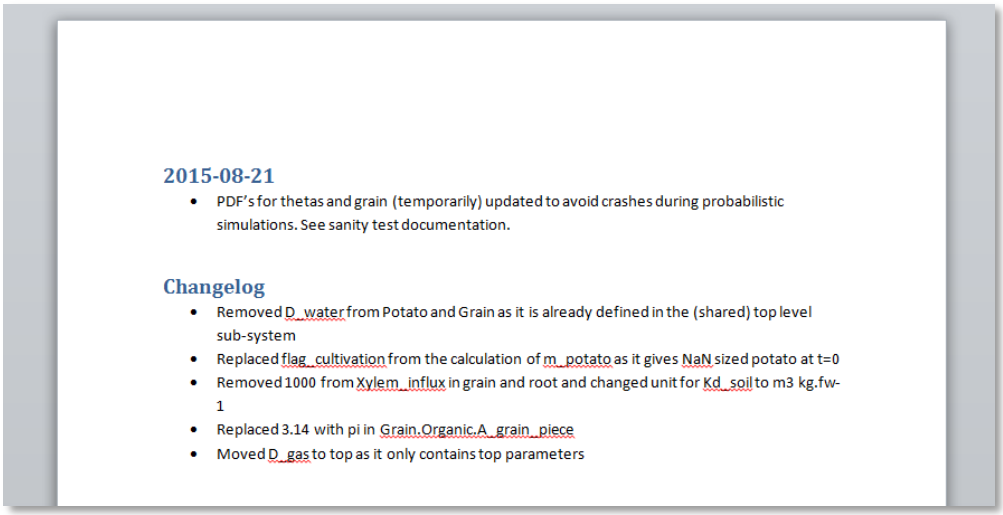
- When verification is completed, the result is sent to the authors and to the developers of model, they are responsible to implement necessary corrective actions.

- Once the Ecolego model has been correctly implemented, the model is tested in MERLIN-Expo tool by examining the model output under different input parameters.



	A	B	C	D	E	F	G
1	**Varification**						
2	*To verify that the Ecolego model is a faithful representation of the original mathematical model follows these steps:*						
3	*1) The block in the Ecolego model exists in the documentation (See Level 3 and 4)*						
4	*2) Name, unit and full name of all blocks in the Ecolego model are the same as in the documentation (Level 3, see columns 'Name' and 'Abbreviation and unit'*						
5	*3) The description is correct for all blocks in the Ecolego model (except for transfers and compartments). Descriptions for parameters, lookup tables, expressio*						
6	*4) The category for all parameters, lookup tables and general variables in the Ecolego model is the same as the headings in parameter tables (Level 3)*						
7	*5) The values or expressions correspond to the mathematical information (Level 4)*						
8	*6) All default values in the documentation (Level 3, chapter 5) are in the Ecolego model.*						
9							
10	**Variable name**	**1**	**2**	**3**	**4**	**5**	**Comment**
11	a_SPM	passed	passed	passed	passed	failed	The PDF dose not match. In the Ecolego model is logn(mu=-2.7,sigma=0.76). But a
12	b_SPM	passed	passed	passed	passed	passed	
13	C_dis_water	passed	failed	passed		failed	There is not expression for this variable in the documentation. The full name is n
14	C_gas_atm	passed	passed	passed	passed	passed	
15	C_mass_sed	passed	failed	passed		failed	There is not expression for this variable in the documentation. The full name is n
16	C_mass_sed_0	passed	passed	passed		passed	
17	C_pore_water_sed	passed	failed	passed		failed	There is not expression for this variable in the documentation. The full name is n
18	C_SPM	passed	failed	passed		failed	There is not expression for this variable in the documentation. The full name is n
19	C_water	passed	failed	passed		failed	There is not expression for this variable in the documentation. The full name is n
20	C_water_0	passed	passed	passed		passed	
21	C_water_upstream	passed	passed	failed	passed	passed	The description is unclear and should be unformatted text.
22	conv_d_to_s	passed	passed	passed	passed	passed	
23	D_O2_water	passed	passed	passed	passed	passed	
24	D_water_metal	passed	passed	passed	passed	passed	
25	D_water_organic	passed	passed	passed	passed	passed	
26	Degradation_in_sediment						Check lambda_deg_sed
27	Degradation_in_water						Check lambda_deg_water
28	Delta_sed	passed	passed	passed	passed	failed	The values dose not match. In the model the values are 5.0E-4 and unif(min=1.0E
29	Delta_w	passed	passed	passed	passed	failed	The PDF-value dose not match. In the model the PDF is unif(min=5.0E-5,max=0.0
30	Deposition_dry_aerosol						See Dry_deposition*S_river
31	Deposition_to_sediment						See F_d*C_SPM*S_river

Figure 2 - Example of verification log



2015-08-21

- PDF's for thetas and grain (temporarily) updated to avoid crashes during probabilistic simulations. See sanity test documentation.

Changelog

- Removed D_water from Potato and Grain as it is already defined in the (shared) top level sub-system
- Replaced flag_cultivation from the calculation of m_potato as it gives NaN sized potato at t=0
- Removed 1000 from Xylem_influx in grain and root and changed unit for Kd_soil to m3 kg.fw-1
- Replaced 3.14 with pi in Grain.Organic.A_grain_piece
- Moved D_gas to top as it only contains top parameters

Figure 3 - Example of changelog attached in the Ecolego model

2.2 Result of verification

The Table 1 summarizes the models that have been verified in the Task 4.2 and the result of the verification.

Table 1 - Result of verification

Model		Result of verification
Environment "Environment v1.6 2015-09-16.eco"	Atmosphere	The standard documentation of this model is still pending, so the implementation has not been checked against any standard documentation. The model implementation was verified with basic tests to assure that the models can be run with the default values and simple inputs, and connected to other models.
	River	After auditing the implementation against the standard documentation, errors in equations, units and parameter values were corrected. Missing full names and descriptions were added. General variables D_water, Kd_sed, Kd_SPM were replaced with aggregate blocks. After testing with a case study, slight modifications were introduced. See "tau_d" in section "Critical shear stress for deposition and resuspension".
	Soil	After auditing the implementation against the standard documentation, errors in equations and units were corrected. Matched full names and descriptions with the documentation. Some categories were updated to match the headings in the chapter 5. General variables D_soil, Kd_soil, f_retardation were replaced with aggregate blocks.
Aquatic food Aquatic food v1.4_2015-09-17.eco	Fish	After auditing the implementation against the standard documentation, errors in equations, units and parameter values were corrected. Metabolic half-life of chemicals values for Pentabromodiphenyl ether, Hexabromobiphenyl, Hexachlorobenzene and Hexachlorobutadiene were recalculated and corrected in documentation and software. Missing/wrong full names and descriptions were added or corrected.
	Invertebrate	The standard documentation of this model is still pending, so the implementation has not been checked against any standard documentation. The model implementation was verified with basic tests to assure that the models can be run with the default values and simple inputs, and connected to other models.

	Phytoplankton	After auditing the implementation against the standard documentation, errors in equations and units were corrected. Added connection from phytoplankton to fish and invertebrate. Changes in MERLIN-Expo and models in the aquatic food library to allow adding phytoplankton to the diet of invertebrates and fish.
Terrestrial food Terrestrial food v1.6 2015-09-10.eco	Fruit, Leaf, Potato, Root, Grain	After auditing the implementation against the standard documentation, errors in equations, units, full names and descriptions were corrected. Once all models were implemented, a sanity check was performed. Some issues were corrected in the models. Note: There are still problems to be solved by the model developer. Note: The documentation of the Grain model is not yet finalized.
Human exposure Man v1.5 2015-05-11.eco	PBPK	After verification, some units, names and descriptions were corrected. Minor modifications to the model were necessary.

3 Conclusion and future work

The models of MERLIN-Expo library were verified by assessing the implementation against the standard documentation. The verification procedure included the inspection of the definition and the equations or the values of each model component. A sanity check has been carried out to assure that the models can be run with the default values and pdf's, and simple inputs. This test is confined to check that the results are reasonable to a non-expert, and does not provide expert judgment on the model structure or parameter values.

3.1 Future work

The standard documentation of the Atmosphere and the Invertebrate models are still pending; for that reason, their implementations must be verified entirely once the documentation is complete.

There are still open issues in the terrestrial food models that have to be addressed by the model developer. This has been properly reported in a sanity check report.

The documentation of the Grain model is not yet finalized; therefore, the implementation of Grain model in the terrestrial food library must be verified totally once the documentation of this model is complete.

4 References

1. Ecolego. https://en.wikipedia.org/wiki/Ecolego
2. MERLIN-Expo user guide. http://wiki.merlin-expo.eu/doku.php?id=model_screen