Is MERLIN-Expo tool suitable for the exposure assessment of inorganic active substances in the environment?

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BACKGROUND

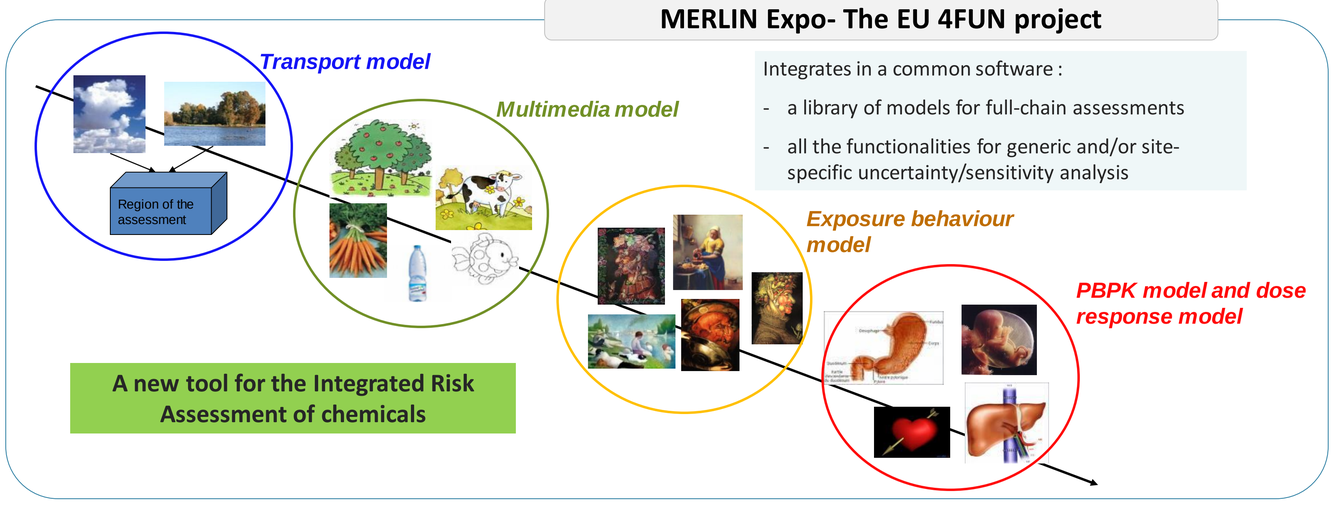
PPPs containing inorganic active substances are widely used to treat important EU crops

The use of standard FOCUS models for inorganic compounds is difficulty accepted by regulators since they are mainly designed for organic substances.

Among the inorganic substances, the case of copper fungicides, which are widely used on several crops, especially tomato, vines and fruit trees, is of great interest.

Copper has raised concerns in view of its persistence and potential harmful impacts to non-target organisms (EFSA, 2013). Copper compounds have been included in the list of substances candidate for substitution (Reg. EU 2015/408). At EU level, the maximum application rate of copper fungicides has been set at 6 kg a.s./ha/year by the Directive 889/2008/EC.

MERLIN Expo- The EU 4FUN project



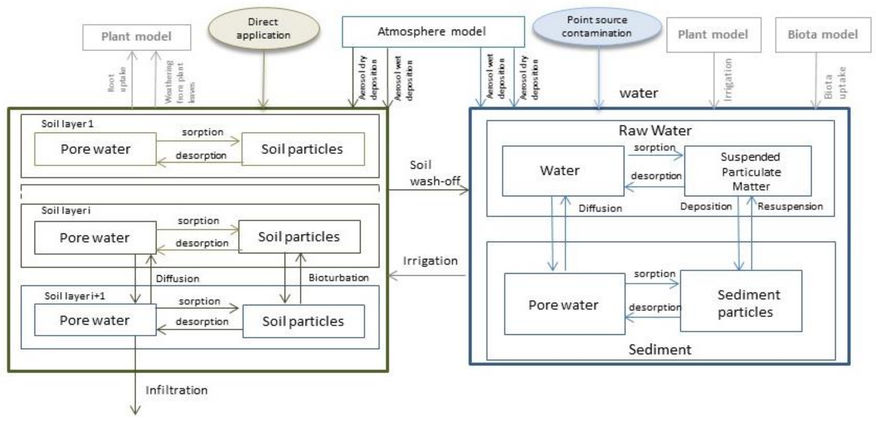
Integrates in a common software :

- a library of models for full-chain assessments
- all the functionalities for generic and/or site-specific uncertainty/sensitivity analysis

A new tool for the Integrated Risk Assessment of chemicals

OBJECTIVE **Can MERLIN Expo be used for environmental exposure of inorganic pesticides?**

MODEL DESCRIPTION



SUBSTANCE PARAMETRISATION

Partition coefficient in m^3/g

	Nominal value	Probability Density Function
Water-soil	3.20E-04	logn(gm=3.2E-4,gsd=4.0)
Water-sediment	7.90E-03	logn(gm=0.0079,gsd=50.0)
Water-SPM	5.00E-02	logn(gm=0.05,gsd=2.51)

Allison and Allison, 2005

SCENARIO DEVELOPMENT

Fungicide application scheme

5 pre-flowering spray applications to apple trees
5 x 1.2 kg Cu/ha - 7 days interval. 1st appl. on 1st February
Total: 6 Kg Cu/ha/y

Meteorological data

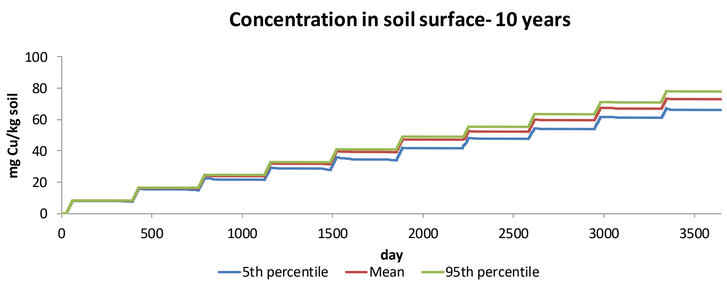
Bologna data (SW FOCUS R3)
Precipitation, wind velocity, radiation, air temperature

Soil and surface water body parametrization

SW FOCUS stream scenario

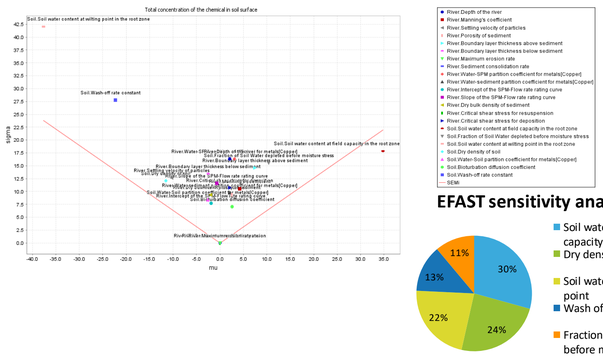
RESULTS AND DISCUSSION

Soil



Concentration in soil surface (soil layer 1) following applications of copper every year for 10 years. The losses of copper from the soil surface are caused by infiltration, diffusion between soil layers and wash off (run off and erosion). Mean and confidential interval (5th and 95th percentile) are shown. The probabilistic assessment takes into account the Probability Density Functions (PDF) associated to the partition coefficients of copper.

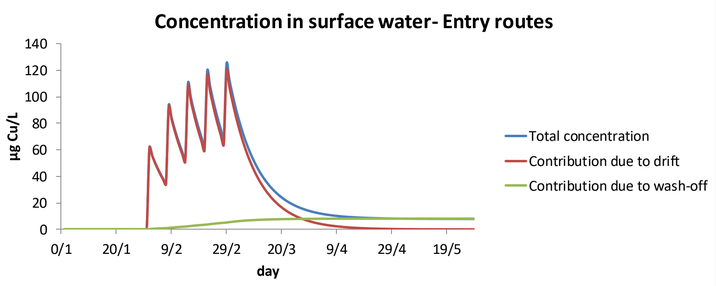
MORRIS Sensitivity analysis



EFAST sensitivity analysis

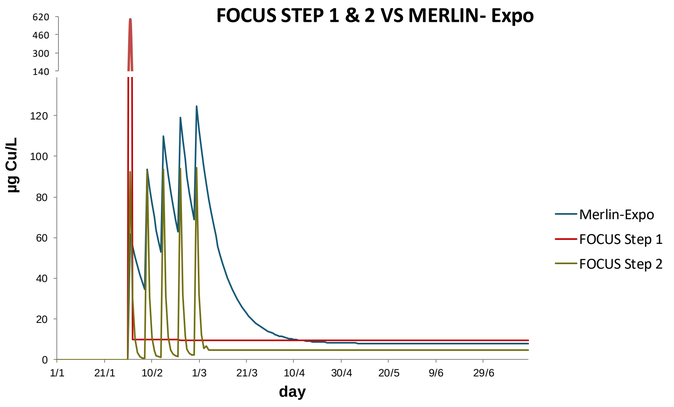
Sensitivity assessment of the parameters associated to PDFs. The screening method MORRIS allows to identify the more sensitive parameters which were further investigated with EFAST (Extended Fourier Amplitude Sensitivity Testing) method. More than 70% of the uncertainties are explained by parameters related to the water budget in the soil root zone.

Surface water



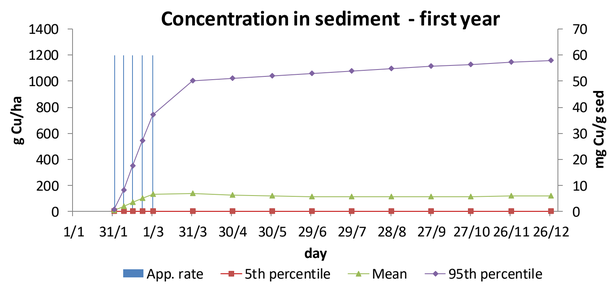
Concentrations in dissolved water refer to the first year of application. The contributions of each entry routs are illustrated. Peaks are caused by spray drift inputs that occur the day of application. The maximum actual concentration occurs to the day of the last application. Wash-off is modelled within MERLIN Expo through a transfer function (using a global wash-off rate constant). This process is responsible of the plateau concentration.

FOCUS STEP 1 & 2 VS MERLIN- Expo



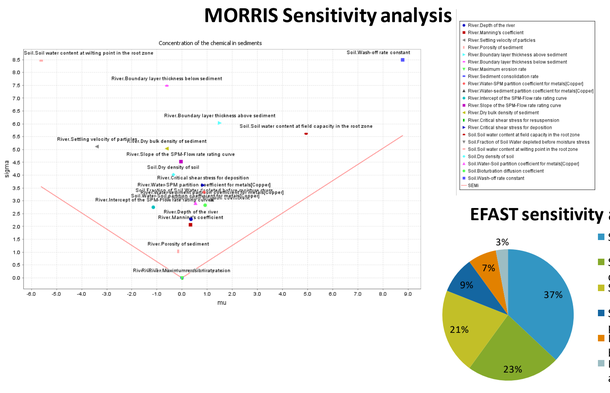
Comparison of MERLIN-Expo outputs vs the standard FOCUS Step 1&2 PECsw (FOCUS, 2001). FOCUS Step 1 is highly conservative compare to MERLIN-expo estimation. In the FOCUS Step 2 modelling, peaks due to spray drift entries are constant, whereas peaks in MERLIN-Expo increase in subsequent applications. The first peak in MERLIN-expo is lower than the maximum Step 2 estimation, on the contrary, the following peaks exceed Step 2 prediction. With regards to the plateau, MERLIN-expo concentration stands in between Step 1 and 2 outputs.

Sediment



Concentrations in sediment refer to the first year of application. Mean and confidential intervals (5th and 95th percentile) are shown. The probabilistic assessment takes into account the probability density functions (PDF) associated to the partition coefficients of copper. The uncertainty associated to these parameters leads to a high variability of the results.

MORRIS Sensitivity analysis



EFAST sensitivity analysis

Sensitivity assessment of the parameters associated to PDFs. The screening method MORRIS allows to identify the more sensitive parameters which were further investigated with EFAST (Extended Fourier Amplitude Sensitivity Testing) method. The wash off rate constant plays a major role in modelling the behaviour of the substance. Other important parameters are the soil water content and the settling velocity of particles in sediment.

CONCLUSIONS

MERLIN-expo is a new tool potentially suitable to predict environmental concentration of inorganic active substances (metals). It allows to calculate actual concentrations and accumulation in years. The sensitivity analysis has allowed to understand which are the most critical parameters and processes driving copper contamination. The MERLIN-expo soil-water model has shown results comparable with FOCUS Step 2.

Features to improve the use of MERLIN Expo for pesticides exposure assessment

The typical pesticides application methods are not specifically included within the scenario description. However, the flexibility of the model has made it possible to overcome this limitation. Mitigation measures are not yet implemented. Groundwater compartment at the moment is not available in the tool.

Potentials for the use of MERLIN-expo tool within regulatory contexts

1. Developed in the frame of the FP7 EU-funded project 4FUN to provide an integrated tool for exposure assessment. The tool combines external exposure (environment, plants and biota) and internal exposure (human intake PBPK). Dose can be referred to organs or biological targets
2. Site-specific assessment (meteorological and pedological data , site-specific dimensions)
3. Probabilistic assessment and sensitivity analysis. The possibility to perform sensitivity analysis on parameters associated to PDFs represents a step forward in the exposure assessment of pesticides
4. Multiple substances can be simultaneously modelled
5. Ability to model organic and inorganic compounds
6. The model documentation has been developed according to a standard documentation protocol resulting from a wide consultation of interested stakeholders and agreed in coordination with CEN (European Committee for Standardisation)

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MERLIN EXPO
www.merlin-expo.eu

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