Evaluation of degradation kinetics of a mobile compound in the field using inverse modelling

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Introduction
- Degradation of pesticides is most realistically studied under field conditions. In a typical field experiment, soil is sampled down to a given depth for a number of time intervals after pesticide application. The standard evaluation procedure requires that total pesticide mass in soil is sampled, i.e. a residue-free lower soil layer is required.
- While this is feasible for less mobile compounds, it is difficult if not impossible for mobile compounds. These may travel below a depth which can be properly sampled due to physical and practical limitations.
- An option to overcome this dilemma is to fit against residues at various depths by inverse modelling. Due to the mechanistic description of all relevant processes, degradation and leaching can be separated. Thus a residue-free lower soil layer is not mandatory any more.
- An example is presented that shows the application of inverse modelling to European field dissipation studies with a mobile compound.

Materials and Methods
- Four European field sites (Germany-1, France-1, France-2, Spain-1)
- Test compound incorporated into soil, sampling down to 30 cm (till day 90), 50 cm (day 120) and 100 cm (from day 180 on)
- Bi-phasic degradation with short fast phase, only slow phase is considered
- Inverse modelling with FOCUS-PEARL and PEST using site specific climate data and soil parameters already set up for standard approach, else FOCUS (2009) defaults (dispersion length and depth dependency of degradation)
- Target function: Residues in 0- 30 cm and 30-100 cm
- Fitted parameters: DegT50 (normalised, topsoil), Kom, initial mass

Results and Discussion
- Generally, the spatio-temporal distribution of the compound in soil could be well reproduced by inverse modelling of transport and degradation which is exemplarily shown for site Germany-1
- According to the simulation, the compound breaks through a depth of 30 cm relatively early. The residues in the subsoil are especially well fitted in the second year.
- Leaching out of the sampled layers could be shown to be small
- Uncertainty of the optimised DegT50 is similar or lower in one case if inverse modelling is used
- For the trials investigated, the effect of leaching on DegT50 is marginal i) because the amount leached was small, and ii) because the decline of degradation with depth was incorporated into the DegT50 value (valid for topsoil)
- Compared to standard evaluation, effect i) leads to increase and effect ii) to decrease of DegT50

Conclusions
- This example shows that inverse modelling is a powerful method which can exploit valuable experimental information that would otherwise be ignored
- It requires a minimum of additional parameterisation and delivers parameter estimates with the same level of reliability as the standard approach