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

Hammel, K.

Bayer CropScience AG, Monheim, Germany
klaus.hammel@bayer.com

Introduction
Degradation of pesticides is most realistically studied under field conditions. In a typical field experiment, the pesticide is applied and the soil is sampled down to a given depth for a number of time intervals. The established evaluation to determine half-lives employs a simple compartment model considering total pesticide mass as a function of time. To determine the total mass, the soil has to be sampled down to a depth with no residues. 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. In such a case there will not always be a residue-free lower layer and compound may have leached out of the sampled domain. Then a standard evaluation is not permissible anymore because degradation and leaching cannot be separated. An option to overcome these difficulties 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. An example is presented that shows the application of inverse modelling to European field dissipation studies with a mobile compound.

Material and methods
The degradation of a pesticide metabolite was studied on four field sites in Europe (Germany-1, France-1, France-2, Spain-1). The compound was incorporated into the soil. Thus surface processes need not to be considered. Nevertheless the degradation behaviour was strongly bi-phasic with a fast initial decline. Only the slow phase was considered for the inverse modelling applying FOCUS-PEARL and PEST (FOCUS, 2009). The inverse modelling approach is compared to the standard compartment evaluation as described e.g. in the FOCUS kinetics report. The inverse modelling approach requires daily weather data and a parameterisation of the soil including hydraulic and thermal parameters. However, these data are usually available because they are likewise required for the standard approach to enable the normalisation of degradation with respect to soil temperature and moisture. There are only few additional parameters required for the inverse modelling such as the dispersion length and the depth dependency of degradation, for which default values were used as given by FOCUS (2009).

Besides the target parameter which is the normalised half-life (DegT50 for 20°C and 100 % field capacity), the Freundlich coefficient (Kom) was fitted to enable PEARL to adjust to the site specific mobility of the compound. The third parameter to be fitted was the initial mass to allow PEARL to adjust to the level of residues observed. The sum of residues in 0-30 cm and the sum of residues in 0-100 cm (for sampling dates when available) were fitted. For visualisation, the mass in the 30 - 100 cm soil layer was calculated by subtraction. The observed data were not weighted.

Results
As for the standard approach, the inverse modelling has to yield a sufficient goodness of fit to consider the optimised parameters acceptable. 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 (Figure 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.

![Graph showing degradation over time for different sites](image)

Figure 1: Modelled (solid line) and measured (symbols) residues of the test compound in the 0-30 cm soil layer (left) and in the 30-100 cm soil layer (right) at site Germany-1. Note the different scales on the y-axis.

The DegT50 obtained from inverse modelling and the standard evaluation are almost identical (Figure 2). The uncertainty of the optimised DegT50 is also similar or lower in one case if inverse modelling is used.

![Graph showing DegT50 and amount leached](image)

Figure 2: Optimised DegT50 ± standard deviation for standard and inverse modelling evaluation (left), and estimated amount leached below 1 m (right).

For the trials investigated, the effect of leaching on DegT50 is marginal i) because the amount leached was small according to the calculation (Figure 2), and ii) because the decline of degradation with depth was incorporated into the DegT50 value which by definition is valid for the (biologically most active) topsoil. Compared to the standard evaluation, effect i) leads to an increase and effect ii) to a decrease of DegT50.

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.

References