Use of time dependent sorption in combination with field degradation half-lives for higher tier leaching assessment

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Background

Time Dependent Sorption (TDS) of pesticides to soil describes increased sorption with time and is a process that is often observed and that is relevant for the environmental behaviour of many substances.

The available guidance on TDS of pesticides (FOCUS, 2009 and Beulke and van Beinum, 2012) focuses on laboratory degradation studies to derive TDS parameters. It indicates that TDS parameters should be used in combination with the estimated half-lives from the same studies. Since degradation parameters from field studies are often used as more realistic data for the leaching assessments, there is a need for approaches where TDS can be combined with degradation half-lives from field studies.

Proposed approaches

Approach 1) TDS from field studies.

The possibility of deriving TDS parameters from field studies, if additional aqueous extractions of the soil samples are carried out is evaluated. Due to dynamic temperature and moisture conditions, inverse modelling with a numerical leaching model is needed to estimate the TDS parameters as well as the degradation in the equilibrium sorption phase DegT50equiv (e.g. combination of FOCUS-PEARL with PEST). Statistical criteria can be applied as proposed for laboratory studies in the existing guidance. For the exposure assessment the estimated TDS parameters can be used together with the estimated field DegT50equiv. If multiple studies are available appropriate mean values can be used for the exposure assessment (e.g. geometric mean for rate constants such as DegT50equiv and desorption rate; arithmetic mean for all other parameters).

Approach 2) TDS from laboratory studies transferred to field studies.

For the exposure assessment of pesticides important e-fate properties such as equilibrium sorption are exclusively derived from laboratory studies and subsequently transferred to outdoor conditions. It should, therefore, be assumed that the TDS behaviour as observed in laboratory is also representative for outdoor conditions. Methodological studies already have indicated that there are no systematic differences between TDS parameters derived from laboratory and field studies (Hammel, 2010). Preferably, laboratory aged sorption studies should be carried out with soils from field degradation studies.

Examples are available where DegT50equiv values from field degradation studies have been successfully re-evaluated considering TDS as measured in laboratory. The consideration of TDS was, for instance, necessary to explain bi-phasic degradation behaviour observed in both laboratory and field studies for a particular substance (Jene, 2006). As for Approach 1) the DegT50equiv from the field needs to be inversely estimated using a numerical simulation model. Gurney et al. (2007) used a time-step normalisation approach to re-evaluate a field study considering TDS with a model that assumes stationary temperature and moisture conditions. However, this approach is not consistent with the inverse parameter estimation.
using a numerical model which takes into account varying soil moisture and temperature. The TDS approach also includes a rate constant (desorption rate) that will be affected by the time-step normalisation, although it is assumed in the models that this parameter is not influenced by moisture and temperature.

For the exposure assessment the estimated field DegT50equ values can be used together with the laboratory TDS parameters. If multiple studies are available, appropriate mean values can be used as proposed for Approach 1).

Parameter validation

For both approaches the relevance of the estimated TDS parameters for the field can be checked. The measured concentration depth profiles at different sampling times need to be compared with simulated concentrations at respective depths with and without consideration of TDS. This was shown, for instance, by Boesten et al. (1989) as well as by Streck and Richter (1999) where measured concentration profiles of cyanazine, metribuzin and chlortoluron, respectively, were compared with simulated concentrations at different depths with and without TDS. In both papers it was clearly shown that the consideration of TDS was necessary to explain the observations.

A successful validation requires, therefore, that the simulation with TDS sorption should fit the observations better than the simulation based exclusively on equilibrium sorption as measured according to OECD 106.

References


Beulke S; van Beinum, W (2012). Guidance on how aged sorption studies for pesticides should be conducted, analysed and used in regulatory assessments. FERA, Sand Hutton, York, YO41 1LZ, UK.


