Kinetic (aged) sorption in the groundwater exposure assessment of pesticides

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Introduction

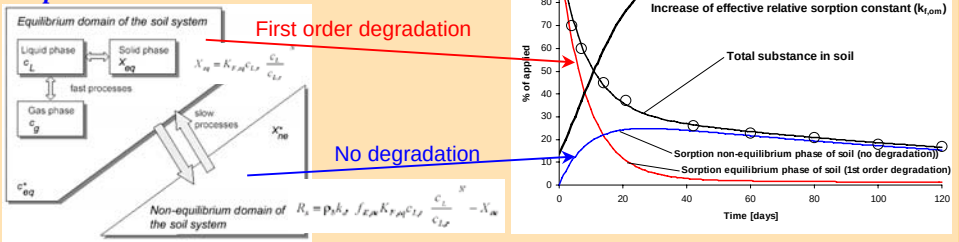
Kinetic or non-equilibrium sorption of pesticides in soil is a frequently observed process in laboratory as well as in field studies.

An approach is shown where kinetic sorption parameters were identified. They were derived from laboratory studies and validated in field degradation studies and could subsequently be used for modelling the transport of a pesticide to groundwater.

Theory

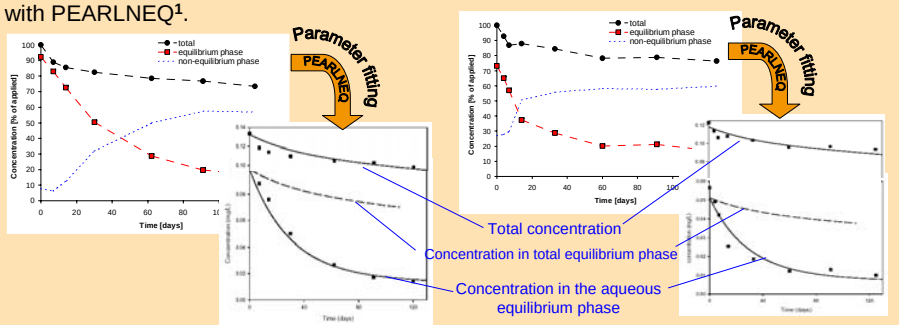
Non-equilibrium sorption results from time-dependent slow sorption and desorption processes. A fraction of the substance is transferred from the equilibrium domain of the soil where exchange is very fast to the non-equilibrium domain. Due to stronger binding to the soil in the non-equilibrium domain it can be assumed that the bio-availability is limited and degradation hardly occurs. This results in an overall bi-phasic degradation behaviour of the substance. Non-equilibrium sorption is implemented in the PEARL[1] model.

Non-equilibrium sorption as implemented in the PEARL model



Step 1) Kinetic sorption in laboratory aged sorption study

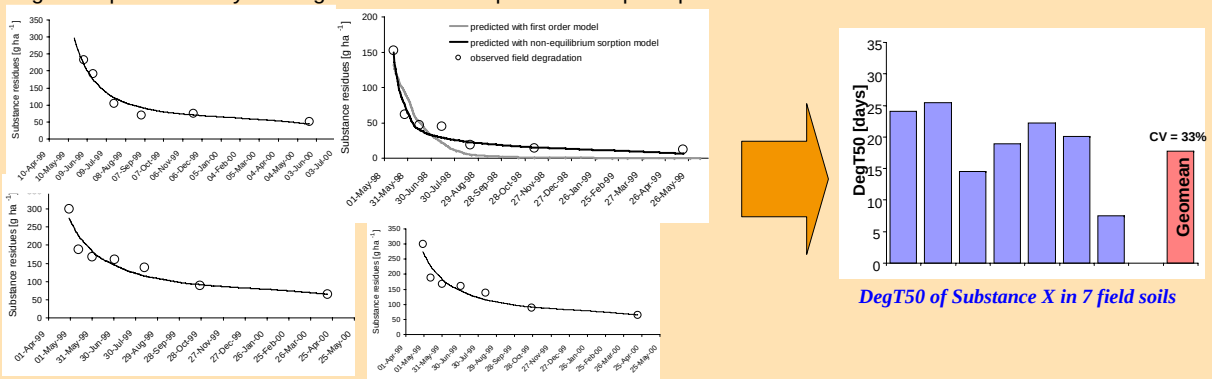
Non-equilibrium sorption can be investigated in laboratory degradation studies. At any sampling time the equilibrium phase fraction is determined by a desorption step with water ($CaCl_2$-solution) and the total degradation is analysed by desorption with organic solvents. The non-equilibrium sorbed fraction is defined as the amount that is not desorbed by water but by organic solvents. The parameter fitting can be carried out with PEARLNEQ[1].



Kinetic sorption of Substance X in two soils fitted with PEARLNEQ: K_d = 0.008 d^{-1}, f_{NE}-value = 2.7

Step 2) Kinetic sorption in field degradation studies

In order to obtain realistic outdoor half-lives that reflects the degradation behaviour of Substance X under field conditions a series of terrestrial field degradation studies was evaluated. For reasons of consistency the PEARL[1] model was again used combined with the inverse modelling tool PEST[2]. The bi-phasic degradation behaviour of Substance X in the field could not be sufficiently fitted with single first order (SFO) but considering non-equilibrium sorption using the kinetic parameters from the laboratory studies. For the evaluation actual soil moisture and temperature was considered. The fitted DegT50 represents only the degradation in the equilibrium sorption phase

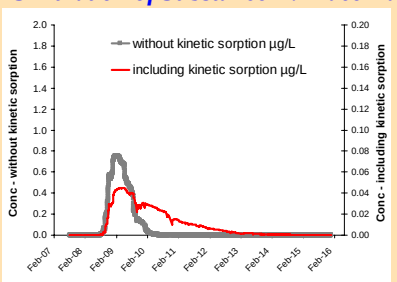


DegT50 of Substance X in 7 field soils

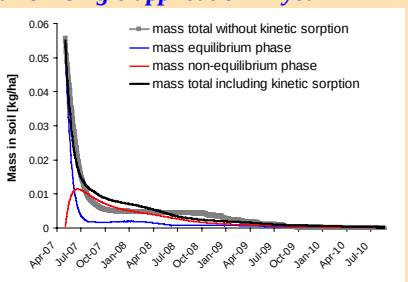
Step 3) Kinetic sorption in groundwater exposure assessment

Non-equilibrium parameters were consistently used in combination with the appropriate DegT50 describing degradation in the equilibrium sorption phase. The PEARL[1] model that was used for the evaluation of the laboratory aged sorption studies and the field degradation studies was also used for the prediction of the leaching of Compound X.

Simulation of Substance X: Piacenza scenario – single application in year 7



BTC with and without kinetic sorption



Mass in soil in different sorption phases

Conclusion: For substances that show pronounced kinetic sorption behaviour it is necessary to consider this process for a good explanation of the experimental behaviour and for a sound assessment of the transport behaviour to groundwater.

References: [1]PEARL: Tiktak, A, F van den Berg, JJJT Boesten, D van Kraalingen, M Leistra, AMA van der Linden (2000) Manual of FOCUS-PEAR (http://www.pearl.alterra.nl)

[2] PEST: Model Independent Parameter Estimation (http://www.waterloohydrogeologic.com/software/visual_pest_asp/visual_pest_ asp_ov.htm)