Comparative Evaluation of Time-Dependent Sorption Data of Pesticides

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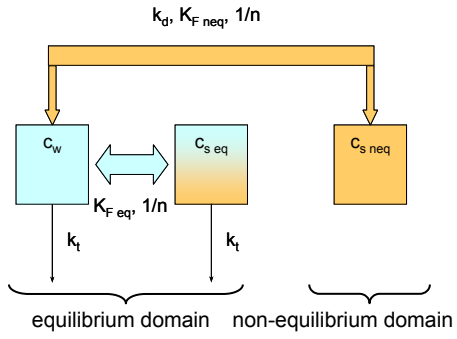
Introduction

The time-dependent sorption (TDS) model is an important higher-tier option for groundwater leaching simulations, e.g. with FOCUS-PEARL, to describe more realistically the mobility of a compound in the vadose zone. The TDS model parameters k_d and f_{ne} were derived from laboratory studies using 78 compound/soil combinations (14 compounds, 23 different soils) and subjected to a comparative statistical analysis.

Methods

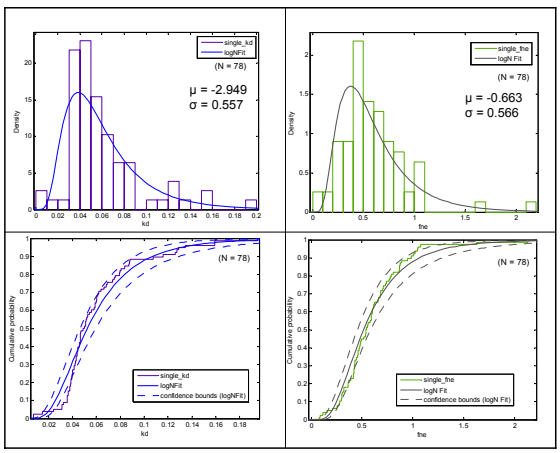
Laboratory TDS Study: The soils were treated with radiolabelled test items and incubated for up to 120 days under controlled laboratory conditions. Samples were first extracted by shaking with calcium chloride solution for 24 h to determine the equilibrium sorbed amount and the non-equilibrium sorbed domain was subsequently extracted with organic solvent mixtures.

Evaluation: The TDS model differential equations following the PEARLneq approach were implemented in MATLAB code for integration and parameter optimization. The degradation rate in the equilibrium domain k_t, the desorption rate constant k_d, the ratio of non-equilibrium to equilibrium domain f_{ne}, and the initial value of the equilibrium sorbed concentration $C_{s\ eq,0}$ were determined by simultaneous fit to the measured concentrations in the equilibrium and non-equilibrium sorbed domain. Significance between TDS parameters and compound/soil properties was tested according to PEARSON (two sided, significance level of 0.01).



Results

Overall Distribution of TDS Parameters

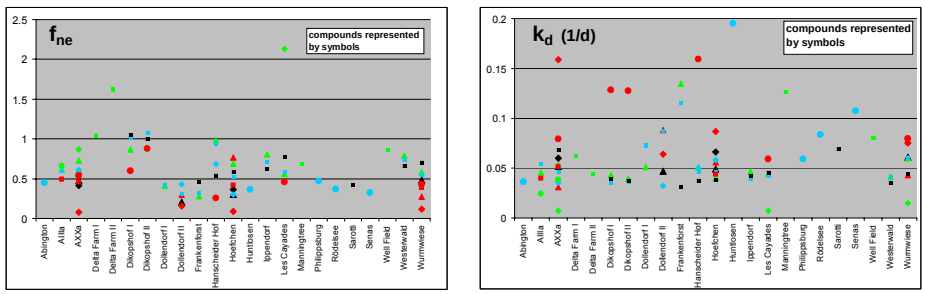


- k_d and f_{ne} were lognormally distributed
- Median values of 0.052 d^{-1} (SD = 0.037 d^{-1}) for k_d and 0.52 (SD = 0.37) for f_{ne} obtained and the following 10th and 90th percentiles:

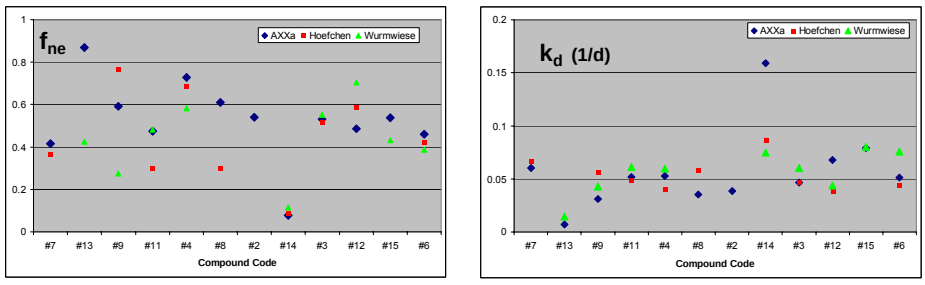
	10th Percentile	Median	90th Percentile
k_d (1/d)	0.026	0.052	0.107
f_{ne}	0.25	0.52	1.1

- The default value for k_d proposed in the draft FOCUS groundwater report II (k_d = 0.01 d^{-1}) represents less than the 1st percentile. The value proposed for f_{ne} (f_{ne} = 0.3) represents the 17th percentile in the distribution of this data set.

TDS Parameters for 14 Compounds on Several Soils



TDS Parameters on 3 Soils for 12 Compounds



Statistical Parameters

Soil		k_d (1/d) Median	k_d (1/d) SD	f_{ne} Median	f_{ne} SD
AXXa	(12 compounds)	0.047	0.051	0.53	0.19
Wurmwiese	(9 compounds)	0.057	0.021	0.44	0.17
Hoefchen	(9 compounds)	0.052	0.015	0.45	0.21

Compound	k_d (1/d) Median	k_d (1/d) SD	f_{ne} Median	f_{ne} SD
# 3 (13 soils)	0.052	0.021	0.60	0.27
# 4 (12 soils)	0.051	0.018	0.68	0.20
# 12 (11 soils)	0.043	0.011	0.64	0.20

Conclusions

- TDS parameters were lognormally distributed (median values: f_{ne} = 0.52 and k_d = 0.052 d^{-1}).
- No systematic influence of soil on the TDS parameters was observed.
- No strong correlations between TDS parameters and compound/soil properties were observed. Only correlations between f_{ne} and k_d (r = -0.41), f_{ne} and OC (r = -0.43), and between k_d and K_F (r = 0.56) were significant.

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