MULTIPHASE MODELLING IN POROUS MEDIA

Sabine Klepsch[1,2], **Andrea Watzinger**[1,2], **Tamara Čoja**[3]

[1]University University of Natural Resources and Applied Life Sciences, Vienna
1190 Vienna, Austria
[2]AIT Austrian Institute of Technology, 2444 Seibersdorf, Austria
Vienna, Austria
[3]Austrian Agency for Health and Food Safety (AGES), 1220 Vienna, Austria
sabine.klepsch@boku.ac.at(Sabine Klepsch)

Abstract

Two chemicals, formaldehyde and allyl isothiocyanate (AITC), have been analysed both experimentally by soil column experiments and theoretically by inverse simulation in order to determine their risk potential and leaching behaviour in porous media. The software products HYDRUS-1D and COMSOL Multiphysics 3.5a coupled to MATLAB (v. 7.0.1) are applied for inverse modelling of the soil column experiments. Due to the viscous properties of AITC, a tool able to simulate multiple phase flow (i.e. COMSOL Multiphysics or STOMP 3.0) has to be used for this substance, while for formaldehyde HYDRUS-1D can be applied. Regarding formaldehyde breakthrough curves, linear adsorption and first-order decay reactions are assumed. AITC reduction in the soil might also be explained by reactions with the soil matrix, biodegradation and partly volatilization. Parameter fitting of the water-oil two-phase flow equations, coupled to equations for solute transport, will be implemented by applying the multidimensional nonlinear minimisation module fminsearchbnd with bound constraints, which uses the Nelder-Mead simplex (direct search) method. Advantages and disadvantages, ease and limits of use, besides flexibility of the respective simulation tools will be pointed out. Results show that formaldehyde is faster degraded than AITC. Thus, the latter will have stronger impact on soil organisms as it is retained longer and migrates slower than formaldehyde.

Keywords: Multiphase flow, Porous media, Inverse modeling.

Presenting Author's Biography

Sabine Klepsch. After finishing the study of Technical Physics, S. Klepsch focused on numerical simulation and modelling of solute transport processes and theories of non-equilibrium phenomena in porous media. Since May 2001 she is research scientist at the Institute of Soil Research, BOKU - University of Natural Resources and Applied Life Sciences, Vienna, funded by the AIT Austrian Institute of Technology, Seibersdorf. Other research topics include linking sorption studies on molecular scale to macroscopic sorption parameters, and rhizosphere modelling.