Estimation of soil concentrations for a localized application of a chemical using Hydrus 2D/3D

Schröder, T. (1), Coquet, Yves (2)

(1) BASF SE, Crop Protection, APD/EF - L444, 67117 Limburgerhof, Germany. E-mail: tom.schroeder@basf.com
(2) University of Orleans, CNRS-INSU, BRGM, UMR 7327, ISTO, 1A rue de la Ferolerie, Orleans Cedex 2, France

Introduction

The development of new formulation types or application techniques for agricultural protection and biocidal products may require innovative approaches for environmental exposure assessments. New application techniques, e.g. seed treatment, require local assessment of exposure, instead of the generally used field-scale spray applications. In the area of biocides local applications are commonly used. In urban pest control for example small areas are treated, e.g. a garden adjacent to or a trench around a house. In these situations, an application of a product, and as a consequence exposure to the environment, is dependent on specific small-scale geometries.

Case study

- Soil injection of a biocidal product around a house that serves as barrier against a pest

Target

- Derivation of a concentration in soil (liquid phase [mg/l], solid phase [mg/kg], total soil [mg/kg]) for a representative soil injection

Methodology

- A chemical can move in vertical and lateral directions. The model Hydrus 2D/3D (Ref. 2) was selected because it can handle water flow and solute transport in 3D for irregular geometries.
- Modified FOCUS GW scenarios (Ref. 3) were implemented along with their upper and lower boundary conditions. Initial conditions were set to: (1) Water potential: linear gradient -200 cm (top) to -700 cm (bottom), (2) Temperature: 20°C throughout the soil profile.
- A 30-year simulation period with 1 application every 10 years was setup. First infiltration 3 months after simulation start.

Concentration in soil [Ref. 1]

Assuming linear sorption:

\[ C_T = C_L \frac{\theta}{\rho} + C_S = C_L \frac{\theta}{\rho} + C_f \cdot f_{om} \cdot K_{om} \]

with:

- \( C_T \) = total concentration in soil [mg/kg]
- \( C_L \) = liquid phase concentration [mg/l]
- \( C_S \) = solid phase concentration [mg/kg]
- \( \theta \) = volumetric water content [m^3/m^3]
- \( \rho \) = dry soil bulk density [kg/l]
- \( f_{om} \) = mass fraction of organic matter [kg/kg]
- \( K_{om} \) = coefficient of sorption on organic matter [l/kg]

Non-linear sorption according to Freundlich:

\[ C_T = \frac{C_L^{1/n}}{1000} \cdot f_{om} \cdot K_{om} \]

Results

Hamburg scenario:

- Number nodes: ~2000
- Number elements: ~14400
- Simulation time: ~1.5h

Conclusions & perspectives

- Based on the modified FOCUS scenarios, suitable (liquid and total) concentrations of a chemical in soil could be derived for a specific ecotoxicological target depth and used for risk assessment of a biocidal product.
- The general setup of the scenarios allows a standardization of localized uses and can easily be extended to other use types. However, the application technique and use scenario, and as such the settings of solute application in the model is case-by-case.
- The usage of higher dimensional models and the proposed methodology, that improves realism, will increase significantly and a commonly agreed evaluation methodology should be strived for.

References