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

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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 application 3 months after simulation start.

Figure 2: 3D soil column of modified Hamburg scenario. Color coded: material distribution after FOCUS.

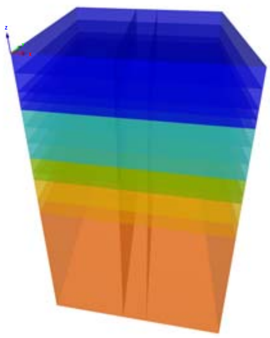
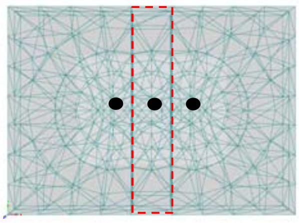


Figure 3: 2D horizontal cross-section at 20 cm depth. Mesh refinement around soil injections (black dots). Red area is evaluation area for concentration derivation.



Key data (Hamburg scenario):

Number nodes:	~ 2000
Number elements:	~ 14400
Simulation time:	~ 1.5h
(1 core, 2.5 GHz)	

Figure 4: Water flow boundary condition at the soil surface.

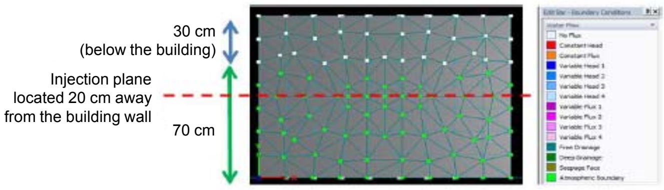
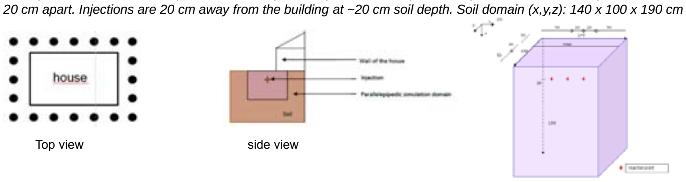


Figure 1: *Soil injection around a house (barrier treatment). One representative injection sequence consists of 3 injections 20 cm apart. Injections are 20 cm away from the building at ~20 cm soil depth. Soil domain (x,y,z): 140 x 100 x 190 cm*



Concentration in soil [Ref. 1]

Assuming linear sorption:

$$C_T = C_L \frac{\theta}{\rho} + C_S = C_L \frac{\theta}{\rho} + C_L f_{om} k_{om}$$

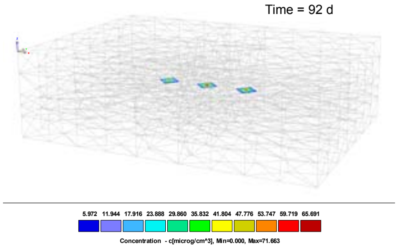
with:
C_T = total concentration in soil [mg/kg]
C_L = liquid phase concentration [mg/l]
C_s = solid phase concentration [mg/kg]
θ = volumetric water content [m³/m³]
ρ = dry soil bulk density [kg/l]
f_{om} = mass fraction of organic matter [kg/kg]
K_{om} = coefficient of sorption on organic matter [l/kg]

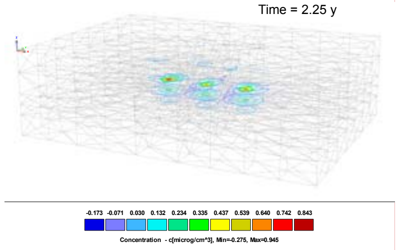
Non-linear sorption according to Freundlich:

$$C_s = \frac{C_L^{1/n}}{1000} f_{om} k_{om}$$

Results

Figure 5: Liquid phase concentration [mg/l] at three simulation times. Vertical and horizontal spreading can be observed.





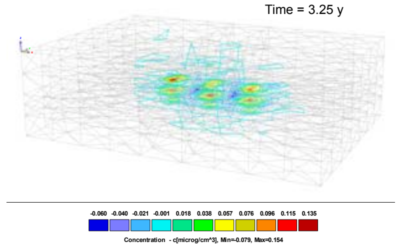
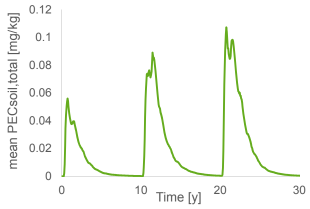


Figure 6: Mean total soil concentration [mg/kg] over time for a soil block (x, y, z) located at the soil surface (Fig. 3; 10 x 100 x 10 cm).



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:
[1] EFSA Panel on Plant Protection Products and their Residues; Scientific Opinion on the science behind the guidance for scenario selection and scenario parameterisation for predicting environmental concentrations in soil. EFSA Journal 2012;10(2):2562. [76 pp]
[2] Šimůnek, J., M. Th. van Genuchten, and M. Šejna (2006) The HYDRUS software package for simulating the two- and three-dimensional movement of water, heat, and multiple solutes in variably-saturated media, Technical Manual, version 1.0, PC progress, Prague, Czech Rep
[3] FOCUS (2014) "Generic Guidance for Tier 1 FOCUS Ground Water Assessments", Version: 2.2, Date: May 2014. Amending report of the FOCUS Groundwater Scenarios Workgroup FOCUS (2000)