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A hydro-geochemical model for variably saturated flow with multi-component gas diffusion: application to predict pollutant fate and transport in Technosols

H. Davarzani (h.davarzani@brgm.fr), S. Coussy, G. Boissard, P. Blanc, P. Bataillard
French geological survey (BRGM), Orléans, FRANCE

Key words: hydro-geochemical modeling, Technosol, pollutants

Introduction

The prediction of the long term trace element transport in Technosols, defined as soils containing at least 20 % of human-made materials within the 100 cm upper soil horizon, would be a way to anticipate land management. These soils, usually abandoned for decades, contain pollutants resulting from industrial processes. The main objective of this study is to develop a model to predict the hydro-geochemical and mechanical evolutions in Technosols.

In this study, the model developments have been made in order to consider the multi-component soil gas phase diffusion whereas the original COMSOL-Phreeqc coupling model [1] does not take it into account. Therefore, the coupling model is able to (i) take into account soil hydro-geochemical heterogeneity (such as permeability and porosity contrasts), (ii) manage multi-component gas diffusion, consumption and generation in unsaturated soil and (iii) take climatic variations, such as rain infiltration, into consideration.

Model concept and validation

The COMSOL® and IPhreeqc procedures alternate for the calculation of liquid water flow, gas and solute transport and reactions using a non-iterative sequential split-operator approach. Data from the output of one procedure is passed back to the Matlab® workspace and reformatted for the following procedure. The gas phase mole numbers and volume are updated using IPhreeqc's method *GAS_PHASE_MODIFY*. As for flow and transport calculations, a function is used to create valid initial conditions for gas transport calculations in COMSOL. The coupling developed model has been validated using CrunchFlow [2] in a 1-D and fixed soil water saturation case.

Model application and results

The coupling model was applied on a case study consisting in a Technosol developed on dredged sediments. The mineralogical compositions of two samples, from fractured oxidation crust and soil block center, were characterized by X-Ray Diffraction spectroscopy. The mineralogical assemblage of the block center sample is used as the composition of the initial sediment deposited 30 years ago. The model axisymmetric geometry consists of a heterogeneous soil profile with a fracture region (about 0.5 m large, 1 m depth). The atmospheric oxygen and carbon dioxide diffuse permanently into the soil and fracture over the time at their respective diffusion coefficients.

The modeling results over 30 years have shown that the Technosol weathering leads to dissolution of galena with consumption of the soil oxygen, as well as precipitation of lead carbonates and formation of ferrihydrite. These mineralogical transformations take place more in poorly saturated zones in the profile such as cracks and soil surface. An example of the results is shown in *Figure 1* for gaseous oxygen diffusion into the soil and related kinetic of galena dissolution after 30 years. The model can capture well the soil evolution trend at least for about 30 years.

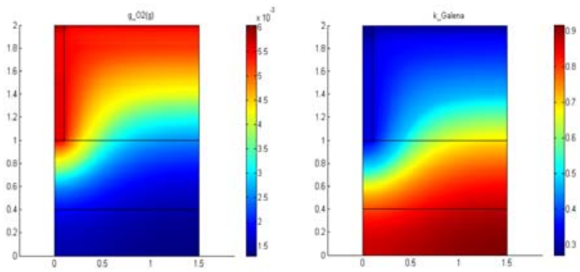

Figure 1: Oxygen concentration in soil air (mol/L) and galena concentration (mol/kgw) after 30 years.

References

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