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A coupled HYDRUS-MT3D-PHREEQC tool for simulating variably-saturated reactive solute transport

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In shallow groundwater environments, fluctuating water tables may induce strong hydrological, physico-chemical and microbial gradients, which will affect the fate of leaching contaminants. Flow-transport-geochemical codes which couple/integrate the vadose and saturated zones at field scale are an important tool to study these processes. However, reactive transport modelling studies most often consider the vadose zone and the saturated zone as separate entities.

In recent years, major advances have been made in the development of numerical codes for continuum subsurface flow and reactive transport simulations. For example, HPx combines the HYDRUS code for water flow and solute transport in variably-saturated conditions with the PRHEEQC code for geochemical reactions. As such, HPx is well-suited for simulating reactive transport in the vadose zone at small scales. Similarly, MODFLOW and PHT3D are used for the modelling of groundwater flow and reactive transport, respectively. PHT3D loosely couples PHREEQC and MT3DMS, which solves the advection-dispersion equation (ADE) for saturated porous media.

The HYDRUS Package for MODFLOW (HPM) is an example of coupling codes for unsaturated and saturated flow at the field scale. It exchanges water fluxes between the HYDRUS and MODFLOW domains; the bottom flux from HYDRUS defines upper boundary fluxes to the MODFLOW model, whereas MODFLOW computes a pressure head boundary for HYDRUS. HPM provides an integrated method for simulating subsurface water flow between the unsaturated and saturated domain. Exchanges of solutes and corresponding geochemical reactions are not incorporated however.

The aim of this research is to construct an integrated tool for simulating water flow and reactive solute transport in the subsurface focusing on the water table interface. This is achieved by loosely coupling the existing HYDRUS, MODFLOW, MT3D-USGS and PHREEQC codes and adding functionalities for the transfer of solute concentrations. Information exchange between the saturated and unsaturated zones occurs at each time step. This results in a comprehensive tool for simulating subsurface water flow and reactive transport in an integrated way while retaining the flexibility of the original codes.

The integrated tool will be developed as a package for the MT3D-USGS code. Prior to the transport simulations, water flow is solved using the HPM code. Subsequently, the transport codes (coupled HYDRUS - MT3D-USGS) are executed to solve the ADE. Here, exchange takes place at the end of either the HYDRUS or MT3D-USGS transport step, depending on which one has the largest length, by exchanging mass-fluxes at the water-table level. Following the approach in HPx, PHREEQC calls are placed at the end of each transport step to solve the geochemical system of the entire domain. The tool is able to simulate water flow and reactive solute transport with an accuracy similar to the codes it is built upon. Simulation results are compared to analytical test cases.