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Numerical investigations of solute transport in bimodal porous media under dynamic boundary conditions

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Quantification of flow and solute transport in the shallow subsurface adjacent to the atmosphere is decisive to prevent groundwater pollution and conserve groundwater quality, to develop successful remediation strategies and to understand nutrient cycling.
In nature, due to erratic precipitation-evaporation patterns, soil moisture content and related hydraulic conductivity in the vadose zone are not only variable in space but also in time. Flow directions and flow paths locally change between precipitation and evaporation periods. This makes the identification and description of solute transport processes in the vadose zone a complex problem.
Recent studies (Lehmann and Or, 2009; Bechtold et al., 2011a) focused on the investigation of upward transport of solutes during evaporation in heterogeneous soil columns, where heterogeneity was introduced by a sharp vertical material interface between two types of sand. Lateral solute transport through the interface in both (lateral) directions was observed at different depths of the investigated soil columns.
Following recent approaches, we conduct two-dimensional numerical simulations in a similar setup which is composed of two sands with a sharp vertical material interface. The investigation is broadened from the sole evaporation to combined precipitation-evaporation cycles in order to quantify transport processes resulting from the combined effects of heterogeneous soil structure and dynamic flow conditions. Simulations are performed with a coupled finite volume and random walk particle tracking algorithm (Ippisch et al., 2006; Bechtold et al., 2011b).
By comparing scenarios with cyclic boundary conditions and stationary counterparts with the same net flow rate, we found that duration and intensity of precipitation and evaporation periods potentially have an influence on lateral redistribution of solutes and thus leaching rates. Whether or not dynamic boundary conditions lead to significant deviations in the transport behavior depends on the magnitude of the flow rates and hydraulic conductivity curves of the materials. Based on the unsaturated hydraulic conductivity at the intersection point of conductivity curves, we are able to define an estimate of flow rates at which the dynamic of the upper boundary condition significantly alters preferential flow paths through the system. If flow rates are low, with regard to the materials hydraulic conductivity at the intersection point, the influence of dynamic boundary conditions is small. If flow rates are in the range of the unsaturated hydraulic conductivity at intersection, solute is trapped in the fine material during upwards transport, which results in a more pronounced tailing. For flow rates exceeding the intersection conductivity, a redistribution at the soil surface can occur.

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