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Modeling solute transport in a heterogeneous unsaturated porous medium under dynamic boundary conditions on different spatial scales

Clemens Cremer (1), Insa Neuweiler (1), and Michel Bechtold (2)

(1) Institute of Fluid Mechanics and Environmental Physics in Civil Engineering, Leibniz Universität Hannover, Hanover, Germany , (2) Thünen Institute of Climate-Smart Agriculture, Braunschweig, Germany

Understanding transport of solutes/contaminants through unsaturated soil in the shallow subsurface is vital to assess groundwater quality, nutrient cycling or to plan remediation projects. Alternating precipitation and evaporation conditions causing upward and downward flux with differing flow paths, changes in saturation and related structural heterogeneity make the description of transport in the unsaturated zone near the soil-surface a complex problem. Preferential flow paths strongly depend, among other things, on the saturation of a medium. Recent studies (e.g. Bechtold et al., 2011) showed lateral flow and solute transport during evaporation conditions (upward flux) in vertically layered sand columns. Results revealed that during evaporation water and solute are redistributed laterally from coarse to fine media deeper in the soil, and towards zones of lowest hydraulic head near to the soil surface. These zones at the surface can be coarse or fine grained depending on saturation status and evaporation flux. However, if boundary conditions are reversed and precipitation is applied, the flow field is not reversed in the same manner, resulting in entirely different transport patterns for downward and upward flow. Therefore, considering net-flow rates alone is misleading when describing transport in the shallow unsaturated zone. In this contribution, we analyze transport of a solute in the shallow subsurface to assess effects resulting from the superposition of heterogeneous soil structures and dynamic flow conditions on various spatial scales.

Two-dimensional numerical simulations of unsaturated flow and transport in heterogeneous porous media under changing boundary conditions are carried out using a finite-volume code coupled to a particle tracking algorithm to quantify solute transport and leaching rates. In order to validate numerical simulations, results are qualitatively compared to those of a physical experiment (Bechtold et al., 2011). Numerical simulations differ in lateral scale reaching from 0.2 m to 1.5 m, while the height of the domain is kept constant to 1.5m. Strong material heterogeneity is realized through vertical layers of coarse and fine sand. Both materials remain permanently under liquid-flow-dominated (‘stage1’) evaporation conditions. Spatial moments as well as the dilution index (Kitanidis, 1994) are used for quantification of transport behaviour. Results show that, while all simulations led to anomalous transport, infiltration-evaporation cycles lead to faster solute leaching rates than solely infiltration at the same net-infiltration rate in both homogeneous and heterogeneous media. Flow and transport-paths significantly differed between infiltration and evaporation, resulting in lateral water fluxes and hence lateral solute transport. Variation of the width of the model domain shows faster leaching rates for domains with small horizontal extent.