Geophysical Research Abstracts
Vol. 16, EGU2014-6074, 2014
EGU General Assembly 2014

Coulombic effects and multicomponent ionic dispersion during transport of electrolytes in porous media

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We study the influence of Coulombic effects on transport of charged species in saturated porous media in advection-dominated flow regimes. We focus on transverse hydrodynamic dispersion and we performed quasi two-dimensional flow-through experiments in homogeneous and spatially variable flow fields to investigate transport of dilute electrolyte solutions. The experiments were conducted at flow velocities (1.0, 1.5 and 6 m/day) where advection is the dominant mass transfer process. High-resolution measurements at the outlet were performed to determine the concentration of different cations and anions. In order to interpret the laboratory experiments we develop a two-dimensional numerical model. The adopted modeling approach is based on a multicomponent formulation, charge conservation, and the accurate description of local transverse dispersion. The latter entails a non-linear dependence of the transverse dispersion coefficient on the flow velocity as well as a compound-specific dependence on the molecular diffusion of the transported solutes. The model was benchmarked by comparing the results of the 2D steady-state multicomponent simulations with 1D transient results of PHREEQC in homogeneous scenarios, and it was successively used to quantitatively evaluate the experimental results in both homogeneous and heterogeneous porous media. Our experimental and modeling results show that Coulombic cross-coupling of dispersive fluxes of charged species in porous media significantly affects the lateral displacement of charged ions in both homogeneous and heterogeneous flow-through systems. Such effects are remarkable not only in diffusion-dominated but also in advection-dominated flow regimes.