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Coulombic effects during conservative and reactive transport of charged solutes in homogeneous and heterogeneous porous media: Experiments and modeling

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Abstract

Transport of charged species in porous media is significantly affected by the electrochemical migration term resulting from charge-induced interactions among dissolved ions. Such electrostatic interactions during multicomponent ionic transport have been investigated both in diffusion-dominated systems [1-3] and, recently, in advection-dominated systems for steady-state plumes [4, 5]. In this work we study the electrochemical effects during transient conservative and reactive transport of ionic admixtures, under advection-dominated conditions, in homogeneous and heterogeneous domains by means of laboratory bench-scale experiments and numerical simulations. Experiments were performed in a quasi 2-D flow-through chamber under transient transport conditions by applying pulse injections of the electrolytes [6]. We performed extensive sampling (600 samples) and measurements of ions'concentrations (1800 measurement points) at the outlet of the flow-through setup, at high spatial (5 mm) and temporal resolution (~0.017 pore volumes). Such sampling approach allowed us resolving the effects of charge interactions on the temporal breakthrough and spatial profiles of the cations and anions. The experimental results show remarkable differences, caused by the Coulombic effects, on the breakthrough curves and on mixing of the different ionic plumes. We evaluated the dilution behavior of individual charged species by experimentally calculating their flux-related dilution index as a metric of mixing.

Modeling of charged species and the interpretation of these experimental results require a Nernst-Planck based formulation with an accurate description of local hydrodynamic dispersion, as well as the explicit treatment of the cross-coupling between dispersive fluxes due to electrochemical migration. We used a recently developed 2-D reactive transport simulator [7], coupling the multicomponent ionic transport with the geochemical code PHREEQC by utilizing the IPhreeqc module, to quantitatively interpret the experimental results. The simulator allows us to reproduce the observed experimental outcomes and to directly quantify and visualize the eletromigration effects by mapping the different components of ionic fluxes and their cross-coupling. Furthermore, we use this 2-D code to explore the impact of charge interactions in large-scale reactive transport scenarios with heterogeneous distribution of both physical and chemical properties.

Key words: electrochemical migration, multicomponent diffusion, breakthrough curves, IPhreeqc coupling, Coulombic interactions, dilution index, flow-through experiments

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