

Multicomponent ionic transport and pH fronts propagation

MASSIMO ROLLE^{1,2*}, MUHAMMAD MUNIRUZZAMAN²

¹ Department of Environmental Engineering, Technical University of Denmark, Miljøvej, Building 115, 2800 Kgs. Lyngby, Denmark. masro@env.dtu.dk

² Center for Applied Geosciences, University of Tübingen, Hölderlinstr. 12, D-72074 Tübingen, Germany. md.muniruzzaman@uni-tuebingen.de

Coulombic interactions are important for the displacement of charged species in porous media not only under diffusion-dominated conditions but also in advection-dominated flow regimes [1-3].

We investigate the propagation of pH fronts during multicomponent ionic transport in saturated porous media. By performing laboratory flow-through experiments we illustrate the impact of Coulombic effects on proton transport in the presence of ionic admixtures [4]. Dilute solutions of hydrochloric acid with $MgCl_2$ are used as tracer solutions to test the effect of electrochemical cross-coupling on the migration of diffusive/dispersive pH fronts.

Numerical transport simulations are carried out to interpret the laboratory experiments. The simulations are based on a multicomponent ionic formulation accurately capturing the Coulombic interactions between the transported ions in the flow-through system (Fig. 1).

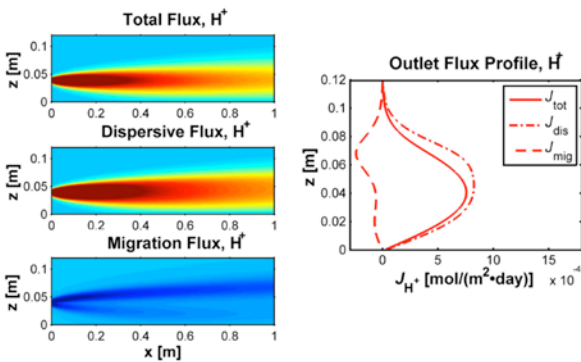


Figure 1: Multicomponent ionic transverse fluxes determining proton displacement.

- [1] Rolle *et al.* (2013), *Geochim. Cosmochim. Acta* **120**, 195-205. [2] Muniruzzaman *et al.* (2014), *Geochim. Cosmochim. Acta* **141**, 656-669. [3] Rasouli *et al.* (2015), *Computat. Geosci.* **19**, 523-533. [4] Muniruzzaman & Rolle (2015), *Water Resour. Res.* **51**, 6739-6755.