

# Multicomponent ionic transport and surface complexation in porous media: Multidimensional experiments and reactive transport modeling

JACOPO COGORNO<sup>1</sup>, LUCIEN STOLZE<sup>2</sup>, MUHAMMAD MUNIRUZZAMAN<sup>3</sup> AND MASSIMO ROLLE<sup>4</sup>

<sup>1</sup>Technical University of Denmark

<sup>2</sup>Lawrence Berkeley National Laboratory

<sup>3</sup>Geological Survey of Finland

<sup>4</sup>Technical University of Darmstadt

Presenting Author: jacogo@env.dtu.dk

Coulombic interactions and surface complexation play key roles in the multicomponent ionic transport of major ions and charged contaminants in porous media [1]. Bench-scale laboratory experiments are standard methods for subsurface investigation and are often performed in one-dimensional flow-through column setups. Thus, little attention is dedicated to the non-intuitive impact of transverse mixing processes on transport of charged species and their interactions in pore water and at surface/solution interfaces [2].

In this study, we present high-resolution experiments and advanced geochemical reactive transport modeling to describe the migration of acidic plumes and major ions in saturated porous media, with particular focus on electrostatic interactions within the pore water and with the charged surfaces. We performed column and quasi two-dimensional flow-through experiments with identical silica porous media and under the same advection-dominated conditions. Equal mass fluxes of different electrolyte solutions (i.e., HCl - pH ~ 2.8, NaBr - 100 mM, HCl - pH ~ 2.8 plus NaBr - 100 mM) were continuously injected and breakthrough curves of pH and major ions were measured at the outlet of the domains. The presence of pronounced ionic strength gradients in the transverse direction in the 2-D setup caused distinct retardation and transport behaviors of protons and major ions which were not observed in the one-dimensional column experiments. An innovative modeling tool, based on the coupling of 1-D and 2-D transport simulators developed in Matlab and the geochemical code PHREEQC, was developed to quantitatively describe the experimental outcomes [3]. The key features of the code are the Nernst-Planck formulation of diffusive/dispersive fluxes [4] and the surface complexation models (i.e., Basic Stern and Triple Layer) to describe the interaction of the charged solutes with the solid surfaces of quartz and metal oxides. The simulations allow reproducing the experimental observations and illuminate the key role of dimensionality effects on transport of charged species in porous media.

- [1] Stolze et al. (2020) *Geochim. Cosmochim. Acta* 277, 132-149. [2] Cogorno et al. (2022) *Geochim. Cosmochim. Acta* 318, 230-246. [3] Muniruzzaman & Rolle (2016) *Adv. Water Resour.* 98, 1-15. [4] Rolle et al. (2018) *Water Resour. Res.* 54, 3176-