Diffusion, Coulombic interactions and multicomponent ionic transport of charged species in saturated porous media

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Diffusion, Coulombic interactions and multicomponent ionic transport of charged species in saturated porous media

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Diffusion and compound-specific mixing significantly affect conservative and reactive transport in groundwater at different scales, not only under diffusion-dominated regimes but also under advection-dominated flow through conditions [1]. When dissolved species are charged, besides the magnitude of their aqueous diffusion coefficients also the electrostatic interactions significantly affect solute displacement. We investigated electrostatic interactions between ionic species under flow-through conditions resulting in multicomponent ionic dispersion: the dispersive fluxes of the different ions in the pore water are cross-coupled due to the effects of Coulombic interactions. Such effects are illustrated in flow-through experiments in saturated porous media. Simple strong electrolytes (i.e., salts and strong acid solutions) were selected as tracers and their transport was studied under different advection-dominated conditions in homogeneous and heterogeneous porous media [2-3]. The model-based interpretation of the experimental results is challenging since it requires a multicomponent ionic formulation with an accurate description of local hydrodynamic dispersion and explicitly accounting for the cross-coupling of dispersive fluxes due to the Coulombic interactions between the ions in the pore water [4-5].

Keywords: Coulombic interactions, flow-through experiments, transport in porous media

References

[1] Rolle M., Chiogna G., Hochstetler D.L. and P.K. Kitanidis (2013). On the importance of diffusion and compound-specific mixing for groundwater transport: An investigation from pore to field scale. *Journal of Contaminant Hydrology*, 153, 51-68, DOI: 10.1016/ j.jconhyd.2013.07.006.

[2] Rolle M., Muniruzzaman M., Haberer C.M. and P. Grathwohl (2013). Coulombic effects in advection-dominated transport of electrolytes in porous media: Multicomponent ionic dispersion. *Geochimica et Cosmochimica Acta*, 120, 195-205, DOI: 10.1016/j.gca.2013. 06.031.

[3] Muniruzzaman M., Haberer C.M., P. Grathwohl and M. Rolle (2014). Multicomponent ionic dispersion during transport of electrolytes in heterogeneous porous media. *Geochimica et Cosmochimica Acta*, DOI: 10.1016/j.gca.2014.06.020.

[4] Muniruzzaman M. and M. Rolle (2015). Impact of multicomponent ionic transport on pH fronts propagation in saturated porous media. *Water Resources Research*, DOI: 10.1002/2014WR017134.

[5] Rasouli P., Steefel C.I., Mayer U. and M. Rolle (2015). Benchmarks for multicomponent diffusion and electrochemical migration. *Computational Geosciences*, DOI:10.1007/ s10596-015-9481-z.