

Technical University of Denmark



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

Rolle, Massimo; Muniruzzaman, Muhammad

Publication date:
2016

Document Version
Peer reviewed version

[Link back to DTU Orbit](#)

Citation (APA):

Rolle, M., & Muniruzzaman, M. (2016). Diffusion, Coulombic interactions and multicomponent ionic transport of charged species in saturated porous media. Abstract from 9th International Association of Hydrological Sciences (IAHS) Groundwater Quality Conference (GQ16), Shenzhen, China.

DTU Library

Technical Information Center of Denmark

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

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

Massimo Rolle¹ and Muhammad Muniruzzaman²

¹Department of Environmental Engineering, Technical University of Denmark, Miljøvej, Building 115, 2800 Kgs. Lyngby, Denmark

²Center for Applied Geosciences, University of Tübingen, Hölderlinstr. 12, D-72074 Tübingen, Germany

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.