A modelling approach for multicomponent ionic transport in heterogeneous clayey-sandy domains

MUHAMMAD MUNIRUZZAMAN[1]* AND MASSIMO ROLLE[2]

[1]Industrial Environment and Recycling, Geological Survey of Finland, Neulaniementie 5, 70211 Kuopio, Finland. (*correspondence: md.muniruzzaman@gtk.fi)

[2]Department of Environmental Engineering, Technical University of Denmark, Miljøvej 115, 2800 Kgs. Lyngby, Denmark. (masro@env.dtu.dk)

Despite the relevance of geologic formations comprising both clay and sandy materials, transport of ionic species in such multidimensional physically, chemically and electrostatically heterogeneous media is still poorly understood.

In this study, we present a 2D multicomponent reactive transport model explicitly taking into account the electrostatic interactions in the free pore water and within the diffuse double layer (DDL), activity gradient fluxes, and the effects of interlayer species. The DDL composition is simulated by considering a mean electrostatic potential following Donnan approach, whereas the interlayer composition is calculated by adopting the Gaines-Thomas convention. Diffusive/dispersive fluxes within each individual sub-continuum (free water, DDL, and interlayer) are calculated solving the Nernst-Planck equation while a zero-charge flux is maintained. Moreover, the model formulation is coupled with PHREEQC, by utilizing the PhreeqcRM module, which enables great flexibility to access all the PHREEQC's reaction capabilities [1 – 3].

The developed code is benchmarked in 1D systems by comparing the outcomes with other software and experimental data from previous studies. Successively, reactive transport simulations are performed in 2D clayey-sandy domains with spatially variable physical and chemical properties. The results reveal the importance of diffusion in DDL and/or interlayer as well as the Coulombic cross coupling between diffusive/dispersive fluxes for the transport and breakthrough of different ionic species.

[1] Parkhurst & Wissmeier (2015) *Adv Water Resour* **83**, 176-189. [2] Muniruzzaman & Rolle (2016) *Adv Water Resour* **98**, 1-15. [3] Rolle et al. (2018) *Water Resour Res* **54**, 3176-3195.