Modelling approach and benchmark experiments for Nernst-Plack-based transport, Coulombic interactions and geochemical reactions in saturated porous media

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The transport of electrolytes in porous media is affected by physical, chemical and electrochemical processes. Coulombic interactions significantly influence the behavior of electrolyte plumes at different scales, not only in diffusion-dominated conditions but also in advection-dominated flow regimes [1-3]. To model the spatial behavior of charge-induced interactions in multi-dimensional homogeneous and heterogeneous domains, we propose a Nernst-Planck based modeling approach for conservative and reactive transport. The model is based on a coupling between COMSOL Multiphysics® and PhreeqcRM [4]. Important features of the proposed approach include transport of chemical species and not of chemical components, the definition of physically and chemically heterogeneous domains and the implementation of electromigration as well as of the flux components arising from the activity coefficient gradients. The model has been benchmarked with numerical simulations in PHREEQC [5], analytical solutions and high-resolution experimental datasets in homogeneous and heterogenous setups for steady-steady state and transient conditions in different dimensions (1D, 2D and 3D). Fully three-dimensional experiments on multicomponent ionic transport were also performed in this study and were used to validate the proposed modeling approach. Simulations show an excellent agreement with the experimental and modeling benchmark problems, thus highlighting the potential of the Nernst-Planck based model for the evaluation of conservative and reactive multicomponent ionic transport.

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