NP-Phreeqc-EK: a Multidimensional Multiphysics Simulator for Electrokinetic Transport and Biogeochemical Reactions in Porous Media

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ABSTRACT. Electrokinetic techniques are used in different fields of science and engineering to enhance the transport of charged species and non-charged compounds in low-permeability porous media. The modeling of electrokinetic transport processes is a challenging task as it requires the description of the interplay between physical, electrostatic and biogeochemical processes occurring upon application of an electric field. In this work we developed a modeling tool, NP-Phreeqc-EK [1], consisting of a coupling between COMSOL Multiphysics and PhreeqcRM [2]. The former is used to solve fluid flow and Nernst-Planck-Poisson-based solute transport in saturated porous media, the latter simulates biogeochemical reactions. The multidimensional multiphysics model uses an operator splitting approach and is implemented in a MATLAB LiveLink interface. The code integrates fluid flow, solute transport including electromigration and electroosmosis, Coulombic interactions between transported species, and a wide range of kinetic and equilibrium reactions. NP-Phreeqc-EK has been benchmarked in different dimensions (1D, 2D and 3D) with analytical solutions, numerical simulations with other software, and data from previously published electrokinetic experiments. This study highlights the flexibility of the proposed approach in simulating electrokinetic reactive transport processes in saturated porous media and emphasizes the importance of charge interactions during electrokinetic transport. The developed modeling tool is suitable to simulate electrokinetic processes at laboratory and field scales and can be applied in a number of studies focusing both on fundamental aspects of electrokinetic transport and on practical electrokinetic remediation applications in homogeneous and heterogeneous media.

References [1] R. Sprocati, M. Masi, M. Muniruzzaman and M. Rolle. Modeling electrokinetic transport and biogeochemical reactions in porous media: a multidimensional Nernst-Planck-Poisson approach with PHREEQC coupling. Advances in Water Resources. 127, 134–147, (2019). [2] D.L Parkhurst, L. Wissmeier. PhreeqcRM: A reaction module for transport simulators based on the geochemical model PHREEQC. Advances in Water Resources. 83, 176–189, (2015).