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Modeling of coupled flow, transport and biogeochemical reactions during electrokinetic bioremediation: model development and application

Riccardo Sprocati and Massimo Rolle
DTU Environment, Technical University of Denmark, Kgs. Lyngby, Denmark

Electrokinetic (EK) remediation is one of the few in-situ remediation technologies that can effectively remove contaminants from low-permeability porous media. Process-based modeling, including the complex multiphysics and biogeochemical processes occurring during electrokinetic remediation, is instrumental to describe EK systems and to assist in their design. In this work we use NP-Phreeqc-EK [1], a multidimensional, multiphysics code which couples a flow and transport simulator (COMSOL Multiphysics) with a geochemical code (PhreeqcRM) through a MATLAB LiveLink interface. The model allows the simulation of coupled fluid flow, solute transport, charge interactions and biogeochemical reactions during electrokinetics in saturated porous media. The process-based code is applied for the modeling of electrokinetic delivery of amendments to enhance bioremediation (EK-Bio) of chlorinated compounds at a pilot test site [2]. We simulate both conservative and reactive transport scenarios and we compute and show the Nernst-Planck fluxes and the velocities of the different species (such as lactate, chlorinated ethenes and degrading microorganisms). To compare remediation performances and model outcomes we define different metrics quantifying the spatial distribution of the delivered reactants and the mass of the organic contaminants in the system. The process-based model allowed the simulation of the key processes occurring during EK-Bio, including 1) multidimensional electrokinetic transport such as electromigration of charged species and electroosmosis, 2) Coulombic interactions between ions in solution, 3) kinetics of contaminant biodegradation, 4) dynamics of microbial populations, 5) mass transfer limitations and 6) geochemical reactions.

[1] Sprocati, R., Masi, M., Muniruzzaman, M., & Rolle, M. (2019). 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.

[2] Sprocati, R., Flyvbjerg, J., Tuxen, N., & Rolle, M. (2020). Process-based modeling of electrokinetic-enhanced bioremediation of chlorinated ethenes. *Journal of Hazardous Materials*, **397**, 122787.