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ABSTRACT. In-situ remediation technologies based on electrokinetically enhanced bioremediation (EK-Bio) have the potential to remove organic contaminants from low-permeability porous media. For chlorinated solvents, which are among the most widespread groundwater contaminants, the technique relies on the delivery of electron donors and, when necessary, also specialized microorganisms to induce and/or enhance microbially mediated reductive dehalogenation. One of the major challenges of such in-situ applications consists in the ability to take into account the complex interplay between physical and biogeochemical reactions to predict the evolution of the system over time. The development of comprehensive numerical models is thus essential to interpret, design and optimize experimental applications under well-controlled laboratory conditions, as well as at pilot and full field scales. In this work we propose a process-based modeling framework for EK-Bio based on NP-Phreeqc-EK [1], a simulator coupling COMSOL Multiphysics and PhreeqcRM. The model accounts for: (i) multidimensional electrokinetic transport in saturated porous media including electromigration of charged species and electroosmosis, (ii) Coulombic interactions with the Nernst-Planck-Poisson equations, (iii) kinetics of contaminant degradation, (iv) dynamics of microbial populations including growth and decay of indigenous and delivered degraders, (v) mass transfer limitations, and (vi) geochemical reactions. The modeling study includes scenario simulations based on an EK-Bio pilot study in a contaminated clayey aquitard at the Skuldelev site (Denmark). The results show that electromigration plays a key role for the delivery of lactate, the charged electron donor used to stimulate the biodegradation activity. The transport of dissolved chlorinated compounds and the delivery of specialized microorganisms (i.e., the KB-1 reductive dehalogenating consortium) was controlled by the induced electroosmotic flow. In the considered geometry, including 9 injection and/or electrode wells, the effective delivery of lactate could be achieved upon application of a sufficient electric potential (110 V) at the electrodes for at least 100 days to ensure degradation of the chlorinated ethenes by the indigenous bacterial population. However, complete reductive dechlorination to the non-toxic product ethane could only be achieved in the zones where the delivered specialized microorganisms were distributed. The simulation outcomes show a great increase of the efficiency in substrate delivery and contaminant degradation when applying an electric field and relying on electrokinetic transport mechanisms compared to cases only based on natural transport processes. To evaluate the results of different conservative and reactive transport scenarios, we used quantitative metrics such as the relative area of substrate distribution and the relative mass of contaminant degraded. In one of the modeling scenarios we also considered the presence of the parent compound, tetrachloroethene (PCE), in the form of free product, as non-aqueous phase liquid (NAPL). When the NAPL product was present it significantly affected the degradation efficiency and the remediation time, as a result of the larger mass to degrade and of the kinetic limitations of the interphase mass-transfer. This study illustrates the potential of electrokinetically enhanced bioremediation and the capability of a newly developed modeling approach to describe the different physical, electrostatic, chemical and biological processes controlling the overall remediation efficiency in field scale applications.

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).