Coupled Hydrochemical Modeling for the Optimal Design of an in-situ Redox Experiment

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Abstract

In the context of deep geological repositories for nuclear waste, field data are essential to develop the scientific understanding of the site, to engineer the repository and to assess the environmental impact and the long-term post-closure safety. In order to maximize the information provided by these data and to optimize the economic impact of the campaigns, field experiments should be properly designed and tailored to the site-specificities. To this end, numerical models offer a powerful framework for the optimal design of these experiments. In this work, we present a number of scoping calculations that have been carried out to design an in-situ redox experiment (Figure 1) focused on assessing potential changes in the pH and redox conditions and in the buffering capacity of the Olkiluoto bedrock (i.e. the site for the Finnish spent fuel repository). A characteristic of these models lies in the need to integrate prior information, computed by a complex surface-subsurface 3D model (i.e. flow velocity field computed over the transmissive zone HZInf7 - see Figure 2), with a number of nonlinear reactions. This coupling has been achieved by using a Java interface (Nardi et al., 2012) that links COMSOL Multiphysics with the geochemical simulator PHREEQC (Parkhurst and Appelo, 1999). The results, which provide interesting insights into the extension of the redox plume as well as the duration of the transient period, can be used to define the optimal configuration of the injection-extraction dipole. COMSOL Multiphysics has been used to assimilate velocity fields computed by a regional hydrological model and to carry out transport simulations. Geochemical reactions are computed using the geochemical simulator PHREEQC. The different processes (i.e. groundwater flow, solute transport and geochemical reactions) are coupled using a sequential non-iterative approach (SNIA). The coupling between COMSOL Multiphysics and PHREEQC is achieved by using a Java interface (Nardi et al., 2012). The coupled model has been shown to be able to integrate the information provided by a complex hydrological model with a number of nonlinear reactions (i.e. mineral dissolution and precipitation treated in equilibrium or kinetic). The results show that both processes are indissolubly connected and the high uncertainty in key hydrogeological parameters has relevant impact on the extension of the redox plume (Figure 3) as well as the amount of mineral that is depleted. The capability to compute the mass balance of the redox mineral over the considered domain provides crucial information about the impact that the redox front has on the buffering capacity of the medium. In this modeling work, three different numerical codes have been coupled (SHYD by WaterHope, COMSOL Multiphysics and

PHREEQC). The resulting model is able to capture their essential features: the accuracy of SHYD to reproduce the flow conditions in the Olkiluoto area, the flexibility of COMSOL Multiphysics to assimilate flow velocities and compute solute transport and the proven reliability of PHREEQC to evaluate complex nonlinear reactions. The model results provide valuable information for the optimal design of the in-situ experiment.

Reference

1. Parkhurst, D. L., and C. A. J. Appelo (1999), User's guide to PHREEQC (version 2)—A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations, U.S. Geol. Surv. Water Resour. Invest.,Rep. 99-4259.
2. Nardi, A., Trinchero, P., de Vries, L., Idiart, A., Molinero, J. Coupling multiphysics with geochemistry: The COMSOL-PHREEQC interface, COMSOL Conference, October 2012 Milan (Italy).

Figures used in the abstract

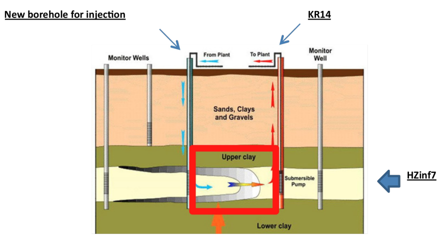

Figure 1: Set-up of the redox experiment. An oxigenetad water is continually being injected (in the injection well) and extracted (in the pumping well).

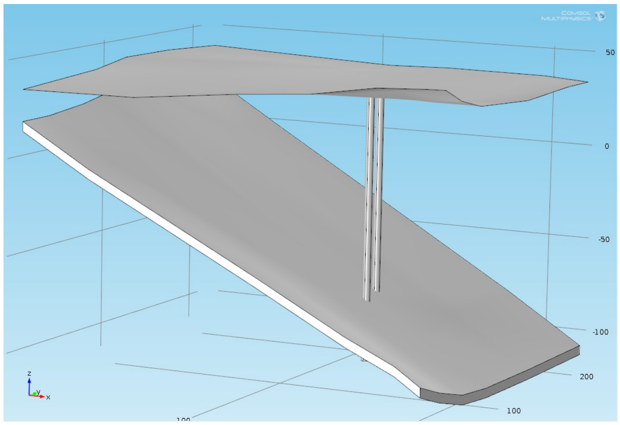

Figure 2: Representation of the soil surface, the transmissive zone HZInf7 and the two boreholes of the in-situ experiment.

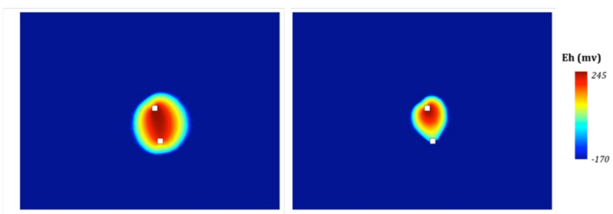

Figure 3: Redox plume after 2 days from the beginning of the experiment for a flow porosity of 6e-4 (left) and 1e-2 (right).