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One-dimensional Reactive Transport Modelling of the Interaction between a High-pH Plume and a Fractured Granodiorite. The GTS-HPF Project

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Introduction

One of the objectives of the GTS-HPF project (Grimsel Test Site - Hyper-alkaline Plume in Fractured Rock) is to study the alteration of the Grimsel granodiorite due to the circulation of high-pH solutions derived from the degradation of cement through the fractures present in the rock. A K-Na-Ca-rich high-pH solution will be continuously injected through a borehole in a fracture. An extraction borehole will be located about one meter away from the injection borehole. The planned duration of the experiment is three years. A laboratory version of the experiment is currently under way at the University of Bern.

Bossart and Mazurek (1991) have given a detailed description of the fractures. The Grimsel granodiorite is characterized by the presence of ductile shear zones, with thicknesses ranging at least up to metre to decametre scales. These shear zones include mylonitic bands, which are bands of more intense deformation, with thicknesses up to several tens of centimetres. They are characterized by being more mica-rich and fine-grained than the surrounding rock. Brittle fractures developed in later stages of deformation, mainly in the mylonitic bands. These fractures, with thicknesses in the millimetre range, are at least partially filled with a highly porous fault gouge (crushed mylonite).

The Model

A modified version of the GIMRT software package (Steefel and Yabusaki, 1996) has been used for the reactive transport calculations. Both diffusive/dispersive and advective solute transport are taken into account in the calculations. Mineral reactions are described by kinetic rate laws. The primary minerals that make up the rock in the simulations are quartz, albite, microcline, phlogopite and muscovite. A number of possible secondary phases have been considered in the calculations (brucite, ettringite, gibbsite, kaolinite, portlandite and several zeolites, CSH and CASH phases). The reaction rate constants for the primary minerals are based on experimentally-determined rates published in the literature. Maximum available mineral surface areas are estimated from BET measurements of fault gouge. Relatively large rate constants have been used for the secondary minerals, so the results resemble the local equilibrium solution for these minerals. The initial surface areas for the secondary minerals in the model are about 10000 times smaller than for the primary minerals. Temperature is 12 ^oC.

The composition (K-Na-Ca-OH) of the solution entering the system corresponds to a solution originating from the degradation of cement (a major component of the engineered barrier system in a repository for low- and intermediate-level waste).

The fluid flow system under consideration is a one-dimensional porous medium simulating a single flow path through a fracture which is filled by fault gouge (30% porosity). The value of the Darcy velocity used in the simulations (192 m/y) is representative of the flow conditions that will be imposed in the fracture during the experiment.

Results and discussion

The model results show that the circulation of the hyper-alkaline solution through the fracture causes the dissolution of albite, microcline and quartz in the fault gouge (the solutions reach saturation with respect to microcline in a relatively short distance). Muscovite dissolves close to the injection borehole and precipitates further away. Phlogopite does not react. Regarding the secondary minerals, there is precipitation of tobermorite (a CSH phase) close to the injection borehole and prehnite (a CASH phase) further away. There is also minor mesolite (a Na-Ca-zeolite) precipitation towards the end of the prehnite zone.

Maximum surface areas in the model are constrained by BET measurements of the specific surface area of fault gouge material (8 m^2/g). However, this measurement provides only maximum available surface areas. It is possible that the solutions do not have access to all the mineral surface area. The extension of the reaction zones and the amount of mineral that reacts depends on the available surface area for reaction. The results (magnitude, mineralogy and extension of the reaction zones) from both the field experiment and the small-scale laboratory experiment should provide constraints regarding the values of the surface areas to be used in the calculations.

All the results show a decrease in porosity close to the injection borehole and an increase in porosity further away. Such an evolution of the porosity of the fracture infill would be beneficial for the performance of a repository.

Bossart P & Mazurek M, *Structural Geology and Water Flow-Paths in the Migration Shear Zone. Nagra Technical Report*, **91-12**, (1991).

Steefel CI & Yabusaki SB, *OS3D/GIMRT, Software for Multicomponent-Multidimensional Reactive Transport: User's Manual and Programmer's Guide. Pacific Northwest National Laboratory Report*, **PNL-11166**, (1996).