LOT A2 TEST, THC-MODELLING OF BENTONITE BUFFER IN A FINAL REPOSITORY OF SPENT NUCLEAR FUEL

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The Finnish spent nuclear fuel disposal is planned to be based on the KBS-3V repository concept. Within this concept, the role of the bentonite buffer is considered to be central. The aim of this study was to model the evolution of the buffer during the thermal phase (heat-generating period of spent fuel), when the bentonite is only partially saturated initially, and the surrounding rock matrix is assumed to be fully saturated. It is essential to study how temperature will affect saturation and also how both of these affect the chemistry of bentonite.

In order to make the modeling more concrete, an example experimental case was considered: Long Term Test of Buffer Materials (LOT) A2-parcel test at the Äspö Hard Rock Laboratory (HRL) in Sweden (Karnland *et al.* 2008). In the A2-parcel the MX-80 bentonite was exposed to adverse (120-150 ºC) temperature conditions and high temperature gradients. The test parcel diameter was smaller than in the actual KBS-3V deposition hole to speed up the saturation. The chemical behaviour of minerals causes their redistribution inside the bentonite. For example, according to the laboratory tests, gypsum dissolves and anhydrite precipitates near the heater-bentonite interface. Also, incoming groundwater affects the bentonite porewater and its properties. These changes may, in turn, influence the mechanical properties of the bentonite.

A coupled Thermo-Hydro-Chemical (THC) model was applied, which means that all mechanical effects were ignored. The purpose of the model was first to achieve a satisfactory match between the model and experimental results, and, therefore, the time frame was limited to ten years (LOT A-2 parcel test lasted approximately 6 years). The system was simplified to 1-D in order to reduce the computational work, which can be very significant due to complex chemical calculations. The 1-D model results are reported in Itälä (2009). The aim is to extend the calculations to 2-D.

TOUGHREACT EOS3 (TOUGHREACT v. 1.0; Xu *et al.* 2004) was applied to model the reactive unsaturated transport processes in 1-D and 2-D on equisized computational grids. The model includes:, Mineral equilibria/kinetics, Gaines-Thomas cation exchange, diffusion and advection, infiltration of groundwater from a granitic rock into unsaturated bentonite under capillary and hydraulic pressure gradients (van Genuchten model) and thermal gradient. The following phenomena were excluded: Surface complexation, mechanical swelling and porosity changes. The results may be used to increase knowledge of the THC evolution of the buffer during the thermal phase. After a good match with experimental data is attained the modeling can be extended to cover the whole thermal phase (a few thousand years). The parameters obtained can also be taken to more complicated models even with other software.

Some of the results from the 1-D model are presented in the figure below. The bentonite was calculated to saturate within approximately one year and the moisture profile does not change after that. The chloride concentration increases with saturation and diffusion continues, although the diffusion profile is slightly anomalous compared to the boundary conditions.

The evolution of exchangeable calcium and sodium (in meq/100 g) is shown in the figures below. According to the model results, the concentration of calcium on the cation exchanger increases while that of sodium decreases. These calcium levels are highest near the bentonite-rock interface due to incoming calcium and there is a significant concentration gradient over the bentonite, indicating that cation-exchange
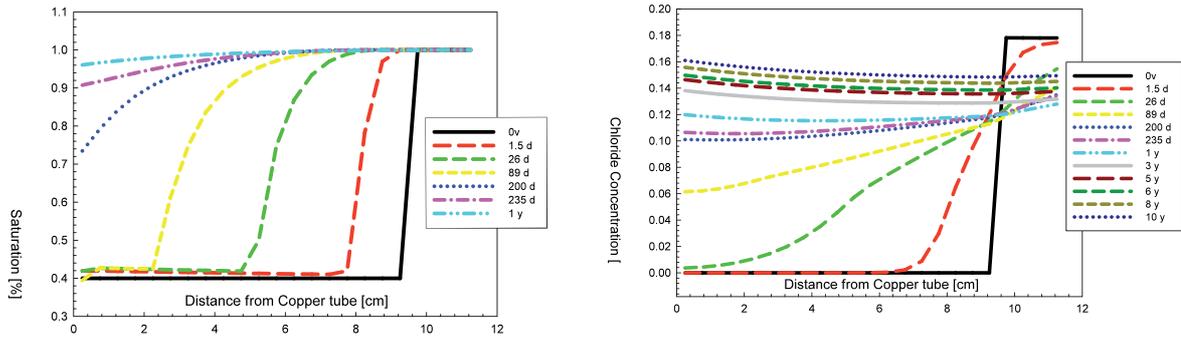
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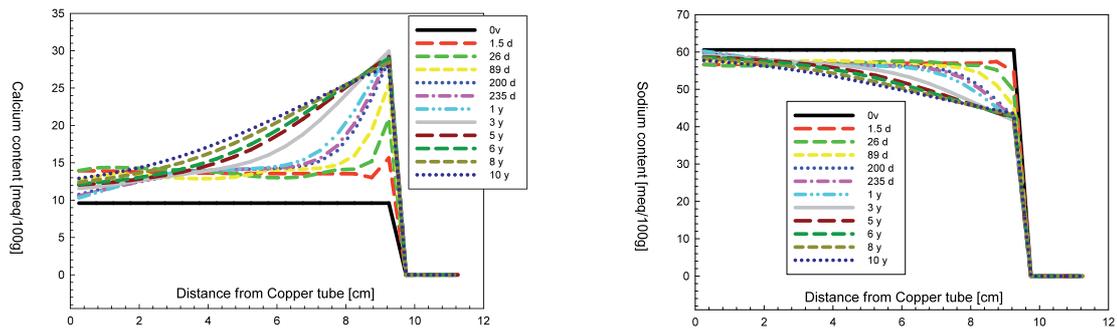
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Figure 1: •••••

Figure 2: •••••

equilibrium is not yet reached. The sodium concentration decreases, with the changes being greatest near the rock surface. The initial 1-D model results indicate a good agreement with the experimental observations.

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