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# Interpretation of geochemical evolution of bentonite at an in situ test and prediction of long-term geochemical change in bentonite

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The most common buffer material for engineered barrier system (EBS) is compacted bentonite, which features low permeability and high retardation of radionuclide transport. The geochemical evolution of bentonite over the course of being heated and hydrated is critical for the long-term safety of EBS. Valuable geochemical data were collected at the two dismantling events of an *in situ* heating (100 ºC) and hydration experiment at the Grimsel test site, which provided two snapshots (5.3 years and 18.3 years) of the porewater concentration profiles within the bentonite. However, interpretation of geochemical data has been challenging because of the complex interaction between thermal (T), hydrological(H), mechanical (M) and chemical (C) processes and measured porewater concentrations cannot be directly used to compare with results from numerical models. After extensive calibration, a THMC model was able to explain the geochemical evolution in the bentonite, which revealed that (1) concentrations of most chemical species along the radial direction were higher near the heater and lower away from the heater, (2) geochemical profiles were strong affected by THM processes such as evaporation/condensation, porosity change due to swelling, permeability change, (3) the shape of concentration profiles for major cations were largely controlled by transport processes (advection and diffusion) but concentration level were regulated by chemical reactions (4) The profiles of some species such as pH, bicarbonate, sulphate were dominated by chemical reactions, and (5) bentonite went through minor degree of illitization, which cannot be confirmed by the data because of the large variation of measured data. Lastly, the THMC model were extended from 18 years to 200 years to evaluate the concentration profiles after bentonite becomes fully saturated and if there is significant mount of illitization. Model results showed the spatial concentration profiles flattened and there was no further illitization.