



## **Long-term Alteration of Bentonite Backfill Used for Waste Disposal: Coupled THMC Modeling of a Full-Scale In Situ Heater Test**

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Compacted bentonite is commonly used as backfill material in emplacement tunnels of nuclear waste repositories because of its low permeability, high swelling pressure, and retardation capacity of radionuclide. To assess whether this backfill material can maintain these favorable features when undergoing heating from the waste package and hydration from the host rock (with temperatures reaching more than 100 degrees C near the waste packages), we need a thorough understanding of the thermal, hydrological, mechanical, and chemical evolution of bentonite under disposal conditions. Dedicated field tests integrated with THMC modeling provide an effective way to deepen such understanding. Here, we present coupled THMC models for an in situ heater test which was conducted at the Grimsel Test Site in Switzerland for 18 years. The comprehensive monitoring data obtained in the test provide a unique opportunity to evaluate bentonite integrity at relevant conditions and test coupled THMC models used to predict the THMC evolution of bentonite over repository time scales. We developed a modeling strategy where conceptual model complexity is increased gradually by adding/testing processes such as enhanced vapor diffusion, thermal osmosis and different constitutive relationships for permeability/porosity changes due to swelling. The final THMC model explains well all the THM data and the concentration profiles of several chemical species. Over the course of modeling the in situ test, we learned that (1) key processes needed to reproduce the THM data include vapor diffusion, as well as porosity and permeability changes due to swelling and thermal osmosis; (2) chemical data provide an important additional set of information for calibrating a THM model; (3) the concentration profiles of cations (calcium, potassium, magnesium and sodium) were largely shaped by transport processes despite their concentration levels being affected by mineral dissolution/precipitation and cation exchange; and (4) the concentration profiles of pH, bicarbonate and sulphate were largely determined by chemical reactions. These findings enable more reliable calculation of the time frame and condition of the early unsaturated phase during bentonite hydration, the porosity and permeability after the bentonite becomes fully saturated, and how transport processes within bentonite and host rock interact with reactions.