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A coupled THC modeling for the geochemical evolution of bentonite buffer using an adaptive process-based total system performance assessment framework

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In deep geological disposal repository (DGR) with multiple barrier systems, complex physicochemical phenomena occur over an entire period of disposal time. These phenomena significantly impact the safety function of the DGR. Specifically, in the case of bentonite buffers which constitute the engineered barrier system, long-term geochemical evolutions can take place due to the changes in host rock groundwater, temperature, and redox condition. Such changes may have direct or indirect effects on radionuclide migration in case of canister failure. Therefore, a modeling tool that accounts for coupled thermal-hydraulic-chemical (THC) processes is necessary for the safety assessment of DGR.

To this end, KAERI developed an adaptive process-based total system performance assessment framework (APro) to conduct safety assessment of DGR. The APro considers coupled THC processes that influence radionuclide migration in DGR consisting of canister, buffer, backfill, and host rock. The solute transport considering thermal and hydraulic processes are calculated using the COMSOL multi-physics, while geochemical reactions are carried out in PHREEQC. The two software are coupled using a sequential non-iterative operator splitting approach under the assumption that the geochemical reaction reaches equilibrium immediately after every time step in the transport calculation. In this study, the transport of non-water H, non-water O, and charge were additionally considered in the coupling to enhance the model stability. Finally, the applicability of APro to simulate long-term geochemical evolution of bentonite was demonstrated through benchmarks with previous studies evaluating the effects of mineral precipitation/dissolution, temperature, redox, and seawater intrusion.