Robust Implementation Of Neumann Boundary Conditions In COMSOL-VIPER For Realistic Bentonite Hydration At Limited Water Supply

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Abstract

The thermo-hydraulically coupled code COMSOL-VIPER (Kröhn and Fromme 2023) based on the balance equations of the experimental VIPER code (Kröhn 2011) for simulating water uptake by bentonite has been further advanced. Bentonite is of particular interest as a geotechnical barrier against access of water to metallic canisters for radioactive waste in deep geological repositories (DGR).

Many modeling approaches still assume unimpeded water access (UA), where the bentonite receives as much water as it can take up. However, experiments at GRS (Noseck et al. 2018) have shown that the hydration behavior of bentonite changes significantly if it is subject to a limited water supply rate (LWSR). Such conditions apply where the external water flux constrains the uptake by the bentonite as in the low-permeable rocks that are foreseen for DGRs. They can be modelled by Neumann boundary conditions that dynamically link the external supply rate to the internal vapor diffusion flux at the bentonite interface thereby allowing for a more realistic representation of water inflow into the bentonite.

Implementing this condition in COMSOL-VIPER presented challenges due to the specific structure of the hydraulic balance equation. In contrast, coupling with the thermal domain was quite straightforward using the appropriate COMSOL Multiphysics node. During the conversion of the original VIPER partial differential equations into the weak form, a surface integral representing the Neumann boundary emerged and was incorporated directly as an additional weak equation with the help of the COMSOL Physics Builder.

In parallel, the robustness of the VIPER interface was increased through targeted improvements. They focused on refining variable definitions, as some were previously not clearly specified and led to solver instabilities. By constraining value ranges and adjusting formulations, model stability and usability were significantly improved.

The updated interface was tested in a one-dimensional simulation against experimental data from a GRS water uptake test (Noseck et al. 2018). This experiment serves presently also as the basis for Task 14a within SKB's Engineered Barrier System (EBS) Task Force. The EBS Task Force is an international collaboration that coordinates research and development to improve the understanding and modeling of engineered barrier components in a DGR.

The improvements presented here not only enhance the robustness and usability of the VIPER interface but also enable more realistic simulations of saturation processes in bentonite under LWSR-conditions. The updated implementation of COMSOL-VIPER is now planned to be applied to other real-world problems, like the recently terminated in-situ experiment "Prototype Repository" at the Hard Rock Laboratory Äspö in Sweden, where a limited water inflow through fractures under natural conditions has been observed.

Reference

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Figures used in the abstract

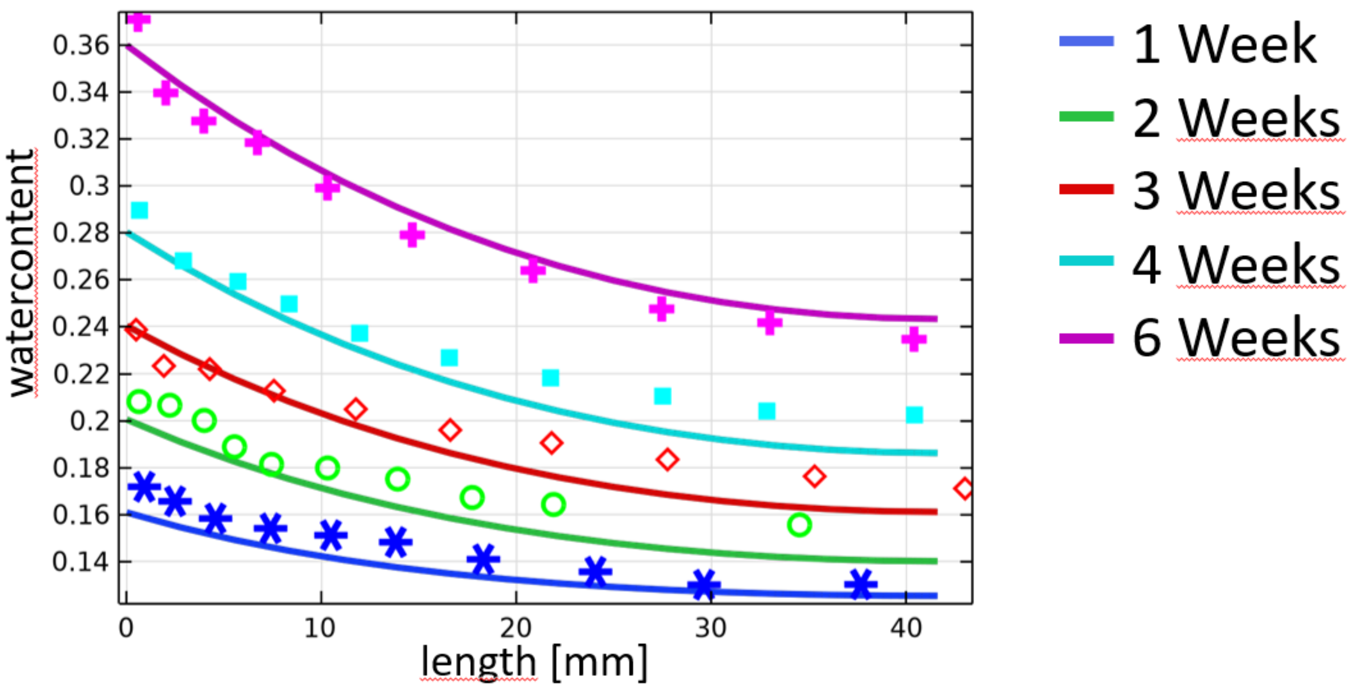

Figure 1 : Comparison of simulation (line) and experimental (symbol) results for an inflow rate of 0.02ml/h