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An alternative thermo-hydraulic model for bentonite re-saturation exclusively based on diffusive water transport and its implementation in 3D

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Bentonite is a versatile material that is, among other things, envisaged for designs for radioactive waste repositories to protect the waste canisters against groundwater. The thermo-hydraulic-mechanical (THM) coupled process of bentonite saturation is commonly based on two-phase flow. As an alternative to the formulations in THM-models, a thermo-hydraulic coupled saturation model for confined conditions (as expected in a repository) has been developed and realised for 1D-problems in the FORTRAN-code VIPER. In order to enhance the inherent limited range of possible applications of this code, the underlying partial differential equations have been transferred to COMSOL Multiphysics®. This has been done for the most simple, isothermal form at first, and subsequently for the non-isothermal formulation by coupling the hydraulics to the heat transfer interface of COMSOL.

The model concept for the hydraulics, qualified for a number of different problems using the VIPER code, is comparatively simple. Vapour diffusion in the pore space is coupled to diffusive water migration in the interlamellar space by instantaneous hydration. This results in a double-continuum model that calculates re-saturation rather efficiently for cases where the bentonite is subject to confined conditions and only little internal swelling occurs.

At first, a COMSOL-model has been developed that matches an isothermal water uptake test performed at GRS as well as the earlier performed simulations with code VIPER. An important motivation for the transfer of the VIPER-concept to COMSOL Multiphysics is broadening the range of possible applications from 1D to 3D modelling tasks.

After successfully completing this first step, further terms in the balance equation as well as equations of state were added which are required for calculating non-isothermal water transport. Furthermore, the simplified treatment of heat flow in VIPER could now be replaced by implementing a full coupling of the hydraulic formulations to the heat flow interface included in COMSOL Multiphysics.

The new implementation in COMSOL has been checked on the basis of temperature and humidity measurements from the FEBEX in-situ experiment performed at the Grimsel hard rock laboratory in Switzerland. The FEBEX-experiment was intended to represent the deposition of heat-producing

nuclear waste canisters that were enclosed in a layer of compacted bentonite blocks in a tunnel in granitic rock. Wetting of the bentonite buffer was provided by the rather highly conductive host rock. Measured and simulated temperature evolution as well as wetting dynamics in the buffer matched each other reasonably well.

The presented work opens up the possibility to apply the alternative re-saturation concept to a wide range of three-dimensional problems not solvable by code VIPER. However, a number of further enhancements of the new model for instance concerning boundary conditions for water vapour or swelling into free space are conceivable as a follow-up.