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Pore-level modelling of cement paste degradation due to cement-clay interaction

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Cement-clay interaction has a significant effect on the integrity of large-scale cement infrastructure as investigated in the Eurad Work Package MAGIC (www.ejp-eurad.eu). The strong geochemical contrast between cement and clay drives dissolution and precipitation reactions (e.g. precipitation of C-S-H phases), altering the local material microstructure at the pore-level. These interactions also lead to non-linear changes in transport properties such as permeability and diffusivity.

In this work, the simulations of mass transport processes at the pore-scale are based on the Lattice-Boltzmann (LB) method. The locality of the LB operator is ideal for highly efficient parallel execution and enables 3D simulations of the microstructure's complex evolutions. To describe the chemical interactions in the system, the LB code needs to be coupled to thermodynamic modelling routines (e.g. GEMS-Selektor [1]). However, due to the high computational costs of thermodynamic calculations, such coupled simulations require significant computational resources. To circumvent the computational efficiency issue, a GPU-based CUDA/C++ LB code is coupled to a surrogate model of the geochemical system. The surrogate model is based on an artificial neutral network (ANN) [2,3] describing the most essential chemical parameters of the system such as the Ca and Si ions' aqueous concentration, pH, the cement phases' saturation. The ANN is trained using a supervised learning approach based on the large array of sample data obtained from a native geochemical solver.

The resulting model is used to investigate C-S-H precipitation taking place at cement-clay interfaces. The reactive transport simulations are applied to investigate the porosity and permeability evolutions resulting from the cement-argillaceous pore water interactions in deep geological radioactive waste repositories. Knowing the mineralogical composition and porosity as function of the reaction progress, the changes in mechanical parameters (e.g. linear elastic moduli) can be evaluated. The model is further used to interpret data from experimental characterisation of cement paste interaction with Opalinus Clay pore water.

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