Application of pore scale modelling approach for long term durability assessment of concrete

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Abstract

Concrete is one of the important materials for the engineered barriers system for nuclear waste disposal system and provides encapsulation to nuclear waste for long period of time. Henceforth, long term integrity of concrete in these waste disposal systems is desirable and adequate assessment of the durability of this system can provide important arguments towards long-term safety of the facility. When the concrete is in contact with aggressive environmental conditions, minerals phases of hardened cement paste undergo chemical alterations. Typical processes of chemical concrete degradation which alter pore scale geometry and change concrete properties are calcium leaching and carbonation. The key to get a good insight in pore scale interactions is the development of an appropriate numerical tool to simulate the interplay between solid phase alterations, pore structural changes and effective transport properties.

In this presentation a lattice Boltzmann based pore scale reactive transport model is described in details. Unlike traditional numerical approaches, lattice Boltzmann method (LBM) provide computationally efficient way of modeling transport through complex pore geometry due to simple local computations used for solving the advective - diffusion equation which can be easily be parallelized and simple bounce back boundary condition at the solid/liquid boundary condition. However, the applicability of LBM to model reactive transport processes is often restricted to small chemical systems. To alleviate this typical restriction of LBM reactive transport codes, the transport LBM code is coupled with well-established geochemical modeling code *PHREEQC* giving flexibility to incorporate complex chemical systems such as the one of cement paste. The applicability of developed code for micro scale modeling of cement paste under chemical degradation is then illustrated with several showcase examples.