Advanced Lattice Boltzmann advection-diffusion-reaction simulations of chloride transport inside hardened cement paste micro-pores

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ABSTRACT

A Lattice Boltzmann model is proposed to simulate advection-diffusion-reaction of species in partial saturated hardened cement pastes (HCP). The approach is intended to capture solid matrix evolution due to chemical precipitation/ dissolution reactions. We focus, in this work, on chloride transport inside HCP's micro-pores. Rather than attacking steel reinforcement chlorides react with cement compounds forming expansive products leading to extra mechanical stresses on the solid matrix that probably leads to failure (cracking).

The cumulant LBM [1] is used to study the fluid flow inside the pores and the multiple-relaxation-time LBM [2,3] is used to account for the transport of chloride inside the pores. A reaction scheme is implemented along with the advection – diffusion to account for the changing solid matrix. A set of benchmarks for flow, advection – diffusion, and reaction are presented. First results for real HCP microstructures obtained from micro-CT X-ray images are used to simulate both fluid flow, and advection – diffusion of chlorides under saturation condition. Comparisons of numerical results and experimental data are shown.

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