Numerical modelling of water isotherms of cement paste: Bridging the gap between the capillary and C-S-H gel pores

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Despite the success of lattice Boltzmann methods in simulating complex flows in a multitude of porous media, their application to cement paste remains very limited [1]. The main reasons appear to be the multi-scale nature of the porosity and the uncertain structure of the calcium silicate hydrate (C-S-H). To overcome these problems, Zalzale *et al.* [2] included the C-S-H gel pores in permeability simulations by using an effective media approach where the C-S-H gel pores are described in terms of averaged transport properties. The simulated permeability span the whole range of experimental measurements (10^{-17} – 10^{-22} m^2) and the results show that the degree of capillary water saturation is a very plausible explanation for the large experimental scatter. The results also show that the role of the weakly-permeable C-S-H, omitted in earlier modelling studies, is critical to determine the permeability at low capillary porosity or low degree of capillary water saturation.

In this work, the effective media approach is extended from single- to multi-phase. The liquid and vapour are linked by a Van der Waals equation of state and the fluid interfaces are tracked implicitly. The algorithm allows the definition of multiple independent surface tensions (*i.e.* contact angles) between the fluid, C-S-H and solid phases. The C-S-H is described in terms of *intrinsic* permeability and *internal* wetting (*effective* Kelvin-Laplace pore radius). The model is first tested and verified on an exemplar system composed of anhydrous cement particles surrounded by nano-porous C-S-H and micron-sized capillary pores. Then, the algorithm is applied to a cement paste model microstructure in order to model the full desorption and adsorption isotherm of water. A two-step isotherm and the ink-bottle effect are clearly observed. Finally, it is discussed how the lattice Boltzmann effective media approach can be used to bridge the gap between state-of-the-art molecular simulations, macroscopic models, and experiments.

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References:

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