A Three-dimensional partial bounce-back method applied to cementitious materials

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(Submitted for the 22nd International Conference on the Discrete Simulation of Fluid Dynamics (DSFD2013), Yerevan, Armenia, 15 – 19 July 2013)

Concrete is the most widely used construction material on Earth and its production exceeds $1m^3$ per person per year. Water transport in cementitious materials significantly affects their durability. Understanding water dynamics is crucial to explaining the link between cement microstructure, performance and durability. In order to model faithfully the water dynamics, cement microstructures are required. Microstructural models have been developed for the purpose of understanding cement hydration and kinetics and are increasingly successful in doing this. In this paper, we demonstrate the application of LB methods for the calculation of the permeability of mature cement paste.

A three-dimensional multi-relaxation-time LB model is used to calculate the permeability of microstructures of cement pastes generated using the numerical model μIC (S. Bishnoi and K.L. Scrivener 2009). It is found that the microscopic capillary pore network is not sufficient to capture the flow complexity (M. Zalzale and P.J. McDonald). Consequently, the simulated permeabilities are larger than experimental values. To overcome this problem, a probabilistic LB algorithm based on the partial-bounceback model (S.D.C Walsh et *al.* 2009) is developed to include the flow inside the nano-porous calcium silicate hydrates (C-S-H). With this homogenization method, the C-S-H average local permeability is an input parameter. By this means, we implicitly include the nano-structure complexity without the high LB computational cost. Using this algorithm, the simulated permeabilities are in very good agreement with experimental measurements.