P3: Lattice Boltzmann modelling of water dynamics

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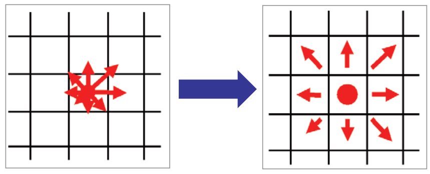
A native of Lebanon, Mohamad Zalzale got his MS in Computational Physics at the University of Montpellier II in France in September 2010. He started to work at EPFL February 1st 2011.

Overview

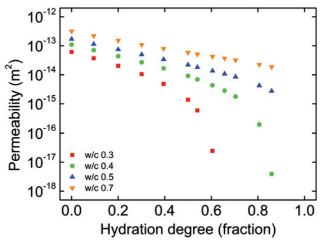
- Lattice Boltzmann (LB) methods are a class of computational fluid dynamics solvers. LB algorithms exist for single and multi-phase flows and are very convenient for the simulation of flow in porous media because they deal implicitly with arbitrarily shaped geometries.



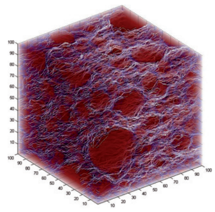
- In this work, cement microstructures with different *w/c* ratios and degrees of hydration are generated using the vector model μIC[Bishnoi & Scrivener 2009]. The water dynamics is simulated with the LB method and the permeability is calculated using Darcy's law.

Results

Months 0 - 18



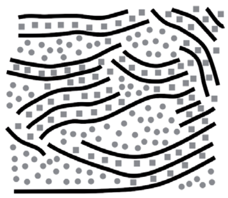
- An LB model of pressure-induced water flow is developed and validated. Although the model captures the expected trend for permeability as a function of degree of hydration, the values are larger than expected from beam-bending experiments ($3*10^{-22} m^2$, *w/c*=0.4, 14 days)[Vichit-Vadakan & Scherer 2002]. These and other results are now published in: M. Zalzale & P.J. McDonald, Cem. Con. Res. 42 (2012) 1601-1610.
- Recently, with improved computing resources, higher resolution simulations were achieved. The computed permeability decreased but remained larger than experimental values.



Flow streamlines in a μIC structure

Months 18 - 24

- To overcome the limitations of standard LB models, a novel algorithm modelling pressure induced flows in partially-permeable media is developed and validated. This new algorithm allows input of an additional partially-permeable phase (*i.e.* C-S-H) by combining the fluid-fluid collision and the fluid-solid collision steps. The new phase is assigned effective medium properties, making it possible to model the flow over a wide range of length scales within achievable computational resources.
- The latest simulations use input data for composition & microstructure from projects 7, 9[Muller et al. 2012] & beam bending experiments. Preliminary results show that the simulated permeabilities are now of the same order of magnitude as those measured in beam-bending experiments and with NMR imaging at Surrey[Zamani 2013].



C-S-H structure as illustrated by Muller et *al.* 2012. Calcium silicates (solid lines), interlayer water (squares) and gel pore water (circles).

Future work

Feb → May → Feb

- Conclude analysis of permeability of μIC structures including C-S-H (+ publication).
- Model the water / vapour transport induced by a relative humidity gradient and validate results against NMR experiments at the University of Surrey (+ publication).
- Write the thesis.

Outstanding questions

- Cement pore structure (answers mostly coming from P7 & P9)
- C-S-H morphology and effective medium properties (answers coming from P2)
- Validation of the simulated cement microstructure (*e.g.* C-S-H density, capillary porosity, shrinkage, voids)

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