Concrete Sustainability Hub@MIT – Research Profile Letter – November 2011

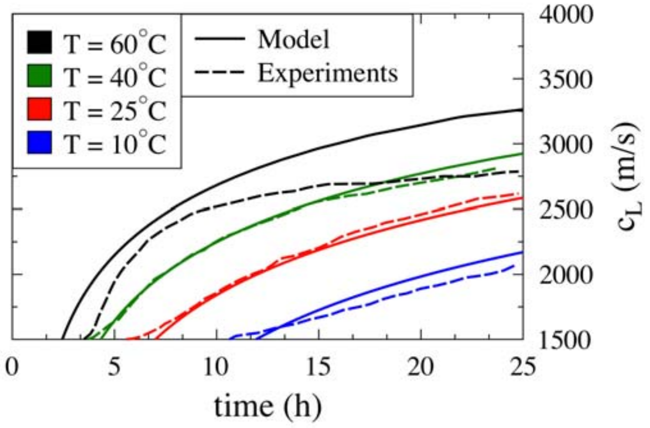
Predicting Setting Times Bottom-Up

Problem

Predicting the time evolution of the mechanical properties of a cement paste during hydration remains a major challenge in cement science. This requires an accurate model for cement setting that is able to capture the inter-grain micron-sizes pore filling due to the precipitation of hydration products. Traditional models address setting based on geometric percolation without considering other aspects of the kinetics of cement hydration, such as the temporal increase of stiffness and strength. In order to predict cement setting, the hardening of the paste must be related to morphology and mechanical properties of the hydration products. A model that couples hydration kinetics, microstructural evolution, and strength development at smaller scales is still lacking.

Approach

To analyze the formation of hydration products within the capillary porosity, we first study the progressive filling of one isolated pore using colloidal simulations of nano-particles (which appear to represent C-S-H and other hydrate phases) in the Grand Canonical Monte Carlo framework. Second, we consider a size distribution of capillary pores with filling kinetics derived from the isolated pore. This yields the time evolution of the solid packing fraction and, consequently, the mechanical properties in each pore. The total bulk modulus of the suspension, obtained via averaging, is translated into acoustic wave speed by elastic continuum theory. The filling rate of the pores is obtained by considering the formation of C-S-H as a two-parameter Arrhenius process that involves an effective energy barrier and a pre-factor. The two parameters are obtained from the scaling of the Vicat setting time with temperature, and depend only on the initial composition of the unhydrated phases.



Longitudinal acoustic wave propagation in Portland hardening cement paste: our setting model and experiments [from Zhang et al., Cem. Concr. Res., 40(7), 2010]. 1,500 m/s is the sound speed in water, and the detection level for a rigid microstructure.

Findings

We find that capillary pore size distribution, morphology and mechanical properties of the hydration products contribute significantly to the evolution of the stiffness of the paste over time. In our simulations we consider low-density C-S-H, modeled as monodisperse colloids. The pore size distribution can be directly measured but, so far, we calibrated it for the reference temperature of T=25°C. The model then gives predictions for other temperatures which are in reasonable agreement with experiments in a temperature range from 10C to 40 C. At temperatures of 60 C, qualitative changes of hydration products and mechanisms have been experimentally observed, and the model reactions would need to be revised to accommodate those changes.

Impact

This model of setting couples hydration kinetics and development of mechanical properties, a combination that allows the prediction of setting times in a bottom-up fashion. Our setting model brings information from atomistic and colloidal simulations to larger length and time scales, suggesting opportunities to link atomic structures of hydration products with engineering properties.

More

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