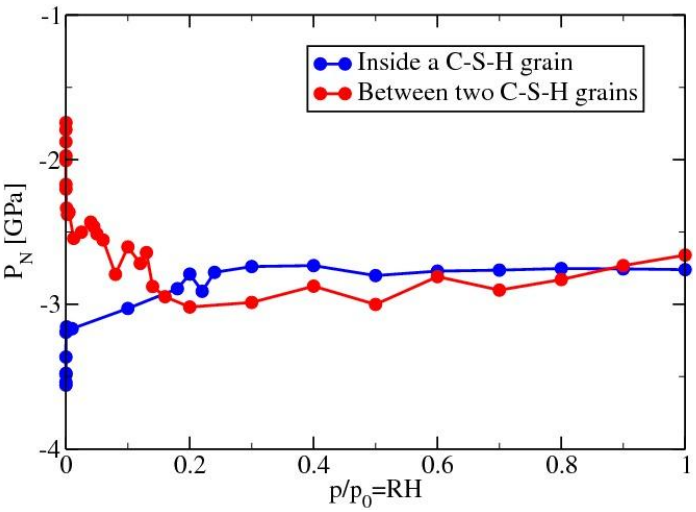
Concrete Sustainability Hub@MIT – Research Profile Letter – December 2011

Holding It Together: C-S-H Cohesion

Problem

To improve the durability of concrete under extreme conditions, it is particularly important to understand damage mechanisms within the cement paste that binds aggregates. The multiscale porosity inherent to cementitious materials implies that water may be present as liquid, solid, and/or gas depending on the thermodynamic conditions (temperature, pressure, ion concentration). It is thus appreciated that water may be both the source and the medium causing damage in cement paste. Here, computational simulations are particularly advantageous because water properties in nanoscale pores (≤1 nm) are challenging to access experimentally.



Pressures applied by the fluid (water and calcium ions) in the direction normal to the grain surface for different relative humidity levels RH=p/p_0, where p_0 is the saturating vapor pressure of water. Intragranular pressure (inside a single C-S-H grain) is indicated in blue. Intergranular pressure (between two C-S-H grains separated by 1 nm) is indicated in red.

Approach

Our study is based on the calcium silicate hydrate phase (C-S-H), the primary binding constituent in cement paste. We employ semi-Grand Canonical Monte Carlo techniques to consider how the water content within and between nanoscale C-S-H volumes or "grains" changes as a function of the relative humidity (% RH) at an ambient temperature of 27°C. To relate the effect of the water content in the cement paste on the cohesion, we computed pressures due to the fluid (water and calcium ions) in the direction normal to the grain surface. Negative pressure indicates cohesion, and positive pressure indicates repulsion. Two situations are considered: (i) inside a C-S-H grain and (ii) between two C-S-H grains separated by a distance of 1 nm, reflecting the close proximity of such grains within cement paste.

Findings

Our first key result is that cohesion within and between C-S-H grains is relatively stable down to about 20% RH, beyond which all nm-scale cement pores are filled with water. The second key result is that below 20% RH, cohesion inside a C-S-H grain is increased (grains shrink) and cohesion between C-S-H grains is decreased.

Impact

Our approach shows that cohesion within cement paste decreases with decreasing water content, specifically at RH<20% and 27°C. This loss of cohesion within the binding phase significantly affects the strength and durability of the material. These calculations help to explain reduced strength and creep resistance of concrete in very dry environments, and also provide insight toward damage mechanisms in concrete at high temperatures (e.g., fire environments) even before heat-induced polymerization of silica chains.

More

Research herein conducted by Dr. Patrick Bonnaud, postdoctoral researcher, in collaboration with Dr. Q. Ji and Prof. R. Pellenq, and supervised by Prof. K. J. Van Vliet.

This research was carried out by the CSHub@MIT with sponsorship provided by the Portland Cement Association (PCA) and the Ready Mixed Concrete (RMC) Research & Education Foundation, as well as the US Army Corps of Engineers and US Department of Homeland Security. The CSHub@MIT is solely responsible for content. For more information, write to CSHub@mit.edu.