

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Understanding the mechanical properties of cement in terms of its early-stage gelation ABHAY GOYAL, CHRISTOPHER TIEDE, Georgetown Univ, KATERINA IOANNIDOU, ROLAND PELLENQ, MIT, EMANUELA DEL GADO, Georgetown Univ — Despite the nearly ubiquitous use of concrete as a construction material, cement hydration is still poorly understood. The variety of hydration products, the non-uniform rate of reaction, and the changing chemical background all contribute to making this a complex process. Recently, a novel statistical physics approach combining Grand Canonical Monte Carlo with molecular dynamics has achieved remarkable correspondence with experimental data. It treats the main hydration product, Calcium Silicate Hydrates (C-S-H), as colloidal particles with a simple effective interaction that varies with the degree of hydration—due to changing pH, ion concentration, etc. Working with this model, I investigate the percolation of the gel structure and the onset of mechanical properties in the early stages of hydration, which end up affecting the material properties at much later times. In particular, I have studied how the tendency of C-S-H to form at the surface of cement grains may affect the gel morphology, its structural heterogeneity, and ultimately its mechanical strength. By varying the effective interaction potential between C-S-H particles, I can rationalize the interplay between the evolution of the gel morphology and the changing physicochemical environment in which the gel forms.

Abhay Goyal
Georgetown Univ

Date submitted: 11 Nov 2016

Electronic form version 1.4