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Seminar Presentation

Continuum Modeling of Reactive Colloids: Transformation of Cement Paste from Sol to Cohesive Gel

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Abstract: A colloid is a collection of nanometer- to micron-sized particles interacting in a fluid or solution. And though colloids have traditionally been defined as fluid-like dispersions that remain suspended on account of the system's thermal fluctuations, the term has become more general, referring to the collective behavior of particles that attract or repulse and interact at varying relative length and time scales. Cement paste, the binding agent in modern concrete, is classified as a colloid. Nearly instantaneously after mixing water with polydisperse cement powder, nanometer-sized grains of calcium-silicate-hydrates (C-S-H) precipitate out of solution and spontaneously gel. It is at this length scale that many of the physicochemical characteristics that lend the paste its mechanical durability are thought to derive. Yet few modeling approaches have been implemented to investigate how the density patterns in such reactive materials evolve and control mechanical behavior.

This talk presents a nonequilibrium thermodynamic theory for the mean-field precipitation, aggregation and pattern formation of colloids. A variable gradient energy coefficient and the arrest of particle diffusion upon "jamming" of clusters in the spinodal region predicts observable gel patterns that, at high inter-particle attraction, form system-spanning, out-of-equilibrium networks with glass-like, quasi-static structural relaxation. For reactive systems, we incorporate the free energy landscape of stable primary particles into the Allen-Cahn reaction equation. We show that pattern formation is dominantly controlled by the Damköhler number --- the ratio of the reaction rate to the diffusion rate --- and the stability of the primary particles, which modifies the auto-catalytic rate of precipitation. As primary particles individually become more stable, bulk phase separation is suppressed.

Throughout our modeling efforts, we relate several results to experimental observations of hydrating cement paste. Firstly, it is hypothesized that curing temperature modifies the thermodynamic landscape of the C-S-H grains, which in turn influences the paste's pore-size distribution: Cements hydrating at higher temperatures produce more capillary porosity and less gel porosity, which adversely affects the materials durability. Secondly, the thermodynamic stress, which derives from the surface interactions of colloidal particles, is proposed as the driving force for cement shrinkage, which was experimentally observed in course of hydration under constant temperature and pressure conditions.

Bio: Over the past year, Thomas has been working as a research engineer at ExxonMobil, investigating technologies that improve the integrity of wells during construction and operation. Prior to moving to Houston, he completed his Ph.D. and Master's degrees in the Civil and Environmental Engineering Department at MIT, and received his B.S. in Civil Engineering at North Carolina State University. His research interests address applied problems concerning the mechanics of reactive materials. In his spare time he enjoys training for marathons, skiing/snowboarding, and trying new restaurants.

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