A Reaction-Diffusion Model to Determine Mesoscale Patterns in Cement Paste

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PROBLEM

Strength and toughness, two important aspects of the durability of concrete structures, are dramatically influenced by the material's nanotexture, but the question of how the building blocks of cement paste organize themselves to create this nanotexture is still being answered.

Recent modelling efforts by CSHub researchers demonstrated a convincing pathway.[1] Upon mixing water with cement clinker, ions dissolve into the pore solution and precipitate out nanometer-sized grains of calcium-silicate-hydrates (C-S-H). These building blocks are the glue that binds sand and gravel together and the primary ingredient for concrete. The organization of these C-S-H grains drastically influences concrete's mechanical performance. By better understanding which parameters influence this organization, we hope to create longer-lasting, more durable materials.

APPROACH

We applied a new technique to model the reaction rate and chemical diffusion of the C-S-H grains during the early stages of cement setting. Rather than track the formation and interaction of the discrete nanograins explicitly, the model predicts how the spatial distribution and packing density of the C-S-H grains change over time. As an example, Figure 1 to the right displays the evolution of these density patterns for several reaction environments that correspond to increasing degrees of supersaturation. Both the local packing density of C-S-H and its connectivity determine the overall strength and toughness of cement.

FINDINGS

We find that the speed and uniformity at which the C-S-H grains precipitate from solution determines the size and contrast of the density patterns. For the same hydration degree, Fig. 1 shows that homogenous reaction rates, which have little chemical diffusion, produce systems with smaller capillary pores and more loosely packed grains. More dramatic phase separation is found in heterogeneously precipitating systems, which have substantial chemical diffusion; here, C-S-H grains pack together and form nuclei more readily. Importantly, these results demonstrate that the interaction of the grains during the initial few hours of the cement reaction control the uniformity of the patterns that form and provide a template upon which C-S-H grains continue to precipitate at later stages of the reaction.

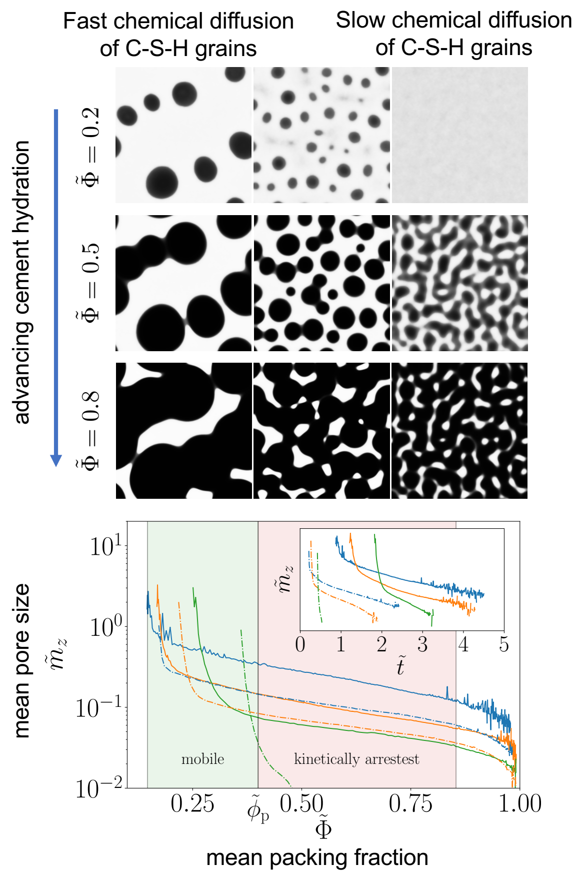

Figure 1: (Top) Cement patterns developing under differing reaction environments. Slower, more heterogeneous reaction rates create more distinct phase separation, causing larger pores to form. (Bottom) Mean pore size plotted against the overall reaction extent (inset- plotted against normalized time); line colors indicate how rapidly C-S-H grains diffuse during the initial period of nucleus formation (blue - fast diffusion, green – slow diffusion), and solid (dashed) lines indicate systems of low (high) supersaturation.

WHY DOES THIS RESEARCH MATTER?

- If the reaction environment and interaction of C-S-H grains during the early stages of cement setting can be controlled, a tougher more resilient material may be engineered by modifying its nanotexture.

[1] *Ioannidou, Katerina, et al. "Mesoscale texture of cement hydrates." Proceedings of the National Academy of Sciences (2016)*

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