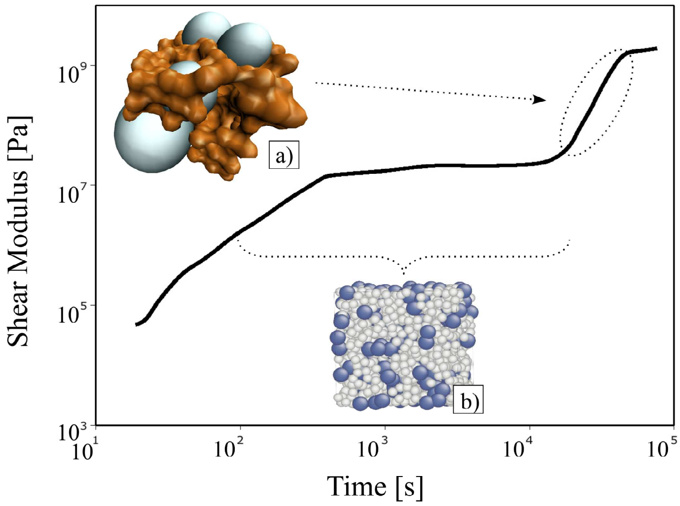
The Hidden Forces of Setting

Problem

Setting of concrete, that is the transition from liquid to stone, is one of the most important parameters of any successful concrete operation. From a cement chemistry point of view, the setting encompasses three phases: the gelation period, the flocculation or dormant period (where the material remains workable) and finally the percolation of the solid phase. Any of these processes affects the setting and thus the success of the operation. From a physics perspective, however, the forces involved in each of these processes remain an enigma, due to the lack of a consistent modeling approach that describes the entire transition from the fluid state to the solid state, from gel formation to jamming. Knowing and manipulating these forces is important to master engineering field quantities (slump, stiffness etc.) critical for meeting demanding construction schedules. Progress on the setting front is also needed to implement novel compositions and components, and in particular lower greenhouse components of concrete.



a) Quantitative clinker–precipitate granular model of jamming and solidification. b) Binary colloidal model that captures qualitatively the three stage process, gelation–flocculation–jamming.

Approach

In contrast to modeling approaches based on reaction kinetics and Finite Element Methods that disregard interparticle forces, we have chosen a statistical mechanics approach that considers these forces explicitly via particle interaction potentials. The inputs to our simulations are formation rates of clinker phases and precipitates. The output is the time history of the particulate microstructure that is amenable to mechanical testing, including shear stiffness and shear strength. By conducting a wide spectrum of such simulations, a consistent model of setting emerges which predicts well the three stage process of setting, from liquid to stone, in terms of critical engineering parameters.

Findings

This is the first elemental statistical mechanics model for cement setting that predicts a 5 order of magnitude stiffness and strength increase over 3-5 orders of time magnitude. It shows that the chemical formation rates determine the time scale of jamming, while the existence of a pronounced gelation and flocculation phase that precede jamming, relates to the clustering of colloidal precipitates.

Impact

This research highlights the importance of the interaction forces between the liquid and solid components of cement hydration (clinker, CH, C-S-H, pore solution etc). The approach holds the promise to become a quantitative bottom-up engineering tool for a science-driven engineering design of the next generation of setting agents including chemical admixtures.

More

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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. The CSHub@MIT is solely responsible for content. For more information, write to CSHub@mit.edu.