Atomistic Modeling of ASR Gel

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PROBLEM

The Alkali-Silica Reaction (ASR), which causes expansion and cracking in concrete, can result in structural problems in concrete infrastructure that can both limit the service life and generate high maintenance costs. The damaging effect of ASR results from expansive pressure within the concrete. ASR gel, formed from a chemical reaction between certain minerals in some aggregates and alkalis in concrete pore solution, is commonly viewed as the origin of this swelling pressure. A better understanding of this reaction and its mechanisms is key to determining solutions that will prolong the life of concrete infrastructure. This brief summarizes an atomistic modeling study of the ASR gel that is meant to better connect the gel's chemical composition to its mechanical properties and swelling characteristics. A parallel experimental study of synthetic gels is in progress to validate this model's predictions.

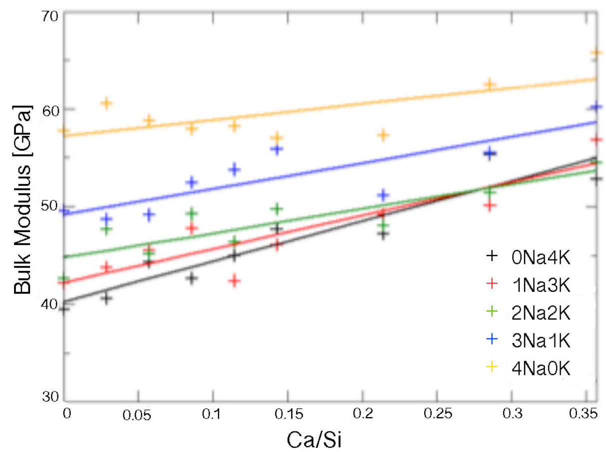

Fig. 1: Bulk modulus (a measure of stiffness) of the glass vs. Ca/Si ratio with various Na-K repartitions.

APPROACH

Researchers systematically studied the relationship between ASR gel composition and its properties. This included mechanical properties and water affinity (which refers to how much water can be imbibed by a system). Gel chemistry was varied to explore the effects. Factors included calcium-silica (Ca/Si) ratio and alkali repartition K/Na. Alkaki repartition refers to method for adjusting the amount of K and Na ions in a way that affects the chemical composition of the material. Evaluation was conducted on model glasses and gels, with the latter being viewed as hydrated glasses. The hydration of glasses was modeled using Grand Canonical Monte-Carlo, a simulation method allowing the insertion of new particles into a system. In this study, water molecules were inserted into model glass matrices.

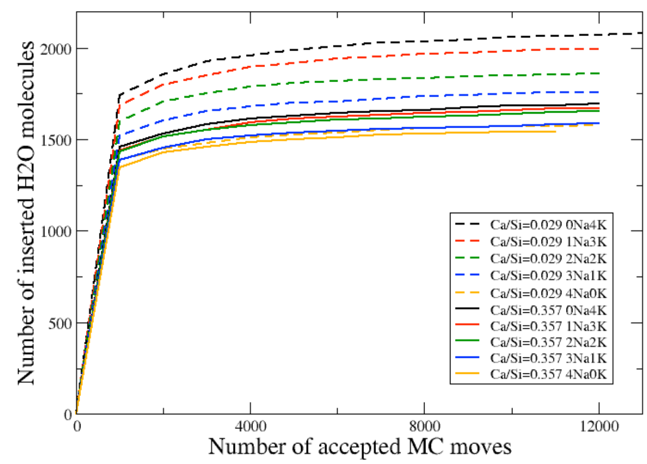

Fig. 2: Water uptake for low Ca/Si ratio (dotted lines) and high Ca/Si ratio, with various Na-K repartitions as a function of the number of accepted Grand Canonical Monte Carlo (GCMC) moves.

FINDINGS

The chemistry of the ASR gel (modeled as glass) had a significant impact on mechanical properties and water affinity. An increased calcium content was found to correspond to a higher bulk modulus, meaning a stiffer material (see Fig. 1) and lower calcium content resulted in higher water affinity (see Fig. 2). Researchers also found that the impact of the alkali repartition on the glass hydration is more important when there is a low Ca/Si ratio than when there is a high Ca/Si ratio. The research shows that, gels with low Ca/Si ratios have lowered mechanical properties, resulting in a gel that behaves more like a fluid. More rigid gels may make a material more prone to cracking whereas a more fluid gel exerts less pressure in the pore space. This perspective on the damaging mechanism can be seen along with what is currently being developed within the CSHub in the scope of freeze-thaw damage meso-scale modeling. Indeed, the driving force for cracking is believed to arise from ionic correlation forces in the pore solution, transmitted to the cement paste when ice or a stiff gel is formed in the pore.

WHY DOES THIS RESEARCH MATTER?

- Study findings supports the idea that gel behavior is strongly dependent on its chemical composition, both for the amount of water it uptakes and its mechanical properties.
- Findings are in agreement with results seen in other CSHub experimental studies of ASR Gels.

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