Bottom-up Modeling of ASR in Concrete

PROBLEM

Alkali–silica reaction (ASR) occurs in some concretes between the highly alkaline pore solution and reactive silica components in certain aggregates. An alkali-silica gel is formed that may, over time, expand in the presence of sufficient moisture. This expansion can generate internal stresses that lead to deformation of concrete and, possibly, cracking and structural failure.

APPROACH

The driving force behind swelling in ASR is largely believed to be alkali-silica gel (ASR gel). The composition of this gel evolves: for example, the calcium content of the ASR gel is known to increase over long time periods. Using knowledge gained from prior studies on C-S-H (calcium silicate hydrate, the binding phase of hydrated cementitious materials, responsible for the material's strength), we aim to develop a model that allows us to understand the reaction at both the atomic and mesoscale.

We adapted existing CSHub models to allow us to examine a potential swelling mechanism for this reaction. Our atomic scale simulations focused on the evolution of C-S-H mechanical properties with increasing sodium content, along with those of the ASR gel with increasing calcium content.

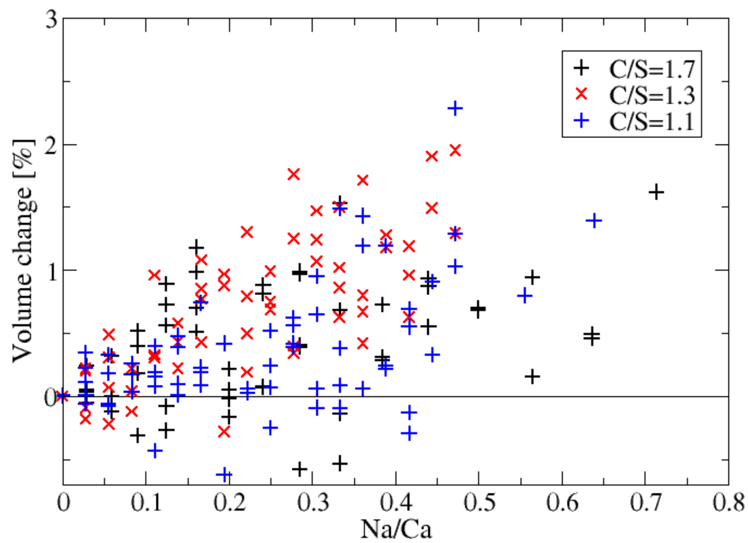

Fig. 1: Simulated C-S-H volume change as a function of the sodium to calcium ratio, for three initial C-S-H compositions at 0K.

We were interested in estimating composition-induced volume changes. By looking at the individual components (C-S-H and ASR gel), and increasing respectively their sodium and calcium content, we were able to observe and understand how the volume of each can change. The ASR gel was modeled as an alkali silicate glass with increasing calcium content because, in glass science, calcium is known to be a glass former (i.e. producing a rigid network at the atomistic scale). As the Ca content increases (upon substitution of 2 Na^+ ions by 1 Ca^{2+}), a more rigid and shrinking ASR phase can be expected; this confirms results obtained by other research groups. This suggests that the driving-force of the swelling of a concrete affected by ASR might have another origin or may be less straightforward than the swelling of the ASR gel itself.

FINDINGS

Based on 0K (absolute zero) calculations at the atomic scale, we observed that sodium enriched C-S-H exhibits significant swelling (Fig. 1), and calcium enriched glass (mimicking the ASR gel) shrinks. These trends imply that the role of the gel would thus be reduced to the delivery of alkalies. Its increased viscosity (on which much of previous research has focused) relates to the fluidity of the gel permeating the C-S-H but not to pressure. (The 0K calculations were used as a first step in the modeling process; in additional research the modeling will be conducted at ambient temperature).

IMPACT

This new ASR modeling strategy allows us to address this very damaging reaction from a fundamental viewpoint. Initial results give possibilities to consider for this reaction: could alkali-enriched C-S-H be the driving-force of the expansion? Could ASR gel be a source of alkalies? As these questions are addressed by further refinements, this would bring to light a new understanding of ASR, leading to the possibility of novel mitigation strategies.

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