



Multiscale hydro-thermo-chemo-mechanical coupling: Application to alkali–silica reaction



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ABSTRACT

Alkali–Silica Reaction (ASR) is a complex chemical process that affects concrete structures and so far various mechanisms to account for the reaction at the material level have already been proposed. The present work adopts a simple mechanism, in which the reaction takes place at the micropores of concrete, with the aim of establishing a multiscale framework to analyze the ASR induced failure in the concrete. For this purpose, 3D micro-CT scans of hardened cement paste (HCP) and aggregates with a random distribution embedded in a homogenized cement paste matrix represent, respectively, the microscale and mesoscale of concrete. The analysis of the deterioration induced by ASR with the extent of the chemical reaction is initialized at the microscale of HCP. The temperature and the relative humidity influence the chemical extent. The correlation between the effective damage due to ASR and the chemical extent is obtained through a computational homogenization approach, enabling to build the bridge between microscale damage and macroscale failure. A 3D hydro-thermo-chemo-mechanical model based on a staggered method is developed at the mesoscale of concrete, which is able to reflect the deterioration at the microscale due to ASR.

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1. Introduction

1.1. Concrete

Good durability to cost ratio renders concrete one of the most widely used construction materials. However, it is an extremely complex heterogeneous material with a random microstructure at different length scales. At the *macroscale*, it is treated as a homogeneous material. One scale lower, the *mesoscale*, includes a binding matrix, aggregates and pores with broad size distributions as well as interfacial zones between the aggregates and the matrix. Finally, the *microscale* constitutes the finest structural scale and is represented by the microstructure of hardened cement paste (HCP), which is comprised of hydration products, unhydrated residual clinker and micropores [1]. The observable or macroscale failure of the concrete caused by various environmental attacks, such as frost [2] and Alkali–Silica Reaction (ASR) [3] as well as severely mechanical loading [4], can be explained by the variation of the underlying microstructure of the concrete. Therefore, it is desirable that a correlation between the macroscopic failure and the variation of the microstructure is established. However, the high cost of the conventional experiment in the laboratory high-

lights the need for an alternative approach. With the continuous improvement of computational power and the development of non-destructive evaluation techniques such as computer tomography, one can obtain the microstructure of the material at the microscale and carry out the analysis numerically.

Over the recent years, multiscale models were developed to analyze the failure in the concrete suffering from various attacks. Hain and Wriggers [2] have evaluated the damage due to frost in HCP using a finite element model that is based on the three-dimensional computer-tomography scans of HCP, and the obtained effective damage was upscaled to the next scale of the concrete via a computational homogenization approach. Cusatis et al. [5] developed an equivalent macroscopic cohesive law reflecting the meso-level failure mechanisms, where the investigation of the fracture behavior at the lower scale was carried out through a lattice-type model. A coupled macro–meso–micro model was described by Nguyen et al. [1] to link the micro-diffusive damage and the macro-crack in the concrete, by incorporating a cohesive zone model (CZM) within an iterative FE² approach. Eckardt and Könke [6] adopted the nonlocal damage model to present the initiation, propagation and coalescence of microcracks at the mesoscale and subsequent formation of a macroscopic crack. In addition, the adaptive domain decomposition method was used to analyze the multiscale failure in the concrete. Ghosh and Chaudhuri [7] developed a multiscale failure model for concrete, where the

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material far from the fracture process zone was described by the homogenized elastic model, while a nonlinear model was used in the fracture process zone. The fracture at the mesoscale was modeled by CZM in the context of an enriched partition of unity meshfree method. Idiart et al. [8] focused on the external sulfate attack on the concrete specimen at the meso-level, where zero-thickness interface elements with fracture-based constitutive laws were adopted. Moreover, the influence of discrete cracks on the transport of ions was explicitly taken into account. While these works successfully capture various features of failure mechanisms, the goal of the present work is to establish a direct link between concrete failure and the microscale driving mechanisms.

1.2. Alkali–silica reaction

ASR, discovered in the 1940s, is a long-term chemical reaction and detrimental to a concrete structure. ASR is characterized by the breakdown of the siloxane bonds (Si–O) in poorly crystallized silica of aggregates, which is attacked by the hydroxyl ions OH^- from the pore solution in the HCP [3,9,10]. It leads to the formation of an alkali–silica gel, which swells in the presence of water and exerts pressure on the surrounding material. It induces micro- and, eventually, macro-cracking of the structure when the tensile strength of concrete is exceeded [3,9,10]. Overall, three factors are indispensable for ASR:

- alkali content in the pore solution,
- poorly crystallized silica in aggregates,
- moisture content.

ASR is a complex phenomenon and it is still a challenging topic from the multiscale modeling point of view due to different manifestations of ASR at the material level of the concrete. A micromechanical approach was proposed by Lemarchand et al. [9], where the *topochemical* and *through-solution* mechanisms were accounted for. The gel was generated at sites of silica dissolution, referred to as *topochemical* mechanism, and the gel was produced in the porous space, referred to as *through-solution* mechanism. McGowan and Vivian [11] have elaborated that a solid layer was formed on the surface of the aggregate to absorb the moisture from the pore solution in HCP, and then the solid substance was transferred to the gel. Some authors [12–14] proposed that the aggregate was tightly packed with an insoluble rim, allowing the penetration of the alkaline solution, rather than the viscous alkali–silica gel. Mutton et al. [15] predicted that the gel was generated inside the aggregates after alkali and hydroxyl ions diffuse into the aggregates to break the silanol bonds. Then the gel permeates through the connected porous volume between aggregates and cement paste. Therefore, the gel was maintained inside aggregates and distributed the expansive pressure to aggregates. Meanwhile, Dunant et al. and Haha et al. [16,17] highlighted the predominant effect of the gel formation in the aggregates, leading to damage in the aggregates themselves and to subsequently damage the surrounding cement paste. Experiments by Ponce and Batic [18] indicated that the different location of the gel from mechanisms reported in [15–17] can be explained by the types of aggregates. The experiment [18] captured that cracking patterns of ASR-affected concrete rely on the mineralogical nature of the aggregates through petrographic examination with a stereobinocular and a polarizing microscope. It was also observed that aggregates such as opal and vitreous volcanic rocks result in the formation of the gel at the interface between aggregate and cement paste, thus causing the cracking in cement paste. On the other hand, mixed mineralogy aggregates formed cracks in both the aggregates and cement paste.

1.3. Review of numerical models on alkali–silica reaction

During the last decade, several numerical models have been developed to predict the ASR induced failure at different length scales of the concrete. Huang and Pietruszczak [28] established the correlation between the expansion strain due to ASR and the mechanical degradation at the macroscale of the concrete, where the expansion strain had a similar formulation with the thermal dilation strain. An advanced thermo–chemo–mechanical model was developed by Ulm et al. [3] in the framework of Biot's theory, where the concrete was conceived as a two-phase material including the expansive gel and the homogenized concrete skeleton. Moreover, the volumetric expansion of the gel was evaluated as a function of the reaction kinetics, which is influenced by the temperature. Comi et al. [31] developed the model based on [3], where not only temperature but also relative humidity contribute to the extent of the reaction. In addition, the investigation on ASR at the macroscale of the concrete was developed by Bangert et al. [30], where the concrete was treated as a mixture of three superimposed constituents through the theory of porous media: skeleton, pore liquid and pore gas. The model was based on converting the mass of unreacted material into the mass of the reacted material in the skeleton. Various analytical models based on empirical equations were also developed to explain ASR at the mesoscale of the concrete, see [10,15]. For instance, Bažant and Steffens [10] proposed that the chemical reaction kinetics was related to the diffusion process of the reactants, leading to the subsequent fracture in the characteristic unit cell of the concrete modeled with one spherical glass particle. Detailed numerical models at the mesoscale were limited. Comby-Peyrot et al. [37] introduced a three-dimensional mesoscopic model, where aggregates are randomly distributed in the cement matrix. The damage in the cement matrix was caused by the isotropic dilatation phenomenon in the reactive aggregates induced by ASR. Dunant and Scrivener [16,34] proposed a 2D finite element/extended finite element framework to qualitatively depict the ASR induced deterioration at the mesoscale of the concrete. The growing gel pockets defined in the aggregates trigger the damage to them, where the geometry of gel swelling is represented by updating the enrichment function. Alnaggar et al. [38] adopted the framework of the Lattice Discrete Particle Model (LDPM) to capture the ASR induced crack patterns at the mesoscale of the concrete. The expansion of the gel occurs at the level of each individual aggregate particle. Due to lack of reliable microscale models and representations, no results were contributed at the microscale of the concrete with the application to ASR. The general review of numerical models on ASR is listed in Table 1. For an overview of ASR with detailed references, see [17,39].

1.4. Scope of the present work

ASR is a complex chemical reaction and its mechanisms at the material level are still in dispute. Some numerical models concerning ASR have already been successfully set up at the macro- and meso-scale of the concrete. The objective of the present work is to establish a multiscale computational framework for predicting ASR induced damage where, for the first time to the best knowledge of the authors'. The analysis on ASR is carried out at the microscale of the concrete and the ASR induced deterioration is up-scaled to the mesoscale. The general scope of the study is as follows:

- to investigate the contribution of the chemical extent of ASR to the expansion strain of the gel at the micropore and the resulting deterioration of HCP,

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