



Lattice Discrete Particle Modeling (LDPM) of Alkali Silica Reaction (ASR) deterioration of concrete structures



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ABSTRACT

A large number of structures especially in high humidity environments are endangered by Alkali–Silica Reaction (ASR). ASR leads to the formation of an expansive gel that imbibes water over time. The gel expansion causes cracking and consequent deterioration of concrete mechanical behavior in the form of strength and stiffness reduction. In the recent past, many research efforts were directed towards evaluation, modeling and treatment of ASR effects on structures but a comprehensive computational model is still lacking. In this paper, the ASR effect is implemented within the framework of the Lattice Discrete Particle Model (LDPM), which simulates concrete heterogeneous character at the scale of coarse aggregate pieces. The proposed formulation, entitled ASR-LDPM, allows precise and unique modeling of volumetric expansion; expansion anisotropy under applied load; non-uniform cracking distribution; concrete strength and stiffness degradation; alkali ion concentration effect; and temperature effects of concrete subjected to ASR. In addition, a unique advantage of this formulation is its ability to distinguish between the expansion directly related to ASR gel expansion and the one associated with cracking. Simulation of experimental data gathered from the literature demonstrates the ability of ASR-LDPM to predict accurately ASR-induced concrete deterioration.

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1. Introduction

Deterioration induced by Alkali–Silica Reaction (ASR) is reported in many concrete structures all around the world, especially those built in high humidity and warm environments [1]. Water is essential for ASR to occur but, in addition, temperature plays a fundamental role in determining the ASR rate of reaction [2], namely the higher is the temperature the faster is the reaction. However, even in countries with average low temperatures ASR is reported to be a serious problem for the durability of concrete structures. The main effect of ASR is a progressive deterioration of concrete stiffness and strength that results from the long term formation and expansion of ASR gel inducing expansive pressure on the internal structure of concrete. This pressure causes nonuniform deformations that eventually lead to cracking and damage. While the chemical description of the reaction was addressed intensively in the literature, the fracture mechanics associated with the progressive expansion has received little attention due to the lack of models describing concrete internal structure satisfactorily. The main

objective of the research reported in this paper is to fill this knowledge gap.

First reports on the effect of ASR on concrete structures are due to Stanton in 1940 [3]. This early research studied ASR chemistry; ASR effects at structure and material level; testing methods to investigate the vulnerability of aggregate and mixes to ASR; and techniques for the mitigation of ASR effects. The assessment of ASR effects has been pursued by several authors in a variety of different experimental programs [4–11,1]. Available ASR experimentation relies often on the analysis of ASR products through Scanning Electron Microscopy (SEM) and Energy-Dispersive X-ray (EDX) techniques [12–14]. For the experimental investigation of ASR in more realistic situations, accelerated ASR tests, such as the Accelerated Mortar Bar Test (AMBT) [15–17] and Concrete Prism Test (CPT) [18,19], are typically used.

Furthermore, in the past, various research efforts focused on studying the different factors affecting ASR, including, but not limited to, pessimum size (particle size associated with the maximum expansion over the test time period compared to both smaller and larger aggregate sizes), type of aggregate, temperature, relative humidity, and stress state [4,20–34]. Other research can be found on the mitigation of ASR problems by using either admixtures, especially fly ash [35–37], or remedial actions such as slot cutting or grouting of cracks [38].

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From the modeling point of view, ASR simulation and its effect on concrete structures have been attempted at various length scales. Theoretical models describing ASR gel evolution based on petrographic measurements were proposed by several authors [39–41,21,42,22,43–45]. These models succeeded in capturing various aspects of ASR expansion such as aggregate pessimum size, ASR induced expansion and pressure but not the fracture mechanics aspects of the deterioration process. A fracture mechanics approach to predict the pessimum size of aggregate was proposed by Bažant [46].

In the literature, one can find macroscopic models trying to describe the global mechanical deterioration due to ASR. One of the earliest models was the phenomenological model presented by Charlwood et al. [47] and Thompson et al. [48]. More refined models [49] and others considering creep [50] were developed later and, although they predict well displacements and stress history in the structure, they completely lack the ability to predict crack patterns as well as to describe the physical phenomena linking ASR to the deterioration of mechanical properties.

Another improvement in macroscopic models was obtained by the formulation of chemo-mechanical coupled models. Huang and Pietruszczak [51,52] and Ulm et al. [53] developed models based on the ASR kinetics. The latter approach, implemented within smeared crack finite element frameworks [54,55], was able to reproduce some ASR expansion data available in the literature [56].

Models considering stress state effects have been also developed. Among others, it is worth mentioning the model by Saouma and Perotti [57] and Multon et al. [58]. Damage models combining in a consistent thermodynamic fashion the chemical and mechanical components of the ASR process were considered by Comi et al. [59,60]. The effect of humidity and temperature was incorporated in the reaction kinetics law by Poyet et al. [61]. While all previous models were deterministic, Capra and Sellier [62] presented a probabilistic model based on the main parameters of ASR and concrete. For very extensive literature reviews of available ASR models, the reader may want to consult Refs. [63] and [2].

Despite some success, the common disadvantage of all aforementioned models is the inability to simulate crack patterns and crack distribution due to ASR. This, in turn, limits the ability to predict the degradation effect of ASR and forces the assumption of phenomenological relationships between ASR gel expansion and concrete mechanical properties. In addition, it also limits the ability of such models to explain complex triaxial behavior of concrete under ASR and also forces the assumption of phenomenological relationships between ASR gel expansion and stress state. These limitations are inherently connected to modeling concrete as an isotropic and homogenous continuum.

Due to lack of reliable mini scale or meso scale models – describing concrete as a three-phase (aggregate, binder, interfacial transition zone) or two-phase (aggregate, binder) material, respectively – very limited results are available on fine scale modeling of cracking induced by ASR. Comby-Peyrot et al. [64] developed a 3D computational tool to describe concrete behavior at mesoscale with the application to ASR. The model predicted well concrete nonlinear behavior up to the peak but was unable to reproduce complete degradation in the softening regime. Dunant et al. [65] proposed a 2D model able to qualitatively reproduce material deterioration of concrete properties by simulating expansive gel pockets inside the aggregates. The 2D character of the model, however, prevented the model from obtaining good results from a quantitative point of view. Shin and colleagues [66,67] used scanning electron microscopy techniques to obtain microstructural images of specimens suffering from ASR and to develop refined, and computationally very intensive, 2D finite element models of damaged internal structure of concrete.

In this paper, all aforementioned limitations are overcome by modeling ASR effects within the Lattice Discrete Particle Model (LDPM) [68,69,91,92]. LDPM, in a full 3D setting, simulates the mechanical interaction of coarse aggregate pieces through a system of three-dimensional polyhedral particles, each resembling a spherical coarse aggregate piece with its surrounding mortar, connected through lattice struts [68] and it has the ability of simulating the effect of material heterogeneity of the fracture processes [69]. ASR-LDPM introduced here is limited to fully saturated conditions as the consideration of water macro diffusion is out of the scope of this paper and will be considered in future work.

2. Alkali Silica Reaction (ASR) modeling

According to the model proposed by Bažant and Steffens [21] – adopted and extended in this section – the overall ASR process can be approximately described by considering that (1) water needs to be available in the pores to act as transport medium for hydroxyl and alkali ions for ASR to occur; (2) the expansion of ASR gel is mostly due to water imbibition; and (3) a continuous supply of water is needed for the swelling to continue over time. As in the original model and consistently with the LDPM formulation, the aggregate particles are assumed to have spherical shape; the whole volume of each particle is assumed to be reactive; and the silica is assumed to be smeared uniformly over each aggregate volume. This is certainly an approximation compared to reality in which shape and size of the aggregate particles may vary widely, as well as the content of reactive silica in flaws, inclusions, and veins. Under this approximation, however, the dissolution of silica may be assumed to progress roughly in a uniform manner in the radial direction inward from the surface towards the particle center. In addition, ASR continues as long as water is continuously provided by macro-diffusion processes. For low values of relative humidity (<60–80%) ASR slows down and eventually stops [70]. However, in this study, only saturation condition is considered. This case has practical relevance in situations in which concrete is continuously exposed to water as, for example, for dams and offshore structures.

2.1. Gel formation

Thermodynamics and kinetics of the ASR reaction were studied in Refs. [71,72] and it was concluded that the chemical reaction rate is much faster than the actual rate of ASR production observed in concrete structures. This led researchers to the conclusion that some other mechanism had to be the dominant one and it was observed that as the reaction progresses, the unreacted silica in the interior of each of aggregate particle is shielded by a spherical layer of the reaction product, the ASR gel. Through this layer further water molecules must diffuse in order to reach the reacting surface of the particle and dissolve more silica. This diffusion slows down the ASR tremendously and becomes the process governing the rate of ASR [71,72]. In comparison the chemical reaction at the silica dissolution front may be considered to be almost instantaneous. Thus, the rate of ASR gel production can be best approximated by solving a diffusion problem.

Consistently, for a steady state diffusion process at constant temperature, one can write [21]

$$M_w = w_s \frac{1 - z/x}{1 - 2z/D} \quad (1)$$

where M_w = water concentration within the layer of ASR gel; x = radial coordinate; z = radius of the remaining unreacted particle; and D = aggregate particle diameter (See Fig. 1a for details). In addition, w_s is the concentration of water in the concrete surrounding the

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