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# A MULTISCALE METHOD TO ANALYZE THE DETERIORATION DUE TO ALKALI SILICA REACTION CONSIDERING THE EFFECTS OF TEMPERATURE AND RELATIVE HUMIDITY

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**Abstract.** This work presents a three-dimensional multiscale framework to investigate the deterioration resulting from alkali silica reaction (ASR) in the concrete. In this contribution, 3D micro-CT scan of hardened cement paste (HCP) and aggregates with a random distribution embedded in a homogenized cement paste matrix represent the microscale and mesoscale of the concrete respectively. A 3D hydro-chemo-thermo-mechanical model based on staggered method is developed at the mesoscale of the concrete, yet taking into account the deterioration at the microscale due to ASR.

## 1 INTRODUCTION

Concrete is an extremely complex heterogeneous material with random microstructures at different length scales. At the macroscale level, it is treated as a homogeneous material. While going down one scale, the mesoscale includes a binding matrix, aggregates and pores with broad size distributions as well as interfacial zones between the aggregates and the matrix. At a lower level, the microscale is represented by the microstructure of HCP, which is comprised of hydration products, unhydrated residual clinker and micropores [1,2].

ASR discovered in the 1940s, is a long-term chemical reaction, while it is detrimental to the concrete structure. ASR is one chemical reaction between reactive forms of silica in the aggregates and alkali ions in the pore solution. The gel as the reaction product can swell in the presence of water and produce internal stresses, which leads to the formation of the micro-crack network in the concrete [3,4,5,6].

## 2 Kinetics of Chemical Reaction

Chemical extent $\xi$ based on first-order kinetics is used to describe the progression of ASR, where $\xi = 1$ denotes the beginning of ASR and $\xi = 0$ indicates the end of ASR. The explicit equation of the chemical extent $\xi$ firstly explained in [6] is expressed through

$$\xi(t) = \frac{1 - exp(-t/\tau_{ch})}{1 + exp(-t/\tau_{ch} + \tau_{lat}/\tau_{ch})} \tag{2.1}$$

where $\tau_{lat}$ is the latency time and $\tau_{ch}$ is the characteristic time, respectively corresponding to the initiation and the development period of ASR from a practical point of view [4,5,6]. In addition, Larive [6] addressed the influences of the temperature and the relative humidity on $\tau_{lat}$ and $\tau_{ch}$. The dependencies of the latency time and the characteristic time on the temperature and the relative humidity are illustrated in Fig.1(a) and Fig.(b) respectively.

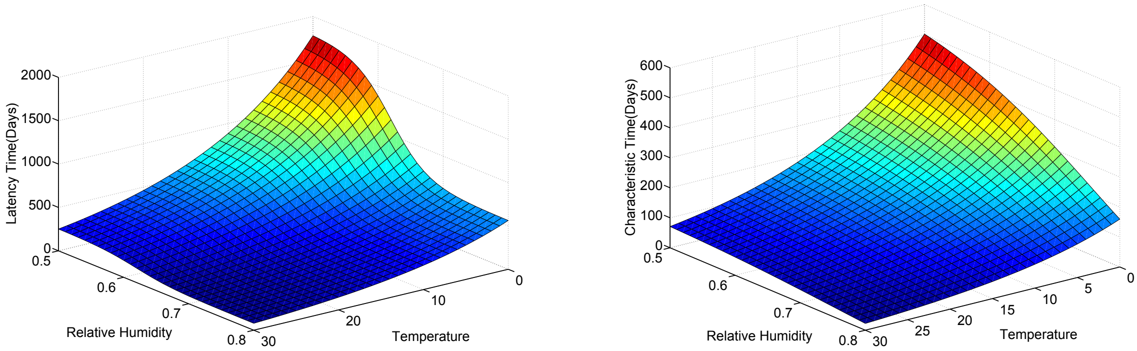


Figure 1: *(a) Latency time with function of temperature and relative humidity (b) characteristic time with function of temperature and relative humidity.*

## 3 Analysis of ASR at Microscale and Mesoscale

In this work, the cement specimen with an length of 1750 $\mu m$ was conducted to obtain the microstructural geometry of HCP using three-dimensional micro-CT scans with a resolution of $1\mu m$. Therefore, the micro-CT scan of HCP is comprised of $1750^3$ data points, where each point corresponds to a voxel of $1\mu m^3$. The natural element to use within

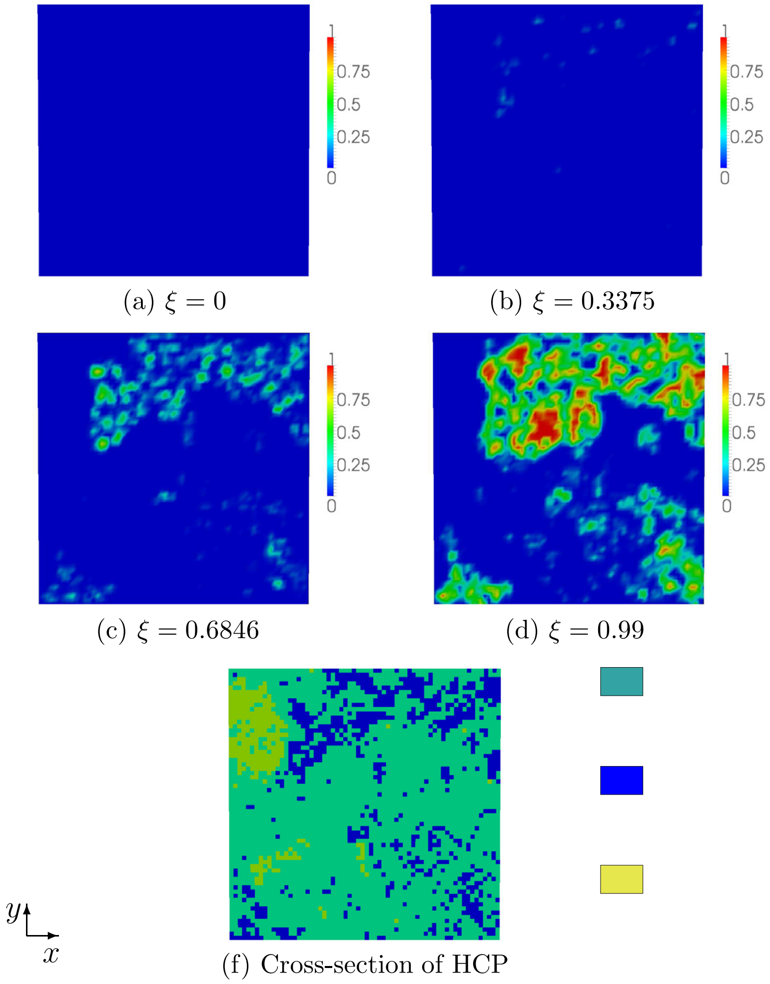


Figure 2: *(a)-(d) damage distribution on cross section of HCP with various values of chemical extent* $\xi$*, (f) material distribution on cross-section of HCP.*

the finite element method to discretize the microstructure is an 8-node brick where each element is assigned to a single material phase [1,2]. Many continuum damage models can depict the failure of HCP, but the simplified constitutive model developed by Hain and Wriggers [1,2] is employed in this work to save the computational cost, due to too complex three-dimensional micro-structural geometry of HCP. In addition, it is only feasible to define the simplified damage model in hydration products because of its high volume fraction in the HCP. The observation that the chemical property of the gel is similar to calcium-silicate-hydrate (C-S-H), enables the gel to be conceived as an incompressible material with the possion ratio of 0.49975. Fig.2 illustrates the distribution and evolution of the damage in HCP with the extent of ASR, where the damage occurs in the hydration products in the vicinity of micropores triggered by the expansion of the gel in micropores. Computational homogenization is an efficient tool to link macro-microscale of the

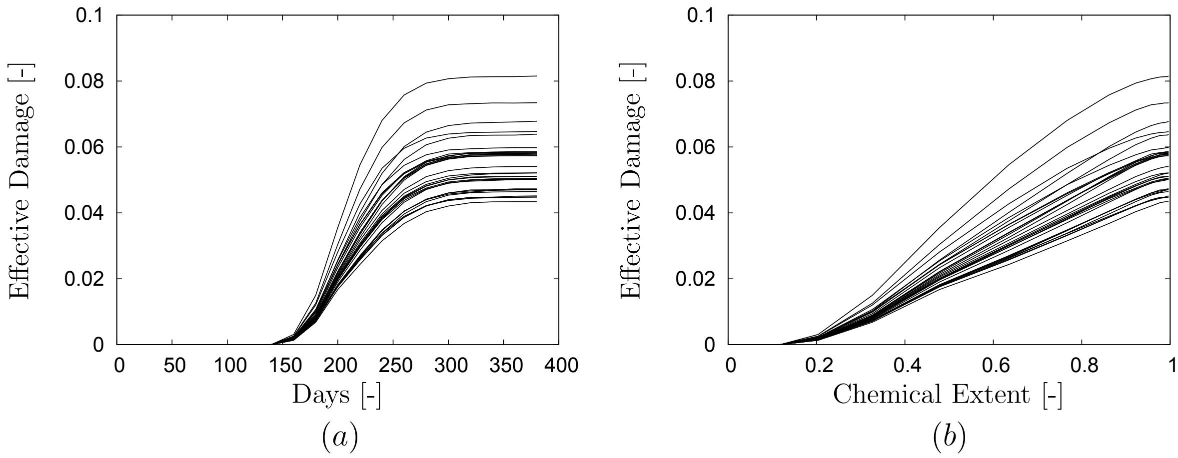


Figure 3: *(a) Effective damage of 30 statistical tests through homogenization with respect to days (b) effective damage of 30 statistical tests through homogenization with respect to extent $\xi$.*

material [7]. In this contribution, 30 randomly obtained representative volume elements (RVEs) from micro-CT scan of HCP are performed and the resulting effective damage of statistical tests due to the expansion of the gel through computational homogenization approach with respect to days and chemical extent are shown in Fig.3(a) and Fig.3(b) respectively. The correlations between chemical extent and effective damage in Fig.3(b) can be approximated by polynomial curve, which can be directly applied to the next legnth scale.

The take-and-place method is employed to generate the three-dimensional geometrical representation of concrete at the mesoscale, where randomly distributed aggregates are embedded in the homogenized HCP [8]. Aggregates are assumed to be elastic material in the present work, and a visco-plastic model of the classical PERZYNA-type combined with an isotropic damage is defined for HCP, in order to capture the experimentally nonlinear phenomenon of the concrete [1,2].

# 4 Coupling

It is observed that ASR is depending on the temperature and the relative humidity from experiments in [6] and the associated influences are explained. The small size of the microstructure can skip over the hydro-thermo-chemo coupling work at the microscale, and the correlation between effective damage and chemical extent $\xi$ is obtained through computational homogenization, which can be applied at the next scale directly. However, the hydro-thermo-chemo coupling has to be carried out at the mesoscale due to its relatively large size, so that the influences of transient temperature and relative humidity on the chemical extent $\xi$ can be analyzed. The obtained chemical extent at the mesoscale enables to obtain the deteroration due to ASR originating from microscale through the

Table 1:

*Multiscale Hydro-Thermo-Chemo-Mechanical Coupling based on Staggered Method in the Concrete.*

1. *Diffusion field.* Update the relative humidity $S^{n+1}$ through the instationary diffusion equation, once the diffusion part can numerically converge.
2. *Thermal field.* Update the temperature $\theta^{n+1}$ through the instationary thermal conduction, once the convergence criterion is satisfied.
3. *Chemical extent.* Adopt $S^{n+1}$ and $\theta^{n+1}$ to calculate the new chemical extent $\xi^{n+1}$ based on the back-Euler approach in a analytical manner, see Eq.(2.1), Fig.1(a) and Fig.1(b).
4. *Upscale damage.* Since temperature and humidity mediated chemical extent as the scalar multiscale variable is projected as constants from upper to the lower scales, the correlation between effective damage and chemical extent can be applied to the mesoscale, see Fig.3(b), therefore, the deterioration due to ASR at the microscale is determined through the value of chemical extent at the mesoscale.
5. *Mechanical field.* Apply the sum of the mechanical damage $D^u$ and chemical damage $D^c$ to the nonlinear constitutive law of HCP in order to obtain $u^{n+1}$, until the convergence is achieved.
6. *Increase time step.* Update all the field variables and set the time step forward to go back to step 1.

correlation between effective damage and chemical extent through computation homogenization, thus presenting the multiscale investigation on ASR in the concrete. Staggered approach adopted in this contribution can overcome the trouble of too expensive cost in the computation while solving the problem of three-dimensional multiphysics, since it permits to solve the equations of all fields sequentially [9]. Supposing that the equilibrium states for diffusion, conduction and mechanical problems have been obtained at time $t_n$, the procedure for searching for the solutions at time $t_{n+1} = t_n + \delta t$ can be described, see Table 1.

# 5 CONCLUSIONS

The objective of the present work is to establish a multiscale model to quantitatively predict the deterioration due to ASR in the concrete structure. In this contribution, 3D micro-CT scan of hardened cement paste (HCP) and aggregates with a random distribution embedded in a homogenized cement paste matrix are used to represent the microscale and mesoscale of concrete respectively. One significant assumption is adopted that gels are evenly produced in micropores of HCP and exert uniform pressure on the surrounding

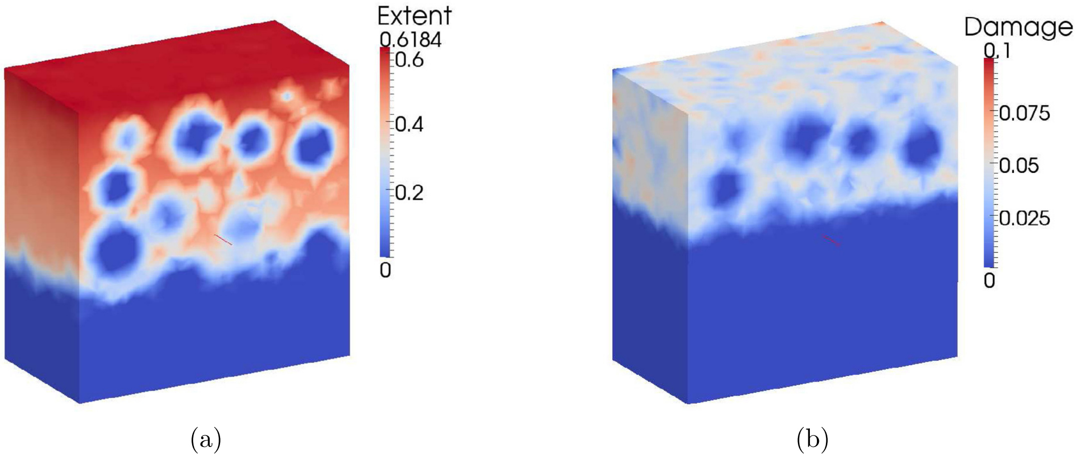


**Figure 4**: *(a) Chemical extent in 200 days (b) damage in 200 days.*

cement paste. The correlation between effective damage and chemical extent is sought through computational homogenization with statistical tests and the obtained expansion coefficient of the gel. Another assumption that temperature and humidity mediated chemical extent as the scalar multiscale variable is projected as constants from upper to the lower scales, ensures the reliability of the transition of the ASR induced damage between two scales.

A visco-plastic model of the classical PERZYNA-type combined with an isotropic damage is defined for HCP. At the mesoscale, hydro-chemo-thermal-mechanical coupling is implemented based on the staggered method, where the transient temperature and relative humidity are upscaled through instationary thermal conduction and diffusion, which contribute to the chemical extent $\xi$ through back-Euler method in a analytical manner. The deteroration due to ASR originating from microscale at the mesoscale is obtained the correlation between effective damage and chemical extent, qualifying the chemical extent. Therefore, a 3D multiscale hydro-chemo-thermo-mechanical is illustrated to predict the faillure due to ASR in the concrete, yet it analyze the reaction at the microscale.

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