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Multiscale Modeling of Alkali Silica Reaction Induced Damage in Concrete: Coupled Hydro-Chemical and Thermo-Mechanical Effects

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Abstract. *In this work, a 3D multiscale investigation on hydro-chemical-thermo-mechanical induced damage in concrete resulting from alkali silica reaction (ASR) is presented. 3D micro-CT scan of hardened cement paste and aggregates with a random distribution embedded in a homogenized cement paste matrix are applied to represent the microscale and mesoscale of concrete respectively. Homogenization approach is utilized to link microscale damage due to ASR and observable deterioration at the macroscale of concrete. A 3D hydro-chemical-thermo-mechanical model based on staggered method is developed.*

Keywords: *Multiscale, Coupling, Concrete, Alkali Silica Reaction.*

1. INTRODUCTION

1.1. Concrete

Concrete is the most widely used construction material in the world because of its good strength and durability. However, it is a complex material and has specific structures at different length-scales. Concrete at the macroscale is assumed to consist of mortar, large aggregates, large pores, and an interfacial zone between aggregates and mortar. The mortar as the mesoscale contains small aggregates, small pores, hardened cement paste (HCP) and an interfacial zone between small aggregates and HCP. At the microscale, HCP includes hydration products, unhydrated residual clinker and micropores [1,2]. The whole multiscale representation of concrete in this contribution is illustrated in Fig.1, in which some components are neglected for simplifications, such as large pores, interfacial zones, small pores and small aggregates. Accordingly, one does not distinguish between cement paste and mortar.

1.2. Alkali Silica Reaction

1.2.1 Chemical Reaction Mechanism

The issue of concrete durability is always of great interest in engineering, and alkali silica reaction (ASR) is harmful to the durability of concrete structures. ASR refers to a multistage process, involving non-instantaneous dissolution of silica and instantaneous swelling.

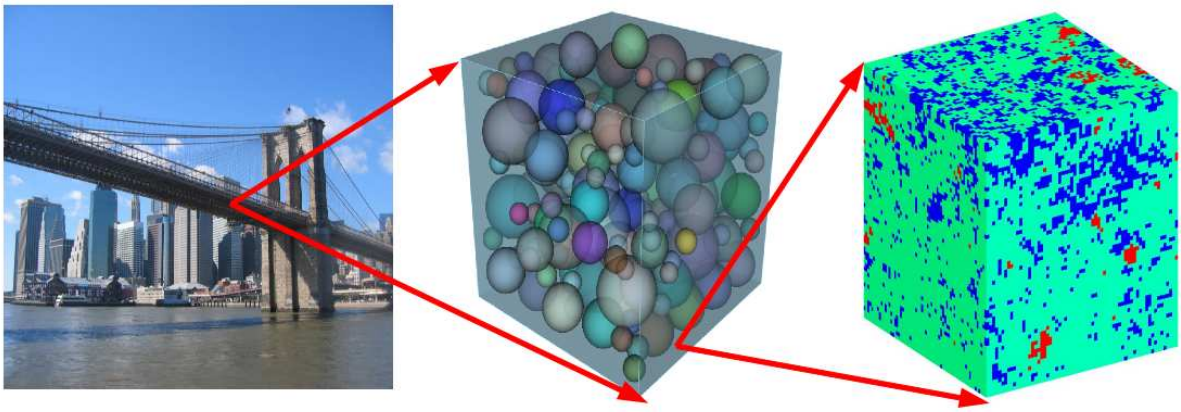

Figure 1. Multiscale Representation of the Concrete

The process of dissolution happens at the interface between aggregates and alkaline solution, where hydroxyl ions attack poorly crystallized silica network. The ions from the dissolution will combine with positively charged ions to form gels, which swell while meeting the water. As long as this free expansion space in pore is filled, the gel can exert locally a pressure on the surrounding cement paste which eventually leads the micro-crack and macro-crack of concrete [3,4].

1.2.2 Chemical Reaction Kinetics

A first order reaction kinetics is defined here

$$\tilde{t}\frac{d\xi}{dt} = 1 - \xi \tag{1}$$

where $\tilde{t}$ is the intrinsic time of the reaction and $\xi \in [0, 1]$ is the extent of the reaction, measuring the progression of the reaction: 0 means no reaction and 1 indicates the termination of the reaction [4,5]. According to the experiment from Larive [6], $\tilde{t}$ is obtained through

$$\tilde{t} = \tau_{ch}\frac{1 + exp[-\tau_{lat}/\tau_{ch}]}{\xi + exp[-\tau_{lat}/\tau_{ch}]} \tag{2}$$

where τ_{lat} is the latency time and τ_{ch} is the characteristic time, which relying on the temperature are expressed as

$$\tau_{lat}(T) = \tau_{lat}(\bar{T})exp[U_{lat}(1/T - 1/\bar{T})]; \quad \tau_{ch}(T) = \tau_{ch}(\bar{T})exp[U_{ch}(1/T - 1/\bar{T})] \tag{3}$$

in which $U_c = 5400 \pm 500K$ and $U_L = 9400 \pm 500K$ [5,6]. The reaction extent ξ is obtained by integrating Eq. (1):

$$\xi(t) = \frac{1 - exp(-t/\tau_{ch})}{1 + exp(-t/\tau_{ch} + \tau_{lat}/\tau_{ch})} \tag{4}$$

Therefore, Fig.2 illustrates the progression of ASR through the term of chemical extent ξ under different temperatures.

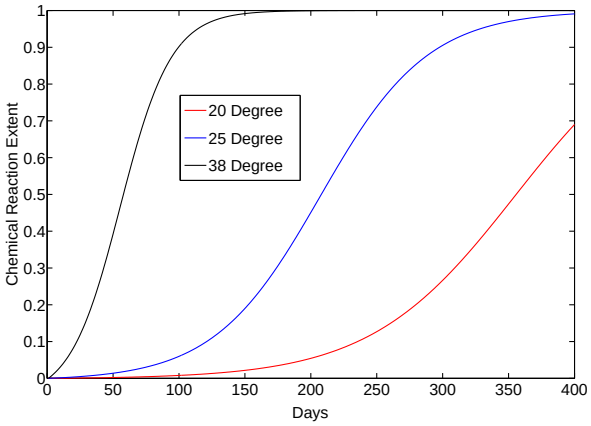

Figure 2. Chemical Extent Affected by Different Temperatures

In the meanwhile, water also plays a very critical role in alkali silica reaction. For example, it can transport ionic species involved in ASR and it is the reactant when the amorphous gel absorbs water for swelling.

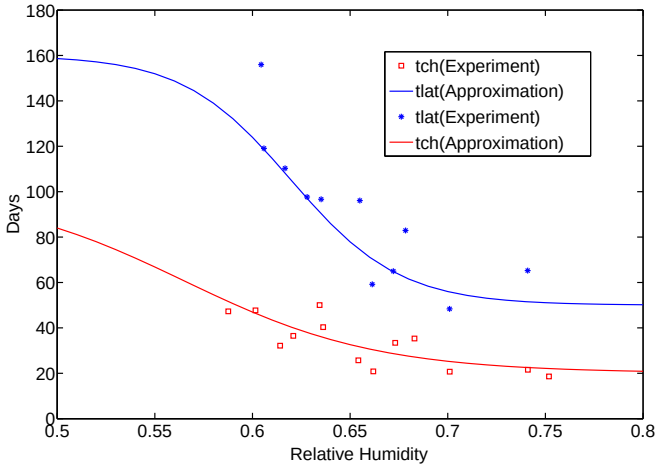

Figure 3. Experimental data and Approximations for Latency Time and Characteristic Time Relating to Relative Humidity

The experimental data in [6] indicate that the latency time and the characteristic time are also affected by relative humidity in Fig.3. Therefore, those experimental data are approximated by polynomial curves

$$\tau_i(T,S) = (\tau_i(\bar{T},1) + \frac{\tau_i(\tau(\bar{T},0) - \tau_i(\bar{T},1))}{1 + a_1 exp[-\frac{a_2(1-2S)}{S(1-S)}]})exp[U_i(\frac{1}{T} - \frac{1}{\bar{T}})] \qquad (5)$$

where lower index i describe the latency time and characteristic time respectively. T is the temperature and S is the relative humidity. Hence, the latency time and characteristic time depend on not only temperature, but also relative humidity, see Fig.4 and Fig.5, which provide the basis for the further coupling framework. The coefficients of approximations are listed in table 1.

1	$\tau(0)$	$\tau(1)$	a1	a2
t_{lat}	160	50	20	-18.5222
t_{ch}	100	20	1	-10.52

Table 1. Coefficients of Approximations for Latency Time and Characteristic Time with Function of Relative Humidity

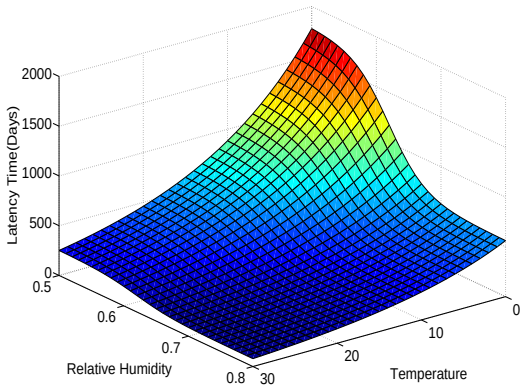

Figure 4. Latency Time Relying on Temperature and Relative Humidity

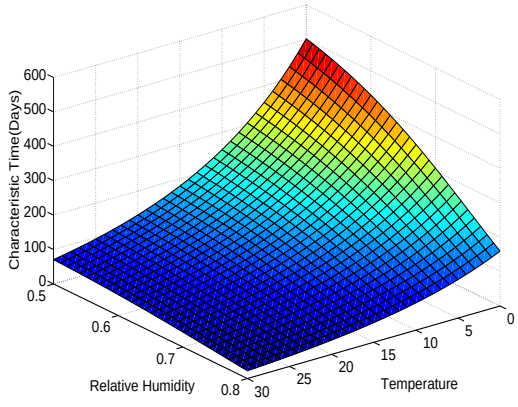

Figure 5. Characteristic Time Relying on Temperature and Relative Humidity

1.2.3 Assumptions and Summary

The purpose of this contribution is to take account of ASR in the microscale of concrete. If doing so, some critical assumptions are proposed:

- All gels are evenly produced in micropores and swell therein
- Gel will be full of micropore once it is produced and the expansion strain of gel is proportional to the chemical extent
- The expansion coefficient of gel does not change with the progression of ASR and environmental parameters such as temperature and relative humidity
- Gel is an incompressible material, the physical property of which is independent of time and location
- Only mild damage is considered

In summary, the coupling framework of ASR in concrete is expressed as:

- The temperature and the relative humidity affect the chemical extent ξ
- The increasing chemical extent enforces the expansion of gel in micropores of hardened cement paste
- The expansion of gel triggers the damage of HCP and results in the macroscale deterioration of concrete

2. MICROSCALE OF CONCRETE

2.1. Representation of Hardened Cement Paste

Micro-CT scan is a non-destructive evaluation technique with a resolution of approximately $1\mu m$ for a three-dimensional specimen. It is of great value to study the microstructure of a material and provide the possibility to implement the numerical simulation in the microscale of material. In this contribution, a micro-CT scan with an edge length of 1750 μm and a resolution of 1 μm was used for hardened cement paste with a water-cement ratio of 0.45 and a hydration degree of 0.945 [1,2]. Each micro-CT scan is comprised of 1750^3 data points, where each point corresponds to a voxel of $1\mu m^3$ and each voxel is a 8-node cubic with only one material identifier. The mesh of hardened cement paste is shown in Fig.6, in which the green sections are hydration products, the blue sections are micropores and the red sections are unhydrated residual clinker.

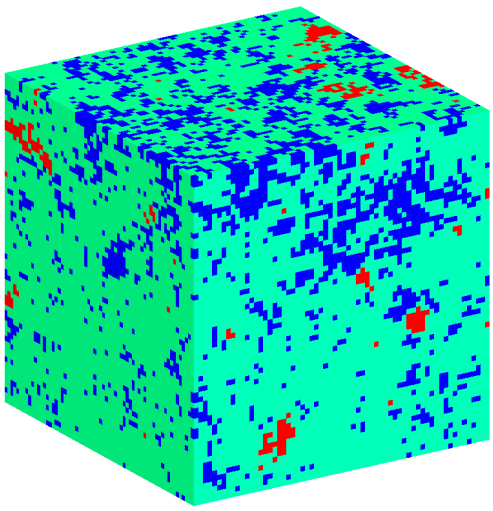

Figure 6. Micro-CT-Scan Image of Hardened Cement Paste with Voxel Dimension of $64 \times 64 \times 64$

2.2. Mechanical Properties of Each Phase in the HCP

Hardened Cement Paste is comprised of hydration product, unhydrated residual clinker and micropore. The idea is to introduce a simplified constitutive model at the micro-scale describing the three-dimensional mechanical behavior basically using the complex three-dimensional micro-structural geometry but not through a complex constitutive equation [2]. The simplified isotropic damage is assumed to exist in hydration products due to the high fractional volume in the HCP and those damage parameters are directly obtained from Hain [2].

The chemical property of gel is similar to the Calcium-Silicate-Hydrate, so that gel is treated as an incompressible material, with a Possion ratio of 0.49975. Standard displacement elements experience locking for incompressible conditions, hence, Q1P0 is launched to solve this problem. In the case of any deformation, there are deviatoric and volumetric strain components. Deviatoric strains determine the shape change of the body and volumetric strains

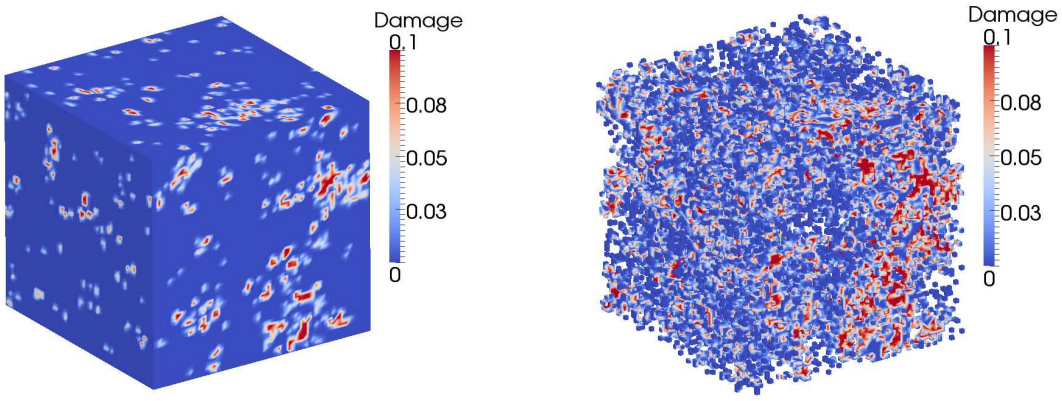

Figure 7. (a) Damage in Hardened Cement Paste (HCP) (b) Damage in Hydration Products of HCP

determine the volume change. The volume change occurs due to a hydrostatic pressure. As a result, Q1P0 element determines the shape change from the deviatoric strains and the pressures from the volumetric strain, where the shape function of pressure in FEM is constant. $\sigma = 2\mu\varepsilon^D + P$ and P is the hydrostatic pressure. Herein, $P = \kappa tr\varepsilon - \kappa\beta\xi$, where β is the expansion coefficient and ξ is the chemical extent.

2.3. Homogenization

Computational homogenization is very efficient tool to bridge the microscale and the macroscale [7]. The resulting effective material behavior can be applied to the mechanical model at the next length-scale through the volume average of representative volume element (RVE). $\langle D\rangle = \frac{1}{V}\int_V DdV$, where $\langle *\rangle$ denotes the volume average of a representative volume element. The size of RVE is very critical for homogenization, which can ensure the statistical representative response under boundary conditions satisfying the HILL's energy criterion. In this contribution, the RVE of 64*64*64 is chosen [1,2]. Then the displacement boundary condition of RVE is fixed and just consider the expansion in the RVE. The damage distributions in hardened cement paste and hydration products of HCP ares shown in Fig.7(a) and Fig.7(b).

2.4. Statistical Tests

Since the representative volume element (RVE) is only a portion of the micro-CT scan of HCP, statistical analysis of a sufficient number of RVEs randomly selected from micro-CT scan can make numerical simulation more reasonable and accurate. 20 statistical tests are carried out with respect to time and chemical extent, see Fig.8(a) and Fig.8(b). The mean value and standard deviation of statistical tests are obtained through:

$$d(\xi)^{med} := \frac{1}{n}\sum_{i=1}^{n} < d(\xi_i) > \qquad d(\xi)^{std} := \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}[< d(\xi)_i > -d(\xi)^{med}]^2} \tag{6}$$

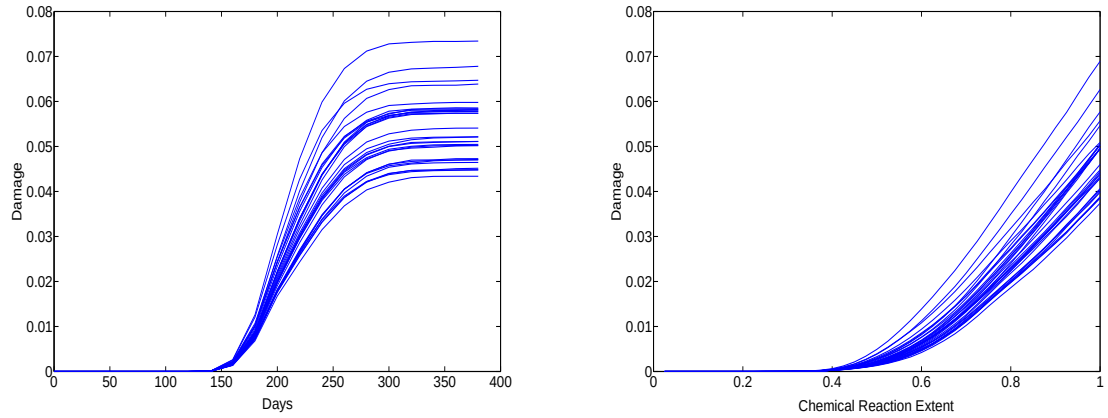

Figure 8. (a) Damage of Statistical Tests Relating to Time (b) Damage of Statistical Tests Relating to Chemical Extent

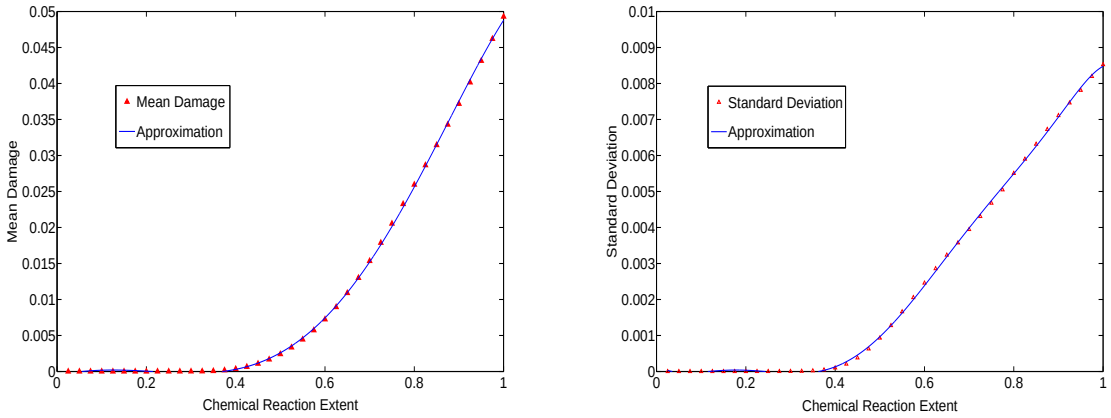

Figure 9. (a) Approximation of Mean Average of Statistical Tests (b) Approximation of Standard Deviation of Statistical Tests

The resulting mean value and standard deviation of statistical tests are approximated through (see Fig.9(a) and Fig.9(b))

$$D(\xi)^{med} := \sum_{i=0}^{i\leq 3} c_i^{med}\xi^i \quad and \quad D(\xi)^{std} := \sum_{i=0}^{i\leq 3} c_i^{std}\xi^i \tag{7}$$

which can be directly applied for the computation in the mesoscale. Table 2 demonstrates the approximation coefficients.

i	c_i^{med}	c_i^{std}
0	0.0809	0.0344
1	-0.1737	-0.0581
2	0.1284	0.0295
3	-0.0016	-0.0002

Table 2. Coefficients of Approximations for Mean Value and Standard Deviation

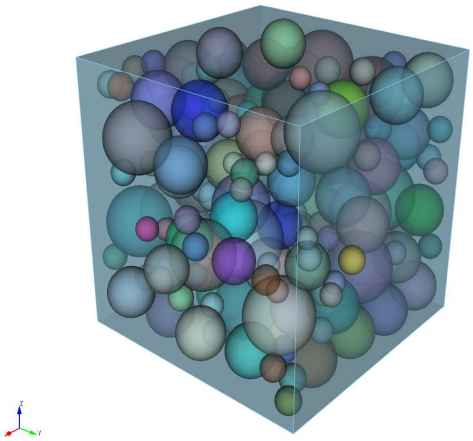

Figure 10. Particles Embedded in Matrix

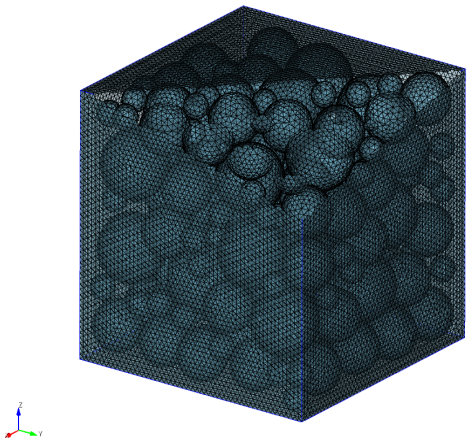

Figure 11. Discretization

3. MESOSCALE OF CONCRETE

3.1. Mesoscale Representation

Concrete is comprised of cement paste and randomly distributed aggregates in the mesoscale. The evaluation of the mesoscale representation of concrete needs the generation of a random aggregate structure where the size and distribution of the coarse aggregates closely resemble real concrete in the statistical sense. This random principle is implemented by taking samples of aggregate particles from a source whose size distribution follows a certain given grading curve and placing the aggregates one by one into the concrete in such a way, which can ensure no overlapping with particles already placed [8], see Fig.10. Once the mesostructure of the concrete is generated, one can discretize the mesostructure by means of conforming mesh in the commercial software CUBIT which offers the option of automatic mesh generation with tetrahedral elements, see Fig.11.

3.2. Effective Inelastic Constitutive Equation

In the mesoscale, aggregates are assumed to be purely elastic and cement paste is assumed to be an inelastic damage material. Since finding an effective inelastic constitutive equation by homogenization is still an unsolved problem, an inelastic effective constitutive equation with the unknown material parameters must be defined through parameter identification. In terms of the cement paste, a visco-plastic model of PERZYNA-type combined with an isotropic damage model is chosen [1]. Considering the definition of elastic energy rate yields

$$D : 0 \leqslant \sigma : \dot{\varepsilon}^{pl} + Y\dot{D}^{u} \tag{8}$$

a constrained optimization problem combined with the Penalty-Lagrange approach can yield an unconstrained optimization problem.

$$P = -\sigma : \dot{\varepsilon}^{pl} - Y\dot{D}^{u} + \frac{1}{\eta}\phi(f) + \dot{\chi}S^{u} \rightarrow stat \tag{9}$$

where the variable $\frac{1}{\eta}$ refers to the penalty-parameter, $\phi(f)$ denotes the penalty function, and χ is the LAGRANGE multiplier. A partial differentiation of P with respct to the elastic energy rate Y yields the evolution equation of damage.

$$\dot{D} = \xi\frac{\partial S(\varepsilon^{eq})}{\partial \varepsilon^{eq}} \tag{10}$$

where $S(\varepsilon)$ is the damage surface determining whether damage increases or not. It depends on the equivalent strain ε^{eq}.

$$S(\varepsilon) := 1 - exp\left[-\left(\frac{\varepsilon^{eq} - a}{b}\right)^{c}\right] - D \leqslant 0 \tag{11}$$

The damage surface is defined by an exponential law and depends on the elastic energy ε^{eq}, in addition, the parameters a, b and c are the material properties of the assumed model. The partial differentiation of P with respect to the σ yields the plastic strain evolution.

$$\dot{\varepsilon}^{pl}_{n+1} = \frac{1}{\eta}\phi^{+}\frac{\partial f}{\partial \sigma} \tag{12}$$

where ϕ^{+} denotes the derivative of the penalty function $\phi(f)$ and the penalty function itself is defined the $(k+1)$ power of the yield surface f. The material property k is assumed to take the value $k = 1$ in order to enable a nonlinear viscous behavior.

$$\phi(f) = \begin{cases} 0 & ;\text{f}\leqslant 0 \\ \frac{1}{k+1}f^{k+1} & ;\text{f>0} \end{cases} \tag{13}$$

The aforementioned penalty function ensures that the constraint f is satisfied which is typical for visco-plastic materials. The yield surface f is assmed to be of VON-MISES-type

$$f := \alpha tr\sigma + \|dev\sigma\| - \sqrt{\frac{2}{3}}k_f \leqslant 0, \tag{14}$$

where $dev\sigma$ denotes the deviatoric part of the stress tensor, $tr\sigma$ is the trace of the stress tensor, and k_f is the material property of the model.

3.3. Parameter Identification

Since the parameters in aforementioned equations can not be obtained from experiments, parameter identification is formulated as an optimization problem, where a least-square function is minimized for providing the best agreement between experimental data and numerical data. The objective function $A(\kappa)$ is defined as a least-square sum between the experimental data [9] and the numerical result: $A(\kappa) := \sum(\langle\sigma(\kappa)\rangle_i - \sigma_i^{exp})^2 \rightarrow min$. The optimization results and resulting parameters are shown in Fig.12 and Table 3.

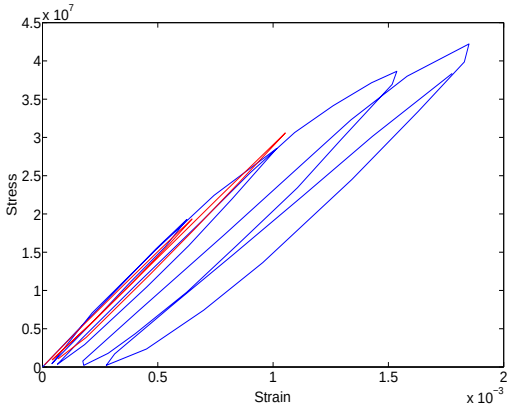

Figure 12. Parameter Identification Results

	κ_0	κ_{min}	κ_{max}	κ^*
k_f	1	1	30	5
η	2500	1000	15000	2513
Δt	0.0015	0.001	0.2	0.0253
b	100	100	5000	3251
a	100	100	2000	504

Table 3. Parameter Identification Coefficients

4. NUMERICAL COUPLING

Since it is expensive to computer 3D coupling problem with so many unknowns on each node of the mesh, a staggered solution strategy permits to solve the equations sequentially, which reduces the size of the discretized problem. It can be specifically expressed as: within a discretized time step, by solving each field equation individually, allowing only the corresponding primary field variable to be active. After the solution of each field equation, the primary field variable is updated, and the next field equation is solved in a similar manner, with only the corresponding primary variable being active. Usually, after this process has been applied only once to all of the field equations, the time step is incremented and the procedure is repeated [10]. Supposing that the equilibrium states for diffusion, thermal conduction and deformation problems have been obtained at time t_n, we explain the procedure for searching for a set of the solutions at time $t_{n+1} = t_n + \delta t$ and illustrate the numerical example of ASR in Fig.13(a), Fig.13(b), Fig.14(a) and Fig.14(b).

- Calculate the diffusion of relative humidity as one dof of problem, solve this equilibrium problem and get new h^{new}
- Calculate the thermal conduction as one dof of problem, solve this equilibrium problem and get new θ^{new}
- Make use of h^{new} and θ^{new} to calculate the chemical extent based on back Euler approach
- Use the new chemical extent ξ^{new} to perform the damage and deformation
- Update all the field variables and set the time step forward to go back to the initial step

5. CONCLUSIONS

ASR is a time-dependent long-term degradation that occurs during the life of a concrete structure. In this contribution, a 3D multiscale investigation on hydro-chemical-thermo-

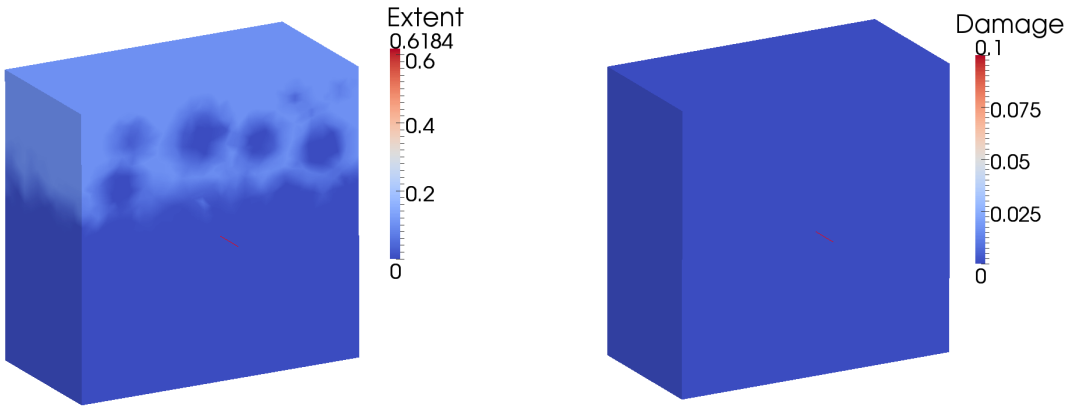

Figure 13. (a) Chemical Extent in 20 Days (b) Damage in 20 Days

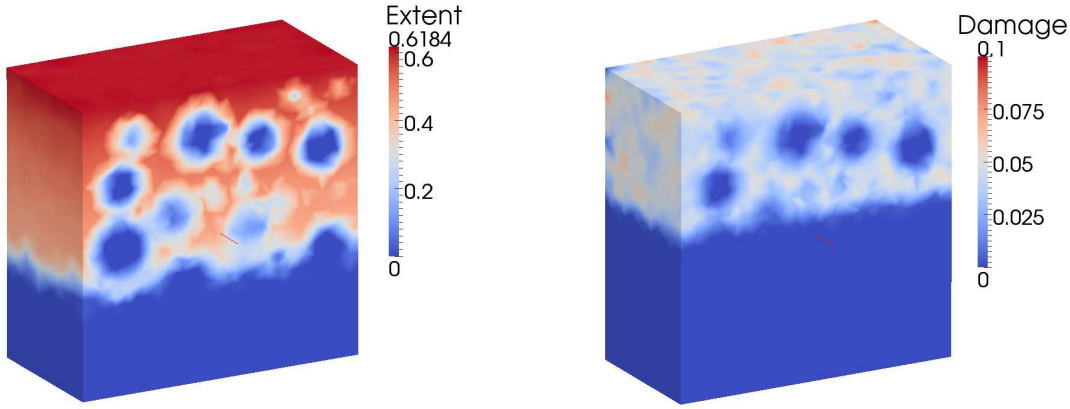

Figure 14. (a) Chemical Extent in 200 Days (b) Damage in 200 Days

mechanical induced damage in concrete resulting from alkali silica reaction (ASR) is presented. 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. Herein, a simple but reasonable idea is assumed that all gel are evenly produced in micropores of HCP and swell therein. Furthermore, the concept of chemical reaction extent is utilized to describe the progression of ASR, which relies on temperature and relative humidity. Computational homogenization approach is used to upscale the damage in HCP resulting from ASR to the mesoscale of concrete. The model of Perzyna including isotropic damage is set for the cement paste, in which parameters are obtained through parameter identification, however, the aggregates are assumed to be elastic. Eventually, 3D multiscale hydro-chemical-thermo-mechanical coupling based on a staggered method is demonstrated, which explicitly describes the damage evolution originating from the chemical reaction in the microscale and the dependence on environmental factors.

6. Acknowledgements

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