

## MODELING OF ALKALI-SILICA REACTION IN A TWO-PHASED MATERIAL MODEL

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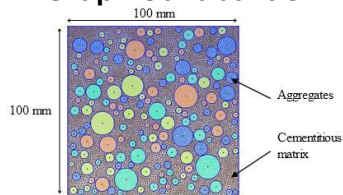
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### Graphical abstract



### Abstract

Alkali-silica reaction causes major problems in concrete structures due to the rapidity of its deformation. Factors that affect ASR include the alkali and silica content, relative humidity, temperature and porosity of the concrete, making the relationship a complex phenomenon to be understood. Hence, the finite element technique was used to build models to study the damage propagation due to ASR. Seeing that ASR initializes in the mesoscopic regions of the concrete, the damage model for ASR at the mesoscale level is studied. The heterogeneity of the mesoscale model shows how difference in material properties between aggregates and the cementitious matrix facilitates ASR expansion. With this model mesoscopic, two-phased material model, the ASR phenomenon under thermo-chemo-hygro-mechanical loading can be understood.

Keywords: Finite element, alkali-silica reaction

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## 1.0 INTRODUCTION

ASR deformation can be identified by a random network of crack patterns on its surface known as map cracking and leaching of the ASR gel. ASR expansion in an affected concrete structure may happen rapidly and cause deformation to the structure well before its serviceability limit is reached, making the understanding of its process crucial.

Factors that affect ASR vary, although it is unanimous that ASR occurs between deleterious silica from aggregates and hydroxide ions in the pore solution that result from cement hydration. Other factors include the relative humidity, temperature and porosity of the cementitious matrix. Temperature influences the kinetics of silica disintegration. Moisture works as a swelling agent for the gel which is hydrophilic in nature. The resultant gel flows into the voids or accumulates on the aggregate surface. The gel expands with the availability of moisture, exerting internal pressure onto the surrounding matrix and lowering the concrete stiffness to the point of cracking.

ASR damage model differs from other concrete damage models through its heterogeneity, occurring at different regions at different rates depending on the concrete composition and external influences, making predicting its behaviour difficult. The heterogeneity of the process depends on the pore distribution and the rate of water diffusion. ASR is studied at the mesoscale level to gain an explicit insight on what happens at the material level. Modeling on this level allows the matrix adjacent to the aggregate surface to be developed. This makes the study of the different phases separately, for instance, the effects of ASR gel expansion on the aggregates as well as the bulk matrix possible.

Numerical simulation has enabled the building of models for the representation of different physical phenomena in so many engineering problems. The potential of ASR simulation in detecting the possibility of expansive pressures and damage propagation due to ASR at a fine scale gives new perspective to this phenomenon.

## 2.0 THE THEORY BEHIND ASR SIMULATION

Two main aspects to be considered in ASR modeling is the kinetics of chemical reactions and the mechanical damage caused by the resulting expansion. Li and Coussy [3] developed a thermo-hydro-chemo-mechanical model to study the behavior of ASR affected concrete based on the Biot-Coussy theory on mechanics of reactive porous medium. Moranville-Regourd [5] suggested that the use of thermodynamics as an irreversible process associated with the continuum damage theory will enable ASR deteriorated zones to be identified. Capra and Bournazel [1] suggested that ASR gel composition is heterogeneous from one reactive site to another, depending on time and the initial content of silica and alkali.

Numerical simulation of stress anisotropy due to ASR is performed by taking into consideration thermoactivation of alkali-silica reactivity and its dependency on relative humidity. In investigating the mechanical deformation of the structure, the theory of continuum damage mechanics can be used to predict the physical and chemical behavior of a structure, making it appropriate to study the behavior of the structure under the influence of alkali-silica reactivity.

Assuming that damage at a given temperature and relative humidity has isotropic behavior, the determination of the local ASR reaction extent,  $\xi$  is performed with a stable time integration method, for instance, the Backward Euler method, taking into account the corresponding moisture and temperature profiles for each time step of the numerical procedure. The stress and damage states from the mechanical response are obtained from the rheological modeling coupled with the damage law and adding the effect of thermal strain,  $\varepsilon^{th}$ , ASR strain,  $\varepsilon^a$ , pore pressure,  $P^f$ . The constitutive equation can be modified into Eq. 1:

$$\sigma = (1 - \omega) \left[ C(\varepsilon - \varepsilon^a - \varepsilon^{th}) - P^f \mathbf{1} \right] \quad (\text{Eq. 1})$$

Where  $C$  is the fourth order linear elastic material tensor and  $\omega$  denotes the scalar damage parameter.

Lund [4] stated that the total thermal strain increment could be summed up over the current and history temperature range:

$$\varepsilon_{ij}^{th} = \left[ \int_{T_0}^T \alpha_T (T - T_0) \right] \delta_{ij} \quad (\text{Eq. 2})$$

The post-computation of the thermoelastic strain starts with the iteration of Eq. 2, resulting in thermal strain values,  $\varepsilon^{th}$ . The numerical solution of the equation for temperature  $T + dT$  can be solved using the Backward Euler method:

$$\varepsilon_{ij}^{th}(T + dT) = \varepsilon_{ij}^{th}(T) + \alpha_T (T + dT) dT \delta_{ij} \quad (\text{Eq. 3})$$

Where  $\alpha_T$  is a thermal expansion coefficient matrix,  $T$  is the temperature at a given point and  $T_0$  is the temperature at which the structure is free of thermally induced strain.

ASR strain can be represented in an equation for free linear expansion,  $\varepsilon^a$  as shown in Eq. 4:

$$\varepsilon^a(t) = \varepsilon_{\infty} \xi(t) \quad (\text{Eq. 4})$$

Where  $\varepsilon_{\infty}$  is the asymptotic ASR expansion. Eq. 4 shows that ASR strain evolution is only governed by the noninstantaneous kinetics of the chemical reaction. In a stress-free condition, the only unknown is the reaction extent,  $\xi$ . The reaction extent,  $\xi$  is determined from:

$$\xi(t) = \frac{\varepsilon}{\varepsilon_{\infty}} = \frac{1 - \exp(-t/\tau_c)}{1 + \exp(-t/\tau_c + \tau_L/\tau_c)} \quad (\text{Eq. 5})$$

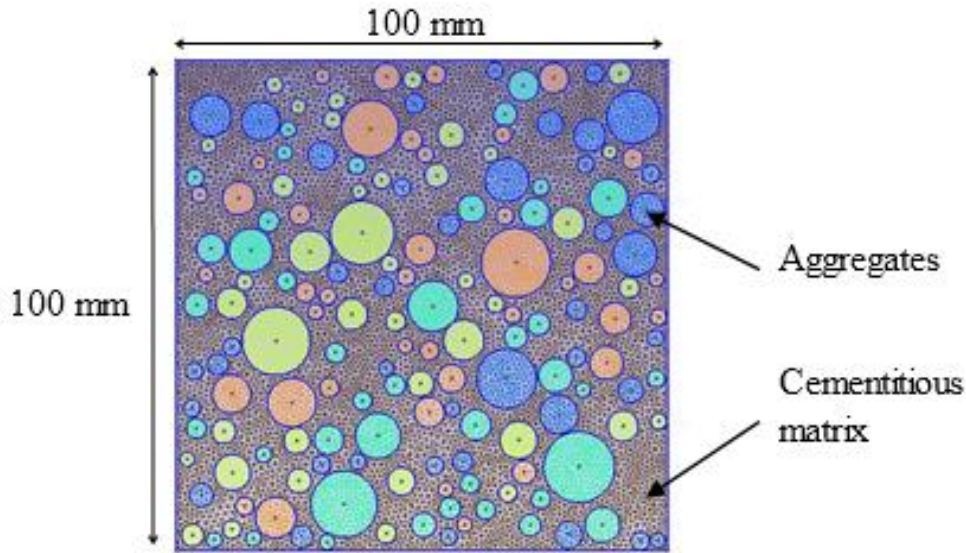
Ulm [6] defined  $\tau_L$  as the latency time as the time needed for the initial expansion of the gel in the presence of water.  $\tau_c$  is the characteristic time that is defined by the intersection of the tangent at  $\tau_L$  with the asymptotic unit value of the reaction extent,  $\xi$ .  $\tau_c$  and  $\tau_L$  are thermally dependent and can be expressed in terms of absolute temperature ( $TK = 273 + T^{\circ}C$ ) and the corresponding activation energies that abide the Arrhenius concept:

$$\tau_L(T) = \tau_L(T_0) \exp \left[ U_L \left( \frac{1}{T} - \frac{1}{T_0} \right) \right], \quad \tau_c(T) = \tau_c(T_0) \exp \left[ U_C \left( \frac{1}{T} - \frac{1}{T_0} \right) \right] \quad (\text{Eq. 6})$$

The variables  $U_L$  and  $U_C$  are the activation energies which represent the minimum energy required to trigger the reaction for the time constants and were determined to be  $U_L = 9400 \pm 500K$  and  $U_C = 5400 \pm 500K$  [2]. The time constants,  $\tau_c$  and  $\tau_L$  tend to have different intensities for drying, sealed, humid and immersed in water conditions, proving that ASR reaction extent is influenced not only by temperature as can be seen in Eq. 5, but also by the relative humidity.

## 3.0 METHODOLOGY

The numerical example in Figure 1 illustrates the performance of a decoupled thermo-chemo-hygral model of a concrete prism that evaluates the evolution of ASR resulting in a damage model for alkali-silica reactivity. The model is made up of a two-phased heterogeneous material consisting of aggregates and the cementitious matrix with interstitial pores. The model is tested for different relative humidity ranging from 60%, 80% and 100% for an isothermal case of 45°C to determine damage intensities under such circumstances. Due to the small dimensions of the mesoscopic models, the relative humidity and temperature are taken as constant throughout the cross-section.



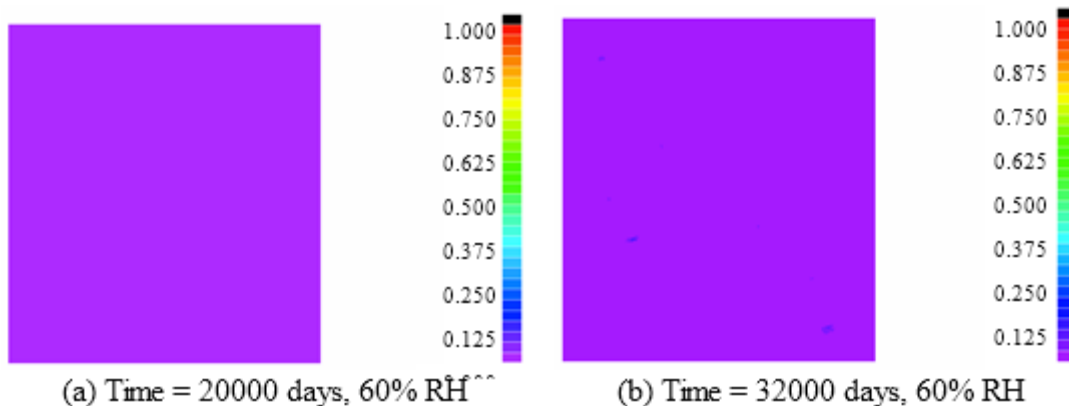
**Figure 1** Finite element model of the two-dimensional three-noded plane elements mesoscale model of a 100 mm x 100 mm concrete prism

The effect of ASR chemical reaction is implemented by using the asymptotic ASR expansion,  $\epsilon_\infty$  which is determined from inverse analysis and taken at an average of 0.22. The material properties used for the simulation are selected as optimal values for alkali-silica reactivity conditions. This research considers exposure of the prism to water only and no other deicing solution. In order to study the orientation of damage in the matrix and aggregates until fully damaged, the Newton-Raphson iterative method was used.

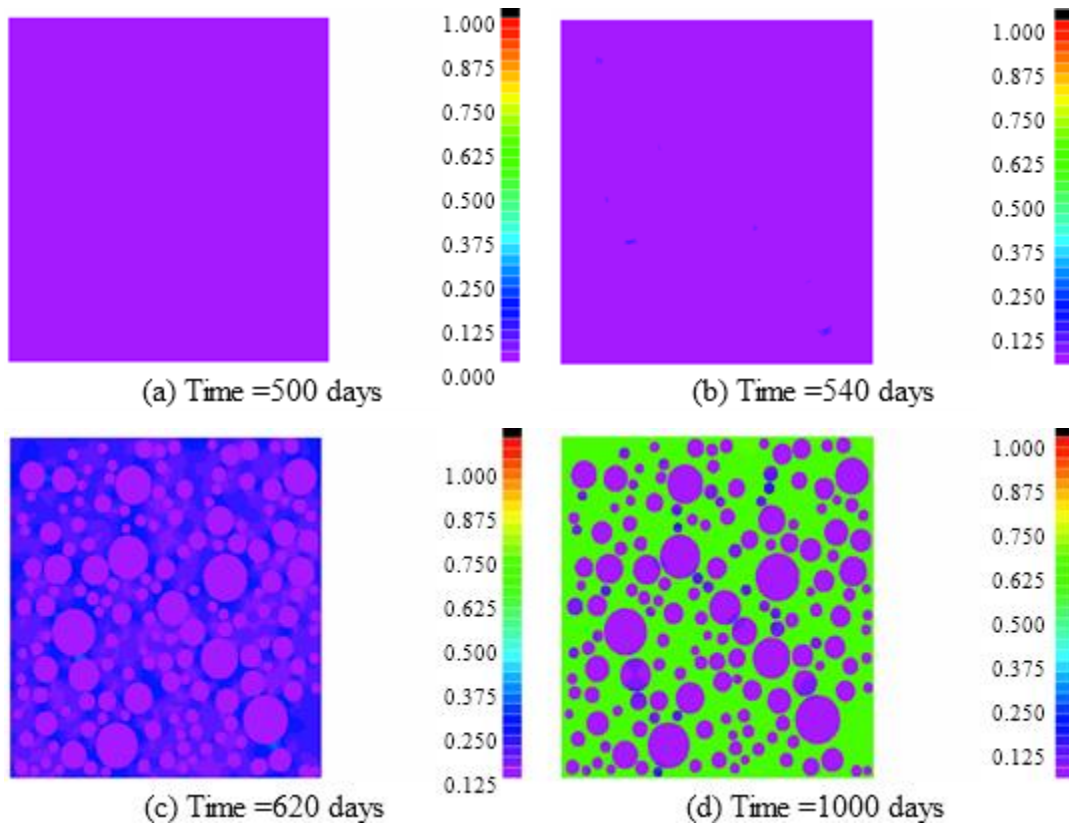
**4.0 FINDINGS FROM ANALYSIS**

Figure 2 to 4 show the damage distributions for 60%, 80% and 100% RH for the mesoscale model. It can be seen that although models with different RH have

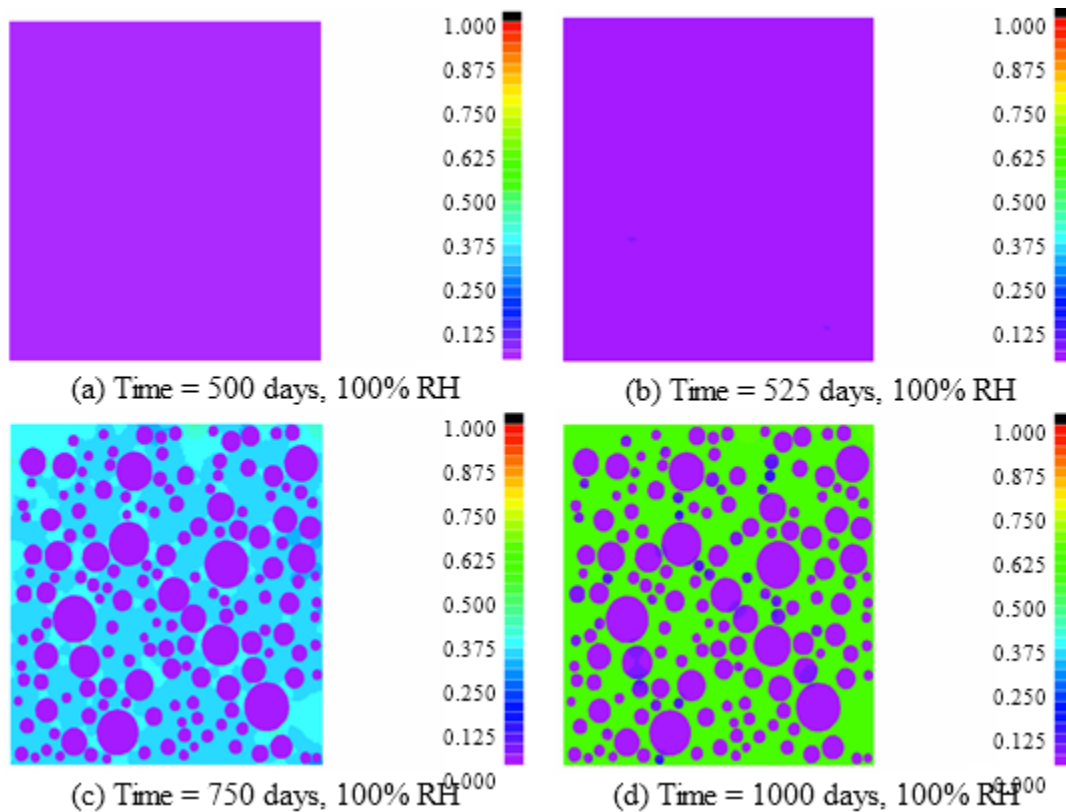
similar damage patterns, the time scale is longer for the lower RH. Damage initiates at approximately 70 days for 100% RH and 400 days for 80% RH. For 60% RH, which is the minimum condition for RH required for ASR to initiate [2], it can be concluded that damage due to ASR expansion did not occur. Damage initializes at the interfacial zones in between matrix and aggregates due to ASR expansion and spreads throughout the whole matrix, which has lower stiffness than the aggregates. Damage in the aggregates initiates at a later time, after the tensile strength value for aggregates have been surpassed, which are approximately 1000 days for the 80% and 100% RH, and no damage was seen in the aggregates with the 60% RH.



**Figure 2** Damage due to ASR expansion for an isothermal condition of 45°C and relative humidity of 60% for a mesoscale model with heterogeneous material properties



**Figure 3** Damage due to ASR expansion for an isothermal condition of 45°C and relative humidity of 80% for a mesoscale model with heterogeneous material properties



**Figure 4** Damage due to ASR expansion for an isothermal condition of 45°C and relative humidity of 100% for a mesoscale model with heterogeneous material properties

## 5.0 CONCLUSION

The mesoscale model was developed to have heterogeneous material properties for aggregates and the cementitious matrix. In order to study the sole effect of ASR chemoelasticity, any mechanical loading has been omitted. It was found that damage initiates at the interfacial transition zones between the aggregates and the matrix. The damage then spreads within the matrix, which has lower stiffness. Damage in the aggregates, which have higher stiffness and tensile strength, occurs at a much later time than for the cementitious matrix which has a lower tensile strength. ASR expansion can be replicated in numerical simulation, provided with the proper material properties and environmental parameters. Therefore it can be concluded that the intensity of damage in a concrete structure due to ASR expansion depends on a lot of factors, most importantly the temperature and relative humidity. Other external factors that influence the damage orientation and structure deflection depend on material properties, boundary conditions and if applicable, external loading.

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