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Z. Itam  
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## NUMERICAL SIMULATION OF THERMO-HYGRAL ALKALI-SILICA REACTION MODEL IN CONCRETE AT THE MESOSCALE

**Z. Itam**

*\* Institute of Structural Mechanics  
Bauhaus-Universität Weimar  
Marienstrasse 15  
99423 Weimar  
Germany*

E-mail: [zarina.itam@bauing.uni-weimar.de](mailto:zarina.itam@bauing.uni-weimar.de)

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**Abstract.** *This research aims to model Alkali-Silica Reaction gel expansion in concrete under the influence of hygral and thermal loading, based on experimental results. ASR provokes a heterogeneous expansion in concrete leading to dimensional changes and eventually the premature failure of the concrete structure. This can result in map cracking on the concrete surface which will decrease the concrete stiffness. Factors that influence ASR are parameters such as the cement alkalinity, the number of deleterious silica from the aggregate used, concrete porosity, and external factors like temperature, humidity and external source of alkali from ingress of deicing salts. Uncertainties of the influential factors make ASR a difficult phenomenon to solve; hence my approach to this matter is to solve the problem using stochastic modelling, where a numerical simulation of concrete cross-section with integration of experimental results from Finger-Institute for Building Materials Science at the Bauhaus-Universität Weimar. The problem is formulated as a multi-field problem, combining heat transfer, fluid transfer and the reaction rate model with the mechanical stress field. Simulation is performed as a mesoscale model considering aggregates and mortar matrix. The reaction rate model will be conducted using experimental results from concrete expansions due to ASR gained from concrete prism tests. Expansive strains values for transient environmental conditions due to the reaction rate will be determined from calculation based on the reaction rate model. Results from these models will be able to predict the rate of ASR expansion and the cracking propagation that may arise.*

# 1 INTRODUCTION

Alkali-Silica Reaction or more known as ASR, occurs between deleterious silica in aggregates and hydroxide ions in concrete pore water. Hydroxide ions attack sites on a reactive silica surface and produce an alkali-silica gel. This gel accumulates on the aggregate and fills the voids, replacing the silica consumed. When moisture diffuses into the affected concrete, this hydrophilic gel expands into the connecting porous media and lowers the concrete stiffness. What sets apart ASR with other concrete damage models is its heterogeneity; occurring at different concrete regions at different rates depending on the concrete composition as well as external influences, making predicting its behaviour difficult.

Numerical simulation has enabled us to build models for the representation of different physical phenomena, based on different theories and finite element methods in numerous occasions. The potential of ASR simulation in detecting the possibility of concrete expansion and cracking at a fine scale level will definitely give new insights and perspective to this deleterious phenomenon. With a reliable simulation, the generation of expansive pressures and crack propagation due to ASR is possible. A benefit of modelling the ASR gel expansion at the mesoscale is that the heterogeneity of the phenomenon can be explicitly modelled. Modelling on the mesoscale allows the matrix adjacent to the aggregate surface to be developed. It allows us to study the different phases separately, for instance, the effects of ASR gel expansion on aggregates as well as bulk matrix due to the difference in material and physical parameters of the phases. For this research, concrete was modelled from two phases; aggregates and bulk matrix.

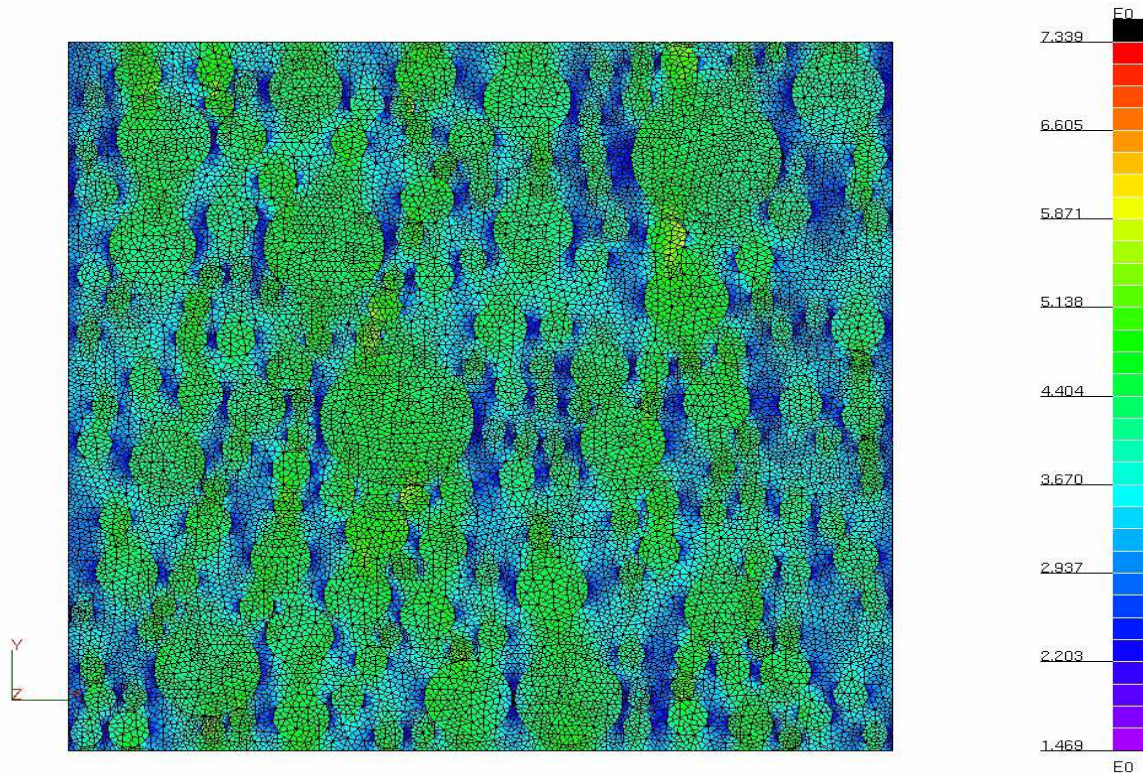


Figure 1: Two-dimensional model of concrete cross-section at the mesoscale.

The ASR process is divided into three separate simulation models based on the main influential parameters, such as temperature, moisture and chemical reactivity model. This will result in the determination of the ASR expansion values in the matrix, after which, the mechanical model could be developed. The importance of moisture in ASR is that moisture provides a medium of transportation for external sources of alkali as well as the swelling agent of the gel, which is hydrophilic in nature. Temperature has an indirect influence on the kinetics of dispersion which can accelerate the silica dissolution process. Both temperature and moisture will be modelled since they affect the diffusivity of the gel dispersion in the porous media.

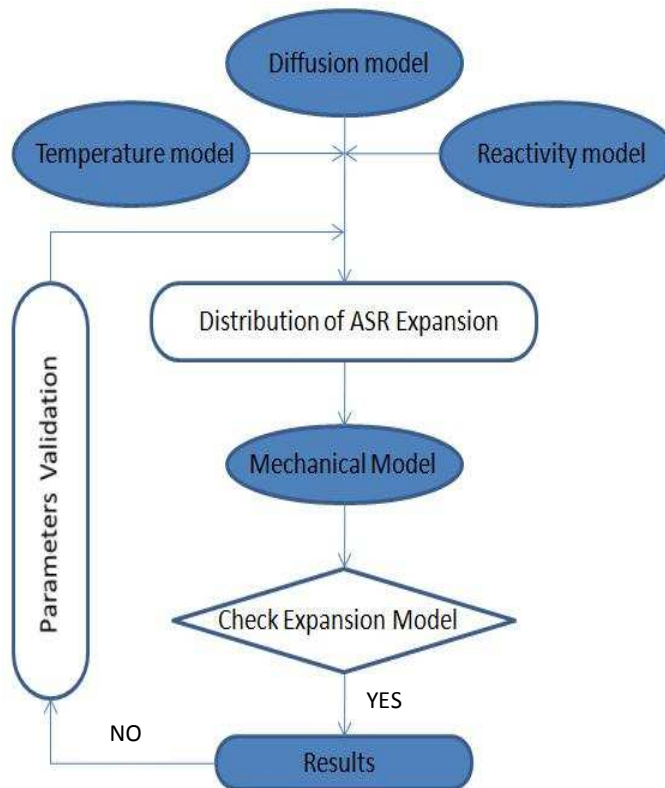


Figure 2: Research flow chart

The research flow chart is shown in the diagram above. Though uncoupled, the temperature gradient results from the temperature model will be linked to the fluid model through the iteration procedure, resulting in a velocity distribution in the bulk matrix. The velocity distribution will then be used to calculate the reaction rate of ASR gel expansion. The reaction rate is calculated using the first order kinetic model with chemical parameter determined from experimental results from concrete prism expansion tests for ASR as conducted by the Finger-Institute for Building Materials Science.

## 2 THE HEAT TRANSFER MODEL

There are two methods of heat transfer in porous media; heat conduction in solid matrix and heat convection in fluid flow in the pores. The finite element heat transfer equation is stated as:

$$\begin{aligned} & \left[ \iint_{\Omega^e} (\rho_o C)_e \Theta \Theta^T dx dy \right] \dot{\mathbf{T}} + \left[ \iint_{\Omega^e} \rho_o C (\Psi^T u_j) \frac{\partial \Theta}{\partial x_j} dx dy \right] \mathbf{T} + \left[ \iint_{\Omega^e} k_{ij} \frac{\partial \Theta}{\partial x_i} \frac{\partial \Theta}{\partial x_j} dx dy \right] \mathbf{T} \\ & = \left\{ \iint_{\Omega^e} \Theta Q dx dy \right\} + \left\{ \iint_{\Omega^e} \Theta \Phi dx dy \right\} + \left\{ \oint_{\Gamma^e} \Theta q ds \right\} \end{aligned} \quad (1)$$

Where  $\rho_o$  is the material density,  $C$  is the heat storage capacity,  $T$  is the temperature,  $u_j$  is the fluid velocity,  $k_{ij}$  is the thermal conductivity, and  $Q$  is the rate of internal heat generation. Natural convection problems are characterized by the fluid motion which is produced by temperature induced buoyancy. Modeling of the heat transfer using the finite element method is developed using the Backward Euler Difference Scheme. The second part of the first term is related to the convective heat transfer and is omitted for conductive heat transfer. The fluid velocity,  $u_j$  will be determined from the fluid transfer model.

## 3 THE FLUID TRANSFER MODEL

ASR gel development begins with the dissolution of the weaker bonds of silicates at the aggregate surface. Fluid transfer through the porous media exposes the silicate ions to the hydroxyl ions, which reacts and disintegrates the silicates, hence producing the ASR gel. The second process involves the imbibitions of the gel with moisture, which is continuously being supplied through fluid transfer. At the mesoscale, the influencing parameters in fluid transfer include the density, porosity and viscosity. The finite element fluid transfer equation in porous media is given as:

$$\begin{aligned} & \left[ \iint_{\Omega^e} \frac{\rho_o}{\phi} \Psi \Psi^T dx dy \right] \dot{\mathbf{u}}_i + \left[ \iint_{\Omega^e} \mu_e \frac{\partial \Psi}{\partial x_j} \frac{\partial \Psi^T}{\partial x_j} dx dy \right] \mathbf{u} + \left[ \iint_{\Omega^e} \gamma_e \frac{\partial \Psi}{\partial x_i} \frac{\partial \Psi^T}{\partial x_j} dx dy \right] \mathbf{u} \\ & = - \left[ \iint_{\Omega^e} \rho_o g_i \beta \Psi \Theta dx dy \right] \mathbf{T} + \left\{ \iint_{\Omega^e} \rho_o g_i \beta T_o \Psi dx dy \right\} + \left\{ \oint_{\Gamma^e} \Psi \mathcal{T} ds \right\} \end{aligned} \quad (2)$$

Where  $\rho_o$  is the density,  $\phi$  is the porosity,  $\mu$  is the viscosity,  $\beta$  is the thermal expansion coefficient,  $g$  is the gravity acceleration and  $\gamma$  is the bulk modulus, which represents the penalty parameter. Equation (2) is the modified version of the Navier-Stokes equation by the penalty function method, in order to decrease the number of unknowns from two (pressure and velocity) to one (velocity). The characteristic body force will also include a buoyancy term, which represents the temperature gradient obtained from the heat transfer model. The benefit of using the penalty method is that the variable P can be easily determined using the equation below:

$$\mathbf{P} = -\gamma_e \mathbf{M}_p^{-1} \mathbf{Q}^T \mathbf{u} \quad (3)$$

The velocity gradient obtained from this model will be used in the reaction rate model in the section below. Porosity of the matrix provides the gel with a dispersion medium; the lack of it

therefore will cause pressure and stain onto the surrounding matrix. Although not modelled explicitly, the porosity of the medium is included in the fluid transfer equation above in a smeared sense.

Modelling of the fluid transfer using the finite element method is developed using the Backward Euler Difference Scheme. Both the heat and fluid transfer models will then be cyclically iterated. This iteration ensures that the energy equation is solved at each iterative cycle before solving the fluid equation.

#### 4 THE REACTION RATE MODEL

The chemical reaction between the silicate and hydroxyl ions is the starting point in the ASR development. For this research however, only the transformation rate of the silica to the ASR gel will be considered. The dissolution process of silica and the moisture imbibitions of the gel can be represented by a chemical reaction that follows the first order kinetic law of the differential rate law where the rate of reaction is directly proportional to the concentration of one of the reactants. Equation (4) represents the expansion rate of the solid as a function of kinetic,  $\xi$ . The product of the reacted matrix will replace the product of the unreacted matrix, but since the material density of the reacted matrix is larger, the product, which is the ASR gel, will swell. The reaction will continue as long as both silica and moisture are available, or  $\xi \neq 1$ .

$$\frac{\partial \xi}{\partial t} = k[1 - \xi] \quad (4)$$

Where  $k$  is the characteristic velocity of reaction, which is dependent on the moisture content and pressure. High moisture content will increase the reaction rate, which will in turn increase the value of  $k$ .  $\xi$  denotes the reaction extent of the silica disintegration or gel formation, where  $\xi \in [0, 1]$  with 0 representing the start of the reaction and 1 representing the end [1].

#### 5 THE ASR EXPANSION MODEL

When considering for the ASR gel development, the total solid matrix is made of two conditions, the unreacted matrix and the reacted matrix. The unreacted matrix is the concrete matrix in initial condition before the silica dissolution and the reacted matrix is the concrete matrix after the dissolution. Expansion strain from ASR gel can be determined from the following equation.

$$\boldsymbol{\varepsilon}_s = \boldsymbol{\varepsilon}_s^a \mathbf{1} + \frac{1}{[1-d]\phi_0^s} [\boldsymbol{\mathcal{C}}^s]^{-1} : p \mathbf{1} \quad (5)$$

With the first term relates to the chemical effects of ASR and the second term relates to the mechanical stresses, with the damage parameter,  $d$  and the effective stiffness tensor,  $\boldsymbol{\mathcal{C}}^s$ :

$$d = 1 - \frac{\kappa_o}{\kappa} \left[ 1 - \alpha_1 + \alpha_1 \exp \left[ \alpha_2 [\kappa_o - \kappa] \right] \right] \quad (6)$$

$$\boldsymbol{C}^s = 2\mu_o \boldsymbol{\mathcal{I}} + \lambda_o \mathbf{1} \otimes \mathbf{1} \quad (7)$$

Where  $\mu$  and  $\lambda$  are Lamé constants,  $\kappa$  in the threshold damage value, and  $\alpha_{1,2}$  are the material parameters which control the post-peak slope of the stress-strain curve where  $\kappa_0$  is exceeded,  $\phi_0^s$  is the initial volume fraction of solid, and  $p$  is the pore pressure of the concrete and is determined from

$$p = P^L s^L + P^g s^g \quad (8)$$

Where  $P^L$  is the pore liquid pressure which is calculated from the fluid transfer model from Equation (3), and the gas and water saturation values,  $s^L$  and  $s^g$  and pore pressure  $P^g$  can be calculated from experimental data. The chemical effects of the equation (4) can be determined from [1]:

$$\varepsilon_s^a = \left[ \frac{\varrho^u}{\varrho^r} - 1 \right] \xi \quad (9)$$

Where  $\varrho^u$  and  $\varrho^r$  are the unreacted and reacted material density respectively. The volumetric expansion,  $(\varrho^u / \varrho^r - 1)$  of the ASR gel can be determined from the variation of the unreacted material to the reacted material in terms of material density, which can be determined from the graph in Figure 3, as with the characteristic velocity of reaction,  $1/k$ .

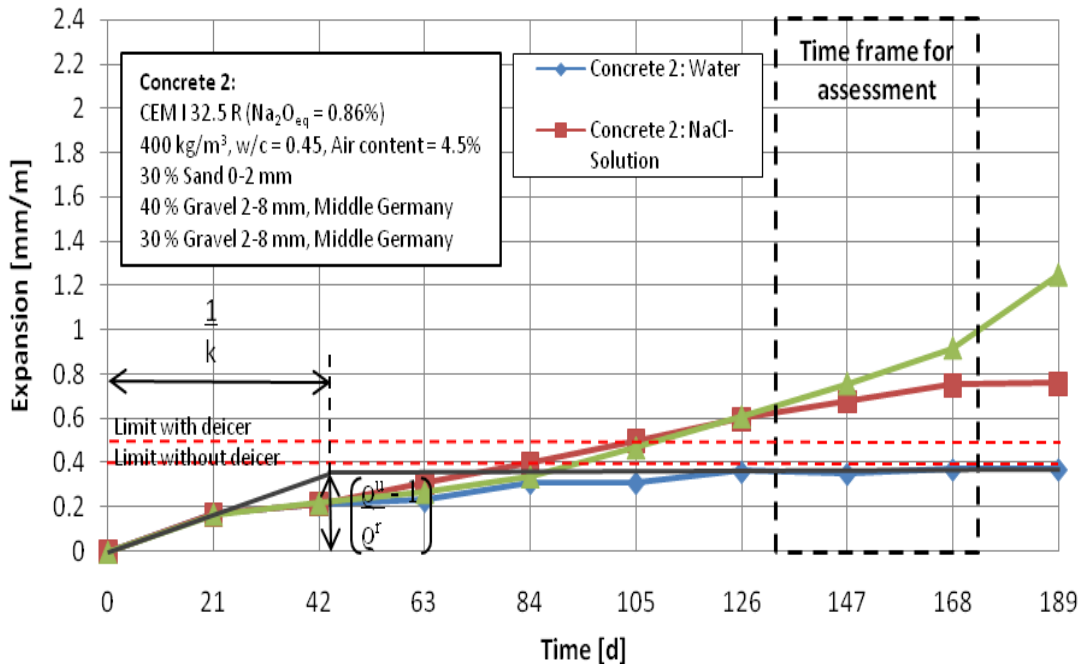


Figure 3: Concrete prism test - Expansion of concrete prism results from the Finger-Institute for Building Materials Science, Bauhaus-Universität Weimar

Expansion tests on concrete prisms tested for ASR yields a curve that shows the evolution of concrete expansion due to the accumulation of ASR gel. The slope of the graph,  $1/k$  controls the slope of the expansion-time relation and is dependent on the silica reactivity, pore liquid alkalinity, temperature and relative humidity. The volumetric expansion is represented with the height of the graph. From the strain calculation, the effect of the ASR gel expansion on concrete can be visualized.

## 6 CONCLUSIONS

- Convective heat transfer and fluid transfer have a direct effect on the reaction rate of ASR expansion. Both these models will be simulated using the finite element method, and then cyclically iterated.
- The reaction rate of ASR is proportional to the volumetric expansion strain produced. A higher expansion rate results in a faster strain rate, which causes damage in the concrete to occur at a more accelerated pace.

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