Diffusion-Controlled and Creep-Mitigated ASR Damage via Microplane Model. I: Mass Concrete

Zdeněk P. Bažant, Hon.M.ASCE¹; and Saeed Rahimi-Aghdam²

Abstract: A diffusion-based and creep-based chemo-mechanical model for calculating the evolution of damage caused in concrete and concrete structures by the alkali-silica reaction (ASR) is developed. First the model of Bažant and Steffens for the diffusion controlled kinetics of ASR is reviewed and used to calculate the rate of production of the ASR gel within the aggregate. The next step is the formulation of a nonlinear diffusion model for the penetration of gel into the micropores and nanopores in a mineral aggregate grain, into the interface transition zone (ITZ) and into the nearby microcracks created in the cement paste of mortar. The gel that penetrates the pores and cracks in cement paste is considered to calcify promptly and stop expanding. A novel point, crucial for unconditional numerical stability of time step algorithm, is that the diffusion analysis is converted to calculating the pressure relaxation at constant gel mass during each time step, with sudden jumps between the steps. The gel expansion in the aggregate and the ITZ causes fracturing damage in the surrounding concrete, which is analyzed by microplane model M7, into which the aging creep of a broad retardation spectrum is incorporated. The gel and the damaged concrete are macroscopically treated as a two-phase (solid-fluid) medium of nonstandard type because of load-bearing but mobile water in nanopores. The condition of equilibrium between the phases is what mathematically introduces the fracture-producing load into the concrete. Depending on the stress tensor in the solid phase, the cracking damage is oriented and the expansion is directional. The creep is found to have a major mitigating effect on multidecade evolution of ASR damage, and is important even for interpreting laboratory experiments. Validation and calibration by experimental data from the literature is relegated to Part II. DOI: 10.1061/(ASCE)EM.1943-7889.0001186. © 2016 American Society of Civil Engineers.

Introduction

The alkali-silica reaction (ASR) afflicts mineral aggregates in concrete if they contain imperfectly crystalline silica. The reaction produces a gel that can imbibe enormous amount of water. The swelling that results, typically during several months to many years or even decades, often causes severe strength degradation and fracturing in concrete structures. Because drying arrests the ASR, the worst damage usually occurs in massive structures such as dams, large bridges, and nuclear power plant structures. Preventing ASR damage is one important goal of sustainable design.

The damage due to alkali-silica reaction (ASR) (also called the alkali-aggregate reaction, AAR) was first identified by Stanton in 1942 (Stanton 1942). Since that time a vast body of literature on this pernicious problem has been accumulated (e.g., Alnaggar et al. 2013; Bažant and Steffens 2000; Bažant et al. 2000; Berra et al. 2010; Clark 1991; Cusatis et al. 2014; Dron and Brivot 1992, 1993; Hobbs 1988; Larive 1997; Mutton et al. 2008, 2010, 2009, 2006; Mutton and Toulmond 2006, 2010; Pan et al. 2012; Poyet et al. 2006; Bažant et al. 2015; Saouma and Xi 2004; Stanton 1942; Steffens et al. 2003; Suwito et al. 2002; Swamy and Al-Asali 1989; Mutton et al. 2005). Comprehensive literature reviews have recently been given by Saouma and Xi (2004) and Pan et al. (2012).

Several chemical relations involved in ASR have been presented and discussed (Alnaggar et al. 2013; Bažant and Steffens 2000; Pan et al. 2012; Saouma and Perotti 2006; Saouma and Xi 2004). A review relevant to mathematical modeling of the chemical reaction kinetics prior to 1999 appears in the introduction of Bažant and Steffens (2000). An excellent recent review relevant to the ASR damage simulation is found in the introduction of Cusatis and Alnaggar et al. (2013). This paper was also the first to provide a general structural analysis of a creep-mitigated ASR damage, in which Cusatis’ lattice discrete particle model (LDPM) was used. All of the ASR gel expansion was in that work assumed to occur in the inter-particle contacts, with no delay attributable to gel diffusion.

A comprehensive model for structural analysis of ASR, capturing the essential physical phenomena and their destructive effects, seems unavailable. Nevertheless, many practical models dealing with the effects of ASR on structure strength and its mechanical properties exist (Swamy and Al-Asali 1988; Clark 1990; Monette et al. 2000; Ono 1990; Siemes and Visser 2000; Swamy and Al-Asali 1986; Swamy 2002), and many more are focused on the effects of ambient temperature and humidity on the ASR-induced deterioration (Jensen et al. 1982; Jones 1988; Kurihara and Katawaki 1989; Larive 1997; Larive et al. 2000; Ludwig 1989; Nilsson 1983; Olafsson 1986; Pleau et al. 1989; Poyet et al. 2006; Salomon and Panetier 1994; Swamy and Al-Asali 1986; Tomosawa et al. 1989; Vivian 1981).

The objective of this work is to develop a comprehensive continuum model capable of capturing the main physical aspects of ASR damage, including: (1) the delay of ASR due to diffusion of ASR gel into the pores and expanding cracks within and very near aggregate grains; (2) fracturing of the solid framework of concrete as a two-phase medium caused by fluid expansion in the pores and cracks; (3) oriented character of damage; (4) mitigation by creep (with chemical aging) of the stresses created by gel expansion; (5) effect of alkali content on ASR-induced damage; (6) effect...
of temperature on ASR kinetics and ASR-induced expansion; and (7) control of the ASR process by variation of pore humidity due to self-desiccation or external drying.

A challenging, though essential, objective is to formulate an unconditionally stable computational algorithm permitting long time steps. To create a model permitting the analysis of ASR in large structures, a macroscopic continuum model (with a localization limiter preventing instability of softening damage) is sought. To capture the oriented character of ASR damage under general (nonhydrostatic) stress states, the microplane constitutive damage (Caner and Bažant 2013a) model is effective and its latest version M7 is used, although most aspects of the present ASR model apply to any constitutive damage model.

To describe the production of the ASR gel in mineral aggregates, the model of Bažant and Steffens (2000) is adopted. This model is considered as a given input, which predicts the gel mass \( M(t) \) per unit area of aggregate surface (kg/m²) extruded into the pores and developing cracks in the aggregate or matrix as a function of time \( t \). The coupling with ASR gel penetration into the pores of the mortar surrounding the aggregate piece is treated as one-way, i.e., the evolution of gel mass \( M(t) \) is considered to be independent of pressure \( p(t) \) developed in the pores surrounding the aggregate piece. This is a simplification, although probably not a major one because the pore pressures sustainable by concrete are apparently not large enough to slow down the alkali-silica reaction appreciably.

Note that the eigenstrain caused by the ASR is different from the thermal eigenstrain or shrinkage eigenstrain. The latter is simply additive to the stress-induced deformation and it causes (or is assumed to cause) no damage to unrestrained concrete. The ASR gel expansion into the pores and microcracks applies, from within, a tensile hydrostatic stress to the porous solid skeleton of the material, producing material damage. It is actually an eigenstrain on a subscale of the material (some previous investigators modeled this eigenstrain by assigning different thermal expansion coefficients to the aggregate and the mortar matrix and imposing a temperature change; this approach is correct only for a certain value of temperature change and could hardly be combined with diffusion or creep effects). The fracturing model formulated in Bažant et al. (2000) is not used because it represents a materials science type approach dealing with local micromechanics of fracture driven by pore pressure. This analytical approach worked well for determining the pessimum size of noncrystalline silica particles that causes maximum damage. But it seems too unwieldy to upscale to a macroscale continuum.

**Review of Simplified Model for Kinetics of ASR Gel Production**

First a model for the kinetics of gel production in mineral aggregates needs to be introduced. To this end, the simplified model of Bažant and Steffens (2000), as improved by Alnaggar et al. (2013) and slightly modified here, is adopted. Because the shape of aggregate grains is not too important, spherical grains of diameter \( D \) are considered.

The ASR reaction occurs at various randomly located discrete sources inside the grain. Penetration of alkali from the cement mortar matrix will first activate the sources near the surface. The time to activate the deeper sources will grow with their depth. To describe the average behavior of many aggregate grains, a smeared continuum model in which water diffuses radially into a spherical aggregate grain is introduced. The ASR reaction is assumed to take place instantly at the spherical front of water penetration, which forms a spherical surface of decreasing radius \( z \) [Fig. 1(c)]. The reaction is slowed down by the diffusion of water through the aggregate piece, and particularly through the layer of ASR gel already formed. The radial diffusion of water through the barrier of the previously formed ASR gel controls the rate of ASR. This diffusion control captures the effect of grain size on the reaction rate, typical of all diffusion phenomena.

For the sake of simplicity, the radial profile of water concentration \( \xi_w \) (water mass per unit volume of aggregate) is considered to be fixed and is assumed to be the solution of the steady-state linear diffusion equation in spherical coordinates (Bažant and Steffens 2000). For the proper boundary conditions, this assumption yields the profile

\[
\xi_w = w_i F(\bar{x}), \quad F(\bar{x}) = \frac{1 - \bar{x}/\bar{D}}{1 - \bar{x}}, \quad \bar{x} = \frac{2x}{D}, \quad \bar{z} = \frac{2z}{D}
\]

where \( x = \) radial coordinate [Fig. 1(c)]; \( \bar{x} = \) dimensionless radial coordinate; \( w_i = \) water concentration at the surface of aggregate grain (kg of water per m³ of aggregate) and can be estimated as (Alnaggar et al. 2013) \( w_i = (w/c - 0.188\alpha_c^\infty)c; \quad \alpha_c^\infty = (1.031w/c)/(0.194 + w/c); \quad w/c = \) water-cement ratio; and \( c = \) cement content. In addition, \( F(\bar{x}) = \) dimensionless concentration profile obtained as the solution of Laplace equation for spherical geometry (Bažant and Steffens 2000). The condition of mass balance at the reaction front \( x = z \) requires that

\[
r_{ws}c_i dz = -a_i [d\xi_w/dx]_{x=z} dt
\]

**Fig. 1.** ASR gel formation due to water diffusion into reactive aggregate: (a) early stage of diffusion; (b) late stage of diffusion; (c) idealization with spherical diffusion
where \( r_w = \) water-to-silica stoichiometric ratio (mass conversion ratio); \( c_r = \) reactive silica concentration (mass of reactive silica per unit volume of aggregate); and \( c_r = \) permeability of water through ASR gel and the aggregate. The permeability dependence on temperature follows the Arrhenius equation, and at reference temperature is \( 1.44 \times 10^{-8} \text{ kg/m}^2 \text{ s}. \) The reactive silica typically is only a part of silica content (assumed in this paper as 25%). Because two water molecules are necessary to dissolve one silica atom, \( r_w = 2m_w/m_s, \) where \( m_w = 18 \text{ g/mole} \) and \( m_s = 60.09 \text{ g/mole} \) are the molar masses of water and silica. The gel as produced at the reaction front \( z \) is called the basic gel. Its total mass in one aggregate grain of diameter \( D \) is

\[
w_{bg} = \frac{\pi}{6} \left[ D^3 - (2z)^3 \right] c_r f_{alk} \frac{m_g}{m_s} \tag{3}
\]

where \( f_{alk} = \) parameter specifying the availability of alkali (sodium and potassium ions); and \( f_{alk} = 1 \) when the alkali content \( C_{alk} \) in permeating water is high enough to give the maximum gel production (the ASR experiments are usually carried out under such conditions). In Part II of this paper an empirical equation for the cases where the alkali content is not high enough to give maximum gel production will be proposed and calibrated.

To calculate the mass of imbibed water, \( w_i, \) its increment is approximated as

\[
\dot{w}_i = \frac{A_i}{\tau_i}, \quad A_i = k_i w_{bg} - w_i, \quad \tau_i = \frac{\delta_w}{C_i} \tag{4}
\]

where \( k_i = \) empirical constant; \( \delta_w = \) average (or effective) distance of water transport process from the concrete around the aggregate into the ASR gel; \( A_i = \) thermodynamic affinity (proportional to the difference in chemical potentials); \( \tau_i = \) time characterizing the imbibition rate; and \( C_i = \) diffusivity of cement mortar around the aggregate, which depends on the relative humidity \( h \) in the pores and obeys Arrhenius temperature dependence. As the reaction goes on and the mass of imbibed water increases, the pore relative humidity around the aggregate (locally dominated by the ASR) decreases. Moreover, the average distance of water transport process \( \delta_w \) to reach the unreacted parts of aggregate increases. Therefore, the characteristic time, \( \tau_i, \) of imbibition [Eq. (4)] increases. In this study (in analogy to the Bažant-Najjar model (1972) for the diffusivity dependence on relative humidity), the following empirical equation for calculating the characteristic time of imbibition as a function of \( w_i \) is considered

\[
\frac{1}{\tau_i} = \frac{C_i}{\delta_w^2} = \frac{C_i^0}{(\delta_{w0}^2)} \left[ \alpha_0 + \frac{(1 - \alpha_0)}{1 + (\eta_{w0}w_i)} \right] \tag{5}
\]

where \( C_i^0 \) and \( \delta_{w0}^2 = \) initial values of \( C_i \) and \( \delta_w, \) respectively; \( \eta_{w0} = \) empirical constant; \( \alpha_0 = \) another empirical constant that is set in this paper as \( \alpha_0 = 0.05. \) Furthermore, \( C_i^0 = 2.2 \times 10^{-3} \text{ m}^2 \text{ s}^{-1} \) and \( \delta_{w0}^2 = \) 0.02D for concrete samples; and \( \delta_{w0}^2 = 0.02D \) for mortar samples.

Production of the basic ASR gel is assumed to cause no volume increase. Rather, the increase of gel volume, or swelling, is attributed solely to water imbibition into the gel. The volume increase of ASR gel per aggregate grain due to imbibing the volume, \( V_i, \) of water of mass density \( \rho_w \) (which is considered as pressure dependent), may be calculated as

\[
V_i = \frac{w_i}{\rho_w} \tag{6}
\]

In what follows, all the quantities will preferably be given as the content fractions (or densities) per unit volume of concrete. When all the aggregate grains are considered as identical spheres of diameter \( D, \) the increase of gel volume fraction in concrete above the initial volume of silica and reacted water is

\[
v_i = n_D V_i, \quad \text{where} \quad n_D = 6/\pi D^3 \tag{7}
\]

where \( n_D \) (of dimension \( \text{m}^{-3} \)) = number of aggregate grains of size \( D \) per \( \text{m}^3 \) of concrete; and \( v_i \) as a function of time \( t \) is used in the following as the input into the ASR damage analysis.

To simplify the equation system, Eqs. (1) and (2) may be combined to yield the differential equation

\[
d\bar{r} = \left( z^2 - \bar{z} \right)d\bar{z}, \quad \text{where} \quad \bar{t} = \frac{4a_i w_i}{D^2 r_{e0} \sigma_i} \tag{8}
\]

Integration with the initial condition \( \bar{z} = 1 \) at \( \bar{t} = 0 \) gives the cubic equation \( 2\bar{z}^3 - 3\bar{z}^2 + 1 = 0, \) which can be solved for \( \bar{z} \) either analytically or numerically to obtain the function \( f(\bar{t}). \) Alternatively, one can use Alnaggar et al.'s (2013) approximation \( \bar{z} = 1 - k_m \bar{t}^{0.6} \) for \( \bar{t} < 1/12 \) and \( \bar{z} = k_m(1/6 - \bar{t})^{0.6} \) for \( 1/12 < \bar{t} < 1/6 \) with \( k_m = 120^{0.6}/2. \) Combining Eqs. (3–5), one gets

\[
\dot{w}_i = C_i^0 \left[ \alpha_0 + \frac{(1 - \alpha_0)}{1 + (\eta_{w0}w_i)} \right] C_i \bar{z} D^3 - w_i \], \quad \text{where} \quad C_i = \frac{\pi}{6} k_i f_{alk} c_r \frac{m_g}{m_s} \tag{9}
\]

In deriving the equations in this section, the effects of three significant parameters have been neglected: (1) alkali content, (2) temperature, and (3) external drying. In Part II of this paper all three will be taken into account.

**Diffusion of ASR Gel into Pores in Aggregate and Concrete**

The expulsion of gel from a gel source into adjacent pores is another mechanism that controls the rate of ASR. It may be treated as a diffusion flow obeying the Darcy law. The flow velocity \( z = b_D \nabla p, \) where \( \nabla = \) gradient and \( b_D = \) Darcy permeability (dimension \( \text{m}^2 \cdot \text{s}^{-1} \cdot \text{kg}^{-1} \)). In detailed analysis, one could now proceed to a pointwise differential equation for the diffusion in coordinate \( x. \) However, in view of all the uncertainties and inevitable simplifications, it should suffice to replace \( z \) with the velocity \( dx/dt \) of the diffusion front at distance \( x \) from the gel source, and the pressure gradient with the average pressure gradient \( \nabla p = p/x. \) This leads to the simplified Darcy diffusion equation

\[
\frac{dx}{dt} = b_D p \frac{p}{x} \tag{10}
\]

The pressure profile over the gel penetration zone \( x \in (0, x) \) is doubtless nonlinear. What matters is the flux of mass into the pores at the penetration front, \( x = 0. \) Generally, it is a good approximation to consider the pressure distribution within \( (0, x) \) to be a power law, proportional to \( (x - x')^u \) (where \( u = \) positive constant). Then the pressure gradient at the front, \( (x' \to x), \) is \( \nabla p = p/ux. \) Thus Eq. (10) may be generalized as

\[
\frac{dx}{dt} = b' D p \frac{p}{x}, \quad b' = \frac{b_D}{u} \tag{11}
\]

So the form remains the same for every fixed profile of \( p, \) and the fact that the permeability \( b_D \) changes to \( b' \) does not matter because its value is a fitting parameter anyway. Frequently considered is a parabolic profile, for which \( u = 2, \) which corresponds to linear diffusion theory.

If \( p \) at the gel source were constant, integration of this differential equation would yield \( x = \sqrt{2b_D p t}, \) which is the well known penetration depth \( x \) of the filling front at constant pressure. Thus it
is verified that this fundamental feature of diffusion theory is exhibited by the simplified Darcy equation.

When the ASR gel pressure increase causes the surrounding concrete to crack, the permeability of concrete will increase significantly. Thus, while at first the diffusion gets accelerated by pressure increase, later, once the surrounding concrete cracks, the diffusion gets accelerated by a large increase of permeability, despite pressure relief.

The ASR gel first enters the pores of volume fraction \( v_0 \) that are empty and easily accessible at near-zero pressure \( p \). They are of three kinds: (1) pores inside the aggregate, whose number and volume depend strongly on the aggregate type; (2) pores inside the cement paste (the paste always contains empty pores because of self-desiccation caused by the chemical reactions during hydration); and (3) pores in the interface transition zone (ITZ), which surround each aggregate grain, typically have the thickness of 0.1 \( \mu \text{m} \), and have a reduced mass density and elevated porosity. The filling of empty pores of volume fraction \( v_0 \) can take years or even decades. After they get filled, further imbibition of water will cause the gel to develop a significant pressure \( p \) and diffuse into adjacent voids and cracks [Fig. 3(a)]. For each gel infiltration path one can write [Fig. 3(b)]

\[
dv_1 = a_f dx = a_f b_D \frac{p}{x} \frac{dx}{dt} \tag{12}
\]

where \( v_1 \) = volume fraction of one gel infiltration path; and \( a_f \) = average cross section area of infiltration path. Because an easily accessible volume fills at zero pressure with no pressure gradient, it will likely have a uniform, though nonzero, pressure after it fills completely. Thus, \( x = [v_1 - v_0]/a_f \) in Eq. (12) can be considered and may be rewritten as

\[
dv_1 = a_f b_D \frac{p a_f}{v_1 - v_0} \frac{dx}{dt} \tag{13}
\]

where \( v_{01} \) = volume fraction of easily accessible pores per infiltration path.

One or several basic gel sources are imagined to develop in each aggregate grain with reactive silica. From each source, the gel diffuses in several directions [Fig. 3(a)] into pores, interfaces, and microcracks in the aggregate grain, and into the ITZ (some of the gel gets expelled into cracks in the surrounding cement paste but will not be harmful because it will calcify and thus will not imbibe water and swell). The distances \( x_n (n = 1, 2, \ldots, n_f) \) from the numerous gel sources to the fronts of all these diffusion paths vary randomly (Fig. 2). On average, \( n_f \) equivalent infiltration paths per unit volume of concrete can nevertheless be assumed

\[
dv = \frac{a_f^2 b_D n_f^2}{v - v_0} \frac{p}{v_0} \frac{dx}{dt} \tag{14}
\]

Finally, on denoting \( b/v_{ef} = a_f^2 b_D n_f^2/(v - v_0) \), one gets

\[
\frac{dv}{dt} = b \frac{p}{v_{ef}} \tag{15}
\]

where \( p \) = average gel pressure; \( b \) = effective Darcy permeability (dimension \( \text{m}^2/\text{N s} \) or \( \text{m s/kg} \)), which is proportional to the actual Darcy permeability \( b_D \); and \( v_{ef} \) = effective volume fraction. In Eq. (15), the ratio between effective permeability and the effective volume fraction is the only unknown parameter to estimate, based on empirical data. The permeability, \( b \), is sure to increase with the opening \( \delta_c \) of the cracks. According to the crack band model (Bažant and Oh 1983; Bažant and Planas 1997), \( \delta_c \approx l_0 \epsilon'' \), where

![Fig. 2. ASR reaction process and schematic illustration of ASR induced damage: (a) alkali-silica reaction; (b) formation of swelling and nonswelling ASR gel; (c) ASR-induced damage and cracking](image)

![Fig. 3. ASR gel transport: (a) ASR gel infiltration and produced global damage; (b) one ideal gel infiltration path](image)
\( l_0 \) = material characteristic length, and \( \epsilon'' \) = inelastic part of average strain across the band (if it is tensile).

Because the gel-induced cracks run randomly in any direction, their effect is expansion in all directions, i.e., a volumetric inelastic strain, \( \epsilon'' \), which is considered to be a function of the principal inelastic strains. Among them, permeability increase can be caused only by those that are tensile and exceed a certain empirical finite threshold, \( \epsilon'' \) (taken in this paper as 0.01%). Thus, the inelastic strain effect on gel permeability may be introduced as

\[
\text{for } v \leq v_0: b = b_0 \\
\text{for } v > v_0: b = b_0[1 + \beta((\epsilon'' - \epsilon_0''))]^{n}
\]

Here \( b_0 \) = initial permeability for filling the empty pores; \( \beta \) = empirical dimensionless constant; \( \langle \rangle \) = max(x,0) (Macaulay brackets); and \( n = 2 \) if the flow related to \( \delta^2 \) is assumed. To define the effective volume fraction \( v_{ef} \), the volume fraction \( v \) may be divided into two parts:

\[
\frac{dv_{el}}{dr} = b_0 \frac{p}{v_{ef}}
\]

\[
\frac{dv_{fr}}{dr} = (b - b_0) \frac{p}{v_{ef}}
\]

where \( v_{el} \) = volume fraction of the transported gel as long as permeability remains equal to the initial permeability (i.e., for no damage); and \( v_{fr} \) = volume fraction of the extra transported gel accommodated by fracturing damage. In this study, \( v_{ef} = v_{el} \) is considered. Therefore, all of the parameters to calculate the volume fraction via Eq. (15) are now known, and the final equation can be written as

\[
\frac{dv}{dr} = b_0[1 + \beta((\epsilon'' - \epsilon_0''))] \frac{p}{v_{el}}
\]

During the initial filling of empty, easily accessible pores, the pressure is nearly zero. Thus the initial condition for ASR gel diffusion is

\[
p = 0 \text{ at } v = v_0
\]

### Unconditionally Stable Algorithm with Gel Pressure Relaxation at Constant Gel Mass during Time Step

Because the transport of ASR gel is considered in the average sense and the different infiltration paths are not treated individually, it is reasonable to assume the volume fraction of calcified gel to depend on the volume ratio of aggregate and cement content, \( v_{calc} \), and for simplicity, the dependence to be linear. So, the calcified and pressurized pore volume fractions may be calculated as

\[
v_{calc} = (1 - v_{calc})v_{fr} \text{ and } v_p = v - v_{calc}
\]

Here the elastic part of diffused gel, \( v_{el} \), is assumed to remain inside or very near the aggregate, and be expansive.

Another issue to address is the pressure profile of pressurized pore volume fraction \( v_p \) [Fig. 3(b)]. As already discussed, a zero pressure gradient is considered for the easily accessible volume. For the remaining part of \( v_p \), a reasonable pressure profile should be chosen. A parabolic profile seems appropriate. Accordingly

\[
p = \kappa \frac{v_p v - v}{v_0 + \frac{3}{2} v_p}
\]

where \( \kappa = \) bulk modulus of the gel, which can be considered to be approximately equal to that of water; and factor 2/3 refers to the area under a parabola (it would be 1/2 for a linear profile). Also, because all \( v, v_i, \) and \( v_p \) depend on the pressure \( (v_i \text{ because the density is pressure dependent}) \), the usual time step integration algorithm will require very small time steps to remain stable. But ASR evolves slowly over decades.

Predicting ASR for hundred-year lifetimes, normally desired for dams or large bridges, necessitates an algorithm that remains stable for progressive increase of the time step to many months of duration when the variation of the state variables becomes very slow. Two well-known phenomena that require an unconditionally stable algorithm are the concrete creep and the drying of structure. For concrete creep, stability without accuracy impairment is achieved by Bažant’s exponential algorithm (Bažant 1971; Jirásek and Bažant 2002), and for drying by the Cranck-Nicholson implicit algorithm. However, a third such phenomenon turns out to be the pressure evolution in ASR gel diffusion.

In analogy with the unconditionally stable exponential algorithm for creep (Bažant 1971; Jirásek and Bažant 2002) the volume fraction of fluid \( v_i \) is held constant during the time step \( dr \), and the pressure is allowed to relax due to diffusion. At the end of time step, a sudden increase of pressure is calculated. Differentiation of Eq. (23) yields the pressure increment in the time step

\[
dp = -\kappa \left( \frac{v_0 + \frac{2}{3} v_p}{v_0 + \frac{3}{2} v_p} \right) (v_0 + \frac{2}{3} v_p) \frac{dv}{dr} \left( (v_0 + \frac{2}{3} v_p)^2 \right) (v_0 + \frac{3}{2} v_p)^2
\]

Eqs. (18), (20), and (22) are used to find the increments \( dv \) and \( dp_p \). Their substitution into Eq. (24) furnishes the differential equation:

\[
\frac{dp}{dr} + \frac{p}{\tau_p} = 0
\]

Here \( \tau_p \) plays the role of characteristic time and can be calculated as

\[
\tau_p = \frac{v_{el}}{\kappa b(v_0 + \frac{2}{3} v_p) + \frac{3}{2} (v_i - v)(b - (1 - v_{calc})(b - b_0))}
\]

Eq. (25) describes pressure relaxation at constant gel mass. It is nonlinear because \( \tau_p \) depends on the volume fractions and permeability, which themselves depend on pressure. However, because these dependencies are weak and almost negligible, \( \tau_p \) may be calculated as a constant from the volume fractions and permeability obtained at the end of the previous time step. This allows Eq. (25) to be integrated by separation of variable, and yields the pressure relaxation decrement

\[
dp = -P_{diff}(1 - e^{-\Delta t/\tau_p})
\]

The advantage of this exponential formula is that for arbitrarily long time steps the numerical integration can never yield unbounded \( p \). In other words, the computation of pressure is unconditionally stable. This is important for predicting the ASR effects for hundred-year lifetimes. Typically, after an initial period of short steps, the pressure variation becomes slower and slower. The step duration can be increased in geometric progression even if the step duration becomes many months long. At the end of each time step, Eq. (27) is used to calculate the new pressure \( p \) to make a sudden jumps in volume fractions.

For laboratory experiments whose total duration is not very long, iterative integration method such as Runge-Kutta can be used with small time steps instead of the exponential algorithm, Eq. (27).
For instance, in each time step of two-stage methods: (1) first all the volume fractions are calculated based on the old pressure, \( p_{\text{old}} \), to obtain the iterated pressure, \( p_{\text{new}} \), using Eq. (27); and (2) all the volume fractions are then calculated at pressure \( (p_{\text{old}} + p_{\text{new}})/2 \), and from them the final incremented \( p \) is obtained using Eq. (27). It has been checked that a single iteration always suffices.

### Constitutive Law for the Solid Part of Concrete: Microplane Model M7

In most structures undergoing ASR, the concrete is subjected to multiaxial stress states. Therefore, anisotropic damage must be expected. The anisotropic damage of quasi-brittle materials, concrete included, may effectively be described by the microplane constitutive model. Its basic idea is to express the constitutive law in terms of the vectors of stress and strain acting on a generic plane of any orientation in the material microstructure, called the microplane [Fig. 4(a)]. The use of vectors, rather than tensors, is analogous to the Taylor models used for plasticity of polycrystalline metals, but with important conceptual differences.

Firstly, to avoid model instability in postpeak softening, a kinematic constraint must be used instead of a static one (Caner and Bažant 2013a). Thus, the strain (rather than stress) vector on each microplane is the projection of the macroscopic strain tensor, i.e.

\[
\epsilon_N = \epsilon_{ij} N_{ij}, \quad \epsilon_M = \epsilon_{ij} M_{ij}, \quad \epsilon_L = \epsilon_{ij} L_{ij} \quad (28)
\]

where \( \epsilon_N, \epsilon_M, \) and \( \epsilon_L \) are magnitudes of the three strain vectors corresponding to each microplane; \( N_{ij} = n_i n_j, M_{ij} = (n_i m_j + m_i n_j)/2 \), and \( L_{ij} = (n_i l_j + l_i n_j)/2 \) (\( i, j = 1, 2, 3 \)); and \( n_i, m_i, \) and \( l_i \) are three unit, mutually orthogonal, normal and tangential vectors characterizing the microplane.

Secondly, the principle of virtual work is used to relate the stresses on the microplanes \( (\sigma_N, \sigma_M, \) and \( \sigma_L) \) to the macrocontinuum stress tensor \( \sigma_{ij} \), to ensure equilibrium. This gives (Bažant and Oh 1983; Caner and Bažant 2013a)

\[
\sigma_{ij} = \frac{3}{2\pi} \int_{\Omega} (N_{ij} \sigma_N + M_{ij} \sigma_M + L_{ij} \sigma_L) d\Omega \quad (29)
\]

where \( \Omega = \) unit hemisphere, over which the integration is carried out numerically, by an optimum Gaussian integration formula [Fig. 4(a)].

![Fig. 4](image)

**Fig. 4.** Microplane model: (a) set of integration points for 37-point formula integrating exactly a 13th degree polynomial; (b) vertical return to stress-strain boundary at constant strain when the boundary is exceeded by elastic stresses in finite load step.
chain. The former is more convenient because model B4 specifies the compliance, rather than relaxation, function [Fig. 5(a)].

The spring and dashpots moduli of the Kelvin units in the chain are obtained by discretizing the continuous retardation spectrum (Bažant and Xi 1995) [Figs. 5(b and c)]. Because of aging, the spectrum is different for every time step and every integration point. The retardation times are selected to form a geometric progression with quotient 10 and must cover the entire time range of interest. The time step as the creep rate decays. On the tensorial level, this algorithm leads to the incremental stress-strain relation

\[ \Delta \sigma_{ij} = \tilde{E}(\Delta \epsilon_{ij} - \Delta \epsilon_{ij}') \]  

(30)

\[ \Delta \epsilon_{ij}' = \Delta \epsilon_{ij} + \delta_{ij}(\Delta \epsilon^{sh} + \alpha \Delta T) \]  

(31)

where \( \epsilon_{ij}' \) = creep strain increment tensor calculated from the exponential algorithm for Kelvin chain model; \( \tilde{E} \) = incremental modulus obtained from the exponential algorithm; \( \epsilon^{sh} \) = shrinkage strain increment; and \( \alpha \Delta T \) = thermal strain.

When the microplane model is used, the creep strain increments should properly be introduced within the microplane algorithm because their effect on the stress changes is different on microplanes of different orientations, thus creating incremental anisotropy. To this end, tensor \( \epsilon_{ij}' \) is projected as a creep strain vector on each microplane, with the normal and shear components

\[ \epsilon_{ij}' = \epsilon_{ij}'N_{ij}, \quad \epsilon_{ij}' = \epsilon_{ij}'M_{ij}, \quad \epsilon_{ij}' = \epsilon_{ij}'L_{ij} \]  

(32)

Based on the microplane elastic stiffness scaled for aging, the trial microplane stress increment gets changed from \( \Delta \sigma_{N} = \tilde{E}_{N}\Delta \epsilon_{N} \), etc., to

\[ \Delta \sigma_{N} = \tilde{E}_{N}(t)(\Delta \epsilon_{N} - \Delta \epsilon_{N}') \]  

(33)

\[ \Delta \sigma_{M} = \tilde{E}_{T}(t)(\Delta \epsilon_{M} - \Delta \epsilon_{M}') \]  

(34)

where \( \tilde{E}_{N} \) and \( \tilde{E}_{T} \) = elastic moduli for the normal and shear components. If these stress increments exceed the stress boundary, a drop to the boundary is executed at constant strain. The microplane elastic moduli at age \( t \) are calculated as

\[ \tilde{E}_{N} = E_{N} \frac{\tilde{E}}{E}, \quad \tilde{E}_{T} = E_{T} \frac{\tilde{E}}{E} \]  

(36)

where \( E(t) \) = Young’s modulus, increasing with concrete age \( t \) due to chemical hydration of cement and micropressure relaxation; and \( E_{N}, E_{T} \) = elastic normal and shear moduli for the microplane calculated from Young’s modulus at the reference age of 28 days and the Poisson ratio.

**Two-Phase Medium for Loading of Concrete by Pressure in Pores and Cracks**

It has been standard to treat porous solids with fluid in the pores and microcracks as the Biot two-phase medium, exemplified by saturated sand. Its volumetric equilibrium relation reads \( S_{V} = \sigma_{V} - \alpha \rho \), in which \( \sigma_{V} \) = volumetric stress in the solid phase, calculated from the constitutive model for the solid (the solid phase is the concrete, consisting of aggregate and mortar); \( S_{V} \) = total volumetric stress in the two-phase medium, which is used in finite element analysis to calculate the nodal forces; and \( \alpha \) = Biot coefficient approximately equal to the porosity but usually defined such that \( 1 - \alpha \) represents the bulk moduli ratio of the solid without and with the pore fluid (Detournay and Cheng 2014).

However, concrete is a nonstandard two-phase solid-fluid medium—nonstandard because much of evaporable water is contained as hindered adsorbed water in nanopores only a few atoms wide. Such water behaves simultaneously as a load-bearing solid. Thus it would be incorrect to use the same Biot coefficient as for saturated sands. Therefore, instead of Biot coefficient, the effective porosity \( \phi \) is used. It is defined as the area fraction of gel in a plane

---

**Fig. 5.** Aging creep: (a) Kelvin chain; (b) continuous retardation spectrum; (c) discrete retardation spectrum
cross section of the material [Fig. 3(a)]. Note that φ must be distinguished from the boundary porosity used to define Terzaghi effective stress (which considers pressure resultant from a statistically planar but microscopically rough cross section passing around microscopic grains). Considering that there are $n_i$ equivalent gel sources per a unit volume, and $m_{eq}$ per unit cross section, the porosity can be roughly estimated as

$$\phi = C_0 v_p, \quad C_0 = \frac{m_{eq}}{n_i h_{eq} A_i}$$  \hspace{1cm} (37)

where $v_p =$ pressurized volume fraction; $A_i =$ area fraction of the cross section for which the equilibrium condition is written; and $h_{eq}$ = equivalent width of the gel infiltration path. The unknown parameters in Eq. (37) are lumped into one parameter $C_0$ to be found empirically. In data fitting, $C_0 \approx 10$ appeared to be optimum. In initial calculations the effective porosity $\phi$ was defined as the volume fraction of gel, but the calculated gel pressures were much too high compared with experiments.

Using effective porosity $\phi$ instead of Biot coefficient $\alpha$, the incremental volumetric and tensorial two-phase equilibrium relations can be written as follows:

$$\Delta S_{V} = \Delta[(1 - \phi)\sigma_v] - \Delta(\phi p)$$  \hspace{1cm} (38)

$$\Delta S_{ij} = \Delta\sigma_{ij} - \delta_{ij}\Delta(\phi p)$$  \hspace{1cm} (39)

$$\Delta(\phi p) = \phi\Delta p + p\Delta\phi$$  \hspace{1cm} (40)

where $i$, $j = 1$, 2, 3 are Cartesian tensorial subscripts; $\delta_{ij} =$ Kronecker delta (unit tensor); and $\sigma_v = \sigma_{eq}/3$ (note that $S_v$ and $\sigma_v$ are positive for tension, unlike $p$). Although Eq. (38) has the form of Terzaghi’s effective stress, its physical meaning is different. The effective stress, based on the boundary porosity, is appropriate only for the failure criterion, while Eq. (38) applies at all stages of loading.

**Effect of Various Aggregate Sizes**

For simplicity, the preceding equations, as well as Bažant and Steffens’ (2000) model for gel production function $w_i(t)$ serving as the input to the present analysis, are formulated for only an equivalent aggregate grain of one size $D$ and of spherical shape. But the sizes (or diameters) of reactive aggregate grains are statistically distributed over a broad range, from $D_0$ to $D_1$. Let $f(D)$ be the frequency distribution function of aggregate concentration ratio $\xi_D$, such that the volume of aggregates of size $D$ (per unit volume of concrete) lying within the infinitesimal interval $(D, D + dD)$ is $dV_D = f(D)dD$. Function $f(D)$ must be normalized such that

$$\int_{D_0}^{D_1} f(D)dD = 1$$  \hspace{1cm} (41)

The reaction kinetics depend significantly on aggregate size. The small aggregates react much faster than big ones. The easiest approach would be to consider one effective aggregate size that produces the same expansion as the entire aggregate size distribution. However, although this easy approach gives a realistic estimate of the ASR-induced expansion and damage for long times, the initial expansion gets underestimated. This initial error stems from the fast reaction of small aggregates. To mitigate this error, two different aggregate sizes are considered, with different computational weights $w_s$ and $w_b$ for small and big aggregate sizes, $D_s$ and $D_b$. Thus, the total mass of imbibed water $w_i$ is calculated as

$$w_i = w_s w_i(D_s) + w_b w_i(D_b), \quad \text{where } w_s + w_b = 1$$  \hspace{1cm} (42)

where $w_i(D_s)$ and $w_i(D_b) =$ masses of imbibed water for aggregate sizes $D_s$ and $D_b$. Fig. 6 illustrates the comparison of computer results for one versus two aggregate sizes. The model with two aggregate sizes is found to give a much better match of the test data, especially for the initial expansion (for details, see Part II).

**Stable Algorithm for a Time Step of Explicit Finite Element Analysis**

The steps for the analysis are as follows:

1. For concrete age $t_{old} + \Delta t/2$ at the middle of the current time step, and for each integration point of each finite element, use Widder’s formula for inverse Laplace transform to calculate from the given compliance function of concrete the continuous retardation spectrum for the current age, pore humidity, and temperature, and then convert it to a discrete, retardation spectrum;

2. For each integration point of each finite element, use the exponential algorithm for aging linear creep to calculate for each microplane the inelastic strains and incremental moduli according to Eqs. (33)–(35);

3. Using the new nodal displacements and strains furnished by the finite element analysis of the previous time step, calculate the new $\sigma_v$-value for each integration point from the constitutive law for the solid (in this paper, based on microplane model M7);

4. In the current time step at each integration point of each finite element, compute the mass of imbibed water and its increment Eq. (9). Then, using the old value of $p$, compute the volume fraction of imbibed water Eq. (6);

5. In the current time step, at each integration point of each finite element, compute the permeability $b$ from Eq. (17). Then compute volume fraction of diffused water and of the elastic and inelastic parts from Eqs. (15), (18), and (19);

6. In the current time step, at each integration point of each finite element, calculate the pressurized and calcified parts of diffused gel and then compute the pressure and pressure change due to diffusion at constant gel mass from Eqs. (22) and (27);

7. Calculate the total volumetric stress $S_V$ and its increment for each integration point of each finite element from Eq. (38); and

8. Use the total stress tensor $S_{ij}$ as the input for an explicit finite element program, to calculate from $S_{ij}$ the equivalent nodal forces according to the principle of virtual work. Then, solve the finite element system for these forces and given applied loads to obtain the new strain tensors $\epsilon_{ij}$ and their increments at all
integration points, which are needed to begin the analysis of the next time step.

Conclusions

Based on the results that have been presented in this study, followings could be concluded:

- Analysis of the ASR gel diffusion into pores and cracks in the aggregate and the surrounding cement paste and mortar is important for a fully realistic model for the ASR damage in concrete;
- The diffusion analysis must distinguish: (1) empty pores fillable at no pressure, (2) pores requiring high pressures to penetrate, (3) microcracks whose opening reduce the required pressure, and (4) pores in cement paste beyond the interface transition zone in which the gel combines quickly with calcium hydroxide and solidifies;
- In view of the complexities and uncertainties involved, the partial differential equation for diffusion may be replaced by an approximate ordinary differential equation for the evolution of the average depth of gel penetration front, characterized by the gel volume fraction in concrete;
- To achieve an unconditionally stable explicit algorithm for time step integration permitting long time steps, the diffusion problem is inverted to gel pressure relaxation during the time step at constant gel mass. The gel mass is then increased suddenly at the end of time step;
- The directionality of damage when ASR evolves under various triaxial stress states can be captured by using the microplane model;
- Although concrete with the ASR gel represents a two-phase medium, the standard Biot’s form must be eschewed because the evaporable adsorbed water in the nanopores, while mobile, is load-bearing and acts as part of the solid skeleton; and
- The creep of concrete, which significantly reduces the stresses produced by ASR, may be incorporated into the microplane model as additional inelastic strains on microplanes of various orientations.

Acknowledgments

Partial financial supports from the NEUP Program of the U.S. Department of Energy under grant DE-AC07-05-D14517, and from the U.S. National Science Foundation under grant CMMI-1153494, both to Northwestern University, are gratefully acknowledged.

References

concrete beams.” Proc., 11th Int. Conf. on Alkali-Aggregate Reaction, ICON/CANMET, 999–1008.
Diffusion-Controlled and Creep-Mitigated ASR Damage via Microplane Model. II: Material Degradation, Drying, and Verification

Saeed Rahimi-Aghdam¹; Zdeněk P. Bažant, Hon.M.ASCE²; and Ferhun C. Caner, Aff.M.ASCE³

Abstract: The theory for the material and structural damage due to the alkali-silica reaction (ASR) in concrete is calibrated and validated by finite element fitting of the main test results from the literature. The fracture mechanics aspects, and particularly the localization limiter, are handled by the crack band model. It is shown that the theory can capture the following features quite well: (1) the effects of various loading conditions and stress states on the ASR-induced expansion and its direction; (2) degradation of the mechanical properties of concrete, particularly its tensile and compressive strength, and elastic modulus; (3) the effect of temperature on ASR-induced expansion; and (4) the effect of drying on the ASR, with or without simultaneous temperature effect. The finite element simulations use microplane model M7. The aging creep, embedded in M7, is found to mitigate the predicted ASR damage significantly. The crack band model is used to handle quasi-brittle fracture mechanics and serve as the localization limiter. The moisture diffusivity, both the global one for external drying and the local one handled by the crack band model. It is shown that the theory can capture the following features quite well: (1) the effects of various loading conditions and stress states on the ASR-induced expansion and its direction; (2) degradation of the mechanical properties of concrete, particularly its tensile and compressive strength, and elastic modulus; (3) the effect of temperature on ASR-induced expansion; and (4) the effect of drying on the ASR, with or without simultaneous temperature effect. The finite element simulations use microplane model M7. The aging creep, embedded in M7, is found to mitigate the predicted ASR damage significantly. The crack band model is used to handle quasi-brittle fracture mechanics and serve as the localization limiter. The moisture diffusivity, both the global one for external drying and the local one for mortar near the aggregate, decreases by one to two orders of magnitude as the pore humidity drops. The fits of each experimenter’s data use the same material parameters. Close fits are achieved and the model appears ready for predicting the ASR effects in large structures.

DOI: 10.1061/(ASCE)EM.1943-7889.0001185. © 2016 American Society of Civil Engineers.

Introduction

After a review of previous studies, Part I of this paper presented the detailed development of a comprehensive mathematical model for predicting the effect of the alkali-silica reaction (ASR) on mass concrete. Part II refines the model and analyzes the effects of temperature, applied stress state, and external drying. Comparisons with experimental data from the literature are used to calibrate and verify the model.

Localization Limiter and Heterogeneity

The material modeling relies on a strain-softening damage constitutive law, for which microplane model M7 with embedded aging creep is adopted. To handle the strain-softening constitutive law objectively, a localization limiter must be used to avoid spurious mesh-size sensitivity. Here this purpose is served by the crack band model (Bažant and Oh 1983; Bažant and Planas 1997) in which the finite element size in a softening damage zone must be fixed and treated as a material property. Generally, if the element size is changed, the postpeak softening of the constitutive law must be adjusted so as to maintain a mesh-independent energy dissipation (Bažant and Oh 1983; Červenka et al. 2005). Such adjustment was not needed in this study, i.e., the element size was kept uniform, because the test specimens were small enough to avoid mesh coarsening. The finite elements were (even for axisymmetric situations) linear 6-node hex-element bricks of a size approximately equal to 15 mm for concrete and 2 mm for mortar. Because usually all of the aggregates are not reactive, it is considered that each large aggregate has a 50% probability to contain reactive silica. Because the size of each finite element is about equal to the maximum aggregate size, one half of finite elements are chosen, by a random number generator, to be reactive.

In this regard, heterogeneity is automatic in the lattice discrete particle model (LDPM) used by Allnagar et al. (2013) to fit part of the data fitted in this paper. In a continuum model such as this one, the heterogeneity must introduced because if the specimen were in a homogenous state, with uniform properties, all the finite elements would be expanding equally, creating no residual stresses and thus no damage. A randomization of strength was tried but omitted because the present randomization of reactive silica proved sufficient to fit the data.

Effect of Various Loading Conditions on ASR-Induced Expansion

Several experimental and numerical studies show that the type of applied stress state, particularly the ratio of various components of applied stress, has a large effect on the ASR-induced expansion in various directions (Ahmed et al. 1999; Alnagar et al. 2013; Gravel et al. 2000; Larive et al. 1996; Multon and Toutlemonde 2006). However, the effect on the volume expansion of concrete is minimal. For instance, large compression in one direction simply transfers the expansion to another direction under smaller or zero compression.

The ability of the present ASR model to predict ASR-induced expansion and deterioration at different stress states can be checked by various published experimental data. First the accelerated
laboratory tests of Multon and Toutlemonde (2006) are analyzed, considering the deformation and expansion due to ASR during the test period of 450 days to be comparable to those during 5–50 years in actual structures. In these tests, which involved concrete cylinders of 130 mm in diameter and 240 mm in height, with water-cement ratio of 0.5 and cement content of 410 kg/m³, the availability of alkali was ensured by dissolving potassium hydroxide in the mixing water to increase the $\text{Na}_2\text{O}_{\text{eq}}$ content to 1.25% of the mass of cement.

The alkalies present in portland cement are of different types, with different reactivity. Mostly they consist of potassium oxide, $\text{K}_2\text{O}$, and sodium oxide, $\text{Na}_2\text{O}$, the latter being more damaging. For the sake of simplicity, they are here characterized by one combined quantity, the equivalent sodium oxide content, labeled by subscript eq.

Because the moisture content has a strong effect on the ASR (Larive 1997; Olafsson 1986), all the specimens were sealed by a watertight jacket to obtain a statistically homogeneous state of moisture in each specimen. Minor defects in the jackets caused water losses $\leq 0.5\%$ after 450 days for unconfined cases. For these cases, in addition to autogenous shrinkage, drying shrinkage is also considered. After 28 days of curing, nine different uniform stress states were applied to the cylindrical specimens. Each stress state involved three different cases: (1) free expansion, (2) expansion confined by a tubular 3 mm-thick steel envelope, and (3) expansion confined by a tubular 5 mm steel envelope. The yield stress of steel was 206 MPa, and Young’s modulus was 193 GPa. For each case three axial loading conditions were used: 0, 10, and 20 MPa. Fig. 1 illustrates the simulated specimens for both unconfined and confined conditions.

First calibrated was the case of free expansion; see Table 1 for the calibration parameters. For simplicity, only 2 aggregate sizes were considered in this study: $D = 9$ mm for 85% of aggregates, and $D = 4.2$ mm for 15%. The actual aggregate size distribution could not be used because for most tests it was not reported; only the minimum and maximum sizes were reported.

Because there are no externally introduced stresses, only the relative volume change due to ASR is calculated; i.e., $3\epsilon_v = \epsilon_{\text{axial}} + 2\epsilon_{\text{radial}}$. Figs. 2(a–c) compare the measurements and simulations based on calibration for Case c, volume expansion. The predicted radial and axial expansions are seen to be quite close.

Although, in absence of load and radial confinement, the initial progress of ASR and of the initial microcracking damage must be statistically isotropic, later on the measured strains are highly anisotropic. That would surely not occur if the specimen were a sphere. For the cylinder, the explanation of strain anisotropy is that the strains include smeared macroscopic cracking engendered by the ASR expansion. The prevailing macroracks with the biggest opening width ought to be those that maximize the rate of release of strain energy from the whole specimen, and this release depends on the specimen shape. In the test cylinder, the maximizing direction is mostly radial, and the radial macroracks of wider opening doublelessly contribute a large part of the measured overall axial strain; consult the cracking patterns in Fig. 5(a), which are calculated by using microplane model M7 with creep (Caner and Bažant 2013a, b), coupled with the crack band model.

The width of the crack band, which represents the material characteristic length $l_0$, is important to prevent spurious cracking localization. It was 15 mm in the present simulations. Because what matters is the average strain across the crack band, the lowest order elements are suitable. Square elements consisting of four constant strain triangles were used for the band.

The cracking pattern in Fig. 5 could not be obtained if all the elements were considered to contain reactive silica. Of course, in reality not all the aggregates are reactive. As already mentioned, 50% of all finite elements, each imagined to contain at least one aggregate, were randomly chosen to be reactive.

Although the present model was calibrated only for the radial strain in load-free unconfined specimens (a strain that is unaffected by cracking), the microplane model with the crack band model provided good predictions for the axial and volumetric strains, which are strongly affected by cracking. This fact highlights the importance of using a material model that reproduces fracture behavior correctly.

Next, using the same material parameters, the Multon and Toutlemonde’s (2006) tests with various loadings and confinements are predicted. Figs. 3 and 4 show that the computer predictions closely match the measured axial and radial strains. In particular, they confirm that the present model can predict the so-called expansion transfer, i.e., the loading-induced transfer of ASR expansion to another direction.

Table 1. Calibration Parameters for the Experimental Sets That Have Been Used in This Study

<table>
<thead>
<tr>
<th>Author</th>
<th>Material</th>
<th>$b_0$ (N/m² day)</th>
<th>$r_0$ (%)</th>
<th>$\beta$</th>
<th>$c_i$ (kg/m³)</th>
<th>$\eta_w$ (1/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multon and Toutlemonde (2006)</td>
<td>Concrete</td>
<td>$5.3 \times 10^{-14}$</td>
<td>0.75</td>
<td>$3.2 \times 10^6$</td>
<td>700</td>
<td>$1.4 \times 10^7$</td>
</tr>
<tr>
<td>Ben Haha (2006)</td>
<td>Concrete</td>
<td>$3.5 \times 10^{-14}$</td>
<td>0.5</td>
<td>$4 \times 10^6$</td>
<td>700</td>
<td>$1.4 \times 10^7$</td>
</tr>
<tr>
<td>Ben Haha (2006)</td>
<td>Mortar</td>
<td>$3.5 \times 10^{-14}$</td>
<td>0.5</td>
<td>$4.5 \times 10^6$</td>
<td>590</td>
<td>$1.4 \times 10^5$</td>
</tr>
<tr>
<td>Poyet et al. (2006)</td>
<td>Mortar</td>
<td>$1.5 \times 10^{-13}$</td>
<td>1</td>
<td>$4.5 \times 10^6$</td>
<td>800</td>
<td>$1.4 \times 10^5$</td>
</tr>
</tbody>
</table>
In the cylinders confined by tubular steel envelopes, the concrete was considered to slide against the steel. The friction coefficient was not reported. In the simulations it was assumed to be 0.15.

In this study the effect of confining pressure on gel pressure has been neglected. This effect can be considered using the so-called Skempton pore pressure coefficient, $B$. For undrained condition, this coefficient can be defined as (Detournay and Cheng 2014)

**Fig. 2.** Expansion due to ASR for unconfined unloaded specimen: (a) axial expansion, (b) radial expansion, (c) relative volume expansion ($\epsilon_{axial} + 2\epsilon_{axial}$)

**Fig. 3.** Axial strain-reaction time for (a) unconfined under 10 MPa axial load; (b) unconfined under 20 MPa axial load; (c) 3 mm confinement under no axial load; (d) 5 mm confinement under no axial load; (e) 3 mm confinement under 10 MPa axial load; (f) 5 mm confinement under 10 MPa axial load; (g) 3 mm confinement under 20 MPa axial load; (h) 5 mm confinement under 20 MPa axial load
where $\Delta p =$ change of ASR gel pressure; and $\Delta P =$ same confining pressure. As this equation suggests, the pressure of the ASR gel would increase as the confining pressure increases. The Skempton coefficient is negligible for undamaged concrete, but as the specimen is damaged and gets weaker the value of this coefficient may become larger and more significant. This phenomenon may be the reason of the slight underestimation of the ASR expansion in the cases where the confining pressure is significant [Figs. 4(b, g, and h)].

The damage and cracking pattern for various stress states are rather different, as seen in Fig. 5. For the unconfined load-free case, the cracks favor no direction. Adding an axial compressive load will prevent damage bands, or macrocracks, in the axial direction and will force the cracks to propagate primarily radially [Fig. 5(b)]. In other words, an axial load at no lateral confinement will cause the ASR-induced expansion to prefer the direction normal to the load, i.e., radial.

The present model can capture all of the aforementioned cracking patterns and yield good agreement with the strains measured in (Larive 1997).

Degradation of Mechanical Properties Caused by ASR

As shown by many studies, the ASR-induced expansion produces microcracks and cracks that weaken the concrete (Swamy and Al-Asali 1988; Ben Haha 2006; Ben Haha et al. 2007; Clark 1990; Cusatis et al. 2014; Monette et al. 2000; Ono 1990; Siemes and Visser 2000; Swamy and Al-Asali 1986; Swamy 2002). In this paper the effect of ASR on (1) compressive strength, (2) tensile strength, and (3) Young’s modulus is investigated. The model predictions are compared to the experimental data of Ben Haha.

Fig. 4. Radial strain-reaction time for (a) unconfined under 10 MPa axial load; (b) unconfined under 20 MPa axial load; (c) 3 mm confinement under no axial load; (d) 5 mm confinement under no axial load; (e) 3 mm confinement under 10 MPa axial load; (f) 5 mm confinement under 10 MPa axial load; (g) 3 mm confinement under 20 MPa axial load; (h) 5 mm confinement under 20 MPa axial load
(Ben Haha 2006; Ben Haha et al. 2007) from his accelerated tests of concrete prisms of dimensions $70^2 \times 280$ mm, submerged in water. Because the autogenous shrinkage and the swelling were not measured, they are neglected, although they might have had nonnegligible effects, particularly at short times.

First the model is calibrated to fit Ben Haha’s measured ASR-induced expansion (see Table 1 for the calibration parameters). As mentioned previously, 85% of aggregates are considered to have the size of $D = 10$ mm, and 15% to have $D = 4.3$ mm. Fig. 6(a) shows the simulated specimen and Fig. 6(b) compares the experimental and calculated ASR-induced expansions using the aforementioned fitting parameters. Having the model calibrated to predict the measured expansion, its power can be examined in predicting the effect of ASR on the mechanical properties. To this end, the authors analyze the effects of axial load, tensile or compressive, at different stages of the ASR.

Starting with a compressive axial force, it is increased uniformly to reach the strength limit and failure in approximately 10 min. Although it seems logical that ASR reduces the compressive strength because of microcracking and macrocracking, there is a discrepancy among various experimenters. For instance, Clark (1990) and Ono (1990) found that ASR can decrease the compressive strength by up to 40%, while Monette (2000) found the compressive strength not to be affected significantly. However, in this regard it must be noted that the ASR and the aging due to cement hydration have opposite effects, the former decreasing the strength and the latter increasing it. Another source of increase may be the filling of pores outside the aggregate piece by calcified gel. These competing effects must be the root cause of the discrepancy.

To isolate the ASR effect, the relative compressive strengths of specimens with and without the reactive aggregates are considered. Fig. 7(a) shows the compressive strength ratio of ASR affected to unaffected concrete at various reaction times, and shows that the compressive strength decreases by approximately 5% due to ASR. The comparison also demonstrates that the present ASR model with microplane model M7 provides a good match of the experimental data.
To study the tensile strength, tensile load at various times is applied, increasing at constant rate to reach the strength limit in approximately 10 min. While there are disagreements about the compressive strength reduction, virtually all the experiments concluded that ASR reduces the tensile strength (Swamy and Al-Asali 1988, 1986; Swamy 2002). Different experimenters nevertheless reported very different reduction percentages. Siemes and Visser (2000) investigated 25 bridges and found reductions by up to 85%.

To simulate the reduction, the same procedure as described for compressive strength is used. Fig. 7(b) shows the ratios of affected to unaffected tensile strength measured at various times. In this study, the ASR expansion is found to decrease the tensile strength by 15%.

Lastly, consider Young’s modulus $E$, which is readily extracted from the simulations of loading up to the compressive strength. The ratios of $E$-values at various reaction times to the unaffected $E$-values are shown in Fig. 7(c). As seen, Young’s modulus is predicted to decrease by 15%, which agrees with the decrease measured by Ben Haha.

It must be emphasized that the experimental data analyzed in this study are specific to two particular concretes. The behavior of other concretes may be very different. That is why a realistic prediction model has been developed.

### Effect of Alkali Content on ASR-Induced Expansion

The alkali content can have a big effect on the ASR reaction (Guédon-Dubied et al. 2000; Sibbick and Page 1992). The availability of alkali ions and hydroxyl ions is what controls ASR kinetics. In Part I, $f_{\text{alk}}$ was defined for this purpose and used to calculate the gel mass in one aggregated grain: $w_{\text{pg}} = (\pi/6)(D^3 - 8z^3)c_{\text{alk}} f_{\text{alk}} m_{\text{g}} / m_c$ [Eq. (3) of Part I]. However, the alkali content was considered to be high enough for ASR progress, and assumed the alkali ions to be in sufficient supply for complete reaction, in which case $f_{\text{alk}} = 1$ was used.

Often it is necessary to assess ASR for concrete with a lower alkali content that is insufficient for a complete reaction. In that case $f_{\text{alk}} < 1$ must be used. To this end, the following empirical equation, which has led to good data fits, is introduced:

$$f_{\text{alk}} = \left( \frac{C_{\text{alk}}}{\text{C}_{\text{alk}}} \right)^{1/3}$$

where $C_{\text{alk}}$ = alkali content (ratio of the mass of alkali to cement mass); $C_{\text{alk}}^0$ = alkali content at which ASR stops; and $C_{\text{alk}}^*$ = alkali content at which alkali ions are sufficient for complete reaction.

In this study, $C_{\text{alk}}^0 = 0.1\%$ was assumed and $C_{\text{alk}}^*$ was set equal $1.25\%$ for concrete and $1\%$ for mortar because $c/a$ is higher in mortar and the alkali content is calculated as a function of cement ($c/a = \text{cement to aggregate ratio, by mass}$). It would be better to find an empirical equation for $C_{\text{alk}}$ as a function of $c/a$, but experimental data are lacking.

In regard to the effect of alkali content, two sets of experiments are considered. The first is the same as that already considered for examining the ASR effect on mechanical properties, characterized by the calibration parameters in Table 1. The second is Ben Haha’s (2006) and Ben Haha et al. (2007) test of sets of saturated mortar prisms of size $40 \times 40 \times 160$ mm, with aggregate size $\leq 3$ mm [Fig. 8(a)]. Because of lack of information, possible autogenous shrinkage or swelling was ignored. The present model was first calibrated by fitting Ben Haha’s test results for $C_{\text{alk}} = 1.2\%$ and temperature $= 20^\circ\text{C}$. Fig. 8(b) compares the experimental results with the predictions based on the calibration parameters listed in Table 1; $85\%$ of aggregates had the size of $D = 2$ mm, and $15\%$ had $D = 0.75$ mm. Thanks to symmetries, only one $1/8$ of each prism had to be simulated.

After this calibration, the effect of alkali content on the ASR expansion is predicted. The experimental and predicted results for different alkali contents are compared in Fig. 9(a) for concrete, and in Fig. 9(b) for mortar. Good agreement is seen. Further tests of alkali content effect conducted at different temperatures are analyzed in the next section.

### Effect of Temperature on ASR-Induced Expansion

Like all chemical reactions, ASR kinetics changes significantly with temperature (Jensen et al. 1982; Jones 1988; Olafsson 1986; Larive 1997; Salomon and Panetier 1994; Swamy and Al-Asali 1986; Pleau et al. 1989), and this affects the ASR-induced expansion and damage. The temperature effect is considered to follow the Arrhenius equation for permeability, $a_s$, of water through ASR gel, for initial diffusivity, $D_i^0$, of cement mortar around the aggregate, and for permeability, $b$, of the ASR gel:

$$a_s = a_s^0 \exp \left( \frac{E_a}{RT} - \frac{E_a^0}{RT} \right) \quad (3)$$

$$C_{ij}^0 = C_{ij}^0 \exp \left( \frac{E_C}{RT} - \frac{E_C^0}{RT} \right) \quad (4)$$

$$b = b_0 \exp \left( \frac{E_b}{RT} - \frac{E_b^0}{RT} \right) \quad (5)$$

here $T = \text{current absolute temperature}$; $R = \text{universal gas constant}$; $a_i^0, C_i^0$, $b_i = \text{values at reference temperature} T_0 = 293 \, \text{K}$; and $E_a, E_C, E_b = \text{corresponding activation energies}$. The values used in the computations were $E_a = E_C = 42.5 \, \text{kJ/mol}$ and $E_b = 45 \, \text{kJ/mol}$. The temperature effects on $C_i^0$ and $a_i$ translate into temperature effects on the rate of ASR gel production [Eq. (5) of Part I]. Note that if parameter $\eta_w$ were kept constant, the foregoing temperature effects would also apply to the characteristic time $\tau_i$ of water imbibition. However, because the temperature effect on $\tau_i$ is expected to be approximately the same as on $C_i^0$, $\eta_w$ is modified such that $w/\eta_w$ be approximately constant [Eq. (5) of Part I]. Therefore

$$
\eta_w = \eta_w^0 \left( \frac{E_{\eta}}{RT_0} - \frac{E_{\eta}}{RT} \right)^{-1}
$$

(6)

where $\eta_w^0 = \text{value at reference temperature}$; and $E_{\eta} = \text{corresponding activation energy}$, and $E_{\eta} = E_a/2$ was used.

For the experimental comparisons and calibrations, Ben Haha’s tests (Ben Haha 2006; Ben Haha et al. 2007) were used again to predict the effect of temperature on the role of alkali using the same parameters as calibrated for $T_0$; Figs. 10(a and b) for concrete and mortar prisms. The fits are seen to be quite close.

Finally, consider the combined effect of alkali content and temperature when both are different from the calibration experiments. Figs. 11(a and b) compare the experimental and simulated results for concrete and mortar prisms at $T = 40^\circ\text{C}$, with different alkali contents. Fig. 11(c) demonstrates the same for $T = 60^\circ\text{C}$.

**Effect of Drying on ASR**

Availability of water is crucial for ASR. No water, no ASR. The more water, the greater the ASR damage. The role of water is fundamental for three reasons (Bážant and Steffens 2000):

- The pore water acts as the necessary transport medium for the mass transport of hydroxyl and alkali ions required by the reaction;
- The expansion of the gel is essentially governed by the imbibition of water; and
- For the reaction to continue, water must be supplied by macro-diffusion through the pores of concrete.

Many researchers demonstrated that if the water supply is decreased by drying, the ASR expansion diminishes (Kurihara and Katawaki 1989; Larive et al. 2000; Olafsson 1986; Poyet et al. 2006; Tomosawa et al. 1989; Vivian 1981). Below some critical relative humidity, $h^\circ$, depending on temperature, the ASR stops.
For instance, Nilsson (1983) reported that the ASR stops if the humidity drops below $h^\circ = 80\%$; according to Ludwig (1989), $h^\circ = 80–85\%$ at $T = 20^\circ$C; and according to Olafson (1986), $h^\circ = 80\%$ for $T = 23^\circ$C and $h^\circ = 75\%$ for $T = 38^\circ$C.

A decrease of water supply not only reduces the ASR swelling, but also drastically reduces the diffusivity of cement paste or mortar around the reactive aggregate and thus decelerates the swelling, even by one or two orders of magnitude. To model it, Bažant and Najjar’s (1972) empirical equation (embodied in $fib$ Model Code 2010) was adopted for the dependence of local diffusivity $C_i$ on moisture in the mortar or cement paste around the aggregate.

For instance, Nilsson (1983) reported that the ASR stops if the humidity drops below $h^\circ = 80\%$; according to Ludwig (1989), $h^\circ = 80–85\%$ at $T = 20^\circ$C; and according to Olafson (1986), $h^\circ = 80\%$ for $T = 23^\circ$C and $h^\circ = 75\%$ for $T = 38^\circ$C.

A decrease of water supply not only reduces the ASR swelling, but also drastically reduces the diffusivity of cement paste or mortar around the reactive aggregate and thus decelerates the swelling, even by one or two orders of magnitude. To model it, Bažant and Najjar’s (1972) empirical equation (embodied in $fib$ Model Code 2010) was adopted for the dependence of local diffusivity $C_i$ on moisture in the mortar or cement paste around the aggregate.
Fig. 13. ASR expansion at different environmental humidity ratios: (a) RH = 96%; (b) RH = 82%; (c) RH = 76%; (d) RH = 59%

\[ C_i = C_i^{\text{sat}} \left[ \alpha_0 + \frac{1 - \alpha_0}{1 + \left(\frac{C_i^{\text{sat}}}{C_i^{\text{sat}_0}}\right)^n} \right] \]  

where \( C_i^{\text{sat}} \) = value of \( C_i \) at \( h = 100\% \); and \( \alpha_0 \), \( n \) and \( h^* \) are empirical constants. If the concrete is exposed to external drying, the numerical solution of Bažant and Najjar’s (1972) differential equation for global water diffusion through unsaturated concrete is inevitable

\[ \dot{h} = \nabla \cdot (C_g \nabla h) + \dot{h}_{\text{self}} \]  

where \( \dot{h}_{\text{self}} \) = pore relative humidity due to self-desiccation (caused by hydration); and \( C_g \) = global diffusivity, which is assumed to depend on \( h \) in a way similar to Eq. (7), i.e.

\[ C_g = C_g^{\text{sat}} \left[ \alpha_0 + \frac{1 - \alpha_0}{1 + \left(\frac{C_g^{\text{sat}}}{C_g^{\text{sat}_0}}\right)^n} \right] \]

where \( C_g^{\text{sat}} = C_g \) at saturation. Fig. 12 illustrates one example of predicted drying evolution for specimen with external relative humidity \( h = 0.82 \).

Another important issue is the significant effect of shrinkage when the concrete undergoing ASR is exposed to drying. In that case, \( \dot{h} \) varies both in space and time. Thus, in different regions, the ASR gel swells nonuniformly, more in the specimen core than near the surface. The local free drying shrinkage, \( \epsilon_{sh} \), which is also nonuniform, may be assumed to be approximately linear in \( h \) (Jirásek and Bažant 2002), i.e.

\[ d\epsilon_{sh} = K_{sh} dh \]

where \( K_{sh} = 0.004 \) (empirical constant); \( C_i^{\text{sat}} = 3 \text{ mm}^2/\text{day} \); \( n = 3 \); \( h^* = 0.76 \); and \( \alpha_0 = 0.07 \). Here, the approximate formulas for average drying shrinkage in the cross section (Bažant and Baweja 2000; Bažant et al. 2015) are insufficient.

To verify the ASR model for drying concrete, the experiments of Poyet et al. (2006) conducted at various environmental relative humidity ratios are used. The specimens were mortar cylinders, 16 cm in length and 2 cm in diameter, and the tests were done at \( T = 60^\circ\text{C} \). Table 1 lists the calibration parameters. Again, 85% of aggregates were considered to have \( D = 2 \text{ mm} \), and 15% to have 0.75 mm. Fig. 13(a) shows the evolution of expansion in time for sealed condition and Figs. 13(b–d) compares the experimental and simulated ASR-induced expansions at various environmental humidity ratios.

**Closing Comment**

Close agreement with the main data on the ASR effects on laboratory specimens gives the promise that the present ASR model would allow realistic predictions of the multidecade evolution of the ASR damage in large structures.

**Acknowledgments**

Partial financial supports from the NEUP Program of the U.S. Department of Energy under grant DE-AC07-05/D14517, and from the U.S. National Science Foundation under grant CMMI-1153494, both to Northwestern University, are gratefully acknowledged.

**References**


© ASCE


