# Multi-Phase Modeling of Concrete Subject to Alkali Silica Reaction

# C. Comi<sup>1</sup> and R. Pignatelli<sup>1</sup>

**Abstract:** This work focuses on a multi-phase chemo-elastic damage model for the description of the mechanical degradation of concrete induced by the Alkali Silica Reaction (ASR). A threephase and a two-phase simplified versions are considered. The model accounts for ASR kinetics, depending on temperature and humidity conditions, and the swelling pressure exerted by the ASR reaction products on the skeleton. Damage and viscous phenomena are taken into account. The model is used to simulate the experimental tests on concrete reactive beams performed at varying environmental humidity conditions.

Keywords: Alkali silica reaction, concrete, damage, viscosity.

# 1 Introduction

The alkali-silica reaction is a slow reaction occurring in concrete composed by certain type of aggregates and cement paste which forms a hydrous alkali-calciumsilica gel. In the presence of water this gel swells, causing expansion and microcracking, with possible serious consequences on the safety of concrete structures. Many experimental campaigns have been performed to assess the influence of environmental factors, such as temperature and humidity conditions, on the ASR development [Larive (1998); Multon and Toutlemonde (2010)] and several mathematical models have been proposed to simulate the mechanical effects of ASR. Multi-phase models have been developed to model various chemo-physical phenomena in concrete: Gawin, Pesavento, and Schrefler (2008) proposed a multiphase model for concrete affected by calcium leaching, several researchers [Ulm, Coussy, Kefei, and Larive (2000); Comi, Fedele, and Perego (2009)] addressed the mechanical modeling of ASR by considering a two-phase material with the concrete skeleton and the expansive gel acting in parallel. Grimal, Sellier, Le Pape, and Bourdarot (2008) developed a model taking into account concrete creep, the stress induced by the formation of ASR gel and the mechanical damage.

<sup>&</sup>lt;sup>1</sup> Department of Structural Engineering – Politecnico di Milano – Italy

In the present work the phenomenological bi-phase and three-phase isotropic damage models proposed in Comi and Pignatelli (2010, 2011) are compared and extended in order to include creep effects. Unlike the two-phase description, the assumption of three different phases allows to take into account also the effects of shrinkage, but the difference in terms of global structural response is shown to be limited.

#### 2 Multiphase damage model

Within the theory of multi-phase porous materials (see Coussy (2004))), at the meso-scale concrete affected by alkali-silica reaction is interpreted as the superposition of different homogenized layers (Fig. 1): the concrete skeleton (*s*), including cement paste and aggregates, the gel (*g*) and the fluid phase (*f*), including liquid (commonly water) (*w*), aqueous vapor (*v*) and dry air (*a*). We assume that the water and the gel occupy two distinct and not interacting porosities ( $\varphi_w$  and  $\varphi_g$  with  $\varphi = \varphi_w + \varphi_g$  total porosity): the water can fill the initial porosity of concrete, the gel consumes the silica particles necessary for the reaction, making its own space around the aggregates, as confirmed by numerous petrographic investigations. This hypothesis is justified also by the very low permeability of concrete with respect to the gel, which allows to consider locally drained conditions with respect to the water and locally undrained conditions for the gel. Consequently, the degree of saturation for the gel is always equal to one (the gel is assumed to exert its pressure from the beginning of the process).



Figure 1: Schematic representation of the proposed multiphase model

Let *V* be the total volume of the representative volume element and  $V_s$ ,  $V_g$ ,  $V_w$  the volume occupied by the solid, the gel and the water. The degree of saturation for the water is defined as  $S_w = V_w/(V - V_s - V_g)$ . With these definitions, the volumetric fractions of gel and water are expressed as

$$\zeta_g = V_g / V = \varphi_g, \quad \zeta_w = V_w / V = \varphi_w S_w \tag{1}$$

151

Using the mixture theory, the overall macroscopic stress  $\ddot{i}_{\ell}^{1/2}\ddot{i}_{\ell}^{1/2}$  is expressed as superposition of the stresses acting on each phase, as in Comi and Pignatelli (2011)

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}' - b_g p_g 1 - b_w p_w 1 \tag{2}$$

where  $\sigma'$  is the effective stress acting on the skeleton,  $p_g$  and  $p_w$  are the pressures that gel and water exert on the skeleton,  $b_g$  and  $b_w$  are Biot's coefficient, depending on concrete porosities  $\varphi_g$  and  $\varphi_w$  and 1 is the unit second order tensor. Stresses are related to the total strain  $\varepsilon$ , the volumetric fraction of gel and water and the temperature variation  $\theta$  by the following state laws, including both damage and viscous phenomena

$$\sigma' = (1-D)[2G(e-e_v) + K(tr(\varepsilon - \varepsilon_v) - \alpha\theta)1]$$
(3)

$$p_g = -(1-D)M_g(b_g tr(\varepsilon - \varepsilon_v) - \zeta_g - \alpha_g \theta)$$
(4)

$$p_{w} = -(1-D)M_{w}(b_{w}tr(\varepsilon - \varepsilon_{v}) - \zeta_{w} - \alpha_{w}\theta)$$
(5)

In the above equations *D* is an internal isotropic damage variable which depends on two scalar variables,  $D_t$  and  $D_c$ , describing damage mechanisms under prevailing tension and compression conditions:  $D = 1 - (1 - D_t)(1 - D_c)$ ; *e* is the deviatoric strain tensor;  $\varepsilon_v$  and  $e_v$  are the viscous strain and deviatoric strain tensors; *G* and *K* are respectively the shear and bulk moduli of the homogenized concrete skeleton;  $M_g$  and  $M_w$  are the Biot moduli referred to gel and water;  $\alpha$ ,  $\alpha_g$ ,  $\alpha_w$  are the volumetric coefficients of thermal expansion for skeleton, gel and water.

The constitutive model is completed by evolution equations for the variation of fluid volume contents, damage and viscous strains. For the evolution of the water content we assume the simple form  $\dot{\zeta}_w = A\varepsilon_w \dot{S}_w$ , where the constant *A* is calibrated on the basis of experimental data in Baroghel-Bouny, Mainguy, Lassabatere, and Coussy (1999). The evolution of the gel content is assumed to be proportional to the rate of the reaction extent  $\xi$ 

$$\dot{\zeta}_g = c\dot{\xi}, \quad c = \frac{K + M_g b_g^2 + M_w b_w^2}{M_g b_g} \mathcal{E}_{ASR,S_w=1}^{\infty}$$
(6)

where  $\mathcal{E}_{ASR,S_w=1}^{\infty}$  is the free asymptotic volumetric expansion due to the ASR in the fully saturated case  $(t \to \infty, S_w = 1)$ . Considering a first order reaction kinetics as in Ulm, Coussy, Kefei, and Larive (2000), the following form for the rate of reaction is proposed

$$\dot{\xi} = \frac{\langle f_{S_w} - \xi \rangle^+}{\tilde{t}}, \quad f_{S_w} = \frac{1 + b_1 \exp(-b_2)}{1 + b_1 \exp(-b_2 S_w)}$$
(7)

where parameters  $b_1$  and  $b_2$  are calibrated with experimental data and  $\tilde{t}$  is the intrinsic time of the reaction which depends on the local temperature and degree of

saturation histories T(t) and  $S_w(t)$ , and on the reaction extent  $\xi(t)$ . As suggested by experiments and assumed by various authors, we consider the simultaneity of gel formation and swelling. The intrinsic time is expressed in terms of latency time  $\tau_{lat}$  and characteristic time  $\tau_{ch}$  registered for the swelling of reactive specimens. In this work both the dependence on temperature and degree of saturation are introduced

$$\frac{1}{\tilde{t}} = \frac{\xi/f_{S_w} + \exp(-\tau_{lat}/\tau_{ch})}{\tau_{ch}(1 + \exp(-\tau_{lat}/\tau_{ch}))} \text{ with} \\
\tau_i(T, S_w) = \left\{ \tau_i(\bar{T}, 1) + \frac{\tau_i(\tau T, 0) - \tau_i(\bar{T}, 1)}{1 + c_{1i}\exp\left[-\frac{c_{2i}(1 - 2S_w)}{1 - S_w}\right]} \right\} \exp\left[U_i\left(\frac{1}{T} - \frac{1}{\bar{T}}\right)\right], i = ch, lat$$
(8)



Figure 2: Variation of (a) latency time and (b) characteristic time with degree of saturation  $S_w$  and temperature T

The expressions (8) combine the Arrhenius law, describing the dependence on the temperature as proposed in Ulm, Coussy, Kefei, and Larive (2000), with a dependence on the moisture, based on experimental results at the reference temperature  $\bar{T} = 38^{\circ}C$ ,  $U_{lat}$  and  $U_{ch}$  are the activation energies, while the parameters  $c_{1i}$ ,  $c_{2i}$ ,  $\tau_i(\bar{T},0)$  and  $\tau_i(\bar{T},1)$  are calibrated with experimental data. Fig. 2 shows the obtained variation of latency and characteristic time with the degree of saturation and the temperature.

The evolution of the damage variables  $D_t$  and  $D_c$  is governed by loading-unloading conditions defined in terms of the macroscopic stress, the gel pressure and the water pressure through the 'inelastic effective stress'  $\sigma'' = \sigma + \beta_g p_g 1 + \beta_w p_w 1$  as proposed by Comi, Fedele, and Perego (2009). The nondimensional coefficients  $\beta_g \leq b_g$  and  $\beta_w \leq b_w$  govern the damage level achievable in a concrete specimen under free expansion due ASR and the pressure exerted on skeleton by gel and water.

In order to take into account the creep behavior of concrete, a simple Voigt model is considered:

$$\sigma = 2G_{\nu}e_{\nu} + K_{\nu}tr\varepsilon_{e}1 + \eta_{1}\dot{e}_{\nu} + \eta_{2}tr\dot{\varepsilon}_{\nu}1$$
<sup>(9)</sup>

where  $G_{\nu}$ ,  $K_{\nu}$ ,  $\eta_1$  and  $\eta_2$  are elastic and viscosity parameters to be identified with creep tests.

The above formulation can be simplified by considering concrete affected by ASR as a two phase material, composed by the solid (s), including the cement paste and the aggregates, and the wet gel phase (gw), including the dry gel (g), the water (w), the vapor (v) and the dry air (a). If V denotes again the total volume of the representative volume element,  $V_s$  and  $V_{gw}$  are the volumes occupied by the solid and the wet gel, the volumetric fraction of the wet gel can be defined as

$$\zeta_{gw} = V_{gw}/V = \varepsilon S_w \tag{10}$$

The two-phase formulation, introduced here as a particular case of a general threephase formulation, is suggested by the evidence that, in concrete affected by ASR, the swelling of the alkali-silica gel in the presence of water is the overriding phenomenon, especially for the high humidity environmental conditions of the majority of the reactive concrete structures. The mechanical effect due to the water itself (shrinkage) becomes significant for very low humidity conditions only (as obtained in laboratory tests by Multon and Toutlemonde (2010)). Moreover the two-phase approach needs less material coefficients then the three-phase model. This is a relevant point because the experimental information available in literature does not permit to calibrate the parameters necessary for a poro-mechanics three-phase approach accurately enough, especially those regarding the interaction between gel and water filling the concrete porosity.

#### 3 Numerical results

The proposed model, in both the three-and two-phase formulations, has been implemented in a finite element code and has been used to simulate the experimental test reported in the literature.

For the calibration of the hygroscopic behavior the data reported in Baroghel-Bouny, Mainguy, Lassabatere, and Coussy (1999) for nonreactive concrete have been used. For the influence of moisture on the final expansion due to ASR the data by Larive (1998); Multon (2003) for reactive concrete have been employed.

Figure 3 shows the total axial deformation for a reactive-concrete obtained with the bi- and threephase model together with the experimental data. The models have been validated by simulating the experimental tests of Multon and Toutlemonde



Figure 3: Axial deformation of cylindrical specimens of non reactive and reactive concrete with degree of saturation: experimental points from Baroghel-Bouny, Mainguy, Lassabatere, and Coussy (1999); Larive (1998); Multon (2003) and proposed three-phase and two-phase models.

(2010) on reactive cylindrical specimens kept in water for two years and then exposed to drying air at 30% RH. As shown in Fig. 4a with the three-phase model the contribution of the water pressure is taken into account, leading to a higher strain in the first period and allowing to predict shrinkage in the second period. The model is also able to capture the dependence of the expansion due to ASR on the state of stress acting on concrete. As an example, Fig. 4b shows the model prediction of the experimental tests by Multon (2003) on cylindrical specimens with different level of compression axial stress.



Figure 4: (a) Free expansion tests at  $T = 38^{\circ}C$  for reactive specimens kept in water for two years and then in air at 30% RH, (b) tests on free and axially loaded specimens.

To compute the degradation effects of ASR on concrete structures when temperature and moisture gradients vary in time, the mechanical analysis is preceded by the heat diffusion analysis, governed by Fourier law, and by the liquid moisture diffusion analysis. The tests of Multon and Toutlemonde (2010) on reactive plain beams have been simulated with a 2D finite element analysis using the three-phase model, also including creep. The experimental conditions have been reproduced by proper initial and boundary conditions: after curing under aluminium sealing, the lower face of the beam was immersed in water, while the upper face was in contact with air at 30% RH for 14 months and then submitted to permanent water supply for 9 months.

Fig. 5 shows the computed patterns of degree of saturation and reaction extent after 14 and 23 months respectively. The comparison between experimental results and numerical analysis is shown in Fig. 6a in terms of vertical strain evolution at different depths of the beam. A qualitatively good agreement is observed.



Degree of saturation

Reaction extent

Figure 5: Patterns of degree of saturation and reaction after (a) 14 and (b) 23 months



Figure 6: (a)Vertical strains and (b) normalized Young��s modulus evolutions at four depths of the beam (0,08, 0,17, 0,27, 0,37 m from the upper face): experimental points and model prediction

Fig. 6b shows the corresponding damage evolution in terms of Young's modulus reduction at four depths of the reactive beam. In the upper part (0.08m depth) a limited damage develops during the first months due to drying, while damage induced by ASR develops after the water supply. The damage evolution is faster in the lower part of the beam, where the degree of saturation is high.

### 4 Conclusions

A multiphase chemo-elastic damage model for the description of the mechanical degradation of concrete induced by the ASR has been discussed. The model takes into account the influence of temperature and humidity histories on the kinetic of the reaction and on the final expansion produced by the ASR. The consequent mechanical degradation of concrete is described by an isotropic damage variable. The application of the model to beams subjected to moisture gradients shows the capability of the isotropic model to predict the structural degradation due to ASR. With respect to the two-phase model, the three-phase model allows to describe shrinkage effects.

# References

**Baroghel-Bouny, V.; Mainguy, M.; Lassabatere, T.; Coussy, O.** (1999): Characterization and identification of equilibrium and transfer moisture properties for ordinary and high-performance cementitious materials. *Cement and Concrete Research*, vol. 29, pp. 1225–1238.

**Comi, C.; Fedele, R.; Perego, U.** (2009): A chemo-thermo-damage model for the analysis of concrete dams affected by alkali-silica reaction. *Mechanics of Materials*, vol. 41, pp. 210–230.

**Comi, C.; Pignatelli, R.** (2010): On damage modeling of concrete affected by alkali-silica reaction in the presence of humidity gradient. In *XVIII GIMC Conference. Siracusa (Italy)*, pp. 1–4.

**Comi, C.; Pignatelli, R.** (2011): A three-phase model for damage induced by asr in concrete structures. In *Proc COUPLED2011*, Kos, Greece.

Coussy, O. (2004): Poromechanics. John Wiley and Sons, New York.

Gawin, D.; Pesavento, F.; Schrefler, B. (2008): A modeling of cementitious materials exposed to isothermal calcium leaching, considering process kinetics and advective water flow. part 1: Theoretical model. *International Journal of Solids and Structures*, vol. 45, pp. 6221–6240.

**Grimal, E.; Sellier, A.; Le Pape, Y.; Bourdarot, E.** (2008): Creep, shrinkage, and anisotropic damage in alkali-aggregate reaction swelling mechanism – part i. *ACI Mat. Journal*, vol. 105, no. 3, pp. 227–235.

**Larive, C.** (1998): Apports combinés de l'expérimentation et de la modélisation la comprehénsion de l'alcaliréaction et de ses effets méchaniques. Phd thesis, LCPC, 1998. **Multon, S.** (2003): Evaluation expérimentale et théorique des effects mechaniques de l'alcali-réaction sur des structures modéles. Phd thesis, LCPC, 2003.

**Multon, S.; Toutlemonde, F.** (2010): Effect of moisture conditions and transfer on alkali silica reaction damaged structures. *Cement and Concrete Research*, vol. 40, pp. 924–934.

**Ulm, F. J.; Coussy, O.; Kefei, L.; Larive, C.** (2000): Thermo-chemo-mechanics of asr expansion in concrete structures. *ASCE Journal of Engineering Mechanics*, vol. 126, no. 3, pp. 233–242.