AN RVE-BASED MULTI-SCALE APPROACH FOR CONCRETE AFFECTED BY ALKALI–SILICA REACTION

Martín E. Almenar[a]**, Felipe López Rivarola**[b]**, Nicolás A. Labanda**[a,b,c] **and Guillermo J. Etse**[a,b]

[a]*CONICET - Universidad Nacional de Tucumán, Facultad de Ciencias Exactas y Tecnología.
malmenar@facet.unt.edu.ar; getse@herrera.unt.edu.ar;*

[b]*Universidad de Buenos Aires. Facultad de Ingeniería. LMNI-INTECIN (UBA-CONICET).
felipelr@gmail.com;*

[c]*SRK consulting, Buenos Aires. nlabanda@srk.com.ar*

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Abstract. The alkali-silica reaction (ASR) is a deleterious reaction that occurs in cementitious mixtures like concrete due to the combination of the alkaline solution of the cement paste with the amorphous silica of the aggregates. As a consequence of this reaction a gel is generated that expands through water absorption, leading to pore filling and pore pressure increment. Experimentally, the consequences of ASR are observed in both the micro-cracking path around the aggregate and the stiffness reduction of the overall skeleton or solid phase. To get a proper prediction of the aforementioned effect, it is necessary to consider the kinetics of the chemical reaction and its effect on the mechanical behavior. In this paper, the ASR is modeled introducing a variable that quantifies its progress through a first order kinetic law. This variable affects the volumetric component of the Helmholtz free energy which now shall account for the chemo-mechanical behavior of the material. Thus, an additional term is introduced in the microscopic free energy density related to the chemical reaction process. The proposed free energy equation is implemented in a thermodynamically consistent multi-scale framework accounting for the chemo-mechanical degradation of the micro-structure due to the volumetric expansion of the gel. The cement mortar constitutive relation is reformulated using Biot's poromechanics theory to include the pore pressure in the mechanical description, and a damage model to reproduce the solid phase degradation. Finally, some numerical examples showing the potential of the presented formulation are discussed.

1 INTRODUCTION

The ARS is a deleterious chemical reaction that occurs in the mesoscopic level of the concrete when an alkaline solution, presented in the pores of the cement paste, is combined with the amorphous silica of the aggregates. As a consequence of this reaction, a gel is produced and expands by water absorption, filling the pores and increasing the neutral pressure of the material. Experimentally, the consequences of ASR are observed in both, a meso-cracking path around the aggregate and the stiffness reduction of the overall skeleton or solid phase. The chemical reaction depends mainly on three elements, which must exist simultaneously: reactive aggregates, high level of alkalinity and high humidity (at least an 80% of the relative humidity must be present in the concrete pores). The product of this reaction is an expansive gel that fills the pores of the material. Depending on the mineralogy and aging of the concrete material at the beginning of the reaction, this phenomena can produce a matrix and aggregate cracking.

The ARS plays an important role in the structural integrity, so it is an important element which must be taken into account to avoid or mitigate undesirable effects. From the numerical point of view, there are several approaches based on meso-micro mechanics to study this physical effect. Micro models are generally used to prove different hypothesis relating the expansion mechanism, being purely mechanical model (Charpin and Ehrlacher, 2012), chemical models (Saouma et al., 2015) or mixed models (Bazant, 2000; Suwito et al., 2002; Poyet et al., 2007). Mircomodels are generally based on the representative volume element concept (**RVE**), composed by spherical particles surrounded by the cement paste and coupling the meso mechanical behavior with the macro structure. In this sense, the material anisotropy is represented explicitly. In meso mechanical models, the expansion due to ASR can be modelled as an aggregate expansion (Comby-Peyrot et al., 2009) or as a gel expansion randomly distributed in the aggregate (Dunant, 2010).

Various macroscopic approaches have been formulated to simulate realistically the ARS induced expansion in the structure. The models are generally formulated in a finite element framework, combining the kinetic of the chemical reaction with the constitutive mechanics, considering the material degradation experimentally observed. A deep review of the macro models is presented in Almenar et al. (2016c). Phenomenological models are generally used for engineering applications due the low computational requirement. Material degradation can be considered using plastic constitutive models or models based in isotropic or anisotropic damage models (Pietruszczak, 1996; Ulm et al., 2000; Huang and Pietruszczak, 1999; Comi et al., 2009; Almenar et al., 2016b). Some models, more sophisticated, include the creep and shrinkage phenomena during the ARS process (Grimal et al., 2008a,b; Pesavento et al., 2012). For the reaction kinetics, the proposal of Larive (1997) is generally adopted, or its subsequent modifications proposed by Steffens et al. (2003), considering the temperature effect, the humidity, and the stress state, among others.

The great variety of models in different scales unfolds the possibility to approach the problem from the numerical point of view. Recently, some multiscale models have been proposed, as can be seen in (Puatatsananon and Saouma, 2013; Wu et al., 2014). In these works, the ARS is simulated within the cement paste of the micro structure, homogenizing the response to capture the damaged constitutive behavior.

In this paper a thermo-poro-mechanical multi-scale problem to model concrete degradation under ASR is presented. The multi-scale model is stated within the semi-concurrent formulations (Blanco and Giusti, 2013) where the strain tensor ε, the temperature θ and its gradient $\nabla\theta$ are transferred from the coarse scale to the fine scale. The mortar in the micro-scale (or repre-

sentative volume element **RVE**) is considered a porous media. Biot's poromechanics theory is considered for the mortar simulation affected by chemical reactions, while the aggregate is simulated as a simple elastic material. After solving the boundary value problem in the fine-scale the macro-stress $\boldsymbol{\sigma}(x, t)$, the macro-heat flux $\boldsymbol{q}(x, t)$ and the macro-pore pressure $p(x, t)$ are obtained. The paper is organized as follows: a thermo-poro-mechanical problem is presented for the coarse scale in section 2, the multi-scale framework is presented in section 3, the micro constitutive behavior is introduced in section 4. Finally the model is validated using numerical examples in section 6 and the conclusions are drawn in section 7.

2 THERMO-PORO-MECHANICAL PROBLEM IN THE COARSE SCALE

In the following section, the equilibrium equations for thermo-poro-mechanics with undrained hydraulic conditions are presented. It is important to note that all variables with sub-index μ, are those acting in the fine scale.

The thermal problem can be expressed as: *Given a thermal source f, find $\theta \in \Theta$ such that the heat flux $\boldsymbol{q}$ fulfil*

$$\int_{\Omega} \boldsymbol{q} \cdot \nabla_{\boldsymbol{x}} \delta\theta \, d\Omega = \int_{\Omega} f \delta\theta \, d\Omega, \quad \forall \delta\theta \in \Theta. \tag{1}$$

The poro-mechanical problem can be expressed as: *Given a temperature field θ that satisfied (1) and a load in the Neumann boundary $\boldsymbol{f}$, find $\boldsymbol{u} \in \mathscr{U}$ such that the stress field $\boldsymbol{\sigma}$ fulfil*

$$\int_{\Omega} \boldsymbol{\sigma}(\boldsymbol{u}_{\mu}, p_{\mu}, \theta_{\mu}) \cdot \nabla_{\boldsymbol{x}}^{s} \delta\boldsymbol{u} \, d\Omega = \int_{\Gamma} \boldsymbol{f} \cdot \delta\boldsymbol{u} \, d\Gamma, \quad \forall \delta\boldsymbol{u} \in \mathscr{U} \tag{2}$$

where

$$\Theta = \left\{ \theta \in \boldsymbol{H}^1(\Omega) : essential \ boundary \ conditions \right\} \tag{3}$$

$$\mathscr{U} = \left\{ \delta\boldsymbol{u} \in \boldsymbol{H}^1(\Omega) : essential \ boundary \ conditions \right\} \tag{4}$$

In equation 2 it can be seen that the macro stress tensor $\boldsymbol{\sigma}(\boldsymbol{u}_{\mu}, p_{\mu}, \theta_{\mu})$ depends on three micro scale variables: the micro-scale displacement $\boldsymbol{u}_{\mu}$, the micro-scale pore pressure p_{μ} and the micro-scale temperature θ_{μ}.

3 MULTI-SCALE FRAMEWORK

Given a point $\boldsymbol{x} \in \Omega$ in the macro scale and being $\boldsymbol{y} \in \Omega_{\mu}$ the coordinate system in the **RVE**, the following scale bridging equations can be formulated. A brief summary is presented in this paper, and further details of the multi-scale setting can be found in López Rivarola et al. (2017). Table 1 shows the assumed axioms for thermal problem, on the one hand, and for the mechanical problem on the other. The former, assumes an injection of the macro temperature θ and its gradient $\nabla_{\boldsymbol{x}}\theta$ in the RVE domain, and considers a energetic balance between the scales using the Hill-Mandel principle (Blanco and Giusti, 2013). The latter, considers a strain injection in the RVE and the classical form of the Hill-Mandel principle. The stress field in the micro scale depends on the micro strain field $\boldsymbol{u}_{\mu}$, but also on the micro temperature θ_{μ} and the micro pore pressure p_{μ}. The calculation of $\boldsymbol{\sigma}_{\mu}$ will be discussed in section 4.

The consequences produced by the considered axioms are presented in Table 2. In both problems, an homogenized operator for dual variables and the micro-scale equilibrium problem are obtained.

The thermal flux in the micro scale is characterize by Fourier's law

$$\boldsymbol{q}_\mu\left(\theta_\mu\right) = -\boldsymbol{K}_\mu \nabla_{\boldsymbol{y}} \theta_\mu. \tag{5}$$

	Axioms
Thermal problem	$\nabla_{\boldsymbol{x}}\theta = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\nabla_{\boldsymbol{y}}\theta_\mu\,d\Omega_\mu$ $\theta = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\theta_\mu\,d\Omega_\mu$ $\theta_\mu\left(\boldsymbol{y}\right) = \theta + \nabla_{\boldsymbol{x}}\theta\cdot\left(\boldsymbol{y}-\boldsymbol{y}_0\right)+\tilde{\theta}_\mu\left(\boldsymbol{y}\right)$ $\boldsymbol{q}\cdot\nabla_{\boldsymbol{x}}\delta\theta = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\boldsymbol{q}_\mu\left(\theta_\mu\right)\cdot\nabla_{\boldsymbol{y}}\delta\theta_\mu\,d\Omega_\mu$
Thermo-Poro-Mechanical problem	$\boldsymbol{\varepsilon} = \frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}\boldsymbol{u}_\mu\otimes^s\boldsymbol{n}\,d\partial\Omega_\mu$ $\boldsymbol{u}_\mu = \boldsymbol{u}+\boldsymbol{\varepsilon}\left(\boldsymbol{y}-\boldsymbol{y}_0\right)+\tilde{\boldsymbol{u}}_\mu$ $\boldsymbol{\sigma}\cdot\nabla_{\boldsymbol{x}}^s\delta\boldsymbol{u} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\boldsymbol{\sigma}_\mu\left(\boldsymbol{u}_\mu,p_\mu,\theta_\mu\right)\cdot\nabla_{\boldsymbol{y}}^s\delta\boldsymbol{u}_\mu\,d\Omega_\mu$

Table 1: Multi-scale axioms for a thermo-poro-mechanical problem.

	Consequences
Thermal problem	$\boldsymbol{q} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\boldsymbol{q}_\mu\left(\theta_\mu\right)\,d\Omega_\mu$ $\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\boldsymbol{q}_\mu\left(\theta_\mu\right)\cdot\nabla_{\boldsymbol{y}}\delta\tilde{\theta}_\mu\,d\Omega_\mu = 0$
Thermo-Poro-Mechanical problem	$\int_{\Omega_\mu}\boldsymbol{\sigma}_\mu\left(\boldsymbol{u}_\mu,p_\mu,\theta_\mu\right)\cdot\nabla_{\boldsymbol{y}}^s\delta\tilde{\boldsymbol{u}}_\mu\,d\Omega_\mu = 0$ $\boldsymbol{\sigma} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\boldsymbol{\sigma}_\mu\left(\boldsymbol{u}_\mu,p_\mu,\theta_\mu\right)\,d\Omega_\mu$

Table 2: Multi-scale consequences for a thermo-poro-mechanical problem.

4 HELMHOLTZ FREE ENERGY IN THE RVE

Biot's theory is used to simulate the constitutive behavior of the paste affected by ASR in the **RVE** (Coussy, 2004; Ulm et al., 2000; Comi et al., 2009). The concrete mortar micro-scale is considered as a combination of two phases: a solid skeleton and a gel phase filling the pores. The pore pressure induced by the gel expansion is noted as p^g. In a free expansion test, the pore pressure of the gel is balanced by the stress of the solid skeleton σ^s. In this sense, the total stress in the mortar $\boldsymbol{\sigma}_\mu$ is null, which means that the gel pressure tensor $\boldsymbol{P}^g$ is equal and opposite to the effective stress $\boldsymbol{\sigma}^{ef}$. The considered model is showed in Figure 1, where the thermal dilatation of the material is also considered.

The energy function used in this paper is based on the proposal of Almenar et al. (2016b), and is suitable to simulate the mortar behavior under ASR attack, considering mechanical and thermal effects. Function $\psi(\nabla_{\boldsymbol{y}}^s\boldsymbol{u}_\mu,\beta_\mu,\xi_\mu,\theta_\mu)$ is introduced as

$$\psi_\mu(\nabla_{\boldsymbol{y}}^s\boldsymbol{u}_\mu,\beta_\mu,\xi_\mu,\theta_\mu) = R(\beta_\mu)\left[\psi_{pm}(\nabla_{\boldsymbol{y}}^s\boldsymbol{u}_\mu,\xi_\mu)+\psi_T(\nabla_{\boldsymbol{y}}^s\boldsymbol{u}_\mu,\xi_\mu,\theta_\mu)\right]+\psi_q(\xi_\mu), \tag{6}$$
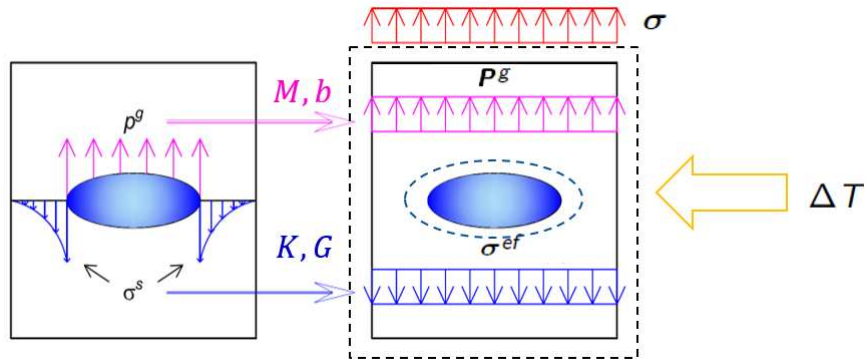
Figure 1: ASR model based in a themo-poro-mechanical philosophy.

$$\psi_{pm}(\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu, \xi_\mu) = \frac{1}{2}\,\mathbb{C}_\mu\left(\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu\right)\cdot\left(\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu\right) + \frac{1}{2}Mb^2\left(tr\left(\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu\right) - \frac{\epsilon^\infty\xi_\mu}{B\,b}\right)^2, \qquad (7)$$

$$\psi_T(\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu, \xi_\mu, \theta_\mu) = \frac{1}{2\,R(\beta_\mu)}\left(-\frac{\mathscr{C}}{T_0} + M\alpha_s^2\right)\theta_\mu^2$$

$$- Mb\left(tr\left(\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu\right) - \frac{\epsilon^\infty\xi_\mu}{B\,b}\right)\alpha_g\theta_\mu - \boldsymbol{B}_\mu\left(\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu\right)\theta_\mu, \quad (8)$$

$$\psi_q(\xi_\mu) = \frac{1}{2}A_0^g(1-\xi_\mu)^2. \qquad (9)$$

where: $\psi_{pm}(\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu, \xi_\mu)$ is the free energy of the porous media, $\psi_T(\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu, \xi_\mu, \theta_\mu)$ is the free energy of the mechanical source, and $\psi_q(\xi_\mu)$ is the free energy of the ASR. M y b are the Biot modulus and coefficient, respectively. α_s and α_g are dilatation coefficients of the solid and gel phase, respectively. $\mathscr{C}$ is the heat capacity. T_0 is the reference temperature. ξ_μ is a variable that measures the ASR progress, being 0 when the reaction is not active and 1 when the reaction is fully activated. ϵ^∞ is the maximum volumetric expansion. $B = Mb/K + Mb^2$, where K is the volumetric modulus. The material degradation produced by chemical and mechanical effects are considered by the function $R(\beta_\mu)$, which depends on the non local damage variable β_μ (Almenar et al., 2016a).

Considering Coleman's relations, from equation (6) the following relations can be obtained

(a) $\quad\boldsymbol{\sigma}_\mu\left(\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu, p_\mu, \theta_\mu\right) = \frac{\partial\psi_\mu}{\partial\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu} = \boldsymbol{\sigma}^{ef} + \boldsymbol{P}^g = R(\beta_\mu)\left[\mathbb{C}_\mu\left(\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu\right) - \boldsymbol{B}_\mu\theta_\mu\right] - b\,p^g\boldsymbol{I},$

(b) $\quad p^g = -R(\beta_\mu)\,M\left\{b\,tr\left(\nabla^s_{\boldsymbol{y}}\boldsymbol{u}_\mu\right) - \left[\frac{\epsilon^\infty\xi_\mu}{B} + \alpha_g\theta_\mu\right]\right\},$

(c) $\quad V = -\frac{\partial\psi}{\partial\beta_\mu} = -R'\left[\psi_{pm} + \psi_T\right],$

(d) $\quad A^g = -\frac{\partial\psi}{\partial\xi_\mu} = -\frac{\epsilon^\infty}{B}p^g + A_0^g(1-\xi) \approx A_0^g(1-\xi_\mu),$

(e) $\quad S = -\frac{\partial\psi}{\partial\theta\mu} = f(\boldsymbol{\varepsilon}, \xi_\mu) + \left[\frac{\mathscr{C}}{T^0} - M\alpha_g^2\right]\theta_\mu \approx \left[\frac{\mathscr{C}}{T^0} - M\alpha_g^2\right]\theta_\mu.$

$$(10)$$

where S is the thermal entropy. Following (Saouma and Perotti, 2006; Grimal et al., 2008a; Comi et al., 2009, 2012), the first terms in (10) (d) y (e) are neglected. This, allows to solve chemical and mechanical effects as uncoupled problems. The computation procedure of the micro-scale problem is proposed as follows: 1) the thermal problem is solved; 2) considering the obtained thermal field, the chemical ASR problem is solved; 3) the mechanical problem is solved, considering the thermal field and the chemical reaction.

Equation (10)(a) shows the equilibrium of all the considered ASR problem (Figure 1).

5   PROGRESS VARIABLE ALKALI SILICA REACTION

The ASR is considered using a variable ξ_μ that measures the global progress of the reaction. The variable ranges from 0, when the reaction has not yet started, to 1 when it is fully exhausted. Following Larive (1997) and Ulm et al. (2000), variable ξ_μ is stated using the associated thermodynamics variable A^g, called reaction affinity.

$$A^g(\xi) = k^d \dot{\xi}_\mu, \tag{11}$$

$$A^g(\xi_\mu) = A^g_0(1 - \xi_\mu), \tag{12}$$

where $k^d > 0$ y A^g_0 is the initial reaction affinity. Combining equations (11) and (12) the following expression is obtained

$$1 - \xi_\mu = t^i \dot{\xi}_\mu, \tag{13}$$

where $t^i = \frac{k^d}{A^g_0}$ is the reaction intrinsic time, calibrated using experimental results. This parameter depends on factors such as the temperature, saturation degree, stress state, and aggregate size, among others (Larive, 1997; Haha et al., 2007). The variation of t^i is considered by the following equation

$$t^i = \tau_c(T) \frac{1 + exp\left(-\frac{\tau_l(T)}{\tau_c(T)}\right)}{\xi_\mu + exp\left(-\frac{\tau_l(T)}{\tau_c(T)}\right)} \tag{14}$$

where $\tau_l(T)$ y $\tau_c(T)$ are the latency and characteristic time, which are function of the temperature. For a given constant temperature $\overline{T}$, the variables take a constant value and define the progress of the ASR in time (see Figure 2). The parameters are obtained by free expansion tests ($\sigma_\mu = \mathbf{0}$), and using the equation (10)(a).
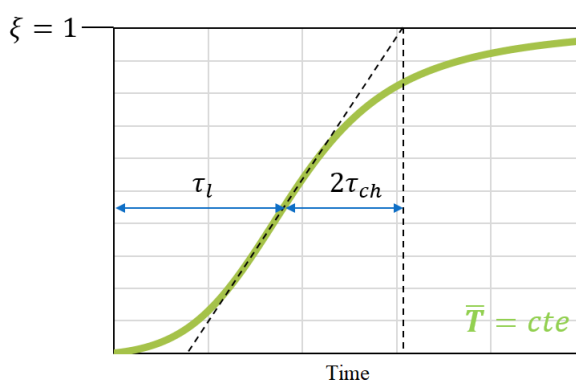

Figure 2: Characteristic time τ_c and latency time τ_l at constant temperature.

Ulm et al. (2000) considers the dependence of ξ_μ with the latency and characteristic time as follows

$$\tau_p(T) = \tau_p(\overline{T})exp\left[U_p\left(\frac{1}{T} - \frac{1}{\overline{T}}\right)\right], \quad p = l, c, \tag{15}$$

where U_l and U_c are the activation energies that must be calibrated using the free expansion test curves at constant temperature.

6 NUMERICAL EXAMPLES

A numerical multi-scale assessment of an ASR in concrete is presented in this example. The **RVE**s considered are plotted in Figure 3 and the model parameters are presented in Table 6. For the mortar phase, a gradient enhanced damage model is used to simulate the damage progression of the ASR (Almenar et al., 2016a). The aggregate phase is considered as an elastic material.
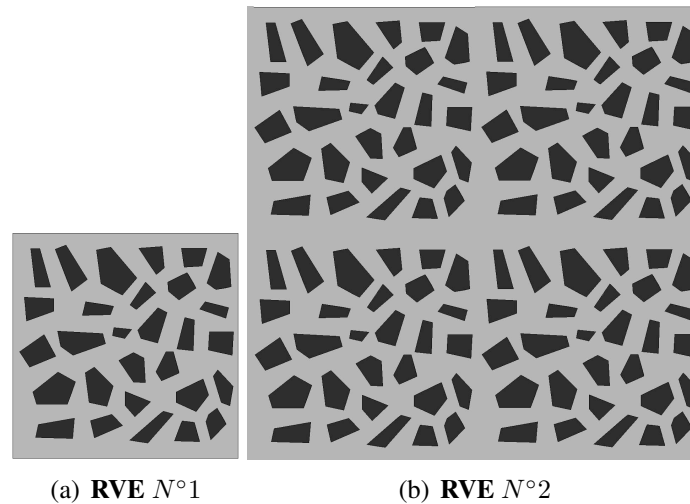

(a) **RVE** $N°1$ (b) **RVE** $N°2$

Figure 3: Proposed **RVE**s for ASR analysis.

	Mortar	Aggregate
Young modulus E [MPa]	9447	386920
Poisson modulus	0.20	0.20
Critical tension σ_c [MPa]	6	-
Fracture energy G_c [N/mm]	0.20	-
Water Biot coefficient b_w	0.40	0.40
Water Biot modulus M_w [MPa]	6000	6000
Latency time τ_l [Days]	-	178
Characteristic time τ_c [Days]	-	87
maximum volumetric expansion ϵ^∞ [%]	-	2.37E-04

Table 3: Properties for concrete.

The chemical attack is taken into account using the ASR variable ξ_μ, and considering that the mortar is the only phase in which the stiffness is degraded. Linear boundary conditions

are considered for the **RVE** kinematics (Neto and Feijoo, 2008). Figure 4 shows the damage progression in **RVE** $N°1$ due to the ASR, and Figure 5 for **RVE** $N°2$. The cell has a negligible damage until day 20, accelerating the expansion from day 50 to day 400. It can be seen that both cells have a similar chemo-mechanical behavior, suggesting that the proposed multi-scale model is independent of the **RVE** size (Gitman et al., 2007). Figure 6 shows the macro volumetric expansion obtained with the proposed mathematical model. The results are consistent with the experimental results obtained by Giaccio et al. (2008).
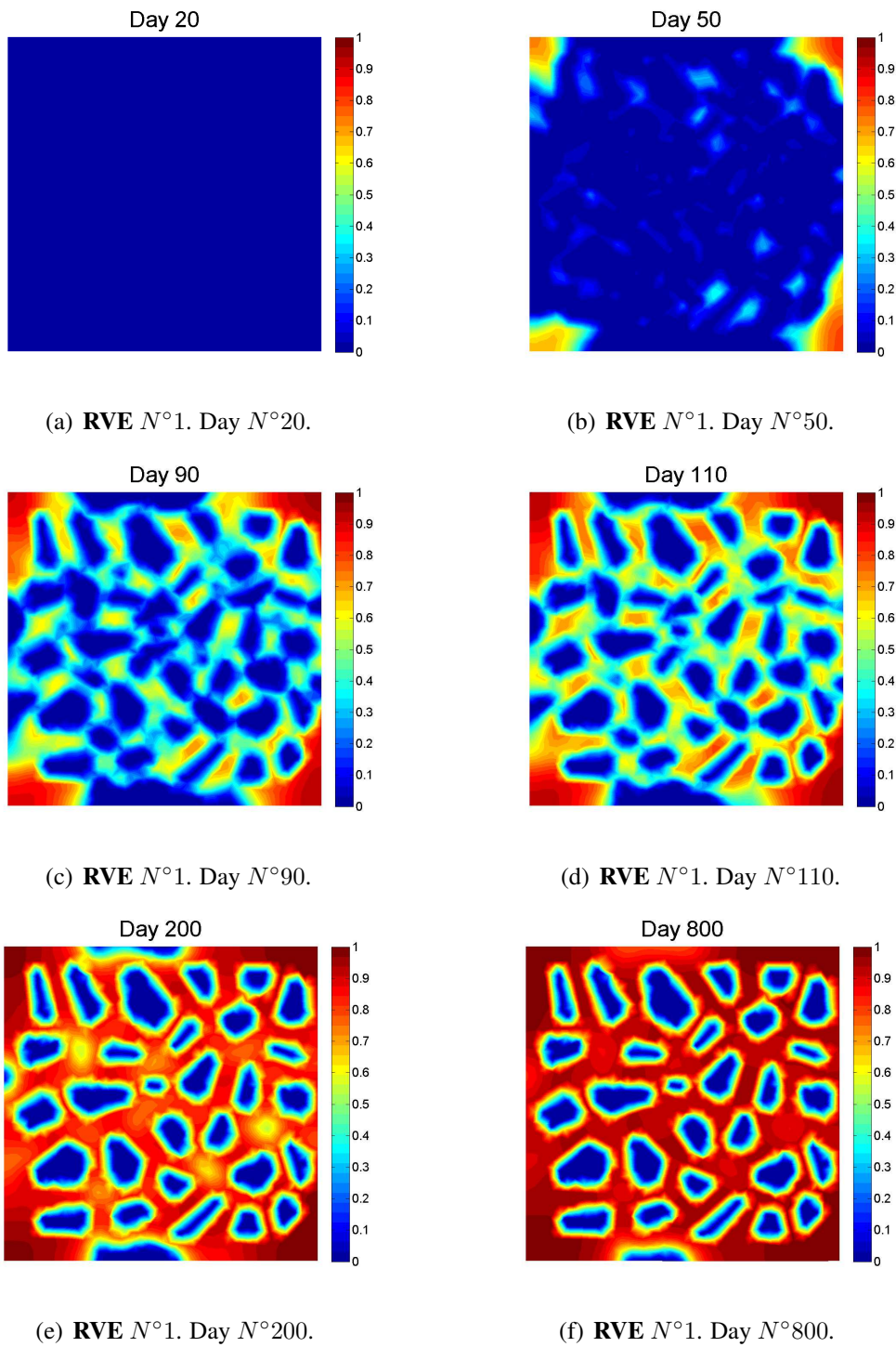
(a) **RVE** $N°1$. Day $N°20$.

(b) **RVE** $N°1$. Day $N°50$.

(c) **RVE** $N°1$. Day $N°90$.

(d) **RVE** $N°1$. Day $N°110$.

(e) **RVE** $N°1$. Day $N°200$.

(f) **RVE** $N°1$. Day $N°800$.

Figure 4: Damage progression due to ASR in **RVE** $N°1$.

(a) **RVE** $N°2$. Day $N°20$.

(b) **RVE** $N°2$. Day $N°50$.

(c) **RVE** $N°2$. Day $N°90$.

(d) **RVE** $N°2$. Day $N°110$.

(e) **RVE** $N°2$. Day $N°200$.
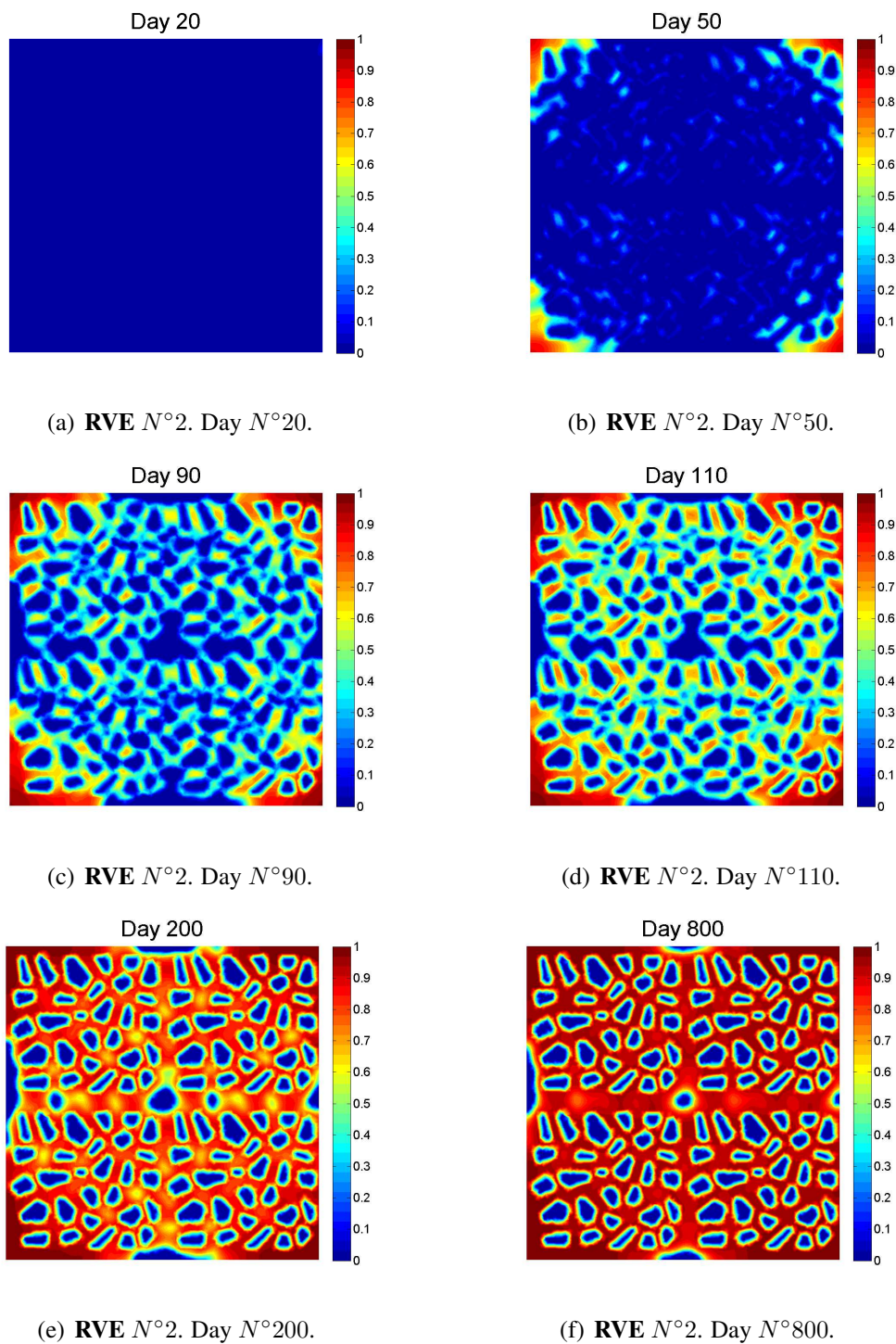
(f) **RVE** $N°2$. Day $N°800$.

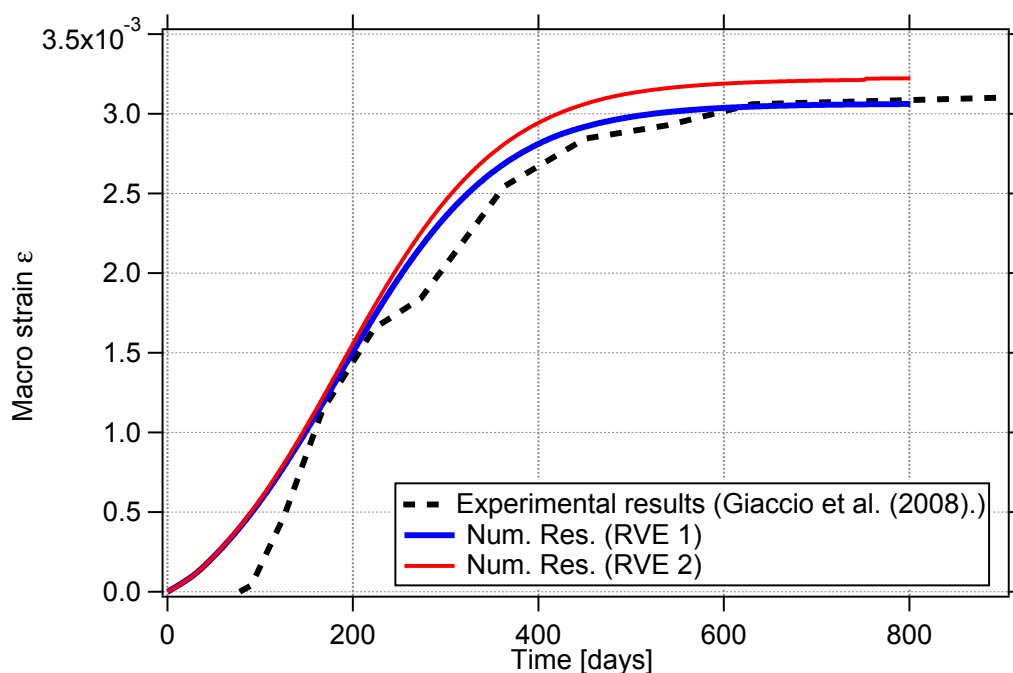Figure 5: Damage progression due to ASR in **RVE** $N°2$.

Figure 6: Numerical volumetric macro-strain versus experimental results.

7 CONCLUSIONS

A multi-scale to model ASR phenomena, based in a thermo-poro-mechanical formulation, has been presented and discussed in this work. Using a semi-concurrent formulation, the Helmholtz free energy of the mortar phase in the micro-scale is reformulated using Biot's theory for porous media in order to consider the effect of the pore pressure induced by the gel expansion. Some numerical examples showing the homogenized response of a concrete like material are presented and discussed. The lost of resistance of the material due a temperature increasing has been numerically reproduced, and the final damage configuration is presented.

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