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Multiscale assessment of damage during hydration of large structures

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Abstract.

This work presents a multiscale framework for damage modeling in cement-based materials (CBM), incorporating the effects of hydration within their heterogeneous microstructure where the degradation occurs within the cement phase. Thus, damage initiation and evolution are influenced by microscale inhomogeneities, resulting in a meso-micromechanical damage formulation. To simulate the thermo-chemo-mechanical behavior of macroscopic structures, a two-scale finite element approach is adopted, the Direct FE^2, in which the heterogeneous microstructure of the CBM is modeled through a representative volume element (RVE) where all the material properties, constitutive and evolution laws are defined. The entire framework is implemented in Abaqus® using a combination of Python scripting and Fortran user subroutines. A L-shaped body is presented to illustrate the evolution of damage. The results provide valuable insights into early-age damage mechanisms induced by hydration, highlighting the relationship between the heterogeneous CBM microstructure and the effective structural performance.

Keywords: cement-based material, damage, dFE^2, hydration, homogenization

1 Introduction

Hydration of Ordinary Portland cement (OPC) is a complex exothermic process. Cement-based materials (CBMs) undergo hydration, resulting in hydrate products that release heat and gain mechanical strength through physical, chemical, thermal, and mechanical interactions [1]. The hydration process and temperature rise may cause problems in massive structures, especially in early ages, when the temperature rise can reach the adiabatic value in the center of the elements while the boundary loses heat, causing a temperature drop. The combination of temperature gradients and autogenous effects can cause structural element cracking and reduce durability [2, 3].

To study these effects the present study focuses on a new damage model to analyze the effects of hydration and the resulting damage due to temperature evolution on early-age of CBMs. This model is based on the work of Mazars [4]. The purpose is to describe the thermo-chemo-mechanical behavior of a structural body (macrobody) using the RVE's microbody description of a CBM to predict cracking zones. The constitutive and evolution rules for each material, as well as thermal, chemical, and mechanical properties, are established at the microscale (RVE level). The method proposed by Tan et al. [5] is used to model the micro and macrobodies of the CBM structure using the software ABAQUS®. The Direct FE^2 (dFE^2) method replaces macro-to-micro and micro-to-macro quantities with multipoint constraint equations (MPCs) that relate the degrees of freedom (DOF) of the RVE and the macrobody element, requiring only one level solution strategy. It is assumed that the damage model occurs solely in cement. However, the damage initiation and evolution are influenced by the presence of inhomogeneities at this level. This work presents the main points of the ongoing research, and more details can be seen in [6].

2 Theoretical formulation: thermo-chemo-mechanical coupling

The mechanical equilibrium and heat conduction problems along with their respective boundary conditions, can be expressed in variational form and solved in terms of the displacement field $\boldsymbol{u} \in \mathcal{U}$ and the temperature field $\theta \in \Theta$. The corresponding virtual fields are denoted by $\delta\boldsymbol{u}$ and $\delta\theta$, respectively. The weak forms of the governing equations are given by:

$$\int_\Omega \boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon} \mathrm{d}\Omega - \int_\Omega \boldsymbol{b} \cdot \delta\boldsymbol{u} \mathrm{d}\Omega - \int_{\Gamma_t} \boldsymbol{t} \cdot \delta\boldsymbol{u} \mathrm{d}\Gamma = 0, \quad \forall\, \delta\boldsymbol{u} \in \mathcal{V}_u \tag{1}$$

$$\int_\Omega \rho c \dot{\theta} \delta\theta \, \mathrm{d}\Omega - \int_\Omega \boldsymbol{q} \cdot \nabla\delta\theta \, \mathrm{d}\Omega - \int_\Omega \dot{r}\delta\theta \, \mathrm{d}\Omega + \int_{\Gamma_q} \bar{q}\delta\theta \, \mathrm{d}\Gamma = 0, \quad \forall \delta\theta \in \mathcal{V}_\theta \tag{2}$$

where $\boldsymbol{\sigma}$ [Pa] is the Cauchy stress tensor, $\boldsymbol{\varepsilon}$ is the infinitesimal strain, such that $\boldsymbol{\varepsilon} = \frac{1}{2}\left(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T\right)$, $\boldsymbol{b}$ [N/kg] is the body force vector, $\boldsymbol{t}$ [Pa] is the tractions vector, $\boldsymbol{q}$ [W/m^2] is the heat flux vector, $\dot{r}$ [W/m^3] is the heat generation rate per unit volume, $\bar{q}$ is the heat flux externally prescribed and Ω represents a body with boundary Γ. Here, $\mathcal{U}$ and Θ are the admissible sets while $\mathcal{V}_u$ and $\mathcal{V}_\theta$ are the variational spaces.

2.1 Constitutive formulation and aging effects

To accurately represent the mechanical, thermal, and chemical behavior of each constituent within heterogeneous CBMs, a characterization of their microstructure is necessary. Adopting the multiscale framework introduced by Bernard et al. [7] and addressing the concrete and mortar scales – referred to as Level IV and Level III, respectively – the evolution of the cement paste microstructure at these scales can be viewed as a homogenized outcome of processes occurring at finer levels, such as Level II (cement paste level), which exhibits significantly complex behavior. Therefore, as an initial step, this study assumes that the aggregates have constant properties and adopts a simplified rheological model for the cement paste, where the total strain $\boldsymbol{\varepsilon}$ can be expressed:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^{th} + \boldsymbol{\varepsilon}^{au} \tag{3}$$

being $\boldsymbol{\varepsilon}^e$ the elastic strain, $\boldsymbol{\varepsilon}^{th}$ the thermal strain, and $\boldsymbol{\varepsilon}^{au}$ the autogenous strain. As the behavior of the hardened cement paste evolves with the hydration process, it can be represented at any stage by means of a conversion variable χ, $\chi \in [0, 1)$, named hydration degree. To account for aging effects, this work adopts the maturity concept M, which relates to χ following the definition proposed by Mazars et al. [8]:

$$M(\chi) = \left\langle \frac{\chi - \chi_o}{\chi_u - \chi_o} \right\rangle_+ \tag{4}$$

where χ_o is the percolation threshold and χ_u is the ultimate degree of hydration. Assuming isotropy, the constitutive model includes the following relations:

- Elastic response:

$$\boldsymbol{\sigma} = \frac{E(\chi)}{1+\nu(\chi)}\boldsymbol{\varepsilon}^e + \frac{\nu(\chi)}{1-2\nu(\chi)}\mathrm{tr}\left(\boldsymbol{\varepsilon}^e\right)\mathbf{I} \tag{5}$$

  where E is the Young's modulus, ν is the Poisson ratio and $\mathbf{I}$ is the second order identity tensor;
- Thermal and autogenous shrinkage strain, respectively:

$$\boldsymbol{\varepsilon}^{th} = \alpha(\chi)(\theta - \theta_0)\mathbf{I}, \qquad \boldsymbol{\varepsilon}^{au} = -\vartheta(\chi) M(\chi)\mathbf{I} \tag{6}$$

  where α is the coefficient of thermal expansion, θ_0 is the reference temperature and ϑ is the coefficient of autogenous contraction.

2.2 Material properties evolution

A water–cement ratio of $w/c \approx 0.5$ was considered and selected experimental data and multiscale predictions from the literature were used to calibrate functional relationships in terms of the maturity function $M(\chi)$. The first step is to define the percolation threshold χ_o and the ultimate degree of hydration χ_u, which were $\chi_u = 0.74$,

following Qian [9], and $\chi_o = 0.25$ according to Bernard et al. [7]. The mechanical properties are presented in eq. (7) to 9, where $\sigma_t(\chi)$ is the tensile strength, $\nu_f(\chi)$ is the Poisson ration, $G_f(\chi)$ is the fracture energy and $\bar{\varepsilon}_d^o$ is the damage threshold. In these equations the quantities $\bullet_u$ are the $\bullet(\chi_u)$.

$$\frac{E(\chi)}{E_u} = [M(\chi)]^{e_E}, \qquad \frac{\nu(\chi)}{\nu_u} = 0.544\exp(-1.743M(\chi)) + 0.919 \tag{7}$$

$$\frac{\sigma_t(\chi)}{\sigma_{t_u}} = 1 - \exp\left(-12.8\,[M(\chi)]^{0.94}\right), \qquad \frac{G_f(\chi)}{G_{f_u}} = [M(\chi)]^{e_G} \tag{8}$$

$$\bar{\varepsilon}_d^o(\chi) = \frac{\sigma_t(\chi)}{E(\chi)} \tag{9}$$

The thermal expansion coefficient α, the autogenous shrinkage coefficient ϑ, the thermal properties such as thermal conductivity k, and specific heat c are assumed constant in this initial study. The mass density ρ =1835 kg/m^3 [10] of the cement paste is also constant at the Level II scale, neglecting any mass loss due to drying.

3 Mazars damage model for early-age CBMs

The damage model proposed by Mazars [4] was used as base for this work, and was originally developed for modeling the damage behavior of brittle and quasi-brittle materials. The original model introduces a continuous isotropic damage variable $d \in [0,1]$, where $d = 0$ represents the undamaged material and $d = 1$ corresponds to complete damage. However, for CBMs, the initiation and evolution mechanisms of damage differ for tensile and compressive states, leading to distinct damage evolution rules for positive (tensile) and negative (compressive) strains. These rules are presented as follow.

3.1 Damage initiation

Assuming that positive principal strains govern damage in the cement paste during hydration, the damage initiation function originally proposed by Mazars [4] is reformulated as:

$$f = \bar{\varepsilon} - \bar{\varepsilon}_d(d;\chi) = 0, \quad \text{with} \quad \bar{\varepsilon} = \left(\sum_{i=1}^{3}\langle\varepsilon_i\rangle_+^2\right)^{1/2} = \left(\langle\varepsilon_1\rangle_+^2 + \langle\varepsilon_2\rangle_+^2 + \langle\varepsilon_3\rangle_+^2\right)^{1/2}. \tag{10}$$

Here, $\bar{\varepsilon}$ is the equivalent strain, where ε_i are the principal strains, and $\langle a\rangle_+$ denotes the positive part of a. The term $\bar{\varepsilon}_d(d;\chi)$ is a strain-like internal variable representing the current damage threshold that becomes active (i.e., $f \geq 0$) only when:

$$\bar{\varepsilon} \geq \bar{\varepsilon}_d(d,\chi) = \max\left[\bar{\varepsilon}_d^o(\chi), \max(\bar{\varepsilon})\right]. \tag{11}$$

In this work, we propose using eq. (9) to define the minimum threshold $\bar{\varepsilon}_d^o(\chi)$. Once the condition for evolution (eq. (16)) is satisfied, the initial threshold value remains fixed in the analysis.

3.2 Traction–compression damage asymmetry and the rate formulation of damage evolution

To capture the distinct behavior under tension and compression of CBMs, Mazars [4] proposed decomposing the total damage d into tensile and compressive components, d_+ and d_-, respectively:

$$d = d_+ + d_- = \epsilon_+\mathcal{F}_+(\bar{\varepsilon}) + \epsilon_-\mathcal{F}_-(\bar{\varepsilon}) \tag{12}$$

where ϵ_+ and ϵ_- are weighting coefficients that depend on the strain state $\boldsymbol{\varepsilon}$.

To distinguish between tensile and compressive effects in the damage evolution, the stress tensor is decomposed into its positive and negative components. A similar decomposition can be applied to the principal strain tensor $\hat{\boldsymbol{\varepsilon}}^e$, that is, $\hat{\boldsymbol{\varepsilon}}^e = \hat{\boldsymbol{\varepsilon}}_+^e + \hat{\boldsymbol{\varepsilon}}_-^e$. The components $\hat{\boldsymbol{\varepsilon}}_+^e$ and $\hat{\boldsymbol{\varepsilon}}_-^e$ are computed by applying Hooke's law to the respective portions of the stress tensor (see eq. (5)):

$$\hat{\boldsymbol{\varepsilon}}_+^e = \frac{1+\nu}{E}\langle\hat{\boldsymbol{\sigma}}\rangle_+ - \frac{\nu}{E}\mathrm{tr}\left(\langle\hat{\boldsymbol{\sigma}}\rangle_+\right) \quad \text{and} \quad \hat{\boldsymbol{\varepsilon}}_-^e = \frac{1+\nu}{E}\langle\hat{\boldsymbol{\sigma}}\rangle_- - \frac{\nu}{E}\mathrm{tr}\left(\langle\hat{\boldsymbol{\sigma}}\rangle_-\right) \tag{13}$$

Given this decomposition, the coefficients ϵ_+ and ϵ_-, used to weight the damage evolution in tension and compression, are defined following Arruda et al. [11] as:

$$\epsilon_+ = \frac{\sum_i \left\langle \hat{\varepsilon}^e_{+_i} \right\rangle_+}{\varepsilon^e_V}, \quad \epsilon_- = \frac{\sum_i \left\langle \hat{\varepsilon}^e_{-_i} \right\rangle_-}{\varepsilon^e_V} \quad \text{and} \quad \varepsilon^e_V = \sum_i \left(\left\langle \hat{\varepsilon}^e_{+_i} \right\rangle_+ + \left\langle \hat{\varepsilon}^e_{-_i} \right\rangle_+ \right) \tag{14}$$

where ε^e_V is the normalization factor.

For the compressive damage evolution ($\mathcal{F}_- (\bar{\varepsilon})$), we adopt the original law proposed by Mazars [4], where A_- and B_- are material parameters, and for the tensile regime ($\mathcal{F}_+ (\bar{\varepsilon})$), we adopt the so-called Oliver's Law [12] as the evolution equation, where κ is related to the specific dissipated energy g_f:

$$\mathcal{F}_- (\bar{\varepsilon}) = 1 - \frac{\bar{\varepsilon}^o_d (1 - A_-)}{\bar{\varepsilon}} - \frac{A_-}{\exp\left[B_- (\bar{\varepsilon} - \bar{\varepsilon}^o_d)\right]}, \quad \mathcal{F}_+ (\bar{\varepsilon}) = 1 - \frac{\bar{\varepsilon}^o_d}{\bar{\varepsilon}} \exp\left[\kappa \left(1 - \frac{\bar{\varepsilon}}{\bar{\varepsilon}^o_d}\right)\right] \tag{15}$$

However, to better capture general loading paths while ensuring the compliance with thermodynamic constraints, we adopt the approach originally proposed by Mazars and Lemaitre [13], rewriting the damage in eq. (12), that is, $\dot{d} = \dot{d}_+ + \dot{d}_- = \epsilon_+ \dot{\mathcal{F}}_+ (\bar{\varepsilon}) + \epsilon_- \dot{\mathcal{F}}_- (\bar{\varepsilon})$ where, for simplicity, we assume that ϵ_+ and ϵ_- remain constant during the increment. The compressive and tensile damage rate in eq. (15) are now, respectively:

$$\dot{d}_- (\bar{\varepsilon}) = \epsilon_- \left[\frac{\bar{\varepsilon}^o_d}{\bar{\varepsilon}^2} (1 - A_-) + \frac{A_- B_-}{\exp\left[B_- (\bar{\varepsilon} - \bar{\varepsilon}^o_d)\right]}\right] \langle \dot{\bar{\varepsilon}} \rangle_+, \quad \dot{d}_+ (\bar{\varepsilon}) = \epsilon_+ \left(\frac{\bar{\varepsilon}^o_d}{\bar{\varepsilon}^2} + \frac{k}{\bar{\varepsilon}}\right) \exp\left[\kappa \left(1 - \frac{\bar{\varepsilon}}{\bar{\varepsilon}^o_d}\right)\right] \langle \dot{\bar{\varepsilon}} \rangle_+ \tag{16}$$

Following Mazars and Lemaitre [13], we define the conditions for damage evolution as eq. (17). If either condition is not satisfied, the damage rate vanishes, i.e., $\dot{d} = 0$.

$$\begin{cases} f = 0 \;\Rightarrow\; \bar{\varepsilon}_d (d; \chi) = \max\left[\bar{\varepsilon}^o_d, \max(\bar{\varepsilon})\right] \\ \dot{f} = 0 \;\Rightarrow\; \dot{\bar{\varepsilon}} > 0 \end{cases} \Rightarrow \; \dot{d} > 0 \tag{17}$$

3.3 Critical damage

In this preliminary study, we do not consider critical damage, that is, $d_c = 1$.

4 Hydration model

The degree of hydration $\chi(t)$ is commonly defined as the ratio between the cumulative heat released by the hydration reaction per unit volume, r [J m^{-3}], up to time t, and the total heat of hydration per unit volume, r_∞:

$$\chi(t) = \frac{r(t)}{r_\infty}, \quad \text{where} \quad r_\infty = -\rho \Delta H = \Delta H_v. \tag{18}$$

In eq. (18), $\triangle H$ [J g^{-1}] is the heat of hydration, and ρ is the cement paste density. The volumetric heat of hydration ΔH_v [J m^{-3}] depends on the cement content C_c [g m^{-3}] and H_u [J g^{-1}], the total specific heat of hydration at complete conversion ($\chi = 1$), by [14–16]:

$$\Delta H_v = H_u C_c \quad \rightarrow \quad H_u = H_{cem} p_{cem} + 461 p_{\text{Slag}} + h_{\text{FA}} p_{\text{FA}} \tag{19}$$

$$H_{\text{cem}} = 500 p_{\text{C}_3\text{S}} + 260 p_{\text{C}_2\text{S}} + 866 p_{\text{C}_3\text{A}} + 420 p_{\text{C}_4\text{AF}} + 624 p_{\text{SO}_3} + 1186 p_{\text{FreeCaO}} + 850 p_{\text{MgO}} \tag{20}$$

In eq. (19), p_{cem}, p_{Slag}, and p_{FA} are the weight fractions of cement, slag, and fly ash, respectively, and h_{FA} the specific heat of hydration of fly ash. In eq. (20) the specific heat of hydration of cement, H_{cem} [Jg^{-1}], is estimated based on the weight fraction of the i-th compound in the total cement content [15]. Here, C_3S =0.59, C_2S=0.12, C_3A=0.07, C_4AF=0.10, SO_3=0.033, MgO=0.017 [3], and Free CaO=0.029 [15]. To calculate the overall χ for a cement paste with $w/c \approx 0.5$, the kinetic model presented by Schindler and Folliard [15] was used, that is,

$$\chi(t_{eq}) = \chi_u \cdot \exp\left(-\left[\frac{\tau}{t_{eq}}\right]^\beta\right), \quad \text{with} \quad t_{eq}(h) = \sum_t \exp\left[-\frac{E_a}{\mathcal{R}} \left(\frac{1}{\theta_r} - \frac{1}{\theta}\right)\right]. \tag{21}$$

In eq. (21), t_{eq} is the equivalent time in $[h]$, χ_u is the ultimate hydration degree, τ is the hydration time parameter $[h]$ and β is the hydration shape parameter. The equivalent time t_{eq} is used to convert the chronological time t at temperature $\theta\ [K]$, in the equivalent time t_{eq} in the reference temperature $\theta_r\ [K]$, being E_a the activation energy of the OPC $[^J/_{mol}]$, $\mathcal{R}$ is the universal gas constant $[^J/_{molK}]$ and Δt is the time variation $[h]$.

Finally, the heat generation rate associated with hydration can be specialized for this model as:

$$\dot{r} = H_u C_c \dot{\chi} = H_u C_c \chi\left(t_{eq}\right) \left(\frac{\tau}{t_{eq}}\right)^{\beta} \frac{\beta}{t_{eq}} \exp\left[-\frac{E_a}{\mathcal{R}}\left(\frac{1}{\theta\left(t\right)} - \frac{1}{\theta_r}\right)\right]. \tag{22}$$

For this application, the model parameters where obtained from Al-Hasani et al. [3] defined for the cement paste as follow: χ_u = 0.74, τ = 22.5, β = 1.03, E_a = 34528 $^J/_{mol}$, $\mathcal{R}$ = 8.314 $^J/_{molK}$ and θ_r = 23 $^\circ C$.

5 Computational homogenization strategy

The thermo-chemo-mechanical problems presented in Sections 2, 3, 4 are solved using the dFE^2 as summarized in the following.

Thermal problem By subdividing the body Ω in n_{el} elements, the discrete finite element formulation of 2 is

$$\delta\boldsymbol{\theta}^T \boldsymbol{q}_{\text{ine}} + \delta\boldsymbol{\theta}^T \boldsymbol{q}_{\text{int}} = \delta\boldsymbol{\theta}^T \boldsymbol{q}_{\text{src}} + \delta\boldsymbol{\theta}^T \boldsymbol{q}_{\text{ext}} \tag{23}$$

and using approach presented by Zhi et al. [17] a relation between the macro and microscopic quantities counterparts in the discrete form by:

$$\delta\theta^T \boldsymbol{q}_{ine} + \delta\theta^T \boldsymbol{q}_{\text{int}} - \delta\theta^T \boldsymbol{q}_{\text{src}} = \sum_{e=1}^{n_{el}} \sum_{\alpha=1}^{n_{int}} \bar{w}_\alpha \int_{\tilde{\Omega}_\alpha} (\tilde{c}\tilde{\theta}\delta\tilde{\theta} - \tilde{\boldsymbol{q}}\cdot\nabla\delta\theta - \tilde{\dot{Q}}\delta\tilde{\vartheta})\,\mathrm{d}V = \delta\tilde{\theta}^T \tilde{\boldsymbol{q}}_{ine} + \delta\tilde{\theta}^T \tilde{\boldsymbol{q}}_{\text{int}} - \delta\tilde{\theta}^T \tilde{\boldsymbol{q}}_{\text{src}} \tag{24}$$

where $\boldsymbol{q}$ are the global "flux" vectors associated to each one of the contributions, n_{int} is the number of integration points, $\tilde{\Omega}_\alpha$ is the RVE body, and $\bar{w}_\alpha$ is the scaling factor, given by $\bar{w}_\alpha = {}^{w_\alpha J_\alpha}/_{|\tilde{\Omega}_\alpha|}$, being $\left|\tilde{\Omega}_\alpha\right|$ the volume of the RVE, w_α is the weight of the α-th integration point of the macro element, and J_α is the respective Jacobian. Variables denoted by $\tilde{\bullet}$ are microscopic quantities.

Mechanical problem The quasi-static mechanical problem is derived from the principle of virtual work (eq. (1)) and solved using the dFE^2 method as proposed by Tan et al. [5]. Its discrete form is:

$$\delta\boldsymbol{u}^T \boldsymbol{f}_{\text{int}} = \delta\boldsymbol{u}^T \boldsymbol{f}_{\text{ext}} \tag{25}$$

Here, $\boldsymbol{u}$ is the global displacement vector. Following the same multiscale approach, the macro-to-micro coupling based on the Hill–Mandel principle yields [5]:

$$\delta\boldsymbol{u}^T \boldsymbol{f}_{\text{int}} = \sum_{e=1}^{n_{el}} \sum_{\alpha=1}^{n_{int}} \bar{w}_\alpha \int_{\tilde{\Omega}_\alpha} \tilde{\boldsymbol{\sigma}} : \boldsymbol{\varepsilon}\left(\delta\tilde{\boldsymbol{u}}\right) \mathrm{d}\tilde{\Omega}_\alpha = \delta\tilde{\boldsymbol{u}}^T \tilde{\boldsymbol{f}}_{\text{int}}. \tag{26}$$

Within each RVE, the mechanical behavior of the cement paste is governed by the constitutive formulation described in Subsection 2.1 and Section 3. As with the thermal problem, the coupling between the microscopic and macroscopic mechanical responses requires a consistent transfer of information between scales, achieved by prescribing appropriate boundary conditions on the RVE.

Equations (24) and (26) link the microbody (RVE) to the macrobody by means of Periodic Boundary Conditions (PBC). As a result, the RVE boundary is linked to each integration point of the macromesh. For a point located at the boundary of the RVE, the following relations apply relating each opposite RVE sides $\{\boldsymbol{y}^+, \boldsymbol{y}^-\}$:

$$\tilde{\theta}^+ - \tilde{\theta}^- = \sum_{I=1}^{n_{int}} \theta_I \boldsymbol{\nabla} N_I \cdot \left(\boldsymbol{y}^+ - \boldsymbol{y}^-\right) \text{ and } \tilde{u_i}^+ - \tilde{u_i}^- = \sum_{I=1}^{n_{int}} u_{iI} \boldsymbol{\nabla} N_I \cdot \left(\boldsymbol{y}^+ - \boldsymbol{y}^-\right) \tag{27}$$

for the temperature and displacement PBC boundary conditions, respectively. Also, to solve the systems in Eqs. 23 and 25, a relationship between the microscopic virtual quantities $\delta\tilde{\bullet}$ and the macroscopic ones $\delta\bullet$ is necessary. This relationship is given by a linear transformation $\mathbf{L}$, such that $\bullet = \mathbf{L}\tilde{\bullet}$, and consequently $\delta\bullet = \mathbf{L}\delta\tilde{\bullet}$. The matrix $\mathbf{L}$ is constructed from the Multi-Point Constraints (MPCs) that couple the scales.

6 Numerical results

This section presents a preliminary result of this research. It is considered an example under semi-adiabatic conditions, where the macrobody can exchange heat with its surroundings through convection. The macrobody is an L-shaped block with the dimensions shown in Fig. 1, which is made up of 300 bilinear quadrilateral elements (Q4). The RVE is an idealized mortar made up of a cement paste matrix and a sand volume fraction variable, which is shown in Fig. 1 as $v_s = 0.40$. The model was constructed inside the software ABAQUS® where the PBC constraints are applied according to eqs. (27) for thermal and mechanical conditions. The thermo-chemo-mechanical coupling were programmed using `UMATH`, `UMAT`, and `UEXPAN` user subroutines [18]. The initial temperature of the body, macro and micro, was $\theta_0 = 20°C$ and the water-cement ratio is $w/c = 0.50$. Other parameters used for analysis were: $\rho_{cp} = 1835\ ^{kg}/_{m^3}$, $c_{cp} = 1224\ ^{J}/_{kgK}$, $k_{cp} = 1\ ^{W}/_{m^2K}$ for cement paste; and $\rho_s = 2650\ ^{kg}/_{m^3}$, $c_s = 734\ ^{J}/_{kgK}$, and $k_s = 2.2\ ^{W}/_{m^2K}$ for sand.

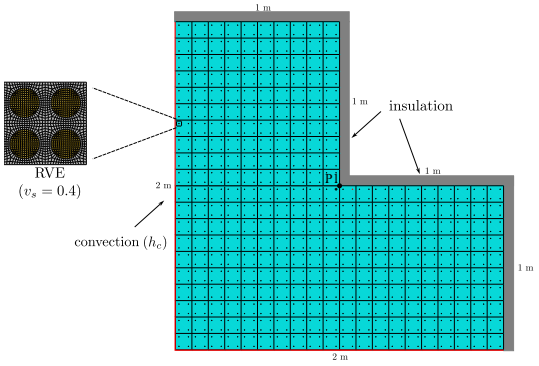
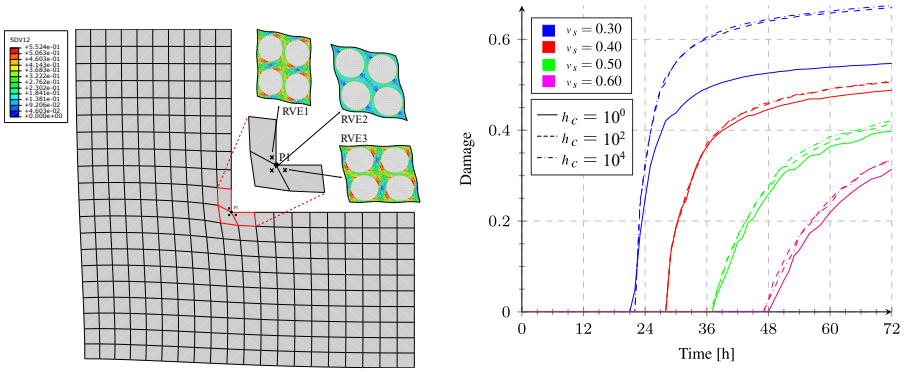


Figure 1. Representation of the L-shaped block for the macro and micromodel used for thermo-chemo-mechanical analysis under semi-adiabatic conditions. Point P1 serves as control point for damage

Figure 2 shows the evolution of the damage with time from 0 to 72 h. In fig. 2a, the isocontours of damage are presented, indicanting the potential local for cracking, and fig. 2b shows the profile for RVE1 chosen, varying the convection coefficient from $h_c = 10^0$, 10^2 e $10^4\ ^{W}/_{m^2K}$ and varying the sand fraction v_s between 0.30 and 0.60. It can be seen that, as the fraction of cement paste increases, the damage variable also increases, and it shows similar results for $h_c = 10^0$, 10^2 e $10^4\ ^{W}/_{m^2K}$, with the highest damage values placed closer to point P1.



(a) Isocontours for $v_s = 0.40$ and $h_c = 10^2\ ^{W}/_{m^2K}$

(b) Damage profile for RVE1

Figure 2. Evolution of damage for $t = 72\ h$ of hydration, indicating the zone of stress concentration and the damage profile. The isocontours in (a) are associated with the damage variable.

7 Conclusions

This study presents a novel microscale Mazars-type damage model tailored for the early-age analysis of heterogeneous cement-based materials, with a particular focus on predicting damage initiation and propagation

within the cement matrix. The numerical results confirm the model's ability to capture key features of early-age damage in cement-based materials, including the influence of sand aggregates on the nucleation and development of localized cracks. The dFE^2 implementation was shown to accurately reproduce the micromechanical response of RVEs under consistent boundary and loading conditions. Ultimately, rigorous validation against experimental data – whether from laboratory or field conditions – is essential to strengthen the predictive capacity of the model.

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