# A study on temperature rise in heterogeneous cement materials using the FE² method

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**Abstract.**

The hydration reaction of ordinary Portland cement (OPC) is a complex process that initiates as soon as the OPC meets water. During this process, hydration products are formed, changing the thermal and mechanical properties and releasing heat. Massive structures of cement-based materials (CBMs) such as damns, bridges or foundations of large buildings, tend to present a substantial increase of temperature due the great amount of heat generated by the hydration reaction which together with the mechanisms of heat transfer trough the boundaries can cause significative high temperature gradients and nonhomogeneous dilation/shrinkage, leading to cracking during the early ages. To prevent these damages, the hydration process can be numerical predicted using multi-scale models, once that the thermochemical response and increasing of temperature of the macroscale depends on the microstructural changes due the hydration reaction. In this paper, the recent computational homogenization approach direct FE² method (dFE²) is applied to predict the adiabatic and semi-adiabatic temperature rising in mortars, assuming a simple chemical kinetics law to describe the hydration of the OPC and several sand fractions. The dFE² method is a monolithic method in which the passage information macro to micro and micro to macro is not required as in the usual FE². Instead, by using the concepts of multipoint constrains the macro and micro discretization are linked allowing the imposition of the boundary conditions (linear, periodic, etc.) to the representative volume element (RVE). The implementation was made on ABAQUS finite element software by developing particular user-subroutines used to determine state of cure of cement-based materials. A example of macrostructure under semi-adiabatic conditions, exchanging heat with its surroundings by convection, is presented. The results show the adequacy of the proposed approach.

**Keywords:** CBM, temperature rise, hydration kinetics, Direct FE².

## 1 Introduction

Ordinary Portland Cement (OPC) and other hydraulic binders undergo a complex chemical reaction known as the hydration reaction, an exothermic reaction. As soon as the clinker phases interact with water, the hydration process begins, producing complex hydration products that give cement paste, mortar, and concrete their physical properties. Massive concrete structures may have their structural integrity compromised as a result of the coupled effect of nonuniform thermal expansion, as a consequence of temperature gradients in a semi-adiabatic cure conditions, and chemical/autogenous shrinkage, as the cement hydrates. The accurate assessment of the material's physical characteristics at each phase and scale, as well as the impact of interface interactions that result from the complex evolving microstructures during hydration, are necessary for the prediction of the thermochemo-mechanical response of cement-based structures.

Models to comprehend the evolving cementitious microstructure at first ages and its impact on the mechanical and thermal properties have continuously been proposed, see the works of Bernard et al. [1], Constantinides and Ulm [2], Pichler [3] and Honorio et al. [4]. Another topic of interest has been the numerical prediction of CBM hydration. There are numerous studies that use the Finite Element Method (FEM), primarily by treating the engineering structure as one scale and the mechanical and thermal properties as averaged quantities. For examples, see the works of de Borst and van den Boogaard [5], De Schutter [6], and Cervera et al. [7], to name a few. Numerical analysis based on Representative Volume Element (RVE) are also explored, where the model presented by Bentz have been extensively employed in the literature. In order to capture the coupled effects of the hydration reaction to the thermal expansion and autogenous shrinkage strain, newer numerical methods have recently been proposed; for examples, see the phase field methods in Nguyen et al. [8, 9].

Here, based on recent developments in the computational homogenization approach, we propose a different methodology for modeling the effects of hydration. The main concept is to completely predict the thermal behavior of an engineering structure (macrobody) using the RVE's description of the microbody of a specific CBM. In this regard, all physical properties will be defined at the RVE level, where we are able to establish specific constitutive and evolution laws for each material and also look into the implications of the Interface Transition Zone (ITZ) on the behavior of macrobodies.

Conventional FE$^2$ approaches use nested FEM simulations to solve whole problem, see Matouš et al. [10] for a review. Just lately, the passage of the macro-micro-macro quantities were replaced by multipoint constrains equations (MPCs) relating the Degrees Of Freedom (DOF) of the RVE in terms of the required boundary conditions on the RVE (linear, periodic, etc) and also the relation of the RVE DOF and the macro element DOF. This was coined as direct FE$^2$, see Tan et al. [11], Koyanagi et al. [12], Zhi et al. [13, 14], named here just as dFE$^2$. Using the dFE$^2$ approach Zhi et al. [14] has demonstrated some particular features associated with the so-called microscale thermal inertia effect described in Ramos et al. [15], Ramos and Rossi [16].

In this work we propose to model the thermal behavior of CBMs using the dFE$^2$ to model the thermal behavior of the massive structural engineering body. In this regard, we proposed the use of a very simple empirical chemical kinetics law to describe the hydration of the cement paste, which is assumed to describe in a average sense the behavior of Level II as defined by Bernard et al. [1], see Figure 1.

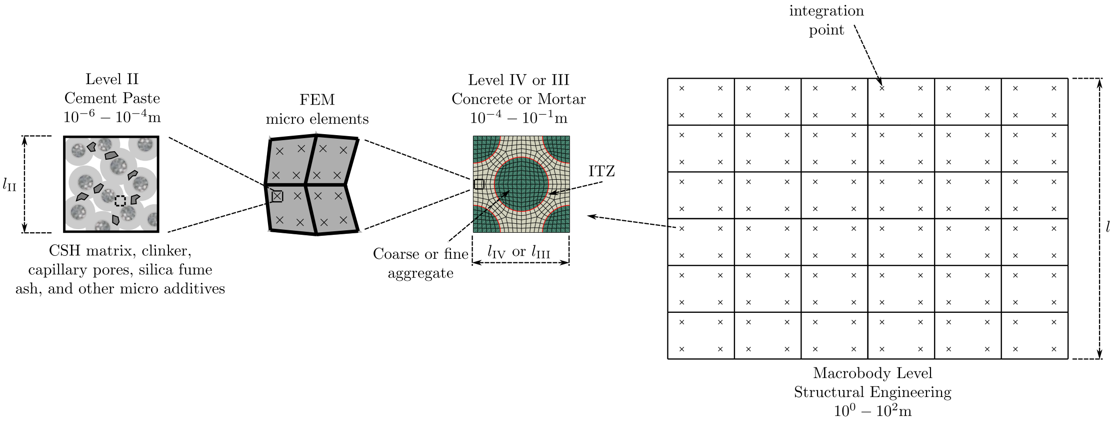


Figure 1. A model for a massive concrete engineering structure's computational homogenization analysis. Level II is an idealization proposed by Bernard et al. [1].

This work is divided into 5 sections, including this introduction. First, in section 2 we present the main ideas behind the dFE$^2$ method applied to the thermal conduction in rigid bodies. After, in section 3, the kinetics of the hydration of the OPC is outlined. Section 4 is devoted to a semi-adiabatic numerical example and in 5 we present the conclusions. In order to give the reader a thorough understanding of the topic, the subject is presented with a primary focus on the most important results.

## 2 Modeling thermal conduction problem by the dFE$^2$ method

The variational form of the heat conduction problem, reads: Find the temperature $\theta \in H^1 \times (0, t_f)$ such that

$$\int_{\Omega} c\dot{\theta}\delta\theta \,\mathrm{d}V - \int_{\Omega} \boldsymbol{q} \cdot \delta\boldsymbol{g} \,\mathrm{d}V = \int_{\Omega} \dot{Q}\delta\theta \,\mathrm{d}V - \int_{\partial\Omega_q} \bar{q}\delta\theta \,\mathrm{d}A, \;\; \forall \delta\theta \in H_0^1 \tag{1}$$

subjected to initial and boundary conditions. In this equation $\rho$ is the density of the material, $\boldsymbol{q}$ is the heat flux vector, which follows Fourier's law, $\boldsymbol{q} = -\mathbf{k}\nabla\theta$, being $\mathbf{k}$ the conductivity tensor, $\boldsymbol{g} = \boldsymbol{\nabla}\theta$, and $\dot{Q}$ is the heat generation rate per unit of volume, a source term which plays a very import role in the hydration of cementious materials problem and will be discussed in section 3.

By subdividing the body $\Omega$ in $n_{el}$ elements, $\Omega = \cup_{e=1}^{n_{el}}\Omega^e$, the discrete equations associated to the standard FEM are

$$\delta\boldsymbol{\theta}^T\boldsymbol{q}_{\text{ine}} + \delta\boldsymbol{\theta}^T\boldsymbol{q}_{\text{int}} = \delta\boldsymbol{\theta}^T\boldsymbol{q}_{\text{src}} + \delta\boldsymbol{\theta}^T\boldsymbol{q}_{\text{ext}} \tag{2}$$

where

$$\boldsymbol{q}^e_{\text{ine}} = \int_{\Omega^e} c\boldsymbol{N}^T\boldsymbol{N}\,\mathrm{d}V\dot{\boldsymbol{\theta}},\ \boldsymbol{q}^e_{\text{int}} = \int_{\Omega^e}\mathbf{B}^T\mathbf{K}\mathbf{B}\,\mathrm{d}V\boldsymbol{\theta},\ \boldsymbol{q}^e_{\text{src}} = \int_{\Omega^e}\dot{Q}\boldsymbol{N}^T\,\mathrm{d}V,\ \text{and}\ \boldsymbol{q}^e_{\text{ext}} = -\int_{\Omega^e} q_n\boldsymbol{N}^T\,\mathrm{d}V.$$

where $\boldsymbol{\theta}$ is the global nodal temperature vector and $\boldsymbol{q}$ are the "flux" global vectors associated to each one of the contributions, $\boldsymbol{N}$ is the shape function vector, $\mathbf{B}$ is the matrix of the derivatives of the shape functions, and $\mathbf{K}$ is conductivity matrix.

### 2.1 dFE$^2$ method

The monolithic method presented by Zhi et al. [14] establish a relation between the macro and microscopic quantities counterparts by

$$\begin{aligned}\delta\boldsymbol{\theta}^T\boldsymbol{q}_{\text{ine}} + \delta\boldsymbol{\theta}^T\boldsymbol{q}_{\text{int}} - \delta\boldsymbol{\theta}^T\boldsymbol{q}_{\text{src}} &= \sum_{e=1}^{n_{el}}\sum_{\alpha=1}^{n_{int}}\bar{w}_\alpha\int_{\tilde{\Omega}_\alpha}\left(\tilde{c}\tilde{\theta}\delta\tilde{\theta} - \tilde{\boldsymbol{q}}\cdot\delta\tilde{\boldsymbol{g}} - \dot{\tilde{Q}}\delta\tilde{\vartheta}\right)\mathrm{d}V\\ &= \delta\tilde{\boldsymbol{\theta}}^T\tilde{\boldsymbol{q}}_{\text{ine}} + \delta\tilde{\boldsymbol{\theta}}^T\tilde{\boldsymbol{q}}_{\text{int}} - \delta\tilde{\boldsymbol{\theta}}^T\tilde{\boldsymbol{q}}_{\text{src}}\end{aligned} \tag{3}$$

where $n_{int}$ is the number of integration points, $\tilde{\Omega}_\alpha$ is the RVE body, and $\bar{w}_\alpha$ is the scaling factor

$$\bar{w}_\alpha = \frac{w_\alpha J_\alpha}{\left|\tilde{\Omega}_\alpha\right|} \tag{4}$$

where $\left|\tilde{\Omega}_\alpha\right|$ is the volume of the RVE, $w_\alpha$ is the weight of the $\alpha$-th integration point of the macro element, and $J_\alpha$ is the respective Jacobian.

Equation 3 can be seen as the bridge from microbody (RVE) to the macrobody and is solved enforcing Linear Boundary or Periodic Boundary Conditions, LBC or PBC respectively, at the microscopic boundary, RVE boundary associated to each integration point of the macromesh. For a point at the boundary of the RVE such conditions read

$$\tilde{\theta} = \sum_{I=1}^{n_{int}}\left(N_I\theta_I + \theta_I\boldsymbol{\nabla}N_I\cdot\boldsymbol{y}\right) \tag{5}$$

for LBC and

$$\tilde{\theta}^+ - \tilde{\theta}^- = \sum_{I=1}^{n_{int}}\theta_I\boldsymbol{\nabla}N_I\cdot\left(\boldsymbol{y}^+ - \boldsymbol{y}^-\right) \tag{6}$$

for PBC.

## 3 Hydration kinetics

The hydration reaction of OPC is an exothermic process and it can be measured by means of the *degree of cure or degree of hydration* of the reaction $\chi$, $\chi \in [0, 1)$, in a specific reference or cure temperature. To obtain the value of $\chi$, experimental or kinetics models are often related to the heat amount released by the hydration reaction $Q$, until time $t$, and the total heat of the hydration reaction $Q_\infty$, respectively, defined as:

$$\chi\left(t\right) := \frac{Q\left(t\right)}{Q_{\infty}} = \frac{\displaystyle\int_{0}^{t} \dot{Q}\mathrm{d}t}{\displaystyle\int_{0}^{\infty} \dot{Q}\mathrm{d}t}, \tag{7}$$

The total heat of the hydration reaction per unit volume at complete hydration $Q_{\infty}$ is a function of the composition of the OPC, the cement content $C_c$ in the material and the water/cement ratio (w/c) [17]. Each compound of the OPC, presents a individual heat of hydration. The total volumetric heat of hydration of OPC can be described as [17, 18]

$$\triangle H_v = H_u C_c \tag{8}$$

where $C_c$ is the cementitious material content and $H_u$ is the total heat of the cementitious at complete hydration ($\chi = 1$) is

$$H_u = H_{\text{cem}} p_{\text{cem}} + 461 p_{\text{Slag}} + h_{\text{FA}} p_{\text{FA}} \tag{9}$$

where $p_{\text{cem}}$ is the cement weight ratio, $p_{\text{Slag}}$ is the slag weight ratio, $p_{\text{FA}}$ is the fly ash weight ratio, and $h_{\text{FA}}$ is the heat of hydration of fly ash. All the rations are in terms of the total cementitious content. The total heat of hydration of the Portland cement and at complete hydration can be estimated using

$$H_{\text{cem}} = 500 p_{\mathrm{C_3S}} + 260 p_{\mathrm{C_2S}} + 866 p_{\mathrm{C_3A}} + 420 p_{\mathrm{C_4AF}} + 624 p_{\mathrm{SO_3}} + 1186 p_{\text{FreeCaO}} + 850 p_{\text{MgO}} \tag{10}$$

where $p_i$ is the weight ratio of the $i$-th compound in terms of the total cement content and these were obtained from the literature, as: $C_3S$ =0.59, $C_2S$=0.12, $C_3A$=0.07, $C_4AF$=0.10, $SO_3$=0.033, MgO=0.017 ([19]), and Free CaO=0.029 ([17]).

The heat generation rate is written in terms of the conversion variable $\chi$ as

$$\dot{Q} = \triangle H_v \frac{\mathrm{d}\chi}{\mathrm{d}t}. \tag{11}$$

### 3.1 Three-parameter exponential hydration model

The so-called three-parameter exponential, modelSchindler and Folliard [17], Al-Hasani et al. [19], Riding et al. [20], have been extensively used in the literature to represent the sigmoid shaped curve and thus approximately describe the chemical kinetics behavior of OPC pastes. This model is

$$\chi\left(t_{eq}\right) = \chi_u \cdot \exp\left(-\left[\frac{\tau}{t_{eq}}\right]^{\beta}\right) \tag{12}$$

where $t_{eq}$ is the equivalent time or age (h), $\tau$ is the hydration time parameter (h), $\beta$ is the hydration shape parameter, and $\chi_u$ is the ultimate degree of hydration, an upper bound for the hydration conversion lower than 1 and strongly dependent of the $^{w}/_{c}$ ratio, see the discussion in Schindler and Folliard [17]. The equivalent age, also known as maturity function, is introduced in the modeling to convert the chronological hydration age $t$ of a cement paste cured at any temperature $\theta$ to an equivalent curing age $t_{eq}$ for a specimen cured at a specific reference temperature $\theta_r$. For an incremental procedure the equivalent age is

$$t_{eq}\left(t\right) = \sum_{0}^{t} \exp\left(-\frac{E_a}{R} \cdot \left(\frac{1}{\theta} - \frac{1}{\theta_r}\right)\right) \Delta t \tag{13}$$

where $E_a$ is the activation energy ($^{\mathrm{J}}/_{\mathrm{mol}}$) and $R$ is the universal gas constant, 8.3144 $^{\mathrm{J}}/_{\mathrm{mol\,K}}$. Since all the requisites of the hydration kinetics are presented, it is possible to specialize the heat generation rate for the cement paste, Eq. 11, associated to hydration kinetics as

$$\dot{Q}_{cp} = H_u C_c \frac{\mathrm{d}\chi}{\mathrm{d}t_{eq}} \frac{\mathrm{d}t_{eq}}{\mathrm{d}t} = H_u C_c \chi\left(t_{eq}\right) \left(\frac{\tau}{t_{eq}}\right)^{\beta} \frac{\beta}{t_{eq}} \exp\left(\frac{E_a}{R} \cdot \left(\frac{1}{\theta_r} - \frac{1}{\theta}\right)\right). \tag{14}$$

# 4 Numerical results

In this section we present an example under semi-adiabatic conditions where the macrobody can exchanges heat with its surroundings by convection. The structure, macromodel, considers a square block of 1m side discretized by 100 bilinear quadrilateral elements (Q4) while the RVE is a idealized mortar composed by a cementitious matrix with sand volume fraction of 40%, see Fig. 2. The model is constructed inside the software ABAQUS where the PBCs constrains are applied according Eq. 6. Also the central point of the RVEs has temperature prescribed. The kinetics model presented in section 3 was programmed inside a UMATH user subroutine. The initial temperature of the body, macro and micro, was considered as $\theta_o = 20$ ºC.

The complete set of physical and chemical parameter used in this work are: $\chi_u = 0.74$, $\beta = 1.03$, $\tau = 22.50$ h, $E_a = 34528$ J/mol, $\theta_r = 23$ ºC for the kinetics model; and $\rho_{cp} = 1835$ kg/m$^3$, $c_{cp} = 1224$ J/kgK, $\lambda_{cp} = 1$ W/m$^2$K, $\rho_s = 2650$ kg/m$^3$, $c_s = 734$ J/kgK, and $\lambda_s = 2.2$ W/m$^2$K for thermal parameters of cement paste and sand, respectively, were $\lambda$ is the thermal conductivity.

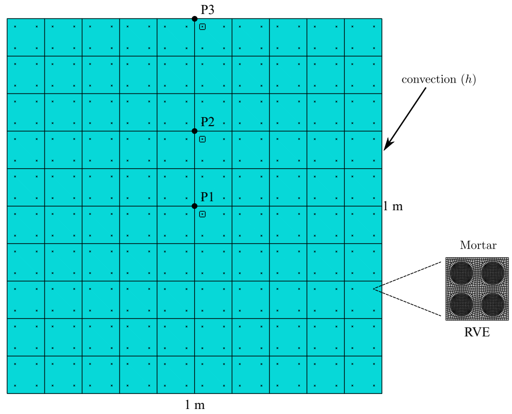


Figure 2. Representation of the square block for the macro and micromodel used for analysis of the temperature rising under semi-adiabatic conditions. Points P1 to P3 serve as control points for measuring $\theta$ and $\chi$.

Figure 3 shows the temperature evolution isocontours for the unitary block at time $t = 24$ h and $t = 72$ h and the REV with $v_s = 0.40$ for points P1, P2, and P3. A coefficient of convection of $h = 10$ W/m$^2$K is considered for all boundary walls.

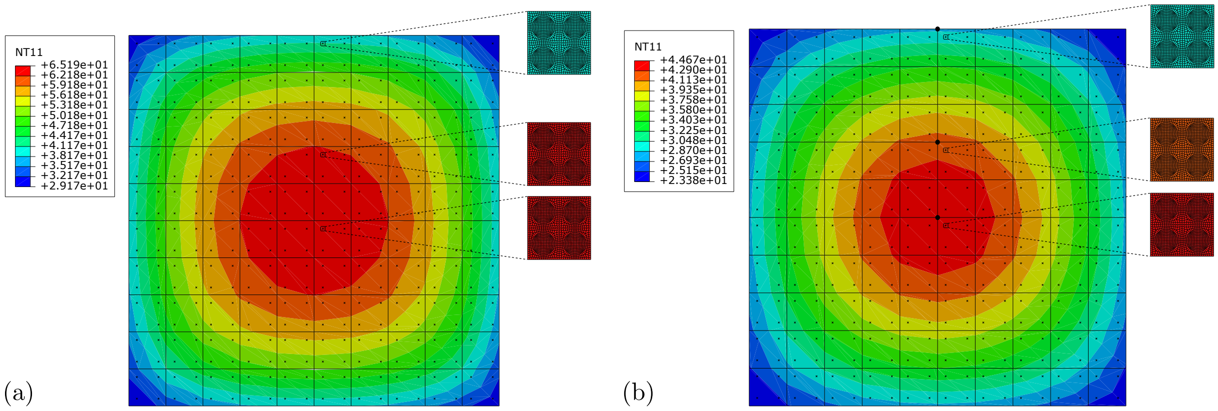


Figure 3. Temperature evolution for the unitary block for points P1, P2, and P3 under semi-adiabatic conditions with $v_s = 0.40$. (a) $t = 24$ h and (b) $t = 72$ h.

The evolution of the $\chi$ along time is depicted in the Fig. 4 for the combination of $h = 10$ W/m$^2$K and $v_s = 0.4$, highlighting the three RVEs close to the selected control points in the macroscale. The points P1 and P2 are closer from the center of the block and presented higher values of $\chi$, which are about 0.68. As expected, the point P3 presented a value of $\chi$ lower than P1 and P2 due the heat exchanged with the boundary, having $\chi = 0.61$.

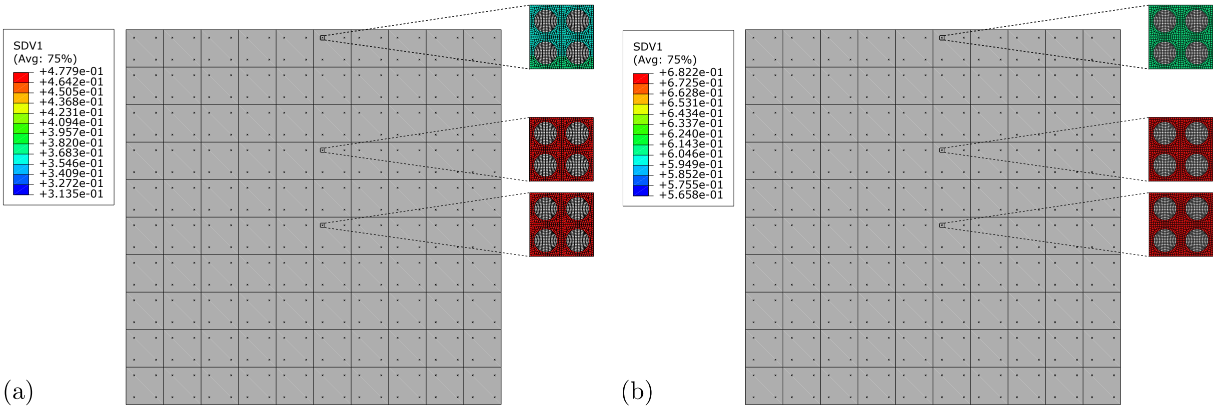
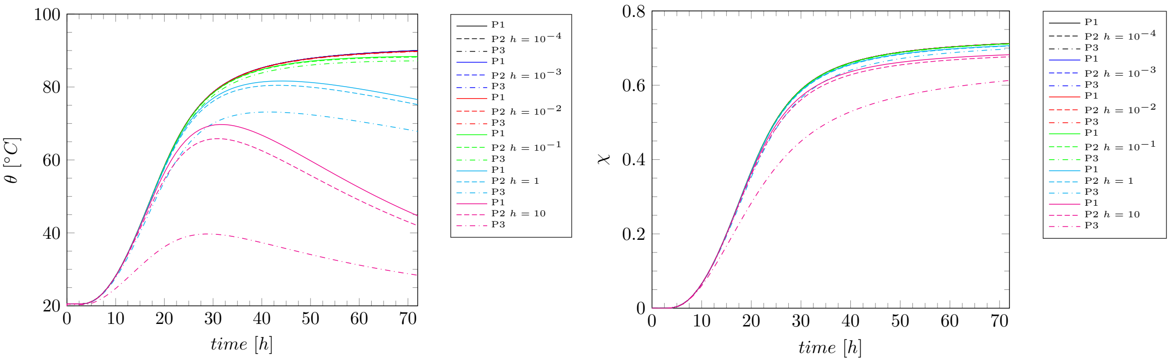


Figure 4. Hydration evolution for the unitary block for points P1, P2, and P3 under semi-adiabatic conditions with $v_s = 0.40$. (a) $t = 24$ h and (b) $t = 72$ h.

Figure 5 shows the temperature (5a) and hydration (5b) profiles for point P1 to P3 in Fig. 2 varying the convection coefficient from $h = 10^{-4}$ W/m$^2$K to $h = 10$ W/m$^2$K. It should be noted that as the convection coefficient varies, the values of the temperature profiles change significantly, mainly for values greater than $10^1$ and having a greater impact for the P3 point, which is closer to the body's border region. Similar results are found for the degree of hydration because it is temperature dependent, indicating that for high values of $h$, the gradient of the degree of hydration can be quite high in the body.



(a) Temperature profile.

(b) Hydration profile.

Figure 5. Temperature and hydration profiles for point P1 to P3 varying the convection coefficient.

## 5 Conclusions

Based on the physical-chemical characteristics of the microscale (RVE), cement matrix and inhomogeneities (sand particles), this paper presented a computational homogenization strategy to determine the semi-adiabatic temperature rise of structures of heterogeneous cementitious materials. For a given RVE the macroscopic temperature and hydration profiles were determined showing the impact of the cooling rate on macroscopic body. These are promising results that aid the understanding the complex interactions that can lead to cracking of the micro-macroscopic body in real applications. Future works will explore the effect of the sand content in heating of the mortars and the effect of the consideration of the interface effect between the cement matrix and the sand, varying the values of conductance in the interface transition zone (ITZ).

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**Authorship statement.** The authors hereby confirm that they are the sole liable persons responsible for the authorship of this work, and that all material that has been herein included as part of the present paper is either the property (and authorship) of the authors, or has the permission of the owners to be included here.

## References

[1] O. Bernard, F.-J. Ulm, and E. Lemarchand. A multiscale micromechanics-hydration model for the early-age elastic properties of cement-based materials. *Cement and Concrete Research*, vol. 33, n. 9, pp. 1293–1309, 2003.
[2] G. Constantinides and F.-J. Ulm. The effect of two types of c-s-h on the elasticity of cement-based materials: Results from nanoindentation and micromechanical modeling. *Cement and Concrete Research*, vol. 34, n. 1, pp. 67–80, 2004.
[3] C. Pichler. *Multiscale characterization and modeling of creep and autogenous shrinkage of early-age cement-based materials*. Phd thesis, Technischen Universität Wien. in English, 2007.
[4] T. Honorio, B. Bary, and F. Benboudjema. Thermal properties of cement-based materials: Multiscale estimations at early-age. *Cement and Concrete Composites*, vol. 87, pp. 205–219, 2018.
[5] de R. Borst and van den A. H. Boogaard. Finite element modeling of deformation and cracking in early–age concrete. *Journal of Engineering Mechanics*, vol. 120, n. 12, pp. 2519–2534, 1994.
[6] G. De Schutter. Finite element simulation of thermal cracking in massive hardening concrete elements using degree of hydration based material laws. *Computers & Structures*, vol. 80, n. 27, pp. 2035–2042, 2002.
[7] M. Cervera, R. Faria, J. Oliver, and T. Prato. Numerical modelling of concrete curing, regarding hydration and temperature phenomena. *Computers & Structures*, vol. 80, n. 18, pp. 1511–1521, 2002.
[8] T.-T. Nguyen, D. Waldmann, and T. Q. Bui. Computational chemo-thermo-mechanical coupling phase-field model for complex fracture induced by early-age shrinkage and hydration heat in cement-based materials. *Computer Methods in Applied Mechanics and Engineering*, vol. 348, pp. 1–28, 2019.
[9] T.-T. Nguyen, D. Waldmann, and T. Q. Bui. Phase field simulation of early-age fracture in cement-based materials. *International Journal of Solids and Structures*, vol. 191-192, pp. 157–172, 2020.
[10] K. Matouš, M. G. Geers, V. G. Kouznetsova, and A. Gillman. A review of predictive nonlinear theories for multiscale modeling of heterogeneous materials. *Journal of Computational Physics*, vol. 330, pp. 192–220, 2017.
[11] V. B. C. Tan, K. Raju, and H. P. Lee. Direct $FE^2$ for concurrent multilevel modelling of heterogeneous structures. *Computer Methods in Applied Mechanics and Engineering*, vol. 360, pp. 112694, 2020.
[12] J. Koyanagi, K. Kawamoto, R. Higuchi, V. B. C. Tan, and T.-E. Tay. Direct $FE^2$ for simulating strain-rate dependent compressive failure of cylindrical cfrp. *Composites Part C: Open Access*, vol. 5, pp. 100165, 2021.
[13] J. Zhi, K. Raju, T.-E. Tay, and V. B. C. Tan. Transient multi-scale analysis with micro-inertia effects using direct $FE^2$. *Computational Mechanics*, vol. 67, n. 6, pp. 1645–1660, 2021a.
[14] J. Zhi, K. Raju, T.-E. Tay, and V. B. C. Tan. Multiscale analysis of thermal problems in heterogeneous materials with Direct $FE^2$ method. *International Journal for Numerical Methods in Engineering*, vol. 122, n. 24, pp. 7482–7503, 2021b.
[15] G. R. Ramos, dos T. Santos, and R. Rossi. An extension of the hill-mandel principle for transient heat conduction in heterogeneous media with heat generation incorporating finite rve thermal inertia effects. *International Journal for Numerical Methods in Engineering*, vol. 111, n. 6, pp. 553–580, 2017.
[16] G. R. Ramos and R. Rossi. A novel computational multiscale approach to model thermochemical coupled problems in heterogeneous solids: Application to the determination of the state of cure in filled elastomers. *Computer Methods in Applied Mechanics and Engineering*, vol. 351, pp. 694–717, 2019.
[17] A. K. Schindler and K. J. Folliard. Heat of Hydration Models for Cementitious Materials. *ACI Materials Journal*, vol. 102, n. 1, 2005.
[18] R. Bogue. *The Chemistry of Portland Cement*. Reinhold publishing corporation, 1947.
[19] L. E. Al-Hasani, J. Park, G. Perez, H. N. Herndon, J. B. Brown, Y. K. Cho, T. R. Gentry, and K. E. Kurtis. Quantifying concrete adiabatic temperature rise based on temperature-dependent isothermal calorimetry; modeling and validation. *Materials and Structures*, vol. 55, n. 7, pp. 191, 2022.
[20] K. A. Riding, J. L. Poole, K. J. Folliard, M. C. G. Juenger, and A. K. Schindler. Modeling hydration of cementitious systems. *ACI Materials Journal*, vol. 109, n. 2, 3.