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MESO-SCALE THERMAL ENERGY STORAGE SIMULATIONS OF CEMENTITIOUS COMPOSITES MADE WITH RECYCLED BRICK AGGREGATES CONTAINING PCM

Christoph Mankel[a], Antonio Caggiano[a,b], Andreas Koenig[c], Mona Sam[a], Gideon van Zijl[d] and Eddie A.B. Koenders[a]

[a] *Institute of Construction and Building Materials, Technische Universität Darmstadt, Franziska-B.-Str 3, 64287 Darmstadt, Germany, mankel@wib.tu-darmstadt.de, caggiano@wib.tu-darmstadt.de sam@wib.tu-darmstadt.de, koenders@wib.tu-darmstadt.de*

[b] *Universidad de Buenos Aires, LMNI, INTECIN, CONICET, Buenos Aires, Argentina, acaggiano@fi.uba.ar*

[c] *Department of Prosthodontics and Dental Materials Science, Leipzig University, Leipzig, Germany akoenig@uni-leipzig.de*

[d] *Department of Civil Engineering, Stellenbosch University, South Africa, gvanzijl@sun.ac.za*

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Abstract. The use of concrete as construction and building material has enormously increased in the last decades. Innovations in the concrete industry are asking for answers in terms of reusing construction demolishing waste, energy saving concepts and cost-effective solutions for CO_2 reductions. Therefore, the concrete industry has committed itself towards developing novel technologies for new materials, which are aimed at reducing its carbon footprint dramatically. One promising solution can be achieved by turning cement-based elements into active energy storing systems via the integration of Phase Change Materials (PCMs), to be accommodated in a concrete's open porosity.

In this regard, this work deals with investigating the advanced coupling of two physical mechanisms represented by the thermal energy storage problem and the effect of mesoscale heterogeneities, where the latter is explicitly taken into account. The thermal response of Cementitious Composites made with Recycled Brick Aggregates (RBAs) containing PCM, along with the occurring phase transformation phenomena will be simulated at the meso-scale level. Particularly, 3D mesostructures considering coarse aggregates with embedded PCMs will provide a fundamental basis for the analysis of the morphological influence on the effective thermal energy storage capacity of such composites. The basic equations, employed for predicting phase transformation phenomena in PCM-based systems, and the corresponding simulations demonstrate the capability of the proposed modelling approach. Laboratory characterization of PCM-RBA-mortars were also performed using several test methods and are used as a benchmark for calibration purposes. The research activities presented are developed within the framework of the "2CENERGY" (A Coupled multiscale approach for modelling ENERGY storage phenomena in Cementitious systems) project founded by the Alexander von Humboldt-Foundation (http://www.avh.de).

1 INTRODUCTION

Building energy consumption could be easily reduced by employing smart materials that passively control the heat flow and temperature fluctuations in residential and commercial buildings (Aidan et al., 2017). Cementitious composites containing Phase Change Materials (PCMs) have been employed in the last years as a way to enhance the energy efficiency and saving of new construction (Ricklefs et al., 2017). A huge Thermal Energy Storage (TES) in PCMs is available in form of latent heat by reversibly changing phase between solid-liquid and vice versa. Therefore, the inclusion of PCMs in concrete could significantly improve the thermal properties of such a material, making it greener and more eco-friendly in construction and building applications (Devaux and Farid, 2017).

Nowadays the concrete industry is asking for innovation and smart materials. In this context, the implementation of components from innovative and sustainable materials using 3D printing technology is of particular importance (Kruger et al., 2019). Experimental activities available in literature, at several scales of observation, aimed at reporting the main benefits in terms of thermal properties of cementitious materials containing PCMs (Shadnia et al., 2015). Some contributions reviewed the effect of the PCMs on the resulting mechanical capacities of concrete (Niall et al., 2017). Other works demonstrated that by employing PCMs in concrete allows to have a certain beneficially reduction in terms of hydration heat during the hardening process of the fresh concrete (Kim et al., 2015).

Plenty of theoretical and numerical formulations have been proposed for analyzing TESs in porous cement pastes, mortar and/or concretes containing phase change materials. The majority of these models arise from an extension of the so-called Stefan problem (Crank, 1984). The solution of this latter has been classically treated in literature by means of three main methods: (i) the fixed grid method (Eyres et al. 1946), (ii) the deformed grid method (Lynch and O`Neill, 1981) and (ii) a combination of these two latter (Udaykumar et al., 1999). Simulation examples related to cementitious composites are those related to the use of the so-called Enthalpy-based Method (EM), which moves into the fixed grid solution. Then, the Apparent Calorific Capacity Method (ACCM) (Šavija and Schlangen, 2016, Thiele et al., 2016) (and the Heat Source Method (HSM) (Rostamizadeh et al., 2012, Fachinotti et al., 1999) represent two main alternatives used for solving the EM.

Concrete and other cementitious materials are multiphase (composite) materials and, for this reason, they can be considered and modelled as homogeneous continuums at the macroscale and/or structural practice-oriented one, while, at lower levels (meso-, micro- or even nano-scale) multi-phase composite approaches can be considered. Available models can be thus categorized in this matter by means of those scales of observation. Structural-scale models allow to capture the essence of heat storage phenomena at the structural (building physics) scale level (Heim and Clarke, 2004).

Macro-scale models are based on the assumption that the schematized material acts as a continuum and homogeneous medium (Tittelein et al., 2015). By considering lower scales of analysis (i.e., meso- and microscale behavior of PCM composite materials), the mechanism of PCMs, affected by external thermal fluctuations, can be better understood. At these lower scales the material can be idealized by considering different phases which together constitute the composite. Thereby, the interaction among the different phases (i.e., matrix, aggregates, PCMs, hydrated products, voids, water and possible interfaces between them) is explicitly considered in these approaches (Aguayo et al., 2017).

This paper shows the results of an experimental research program aimed at investigating the thermal energy storage performance of various mortars made with Recycled Brick Aggregates (RBAs), while filled with Phase Change Materials (PCMs). More specifically, this work presents the possibility of adding a large volume of PCMs (here paraffin waxes) in the high volume of capillary pore space in RBAs (including also cracks). All components i.e., paste, RBA and the used PCM are thermally analyzed with Differential Scanning Calorimetry (DSC). Furthermore a thermal analysis of six different composite mixtures with two different RBAs and three different PCM volume fractions will be performed through specially designed "DKK" spherical specimens (Mankel et al., 2019, Caggiano et al., 2019) which is patented at the *Institut für Werkstoffe im Bauwesen* – TU Darmstadt (Patent 123-0069 AZ 2018/21). Together with this thermal study, corresponding mechanical tests under bending and compression load were also considered.

This work proposes also a theoretical model for simulating the thermal behavior in hardened PCM-RBA mortars. An Enthalpy-based approach formulated in the framework of the Apparent Calorific Capacity Method (ACCM) is solved to accurately analyze the above mentioned phenomena. The model has been validated at macroscale by means of temperature curves, measured from three different mortars without PCMs and with two different amounts of PCM volume fraction contents. Then, the thermal behaviour of the PCM-RBA mortars will be simulated at the meso-scale level. Particularly, 2D meso-structures considering the RBAs as well as air voids will provide a fundamental basis for the analysis of the morphological influence on the effective thermal energy storage capacity of such composite materials.

2 EXPERIMENTAL RESULTS

This section briefly reports the employed materials, the considered tests and results considered as reference for the numerical activities. DSC tests were done for all components, i.e. paste RBAs and PCM. Conductivity, and temperature evolution tests were done for investigating the thermal properties of plain RBA mortars as a reference and PCM-RBA mortars with two different amounts of PCM volume fraction contents. In addition the mechanical behavior in terms of compressive strength and flexural strength were tested.

2.1 Materials and Methods

First, the thermal analysis (DSC) of all components i.e. paste, RBAs, PCM of the composite material (PCM-RBA mortars) is presented showing their heat storage capacity. Afterwards, plain RBA mortars and PCM-RBA mortar samples have been casted and tested for measuring the thermal conductivity, temperature evolutions and mechanical characterizations. The RBAs used in the experimental investigations were supplied by a German recycling company that collects and processes construction and demolition waste in the region. Standard recycled bricks (SB) and highly porous Poroton® lightweight refractory bricks (PB) were considered. A paraffin wax (namely, RT 25 HC by Rubitherm, 2018), was filled in the open pore space of the used RBAs with different volume fractions.

Table 1: *Overview of the six PCM-RBA mortars.*

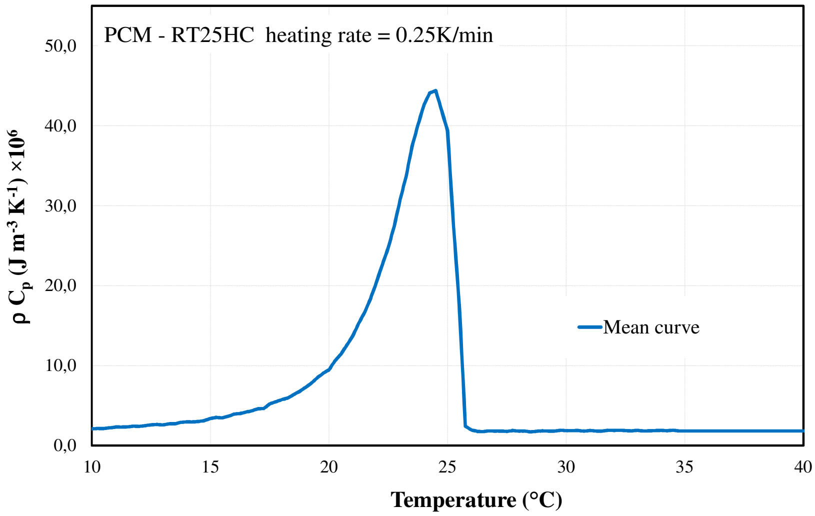
Labels	REF-SB (kg/m^3)	SB-65 (kg/m^3)	SB-80 (kg/m^3)	REF-PB (kg/m^3)	PB-65 (kg/m^3)	PB-80 (kg/m^3)
Cement	701.5	694.2	692.9	700.2	691.7	691.7
Water	350.8	347.1	346.5	350.1	345.9	345.9
PCM-RBA	655.2	719.3	734.0	664.0	728.9	743.9

Air content (V.-%)	2.3	2.9	3.0	2.4	3.1	3.1
w/c ratio	0.50					

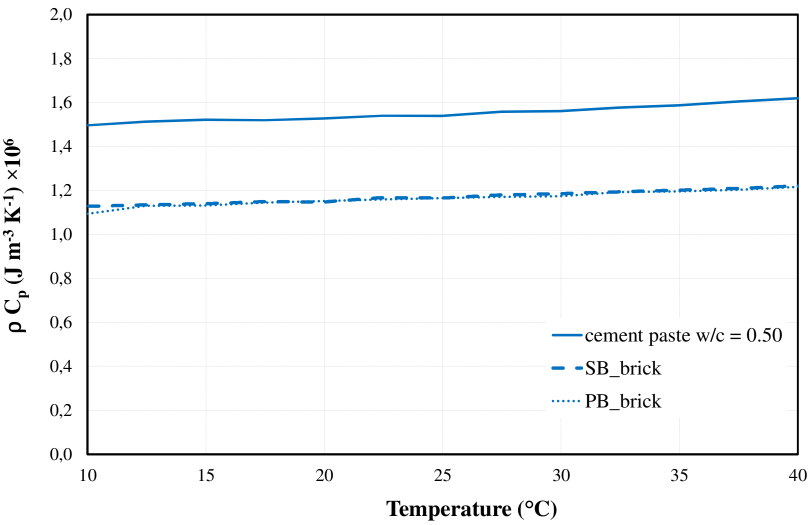
The advanced immobilization technique that was developed and applied is omitted herein for the sake of the brevity, however it is fully documented in the German patented by the *Institut für Werkstoffe im Bauwesen* of the TU Darmstadt (Patent DE 102016123739, 2019). Furthermore a commercial ordinary Portland cement (CEM I 42,5 R) was used and all mixtures were prepared according to EN 196-1. Following the recipes are highlighted in Table 1 (It provides the key information on the amount of PCM filling degrees, the RBA open porosity expressed in V.-% of the open capillary pore space, and the type of RBAs applied. For example, the label ''REF-SB'' refers to the reference mixture (without PCM) using SB RBAs; or "SB-65" indicates a mixture using SB-bricks and a filling degree of PCM of 65 V.-% of the total SB-RBA open capillary porosity).

2.2 DSC test data

Differential scanning calorimetry (DSC) measures were performed for each one of the components. For each component 3 samples were prepared in aluminum DSC pans and tested. The scatter among the mean value is negligible small. The results can be taken from Figure 1.



(a)



(b)

Figure 1: Results of DSC tests obtained with a heating rate of 0.25 K×min^{-1} for PCM (a) and 10 K×min^{-1} for paste and RBAs (b) in terms of ρ×Cp.

DSC results for the PCM (Paraffin) are shown in Figure 1a. It is well known that the heating/cooling rate affects the results strongly. For this reason, a sufficient heating/cooling rate for the used sample size was determined according to (RAL GZ 896) procedure. In this context according to IEA DSC 4229 PCM Standard the representative heating/cooling rate should be chosen verifying that the difference between the peak-temperature from one heating ramp to the next slower one is smaller than ≤ 0.2 K (Gschwander et al., 2015). In this work the adequate (final) heating/cooling rate, which was selected for verifying the aforementioned criterion, was 0.25 $K{\times}min^{-1}$. The PCM is characterized by an almost sensible behavior in the temperature ranges far from the melting point and an evident latent peak in that region close to the temperature of phase changes. Particularly, all curves are characterized by a remarkable peak which mainly represent the solid–liquid melting phase change PCM with a peak temperature of 24.5 °C.

Furthermore the DSC thermogram of Figure 1b shows the $\rho{\times}Cp\text{-}T$ response for the paste and both types of RBAs SB and PB. It can be observed, that the two types of RBAs are characterized by the same kind of sensible behavior, analyzed in the temperature ranges between 10 and 40 °C. It should be mentioned that the cement paste samples have a slightly higher heat storage capacity. As expected, the results also remark an almost temperature independent behavior of the $\rho{\times}C_p$ response with a very low positive slope towards higher temperatures.

2.3 Thermal conductivity

Thermal conductivity tests were performed by means of the Hot-Disk transient plane heat source method and using 40 mm × 40 mm × 160 mm beams. The test procedure was performed according to ISO 22007-2.

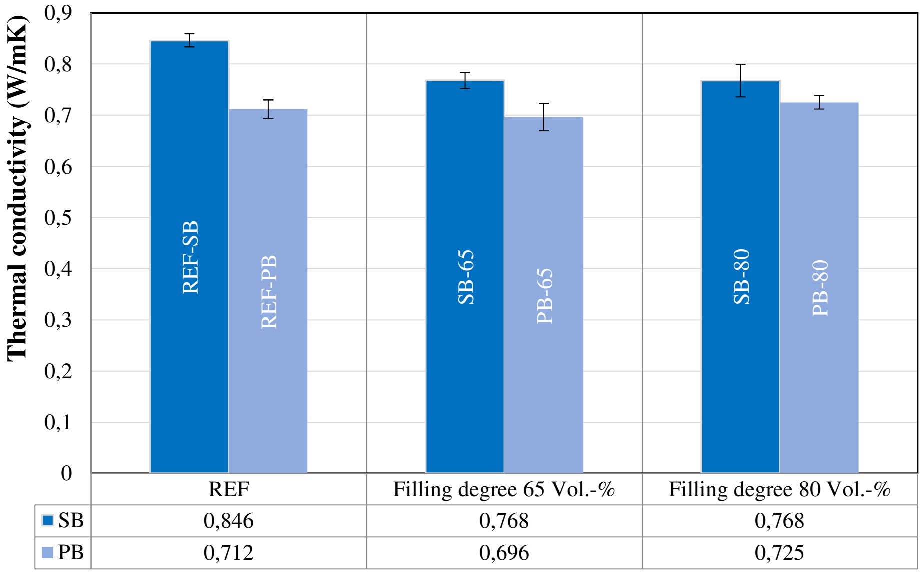


Figure 2: Thermal conductivity of the REF, C-PCM-10% and C-PCM-20% mixtures with different w/c ratios.

Figure 2 reports the results of the conductivity tests for the analyzed PCM-RBA mortars. It can be observed that all mortar mixtures have comparable thermal conductivities, even if higher PCM filling degrees are used. From this it can be deduced that the filling of the RBAs with PCM has only a minor influence on the thermal conductivity of the material. Basically, it can be detected that mixtures with PB RBAs have a slightly lower thermal conductivity compared to SB RBA-based mixtures. This behavior is due to the slightly higher air content in these compounds.

2.4 Thermal tests (DKK) and Mechanical tests

For all PCM-RBA mortar mixtures, temperature evolution measurements were carried out on spherical samples. Particularly, three spheres characterized to have a diameter of about 70 mm and produced with embedded thermocouples were cast to investigate the structural and mesoscale behavior of such shapes and through studying temperature evolutions. The thermocouples allowed to measure the temperature evolution in time in 2 positions, i.e. in the center of the sphere and at the boundary surface, respectively. The samples were cooled down to an initial temperature of approximately 8 °C. Afterwards the samples were placed in a climate chamber and heated up to roughly 50 °C (Mankel et al., 2019). The complete measurement procedure can be taken from the German patent (Patent 123-0069 AZ 2018/21). The thermal experiments were accompanied by mechanical tests to observe the effect which PCMs have on the resulting strengths in both compression and bending. These results are omitted herein for the sake of the brevity, however they are fully documented in ENB_2019_1193 (Mankel et al., 2019).

3 FIRST LAW OF THERMODYNAMICS AND ENTHALPY-BASED METHOD

The basic equations, employed for predicting phase transformation phenomena in PCM cement-based systems, are described in this section.

3.1 Thermodynamics principles

The basic equation describing a heat conduction problem can be written as follows:

$$\frac{\partial Q}{\partial t} = \nabla.(\lambda \nabla T) + \dot{q}_v \qquad \forall \mathbf{x} \in \Omega \tag{1}$$

where Q is the heat of the system under consideration, t the time, λ the thermal conductivity of the material (depending on temperature T and position vector $\mathbf{x}$ of the considered body Ω), $\dot{q}_v$ is the possible source term while $\nabla.$ and ∇ are the divergence and gradient tensorial operators.

In thermodynamics processes, a small amount of heat added to a system (dQ) is defined by means of the *first law of thermodynamics* as:

$$dU = dQ - p\,dV \tag{2}$$

where dU indicates the variation of the internal energy of the system and pdV the rate of the work spent, indicated as dW (under the simplified hypothesis that $dW=pdV$).

By introducing the definition of the enthalpy of a homogenous system, $H = U + p\,dV$, and by combining Eqs. (1) and (2), and adopting the hypothesis of a constant pressure process, the following enthalpy-based equation can be reached:

$$\frac{\partial H}{\partial t} = \nabla.(\lambda \nabla T) + \dot{q}_v \qquad \forall \mathbf{x} \in \Omega \tag{3}$$

which is the mostly used equation for solving phase change responses in construction and building material applications. This is commonly addressed as the enthalpy-based method.

3.2 Enthalpy-based and Apparent Calorific Capacity Method

The Apparent Calorific Capacity Method (ACCM) allows for describing the enthalpy evolution of a system in terms of an apparent (or sometime called effective) heat capacity during the thermal phase change.

The approach is based on following chain rule:

$$\frac{\partial H}{\partial t} = \frac{\partial H}{\partial T}\frac{\partial T}{\partial t} \tag{4}$$

then, by introducing the so-called temperature-dependent apparent (effective) heat capacity, defined as follows:

$$\frac{\partial H}{\partial T} = \rho C_{eff}(T) \tag{5}$$

Eq. (3) modifies into the following non-linear transient heat equation:

$$\rho C_{eff}(T)\frac{dT}{dt} = \nabla.(\lambda \nabla T) + \dot{q}_v \qquad \forall \mathbf{x} \in \Omega \tag{6}$$

To complete the problem statement of the ACCM approach, outlined in Eq. (6), Initial Conditions (ICs) and Boundary Conditions (BCs) need to be employed.

3.3 1D Spherical-based solution for the ACCM

In this work, Eq. (6) is transferred into spherical coordinates for predicting the thermal energy storage in the tested specimens, which had a spherical shape. Particularly the following relation is used:

$$\rho C_{eff}(T)\frac{dT}{dt}=\frac{1}{r^2}\frac{\partial}{\partial r}\left(\lambda r^2\frac{\partial T}{\partial r}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial}{\partial\phi}\left(\lambda\frac{\partial T}{\partial\phi}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\lambda\sin\theta\frac{\partial T}{\partial\theta}\right)+\dot{q}_v \tag{7}$$

In Eq. (7), r, θ, Φ are the radial distance, the polar and azimuthal angle, respectively. In the case of a two-dimensional approach and assuming that the source is independent of Φ the previous Eq. (7) can be simplified, and finally written, as:

$$\rho C_{eff}(T)\frac{dT}{dt}=\frac{1}{r^2}\frac{\partial}{\partial r}\left(\lambda r^2\frac{\partial T}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\lambda\sin\theta\frac{\partial T}{\partial\theta}\right)+\dot{q}_v \tag{8}$$

4 ENERGY STORAGE AND 2D MESOSTRUCTURAL ANALYSIS

This section addresses a numerical modeling approach of heat transport in PCM-RBA mortars. The section only reports a plan for future investigations and shows potential research lines based on the use of virtual 2D-dimensional meso-structures with different porosities, and distribution of PCM-RBAs.

In order to determine the exact meso-structure of the PCM-RBA mortar systems, as well as the volume fractions of PCM-RBA, cement paste and air voids, µXCT-scans of the spherical specimens were also performed. The spherical sample, having a diameter of 70 mm (±2 mm), were voxelized by choosing a size of 34.4 µm resolution. The images of the µXCT-scans can be seen in Figure 3.

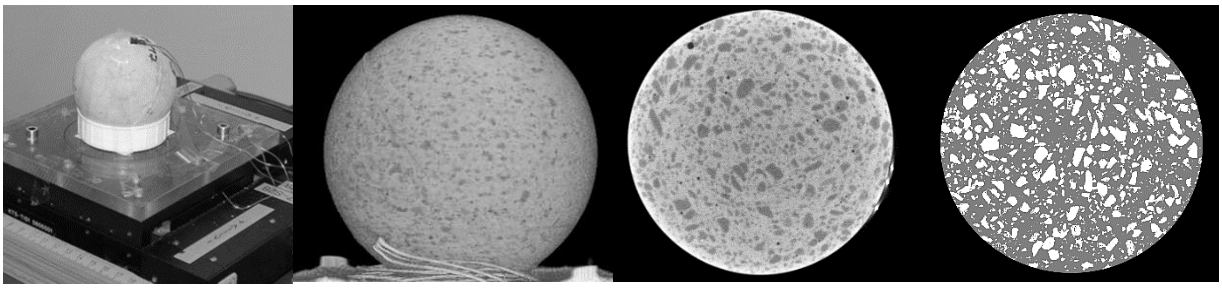


Figure 3: µXCT- setup (top) and slices cross including image-segmentation (down) of the spherical specimens.

2D-meso-structures with the meso-phases, i.e. PCM-RBAs, paste and air voids are taken from the µXCT-scans and implemented in a Finite Element simulation environment. The aim is to determine the macroscopic properties of the PCM-RBA mortar from the generated meso-structures and the thermal properties assigned to each individual meso-phase (Figure 4).

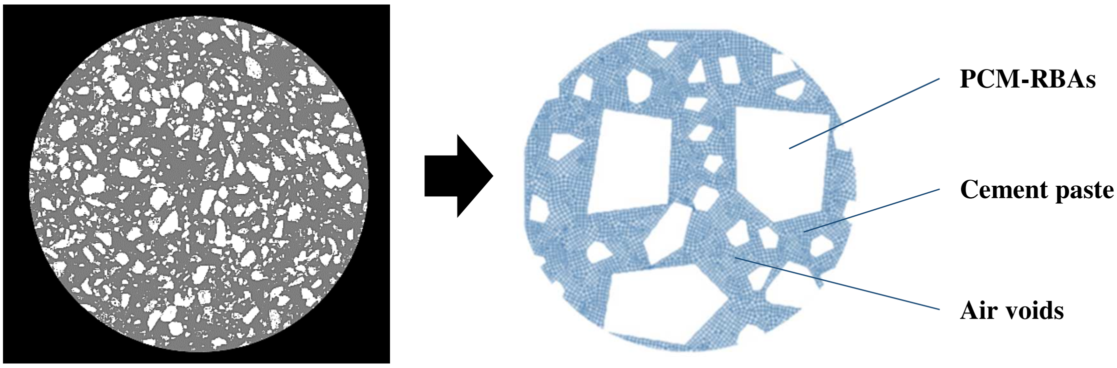


Figure 4: Example of a schematized meso-structure of a PCM-RBA mortar sample.

Homogenization techniques are employed for evaluating the temperature dependent thermal parameters expressed in thermal diffusivity D_{hom} which is the quotient of thermal conductivity and heat storage capacity $D=\lambda/(\rho \cdot C_{eff})$. In the meso-structure D_j was allocated to each meso-phase j, i.e. PCM-RBAs, paste and air voids. Therefore the thermal conductivities, specific heat capacities as well as the bulk densities were taken from the measurement results highlighted in section 2.2. However the effective specific heat capacity C_{eff} of the PCM-RBAs was modeled, by homogenizing the volume fractions of the components such as RBAs and PCM using a parallel approach. More precisely, the model smears out the heat storage capacities expressed in specific heat ones multiplied with the bulk density ($\rho \cdot Cp$) of the two components RBAs and PCM, as reported in section 2.2.

The diffusion-type heat flow in a heterogeneous cementitious composite can be thus described according to the following differential equation:

$$\frac{dT}{dt} = D_j \left[\frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial T}{\partial \theta} \right) \right] \tag{9}$$

where $D_j(T) = \dfrac{\lambda}{\rho C_{eff}(T)}$ is the thermal diffusivity of the j^{th} meso-component (PCM-RBAs, cement paste and air voids).

At the homogenized length scale, the diffusion transport model of Eq. (9) can be written as follows:

$$\frac{d\overline{T}}{dt} = D_{\text{hom}} \left[\frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial \overline{T}}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \overline{T}}{\partial \theta} \right) \right] \tag{10}$$

where $\overline{T}$ is the average temperature of the diffusing meso-phases, D_{hom} the effective macroscopic diffusivity.

By solving Eq. (9) it is possible to define the mean value of the temperature $\overline{T}_{\mathbf{n}j}$ throughout the faces (- and +) and in the mean layer (×) of the REV:

$$\overline{T}_{\mathbf{n}j}^{-} = \frac{1}{A}\int_{\Gamma_{\mathbf{n}j}^{-}} T\, d\Gamma_{\mathbf{n}_j}^{-} \qquad \overline{T}_{\mathbf{n}j}^{\times} = \frac{1}{A}\int_{\Gamma_{\mathbf{n}_j}^{\times}} T\, d\Gamma_{\mathbf{n}_j}^{\times} \qquad \overline{T}_{\mathbf{n}_j}^{+} = \frac{1}{A}\int_{\Gamma_{\mathbf{n}j}^{+}} T\, d\Gamma_{\mathbf{n}j}^{+} \qquad \text{j=x,y.} \tag{11}$$

Thus, by using a backward difference scheme at time $^{n+1}$ and a second-order central difference approach for the space derivative in the x- and y-directions, Eq. (10) can be used for evaluating the D_{hom} as follows:

$$D_{\text{hom},j} = \frac{\dfrac{{}^{n+1}\overline{T}_{\mathbf{n}j}^{\times} - {}^{n}\overline{T}_{\mathbf{n}j}^{\times}}{\Delta t}}{\dfrac{{}^{n+1}\overline{T}_{\mathbf{n}j}^{+} - 2\,{}^{n+1}\overline{T}_{\mathbf{n}j}^{\times} + {}^{n+1}\overline{T}_{\mathbf{n}j}^{-}}{\Delta L_j^2}} \qquad \text{j=x,y} \tag{12}$$

where Δt is the time step and ΔL_j (with $j=x,y,z$) is based on the REV dimension. Finally, the homogenized diffusivity can be evaluated as follows:

$$D_{\text{hom}} = \frac{D_{\text{hom},x} + D_{\text{hom},y}}{2} \tag{13}$$

To validate the numerical procedure of the proposed enthalpy-based two dimensional heat flow model, semi-adiabatic temperature evolutions will be simulated and compared with the experimental data reported in Section 2.4. The set of differential equations described in Section 3 will be solved numerically through the Finite Element Method (FEM). Particularly, the partial differential with spherical coordinates of Eq. (8), which describes the heat-diffusion process throughout the hardening spherical specimens, was solved under a 2D hypothesis, while the space domain was subdivided in n_s spaces (trusses elements), n_s+1 nodes, and, applying a full-implicit Euler Method for solving the transient problem.

The initial conditions was imposed following the initial temperature of 8°C of the spherical samples. Moreover, the calibrated Robin heat transfer coefficient (h) for the oven convection was determined for each mixture.

4.1 Statistical evaluation of RVE

The study of Representative Element Volume (REV) of heterogeneous PCM-RBA mortar meso-structures will be aiming at defining the minimum size of a sample that must employed for determining the corresponding effective properties of a homogenized macroscopic model. The REV dimension should be large enough to contain the necessary information about the microstructure in order to be representative. An indicator proposed by (Guittman et al., 2006) can be estimated for each 3D or in this case 2D meso-structure to find out the most appropriate REV size and particularly to quantify the change of the calculated homogenized (effective) thermal property based on the mean value calculated for the different numerical realizations. The following expression was proposed by Guittman et al. (2006)

$$\chi^2 = \sum_{i=1}^{m} \left(R_{\text{Diff,i}} - R_{\text{Diff,a}} \right)^2 / R_{\text{Diff,a}}{}^2 \tag{14}$$

where $R_{\text{Diff,i}}$ is the investigated effective parameter (i.e., the thermal diffusivity), $R_{\text{Diff,a}}$ is the average of the investigated $R_{\text{Diff,i}}$, and m the total number of numerical realizations performed with different PCM-RBA particle distributions and different volume fractions.

The variability of the results can be estimated with χ^2, indicating that for smaller values of χ*-square*, the closer the volume of the sample under consideration represents the expected REV. In fact, the true REV may only be obtained for a sample with an infinite volume. Nonetheless, a smaller size of a sample can normally be used if the value of χ^2 is acceptably low. Generally, 0.1 is regarded to be an acceptable value (Zhang et al., 2010).

5 CONCLUDING REMARKS

This paper proposes the theoretical basis for simulating the thermal behavior of cement based recycled brick mortar systems made with and without PCMs. A meso-scale based approach formulated through the use of the so-called Apparent Calorific Capacity Method (ACCM) was solved to accurately analyze the above mentioned phenomena. The model considered the experimental data measured from two different RBA mortar systems without PCMs and with two different PCM volume fraction amounts, for a total six different mixtures. The model validation of the proposed method dealt with simulating the experimental tests for given boundary and initial conditions and based on the adopted experimentally-based $\rho \cdot C_{eff}\ (T)$ curves. The proposed study was developed within the framework of the "2CENERGY" project and will be further extended on investigating the 3D thermal-mechanical response in micro and mesoscopic structural specimens.

It may be worth to mention that although a significant research effort has already been done in the field of numerical modelling for heat transfer processes with PCM accumulations, further efforts in the field of cementitious composites embedding PCMs are certainly needed. In this sense, a novel approach, combining a micro-to-mesoscale multiscale poro-analysis model with a multi-physics approach, along with a microstructural response, moisture diffusivity, phase change and thermal analysis, will be developed as next step of the current research.

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