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## **1** Thermal performance of a building envelope including microencapsulated

# phase change materials (PCMs): A multiscale experimental and numerical investigation

Franck Komi Gbekou<sup>1</sup>, Rahma Belloum<sup>2</sup>, Nawal Chennouf<sup>2</sup>, Boudjemaa Agoudjil<sup>2\*</sup>,
Abderrahim Boudenne<sup>3\*</sup>, Karim Benzarti<sup>1</sup>

<sup>1</sup>Laboratoire Navier, Université Gustave Eiffel, Ecole Nationale des Ponts et Chaussées
(ENPC), Centre National de la Recherche Scientifique (CNRS), F-77447 Marne la Vallée,
France.

<sup>2</sup>Laboratoire de Physique Energétique Appliquée (LPEA), Université Batna-1, Les Allées 19
Mai, Route de Biskra, Batna, Algérie

<sup>3</sup>Centre d'Études et de Recherche en Thermique, Environnement et Systèmes (CERTES),
 Université Paris-Est Créteil, France.

### 13 Abstract

- 14 This study aims to assess the thermal behavior of a cement mortar (denoted M15D) incorpo-
- 15 rating microencapsulated biobased phase change materials at both wall and building scales. A
- 16 bi-climatic chamber setup was employed to subject the wall to distinct thermal conditions
- 17 simulating outdoor and indoor environments, using heating and cooling solicitations. Temper-
- 18 ature sensors, strategically positioned at various depths, allowed the monitoring of tempera-
- 19 ture within the walls during the experiments.
- 20 On a building scale, the thermal performance of M15D was predicted using two mathematical
- 21 models describing heat transmission in porous systems incorporating phase-change materials.
- 22 Numerical simulations were carried out using COMSOL Multiphysics and EnergyPlus soft-
- 23 ware. The results obtained were validated against experimental data, at wall scales.
- The outcomes highlighted that the incorporation of microencapsulated biobased phase change materials significantly influences both building energy consumption and interior temperature. The heat storage capacity offered by M15D demonstrated a significant impact on thermal performance, leading to energy savings of up to 33% for heating and 31% for cooling, contingent on climate conditions. In conclusion, the integration of biobased phase change materials in the
- 29 cement mortar (M15D) display benefits in enhancing thermal performance at building scales.

Keywords: phase change materials (mPCM), experimental setups, energy saving, numerical
 model.

## 32 **\*Corresponding author**:

33 Pr. Boudjemaa Agoudjil, email :boudjemaa.agoudjil@univ-batna.dz

- 1 Laboratoire de Physique Energétique Appliquée (LPEA), Université Batna-1, Les Allées 19
- 2 Mai Route de Biskra, Batna, Algérie.

#### 1 1. Introduction

2 Global warming and resource depletion have become central topics in the news, and current 3 trends indicate that we are approaching a crucial decision point. Population growth and over-4 consumption are contributing to increased energy consumption and CO<sub>2</sub> emissions[1]. Ac-5 cording to the Intergovernmental Panel on Climate Change (IPCC) in its latest 2023 report, 6 global surface temperatures have already risen by 1.1°C compared to the pre-industrial period, 7 and this is projected to increase to 1.5°C by 2030. Furthermore, the 2022 Global Status Report 8 for Buildings and Construction, published by the UN Environment Program, reveals that CO<sub>2</sub> 9 emissions from building use reached approximately 10 gigatons in 2022 [2]. One of the most 10 resource-intensive industries is the construction sector, responsible for 36% of global energy consumption. Energy consumption in buildings encompasses the entire energy usage, from 11 12 raw materials to the final building, with a significant portion dedicated to maintaining com-13 fortable living conditions within structures. For instance, in France, heating alone accounts for 14 approximately 65% of energy consumption in the residential sector and 43% in the tertiary 15 sector [3].

16 To overcome the rising trend of energy consumption and global warming, it is crucial to offer 17 alternative solutions to the public while promoting eco-friendly options. There is an urgent 18 need to develop innovative solutions that enhance thermal efficiency in buildings [1, 4]. Nu-19 merous research efforts are currently underway to develop new building materials aimed at 20 improving their thermophysical properties for energy-efficient and environmentally friendly construction alternatives [5-8]. One such solution is passive thermal energy storage systems 21 22 (TES), which enable the storage of a certain amount of energy for later use with minimal en-23 ergy loss between storage and release [8]. Among thermal energy storage systems, latent heat 24 thermal energy storage is particularly well-suited for building applications[9-12]. This tech-25 nology relies on the use of phase change materials (PCMs), which are materials that undergo 26 a change in their physical state (transitioning from solid to liquid and vice versa) in response to temperature fluctuations, thereby storing and releasing energy during these phase transi-27 tions[13, 14]. Combining PCMs with building materials such as concrete or mortar holds 28 29 great promise as it enhances the thermal properties of these materials and provides energy 30 storage capabilities. Studies on PCM walls in building applications have demonstrated signif-31 icant benefits. For example, Bahrar et al. [15] reported a reduction of up to 1.7°C in the max-32 imum temperature recorded when using an additional PCM panel. Al-Absi et al. [16] in their 33 investigation of the addition of a PCM panel to concrete in a test box, observed temperature 34 reductions of up to 6°C compared to the reference box as outdoor temperatures increased. Li 35 et al.[10], reported a dampening effect on indoor/outdoor temperature differences in a room 36 equipped with a multi-layer system of cementitious walls incorporating an insulating PCM 37 layer, resulting in energy savings of up to 30%.

38 The rapid advancements in alternative building materials research have spurred the develop-

39 ment of simulation tools aimed at analyzing the performance of these materials under differ-

40 ent sizes and environmental conditions [13, 14]. These simulation tools rely on mathematical

models to depict heat flow within building materials, enabling them to forecast temperature patterns. Nevertheless, given the extensive range of materials, PCM (Phase Change Material) combinations, and integration techniques accessible for building envelopes, optimizing PCM usage necessitates a comprehensive assessment of factors such as building construction, PCM integration methods, and their specific placement within the structure [17, 18].

6 Several techniques exist for incorporating PCMs into construction materials, facilitating their 7 integration into a wide range of building components [7]. The current methods employed in-8 clude direct embedding, immersion, form-stable and shape-stabilization, as well as micro, 9 macro, and nano encapsulation [7, 19, 20]. In this paper, we focus on the microencapsulation 10 of PCMs, a process where the PCM is encapsulated within microcapsules ranging from 1 µm 11 to 1 mm in diameter. This method involves enclosing a small quantity of PCM within another 12 substance, such as a lipid, polymer, or inorganic component, to create microcapsules that act 13 as a protective barrier between the PCM and its surrounding environment. The resulting mi-14 crocapsules can then be incorporated into various materials, such as mortar or concrete, to

15 form composite materials with enhanced thermal properties.

Numerous tools are currently available for simulating building energy consumption, such as
BLAST, BSim, DeST, DOE, ECOTECT, Ener-Win, Energy Express, Energy-10, EnergyPlus,
eQUEST, IDA-ICE, IES, HAP, HEED, PowerDomus, SUNREL, Tas, TRACE, and
TRNSYS. For our work, we chose the EnergyPlus tool due to its robust validation and ability
to interface with various systems like HVAC and renewable energy [21].

Indeed, despite a good understanding of the physical equations governing PCM behavior, there is a scarcity of numerical models available for its simulation. Most existing numerical models tend to focus on whole-building modeling, using unidirectional heat transmission through walls and an equation for the air energy balance to determine the typical room air temperature [22-24]. However, adapting these models to various building arrangements can be complex.

27 To comprehensively harness the potential of PCM energy storage when integrated with 28 HVAC systems, such as natural night ventilation during the summer, the adoption of a modu-29 lar simulation tool structure becomes imperative. This approach would substantially enhance 30 the optimization and analysis of PCM performance. In fact, one notable effort in simulating 31 PCM walls has been presented by Ibáñez et al. [23] using EnergyPlus. Their method adopts a global energetic perspective, taking temperatures (both wall and air) as inputs and generating 32 33 data for the active layer as outputs. This approach enables the assessment of PCM's impact on 34 the overall energy balance within a room. However, further experimental confirmations are 35 still needed to validate and enhance the accuracy of this approach.

36 In the existing literature, the studies have predominantly investigated the effect of incorporat-37 ing an additional PCM panel within multi-layered insulation systems. Furthermore, to our 38 knowledge, very little research has been conducted on the thermal performance of a homoge-

- 1 neous cement mortar system that integrates microencapsulated PCM distributed throughout its
- 2 thickness. This study aims to fill this research gap by thoroughly investigating a homogeneous
- 3 mortar wall that incorporates bio-based PCM. The wall will be subjected to various thermal
- 4 conditions, and its thermal performance will be systematically compared to that of a reference
- 5 mortar wall. To facilitate this research, a custom-made experimental setup was constructed to
- 6 replicate a bi-climatic environment. This setup exposes each surface of the wall to distinct
- 7 hygrothermal conditions, simulating both indoor and outdoor environments. The incorpora-
- 8 tion of hygrothermal sensors at various depths within the wall has enabled the recording of
- 9 temperature variations throughout its thickness.
- 10 The primary objective of this research is to improve the heat consumption efficiency of build-
- 11 ings by enhancing their thermo-physical characteristics and developing composite walls with
- 12 bio-based microencapsulated phase change material incorporated into mortar. The study em-
- 13 ploys an enthalpy approach and COMSOL analysis to create an unsteady thermal transport
- 14 numerical model of bio-based PCM. This model helps to understand the mechanism of heat
- 15 storage and temperature regulation of PCM within the wall. Moreover, numerical simulations
- 16 are performed to investigate thermal inertia and energy savings.
- 17 The fundamental idea behind this research starts with the experimental characterization of the 18 bio-based PCM at both material and wall scales. The collected data are then used to validate 19 the numerical model developed using COMSOL-Multiphysics, which enables the calculation 20 of the bio-based PCM enthalpy as a function of temperature. Subsequently, this validated model will be integrated into EnergyPlus to provide comprehensive results representing the 21 22 performance of the bio-based PCM at the building scale under real climatic conditions, con-23 sidering aspects like thermal inertia and energy consumption. The goal is to assess the thermal 24 performance and energy-saving potential of the bio-based PCM when incorporated into build-
- 25 ing envelopes.

## 26 **2. Materials and experimental methods**

## 27 2.1 Materials

28 Two cement mortar walls were studied in this work: a reference cement mortar wall (noted 29 M0) and a wall made from the reference mortar with the addition of microencapsulated bio-30 based phase change materials (M15D). The reference mortar is a pre-existing formulation designed for additive manufacturing [25]. It comprises an ordinary Portland cement 31 32 EXTREMAT® CEM I 52.5 N (denoted OPC), a fast-setting sulfo-aluminous cement (denoted 33 CSA), both products by the VICAT company (L'Isle-d'Abeau, France), a superplasticizer 34 VISCOCRETE TEMPO 11 (SP) water reducer from SIKA (Baar, Switzerland), and standard-35 ized sand with a maximum particle size of 2mm, provided by Société Nouvelle du Littoral 36 (Leucate, France).

A commercial bio-based PCM was selected for the study. It's denoted CrodaTherm<sup>TM</sup>
 ME29D and is in the aqueous dispersion form of microencapsulated particles in water (solid

content of about 50 wt.%). The particles are an organic PCM core (from plant-based
 feedstocks) surrounded by a formaldehyde-free acrylic polymer shell. The PCM has a melting
 and crystallization point of 29°C and 24°C, respectively, and heats of fusion and crystalliza tion of 183 kJ/kg and 179 kJ/kg, according to the supplier's technical datasheet [26].

5 In a material-scale study on the effect of the addition of these PCMs on the mechanical and 6 thermophysical properties of the mortar, we have prepared and tested various mortars with 7 PCM content up to 13.5 wt.%. We have shown the beneficial effect of the addition of PCMs 8 on the thermophysical properties of mortars while reducing mechanical performance. A sig-9 nificant improvement in the thermophysical properties is found with the reduction of the thermal conductivity by 72% (0.6 W.m<sup>-1</sup>. K<sup>-1</sup> compared to 2.3 W.m<sup>-1</sup>. K<sup>-1</sup> for M0) with 11 10 11 wt.% of PCMs added. This formulation is denoted M15D and was then chosen to conduct a 12 comparative study at the wall scale to compare the thermal responses of a wall made with 13 mortar to the ones of the reference mortar. The composition of the two mortars (M0 and 14 M15D) is displayed in Table 1.

15

**Table 1.** Composition of the two mortar formulations used in this work.

Type of	Sand	OPC	CSA	SP	Mass of	Total	W/C	Weight frac-	Volume
mortar	(g)	(g)	(g)	(g)	mPCM particles (g)	water (g)	ratio	tion of mPCM particles (%)	fraction of mPCM particles (%)
<b>M0</b>	1350	1059	80	3	-	399	0.4	0	0
M15D	1350	1059	80	3	433	1006	0.9	11	21

16

#### 17 2.2 Thermophysical properties

Several measurements were conducted to determine the thermophysical properties of the two mortars. For this purpose, the Hot Disk method (HD) was employed, using a TPS 2500 S device with a sensor "Kapton ref 5501" having a radius of 6.4 mm. The HD method allows for

21 the simultaneous measurement of thermal conductivity ( $\lambda$  in W.m<sup>-1</sup>.K<sup>-1</sup>), thermal diffusivity ( $\alpha$ 

22 in  $m^2.s^{-1}$ ), and volumetric heat capacity ( $\rho.Cp$  in MJ.m<sup>-3</sup>.K<sup>-1</sup>). Several measurements were

conducted in a controlled moisture environment of 50% RH and a temperature range from

 $10^{\circ}$ C to  $45^{\circ}$ C, covering all states of the core of the phase change material.



Figure 1. Thermophysical properties (at 50% RH) of M0 and M15 were determined by the
HD method (solid and liquid states of the PCM core).

4 The thermophysical properties of the reference (M0) and bio-based PCM mortar (M15D) are 5 presented in Figure 1 as a function of temperature variation, with error bars indicating stand-6 ard deviations based on five measurements for each temperature. The M15D mortar exhibits 7 significantly lower values for all three measured properties compared to the reference materi-8 al, regardless of the temperature considered. For instance, at 20°C, the thermal conductivity of M15D is reduced by approximately 72%, dropping from 2.32 W.m<sup>-1</sup>.K<sup>-1</sup> (for M0) to 0.68 9 W.m<sup>-1</sup>.K<sup>-1</sup>. This decrease can be attributed to the low thermal conductivity of the bio-based 10 PCM itselfs, which typically ranges from 0.25 to 0.35 W.m<sup>-1</sup>.K<sup>-1</sup> depending on the physical 11 12 state of the PCM core [27]. Additionally, the significant increase in porosity of the mortar containing bio-based PCM promotes thermal transfer through convection in the pores rather 13 14 than through thermal conduction [21-23]. These findings agree with the observations of pre-15 vious studies by Dehdezi et al. [21], Hunger et al. [22], and Jayalath et al. [23], where the ad-16 dition of 5 wt.% PCMs into cement composites resulted in respective decreases in thermal conductivity of approximately 36%, 38%, and 45% compared to reference specimens. 17

#### 18 2.3 Experimental setup of bi-climatic test cell

#### 19 2.3.1 Preparation and instrumentation of walls

20 The studied test walls have a dimension of  $50 \times 50 \times 10$  cm<sup>3</sup> and were prepared according to a

21 mixing protocol displayed in our previous work. The walls were prepared and underwent sev-

1 eral months of curing in a laboratory environment at 20°C and under ambient humidity condi-

2 tions.

To record the hygrothermal response of the wall, temperature sensors were installed within the walls. Each wall is equipped with a total of five sensors. One on the external faces and three in the thickness. Three holes of 8mm in diameter were carefully drilled into the wall's thickness at a depth of 25 cm. They are positioned at 2.5 cm, 5 cm, and 7.5 cm, respectively, from the outer surface (Figure 2.a). The holes are spaced 15 cm apart vertically to prevent any interference during the measurements. For precision of sensor position, the holes were performed using a precision's column drilling machine.

## 10 2.3.2 The bi-climatic experimental setup

A homemade experimental setup was constructed to simulate a dual-climate environment fora building. This setup involves the application of two different hygrothermal conditions on

13 opposite sides of the wall, simulating indoor and outdoor environmental conditions.

14 The system consists of a metallic frame built around a climatic chamber (Memmert ICH 260)

15 to connect the wall to both environments (indoor and outdoor). The indoor environment is a

16 laboratory room where the temperature is regulated at 20°C using an air conditioner. The rela-

17 tive humidity of the room is recorded over several weeks of measurements (between 45% and

18 55% RH) but is left uncontrolled to provide a daily-use impression.

19

20 To avoid thermal leaks, an expanded polystyrene (6 cm) is placed between the wall and the 21 frame. The insulation material is recovered with an insulating and vapor-barrier adhesive plas-22 tic film. Therefore, hygrothermal exchanges may happen only in the central open area of 23 40'45 cm2 (Figure 2.b). To ensure unidirectional (1D) hygrothermal transfer, all lateral sur-24 faces were insulated using expanded polystyrene, allowing hygrothermal exchange exclusive-25 ly through the two exposed surfaces. Two additional sensors were positioned within the cli-26 matic chamber and the laboratory room to record the indoor and outdoor temperature condi-27 tions instantly. The insulation of the total setup is checked using a thermal infrared camera to 28 prevent heat loss and have a uniform transfer across the observed surface (Figure 2.c).



Figure 2. (a) Wall preparation with sensors; (b) Experimental setup; (c) IR image of the wall
to check uniform heat transfer and prevent heat losses.

### 4 2.3.3 Experimental hygrothermal case study

After the setup was performed, the two faces of the wall were stabilized at 20°C and 50% RH for approximately one week, until all recorded measurements indicated the set point. Two experimental programs were applied to each wall (Figure 3). The indoor environment is kept constant during the two scenarios. It is set at 20°C with ambient humidity. The outdoor thermal conditions are applied at a fixed humidity of 50% RH. These programs consist of:

- A day/night simulation involves varying temperatures between a heating (40°C) and a cooling (15°C) phase, each lasting 12 hours.
- continuous heating at 40°C until reaching a steady-state condition.



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## Figure 3. Case studies applied to the wall.

## 2 **3. Mathematical model**

The existence of PCMs in three different states (solid, liquid, and solid-liquid coexistence) adds complexity to the phase change heat transfer problem [18]. As latent heat is stored and released over time, the interface between the two phases moves, making the simulation more challenging.

To simplify the complex heat transfer process in mixing mortar and encapsulated PCM, the
following hypotheses are suggested to develop the analytical model [28]:

- Heat transfer is assumed to occur only in the thickness direction since it always
  takes place between the inner and outer surfaces, leading to one-dimensional heat
  transfer.
- Natural convection during the melting process of PCM and the undercooling effect
   during the solidification process of PCM are neglected.
- 14 The physical properties of other solid materials are considered constant.
- 15 The PCM in the phase-change layer is assumed to be homogeneous and isotropic.
- 16 The thermal contact resistance between layers is considered negligible.
- The liquid state of the PCM is assumed to be an incompressible Newtonian fluid,
  following Fourier's heat conduction.

By applying these hypotheses, the analytical model aims to achieve simulation results while reducing the complexities involved in the heat transfer process between mixing mortar and encapsulated PCM.

22 According to the literature, there are two commonly used numerical methods for modeling

23 phase change materials (PCMs): the enthalpy method and the effective heat capacity method.

- 24 For this study, we have chosen to utilize the enthalpy method, which considers the liquid
- state, solid state, and transition phase in PCM using the mixtures law.

To conduct a comprehensive investigation at both the wall scale and the building scale, we employed two different software tools: COMSOL and EnergyPlus. However, the enthalpy model is not readily available in both tools. To overcome this limitation, we utilized the flexibility of COMSOL, which allows us to introduce the enthalpy model and then create a ready-

30 to-use function for EnergyPlus.

The enthalpy model [8, 29, 30] relies on enthalpy and temperature as dependent variables. The advantage of this model is that it does not require the consideration of movement and changes in the transition interface, allowing for the establishment of unified equations in all three states of PCM (solid, liquid, and transition). Where, the enthalpy model is expressed as:

1

$$\rho \frac{dh}{dt} = \nabla(k \, \nabla T) \tag{1}$$

1 The total enthalpy (h) is the sum of the sensible and latent heats of the PCM and is related to 2 the temperature of the PCM as follows:

$$h = \begin{cases} C_{PS}(T - T_m) + C_{PL}(T_m - T_a) - \theta \left( 1 - \frac{T_a - T_m}{T_a - T} \right) - (C_{PS} - C_{PL}) \times (T_a - T_m) \times \ln(\frac{T_a - T}{T_a - T_m}) & T \le T_m \\ C_{PL}(T - T_a) & T \end{cases}$$
(2)

3 where:

- 4  $\rho$ : Density, (kg.m<sup>-3</sup>)
- 5  $\lambda$ : Thermal conductivity, (W.m<sup>-1</sup>.K<sup>-1</sup>)
- 6  $C_{PS}$ : Specific heat capacity of solid state,  $(J.kg^{-1}.K^{-1})$
- 7  $C_{PL}$ : Specific heat capacity of liquid state,  $(J.kg^{-1}.K^{-1})$
- 8  $\theta$ : Liquid fraction
- 9  $T_m$ : Melting temperature (23°C).
- 10  $T_a$ : The end of the non-isothermal melting (28°C).

11 The enthalpy-temperature function of the M15D was determined using COMSOL 12 Multiphysics software, which can solve the unsteady heat transfer problem by the finite ele-13 ment method. The model is supplied by the properties presented in Table 2. The values of 14 thermal capacity in solid and liquid states are obtained using the mixing law according to the 15 results of Gbekou et al. [31]

16

 Table 2. Thermal proprieties of M15 introduced in COMSOL-Multiphysics [31].

Properties	Density $(kg/m^3)$	Thermal capacity solid (j/kg. k)	Thermal capacity Liquid (j/kg. k)	Thermal conduc- tivity (W/m. k)
M15	1710	1026	1073	0.7

17 The results obtained using COMSOL for the enthalpy temperature relationship of M15, as 18 shown in Figure 4, are incorporated into EnergyPlus to feed the PCM model. EnergyPlus, 19 developed by the United States Department of Energy (US DOE), is widely used for whole-20 building energy simulations, and it offers the capability to model PCMs using a Conduction 21 Finite Difference (CondFD) solution algorithm. The CondFD algorithm discretizes the layers 22 of the building envelope into different nodes and numerically solves the heat transfer equa-23 tions using a finite difference method (FDM). In this study, the Fully Implicit Finite Differ-24 ence Scheme, coupled with an enthalpy temperature function to account for the phase change

1 energy, was adopted [32]. The following equations represent the method of the fully implicit

2 schema used in EnergyPlus:

$$c_p \rho \Delta x \ \frac{T_i^{j+1} - T_i^{j}}{\Delta t} = k_W \ \frac{T_i^{j+1} - T_i^{j+1}}{\Delta x} + k_E \ \frac{T_{i+1}^{j+1} - T_i^{j+1}}{\Delta x}$$
(3)

3 With:

$$k_w = \frac{k_{i+1}^{j+1} + k_i^{j+1}}{2} \tag{4}$$

4

$$k_E = \frac{k_{i-1}^{j+1} + k_i^{j+1}}{2} \tag{5}$$

5

$$C_P^{*}(T) = \frac{h_i^{j} - h_i^{j-1}}{T_i^{j} - T_i^{j-1}}$$
(6)

6 Where:

7  $k_i = k(T_i^{j+1})$ : if thermal conductivity is variable.

- 8 T: Temperature
- 9 Cp: Specific heat capacity, (J/(kg·K))
- 10 i: Node being modeled
- 11 i+1: Adjacent node to interior of construction
- 12 i-1: Adjacent node to exterior of construction
- 13 j+1: New time step
- 14 j: Previous time step
- 15  $\Delta t$ : Time step
- 16  $\Delta x$ : Finite difference layer thickness





Figure 4. M15D enthalpy curve variation calculated using COMSOL.

#### 3 4. Results

#### 4 4.1 Thermal response of the walls under cyclic heating/cooling solicitation

5 As mentioned in 2.3.3, a stabilization stage was conducted for one week on both walls before starting the case studies. The first case study is a day/night simulation at controlled hygrome-6 7 try (50% RH) by varying the outdoor temperature between a heating (40°C) and a cooling 8 (15°C) phase, each lasting 12 hours. The cycles were repeated for more than 7 days to validate the repeatability between the daily cycles. Therefore, the comparison between the ther-9 mal responses of the two walls (M0 and M15D) during the heating and cooling phases is pre-10 sented in Figures 5 a,b. The evolution of the temperature during one cycle is presented at var-11 ious sensor positions during the heating and cooling stages. The trend of the evolution of tem-12 13 perature at various depths in the wall is the same for both walls during the heating and cooling 14 stages.



Figure 5. Responses of the walls during 24 hours under temperature solicitation cycles between 40° and 15°C: (a) M0; (b) M15D.

1

5 One noticed the same evolution trends for the temperature during the 24-hour cycle. On the 6 heating stage, the temperature on the outer face of the walls increases rapidly during the first 7 hour and reaches, after 12 hours, a maximum recorded value of 36°C for M0 and 34.8°C for 8 M15D. From the outer face to the inner one, a temperature gradient is observed with decreas-9 ing values. A gap is observed in the recorded temperature between the wall M15D and the 10 reference wall. Except at position 25 mm, which can be an error from the sensor position, M15D exhibits a lower temperature than M0 with a gap up to 1°C at 75 mm. The observed 11 12 reduction in the recorded temperature (~ 1°C) between the two walls may come from the effect of the mPCMs in the wall M15D. The increase in temperature over the melting point of 13 14 PCM (28 °C) may be stored by the PCM core for phase change to a liquid state. It can reduce 15 the temperature increase's kinetics and induce a small delay in the temperature increase in each position between M15D and M0. On the inner face, the indoor temperature is 20°C and 16 17 is above the melting point of the PCM, which does not allow the PCM to be activated. The recorded temperature is almost the same for both walls on the inner face. 18

2 outer face of the wall cools down rapidly. A delayed is observed within the thickness of the 3 wall with the reverse effect in the temperature gradient. On the outer face (position 0 mm), the 4 maximum recorded temperature is 16°C for M0 and 17°C for M15D. Here again, the reduc-5 tion of  $\sim 1^{\circ}$ C is observed on the PCM wall. Within the thickness of the wall at 24h, the tem-6 perature increases nearer the indoor environment (20°C) with recorded value at position 100 7 mm of 18°C for M0 and 19°C for M15D. One can observe a higher temperature for M15D 8 than M0 with the gap of about  $\sim 1^{\circ}$ C for sensor positions. On the inner face the temperature is 9 almost the same for both walls as the PCM are not activated. But when the outdoor tempera-10 ture drops below the phase change range, a reverse effect may happen as the PCM started so-

In the cooling phase, when outdoor temperature rapidly decreases from 40°C to 15°C, the

11 lidification process and the core release the stored energy.

#### 12 4.2 Thermal response of the walls under steady-state heating at 40°C

13 After the cyclic solicitation, the stabilization stage (20°C, 50% RH) is run again before the

- 14 second thermal case study. The second case consists in an increase in temperature from 20 to
- 15 40°C with a continuous heating at 40°C until steady state. Figure 6 presents the comparison
- 16 of the evolution of the temperature during time variation at various sensors positions of the
- 17 two walls.

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18

19

Figure 6. Comparison between M0 and M15D for a steady-state regime at 40°C

The evolution trend of temperature is similar as the one during heating stage of cycling solicitation. One can notice that the temperature rapidly increases during the early hours and almost reaches the maximum value after 12 hours. This result confirms that the highest temperature

23 is reached during the heating stage of day/night solicitation after 12 hours. For the reference

1 mortar wall M0, the steady state is reached from 12 hours and the recorded temperatures re-2 mains constant even after long exposure (values at  $t = 12h \cong$  values at t = 60h). A maximum 3 recorded value of 36 °C is obtained for the reference wall against 35 °C for M15D on the out-4 er face. A temperature gradient is observed from the outdoor face to the indoor across the 5 thickness of the wall.

6 For the wall M15D, there is a small delay between the temperature recorded at 12h and the 7 maximum value at steady state. The same gap of reduction is observed on the temperature 8 within the thickness of the wall. This effect is due to the activation of the PCM as the temper-9 ature increases over the melting point (29 °C), the PCM core store the energy and become 10 liquid, delaying the kinetics of the evolution of the temperature. The indoor temperature is constant at 20°C and lower than the PCM melting point which doesn't allow the PCM to be 11 12 activated. The same temperature is almost recorded on the inner face (position 100 mm) with 13 a value 26°C.

14 Considering all the presented results, the addition of Phase Change Materials (PCMs) has 15 proven effective in mitigating temperature variations in the wall with induce a delay in the 16 kinetic evolution of temperature. Interestingly, more significant effect was anticipated regard-17 ing the thermophysical properties of the two materials, notably the thermal conductivity, with 18 values of  $2.32 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$  for M0 and  $0.66 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$  for M15D at 20°C. It is worth not-19 ing that besides boundary conditions, there are other possible phenomena that reduce the ef-20 fect of the thermal response of the PCM wall.

## 21 **4.3** Numerical study of building under real climatic conditions

The indoor conditions (temperature and energy consumption) seem to be one of the most crucial variables to consider when assessing the envelope building performance. High temperature oscillations increase overheating, which is the discomfort felt by building inhabitants because of heat accumulation. Health problems may occur from overheating, especially in the elderly and small children. Therefore, the purpose of this part is to investigate how incorporat-

27 ing bio-based PCM to mortar affects the building's thermal inertia and energy consumption.

## 28 4.3.1 Model validation

In this part, EnergyPlus and COMSOL Multiphysics PCM models were validated by comparing simulation outcomes with the results of experiments obtained in section 4.1. The heating/cooling test was modeled using both software for the M15D and the simulated temperature was compared with the experimental data.

52 thre was compared with the experimental data.

The overview of the experimental and numerical data which use enthalpy model implemented on COMSOL for a thickness of 5 cm of the wall is shown in **Figure 7**. The numerical output

- 35 results appear to be in good agreement with the experimental data. We notice only a  $0.5^{\circ}$ C
- 36 difference between experimental and numerical data, which can be explained by the sensor
- 37 accuracy used in the experiments. These findings demonstrate that the model provides accu-

- 1 rate results and it takes into account the phase shift of PCM particles, especially when the wall
- 2 temperature is around 29°C, which falls within the temperature range for PCM fusion.



**Figure 8** illustrates a comparison between the experimental measurements and the numerical models for a wall thickness of 10 cm. This thickness was chosen because in EnergyPlus, the numerical simulation enables the prediction of temperature variations solely at the internal and external surfaces. It can be observed that the numerical temperature output closely matches the experimental data except for the initial hours, where a slight lag is evident. This lag primarily arises from the initialization conditions, including the initial temperature and enthalpy, employed to initiate the simulation tools.

Furthermore, the temperature obtained using COMSOL-Multiphysics closely matches the experimental data, showing nearly the same results. However, a slight difference of approximately 0.5°C is noticed when using EnergyPlus. This difference falls well within the experimental error range, indicating that the models are suitable for analyzing the thermal behavior of M15D at the building scale, and the numerical results are considered accurate.

18 Overall, the validation process confirms that both EnergyPlus and COMSOL-Multiphysics 19 models provide reliable results and are appropriate for studying the thermal performance of

20 M15D in building-scale applications.



2

Figure 8. Validation of numerical models using the heating/cooling test.

3 Indeed, the PCM model integrated into the EnergyPlus program has been subject to validation

4 in various research studies [33]. For instance, *Salihi* et al. [34] found that EnergyPlus simula-

5 tion results showed good agreement with the numerical work conducted by Alam et al. [35]

6 when a 0.5 cm thick PCM layer was inserted into the ceiling between the plasterboard and the

7 insulation layer. This validation further supports the accuracy of the PCM algorithm.

Another successful validation of the PCM algorithm was reported by Zhuang et al. [36], who studied two different envelopes with mPCMs: envelope "A" with one layer of PCM and envelope "B" with two layers of PCM. The study showed that the largest relative error in temperature was 12.41% for envelope "A," and the smallest was 0.71%. For envelope "B," the largest relative difference was 8.33%, and the smallest was 0.33%. The study concluded that using the appropriate real weather data and thermal characteristics of the material are crucial factors

14 in reducing differences between simulation and experimental results.

Furthermore, the PCM algorithm has been validated by Campbell et al. [37] and Chan et al. [38] sing experimental data published by Kuznik et al. [39]. In both validation studies, the indoor air temperature predicted by the PCM algorithm in EnergyPlus was found to be in good agreement with the experimental results. These validation studies demonstrate the reliability and accuracy of the PCM algorithm integrated into EnergyPlus, providing confidence in its use for analyzing the thermal behavior of PCM incorporated building envelopes

20 its use for analyzing the thermal behavior of PCM-incorporated building envelopes.

## 21 4.4 Comparison of the thermal behavior of M15D and M0 buildings

To evaluate the effectiveness of Bio-based Phase Change Materials (PCM) in building envelopes, we conduct in this section a numerical comparison of the thermal performances and energy consumption between both formulation M15D and M0 at the building scale. For this investigation, we selected a simple model of a room representing a typical building known as

- the "BESTEST building," as depicted in **Figure 9**. This building is referenced within the framework of the International Energy Agency (IEA). The room is a closed space with a volume of 129.6 m<sup>3</sup> ( $6 \times 8 \times 2.7$  m<sup>3</sup>) and features 20 cm-thick external walls. The south facade of the room includes two double-glazed, identical windows.
- 4 the room includes two double-glazed, identical windows.
- 5 To conduct the comparison, we examine three different climates: a Mediterranean climate
- 6 represented by Algiers, North of Algeria, a hot and dry climate represented by Ouargla, South
- 7 of Algeria, and a degraded oceanic climate represented by Paris, France, which implies rela-
- 8 tively cold winters and relatively hot summers.
- 9 This study is divided into two parts: the first part involves considering the buildings as pas-
- 10 sive, meaning no heating or air conditioning is applied. In contrast, the second part involves
- 11 considering the buildings as air-conditioned to investigate the impact of integrating PCM on
- 12 energy consumption. To facilitate this analysis, a thermal regulation system has been pro-
- 13 grammed with set-point temperatures of 20°C for heating and 24°C for cooling.



15

Figure 9. Geometry of the building model.

16 Indeed, studying the implementation of passive strategies, such as "free-floating" systems, is 17 crucial as it enables the assessment of thermal comfort. Additionally, it facilitates the optimal 18 design of buildings from both architectural and technical perspectives. By exploring passive 19 strategies, it becomes possible to enhance internal thermal conditions, leading to a reduction 20 in the size and energy demands of air conditioning systems. Therefore, in this section, we 21 compare the thermal behavior and inertia of buildings constructed using M15D and M0 mate-22 rials.

To achieve this goal, we employed the enthalpy model to simulate the M15D building, while

24 a basic heat conduction transfer model was utilized for the simulation of the M0 building. Us-

25 ing these simulation approaches, we analyzed the hourly temperature fluctuations for four

representative days during summer conditions, specifically from July 21st to July 24th, in the
 Mediterranean's hot-dry climate and a degraded oceanic climate. The results of these simula-

3 tions are presented in **Figure 10** (a, b, and c).

4 In both Mediterranean and degraded oceanic climates, the incorporation of bio-based PCM 5 leads to a decrease in wall temperature during the morning and less efficient heat dissipation 6 during the night, as compared to conventional concrete walls. The results indicate that when 7 the zone temperature reaches the melting range (25-28°C), the bio-based PCM undergoes a 8 phase change, absorbing energy as latent heat, thereby preventing a rapid increase in indoor 9 air temperature. Conversely, when the outdoor temperature drops below 28°C, the PCM initi-10 ates the solidification process, releasing the stored heat and raising the zone temperature 11 above the reference case.

- 12 Moreover, it is observed that M15D significantly helps to dampen the periodic temperature
- 13 variations in comparison to conventional concrete (M0). The damping rate for M15D is esti-
- 14 mated to be around 34% in the Mediterranean climate, whereas it is approximately 48% for
- 15 M0. Additionally, the integration of M15D leads to a delay of temperature peaks by approxi-
- 16 mately 5 hours, whereas M0 only delays the temperature peak by about 2 hours (see Table 3).

17 We also notice that M15D has a greater ability to dampen periodic temperature variations

- 18 compared to conventional concrete (M0) in the degraded oceanic climate. The damping rate is
- estimated at 34% for M15D and 48% for M0. Additionally, M15D exhibits a remarkable abil-
- 20 ity to delay temperature peaks by 5 hours, while M0 only achieves a delay of around 2 hours
- 21 (Table 3). These results clearly indicate that M15D possesses significant thermal inertia ow-
- 22 ing to its thermal storage capacity and low thermal diffusivity, setting it apart from M0.

These observations hold true even in mild climates, as the melting temperature of the biobased PCM lies within the range of external temperature variations.





Figure 10. Simulated indoor temperature of the M15D and AAC M0 buildings: (a) Mediter ranean climate and (b) hot-dry climate (c) degraded oceanic climate.

3 In the hot and dry climate (Figure 10.b), the findings indeed indicate that the temperature

4 profile obtained with M15D is almost the same to the one obtained without the PCM (M0).

5 The outdoor temperature in this climate exceeds the melting point of the bio-based PCM, re-

6 sulting in the PCM remaining in a liquid state throughout the day.

Therefore, the integration of our bio-based PCM with (29°C of melting temperature) is not
advantageous in hot-dry climates under passive conditions. The combination of high outdoor
air temperatures and intense solar radiation during the day leads to the quick melting of the
PCM. Moreover, without a cooling or ventilation system to expedite the solidification pro-

- 11 cess, the use of PCM becomes unfavorable in such situations.
- 12

13

	Mediterra	anean climate	H c	ot-dry limate	Degraded oceanic climate	
	M0	M15D	M0	M15D	M0	M15D
ξ(%)	48	34	42	40	41	27
η (h)	2	5	2	3	2	5

Most of the time, the primary advantage of using PCM is to achieve a setback of temperature and reduce peak energy demand. In this section, we examine the energy consumption of buildings constructed with M15D and M0 during both winter and summer periods, considering three different climatic regions (Mediterranean, hot-dry climate, and degraded oceanic climate). The energy consumption for both materials over four representative days in winter and summer is depicted in **Figure 11**.

8 The results clearly show that the integration of bio-based PCM has a positive impact on re-9 ducing energy consumption across all scenarios. For instance, during winter, M15D allows for

10 a heating energy saving of 33% in both climates, while the saving in cooling energy amounts

to approximately 31% in the Mediterranean climate and 27% in the hot-dry climate. However,

the energy-saving potential varies significantly depending on the external environmental con-

13 ditions surrounding the building, especially during the summer period.

15 unons surrounding the building, especially during the summer period.

14 The simulation results reveal several key insights. In hot-dry areas characterized by extreme

15 heat during the summer period, the energy demand for cooling is significantly higher com-

16 pared to Mediterranean or degraded oceanic climate zones. However, due to the wide range of

17 daytime temperatures in these hot-dry regions, there is not enough temperature difference be-

18 tween day and night to facilitate or sustain solidification of the PCM. As a result, the impact

19 on energy savings from PCM integration is limited in such cases.

20 Conversely, during the winter, the results demonstrate an interesting contribution of PCM 21 integration to heating energy savings in buildings across all three climate types. For both 22 Mediterranean and degraded oceanic climates, even though the external temperature is lower 23 than the melting range of M15D, substantial heating energy savings are achieved, highlighting

24 the excellent thermal properties of M15D, including its thermal conductivity and diffusivity.

25 Furthermore, in the hot-dry climate, where the outdoor temperature remains within the melt-

26 ing temperature range of the PCM, there is a maximum benefit from the heat charge/discharge

27 processes in M15D, leading to notable heating energy savings.



Figure 11. Energy consumption for M15D and for M0 buildings: (a) Mediterranean climate
 and (b) hot-dry climate (c) degraded oceanic climate.

Table 4. Energy saving using bio-based PCM.

	Saving (%)			
	Heating Cooling			
Mediterranean climate	33	31		
Hot and dry climate	33	27		
Mild climate	33	29		

4

#### 5 **5.** Conclusion

6 This study investigated the thermal responses of two walls: a reference mortar wall and one 7 with bio-based microencapsulated phase change materials (PCM). The bi-climatic testing set-8 up simulated indoor and outdoor conditions, highlighting the PCM's positive influence on 9 cement composite thermal performance. 1 Key findings from our research are summarized in the following.

2 During day/night cycles, both walls showed similar temperature trends, but PCM inclusion 3 introduced a controlled damping effect, absorbing and releasing heat during melting and so-

4 lidification.

5 EnergyPlus simulations conducted at the building scale consistently demonstrated notable 6 effects of PCMs on temperature variation and damping rates within model cells. The im-7 provement in thermal performance was notably impactful in regions marked by substantial 8 daily temperature fluctuations, such as those found in Mediterranean and Degraded oceanic 9 climates. Reduced effectiveness was observed in extremely hot and dry climates, highlighting 10 limitations posed by the swift melting of PCMs in the absence of suitable cooling strategies.

- 11 Overall, the utilization of bio-based PCMs demonstrates advantages in optimizing building 12 envelopes for enhanced energy efficiency. Significant energy savings and diminished peak
- demand were evident, particularly during winter seasons, even in climates where seasonal
- 14 temperatures fall below the melting range of the PCMs.
- 15 The strategic application of bio-based PCM shows potential for promoting energy sustainabil-
- 16 ity in construction, contingent on climate conditions. Challenges exist in hot-dry climates,
- 17 requiring careful consideration of cooling and ventilation strategies.
- 18 Future research should focus on long-term durability and cost-effectiveness of bio-based PCM
- 19 integration, exploring tailored applications for specific climates, optimizing PCM composi-
- 20 tions, and investigating compatibility with other construction materials.
- 21 In conclusion, this comprehensive study underscores the promising role of bio-based PCM in
- 22 enhancing energy efficiency, particularly in regions with favorable climatic conditions. As
- 23 construction trends toward sustainability, the strategic use of PCM offers a tangible solution
- to address both energy demands and thermal comfort in buildings.
- 25
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