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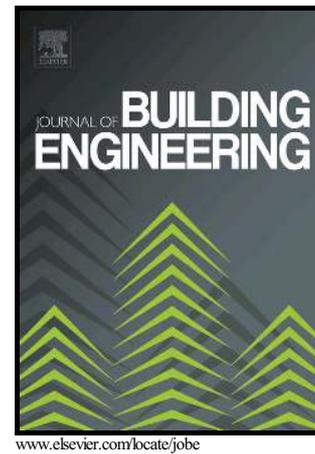
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## Numerical analysis of a micro-encapsulated PCM wallboard:

## Fluxmeter applications

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**Abstract:** In this paper, the thermal behavior of a micro-encapsulated phase change material wallboard is numerically investigated. A physical model coupling the heat transfer inside the wallboard with the heat transfer and the phase change process within micro-encapsulated phase change material (PCM) is introduced. The effect of different parameters such as the heating/cooling rate and the mass fraction of the PCM on the thermal behavior of the wallboard is evidenced. Simulation results are used to determine the variation of temperature and liquid fraction of the PCM and quantify heat fluxes exchanged between the two lateral sides of the wallboard. The physical model presents a methodology to determine the thermophysical properties of materials containing phase change materials (PCM).

**Keywords:** PCM; Heat transfer; Melting/Freezing; Building construction; Energy storage.

**Nomenclature**

$a$  Superficial capsule area per unit bed volume ( $m^{-1}$ )

$c$  Specific heat ( $J kg^{-1} K^{-1}$ )

$d$  Diameter ( $m$ )

$f$  PCM liquid mass fraction

$h$  Heat transfer coefficient ( $W m^{-2} K^{-1}$ )

$L_F$  Latent heat of PCM ( $J kg^{-1}$ )

$k$  Thermal conductivity ( $W m^{-1} K^{-1}$ )

$L$  Thickness ( $m$ )

$t$  Time ( $s$ )

$T$  Temperature ( $K$ )

$x$  Axial coordinate ( $m$ )

**Greek symbols**

$\varepsilon$  Volume fraction

$\rho$  Density ( $kg m^{-3}$ )

$\phi$  Heat flux ( $W m^{-2}$ )

*Subscripts, superscripts*

*B* Building material

*int* Inside

*ini* Initial

*m* Melting

*out* Outside

*PCM* Phase change material

## 1. Introduction

Currently, the building sector is considered as the largest energy-consuming sector with a total of 30% share of the overall energy consumption [1-2]. Thus, improving energy efficiency and reducing energy demand of buildings are widely considered as the most promising, fastest, cheapest and safest means to reduce the dependence on fossil fuel and mitigate climate change [3].

One of the promising methods to ameliorate the energy efficiency of buildings is implementing of thermal energy storage system. It is evidently important to note that the storage of the thermal energy is significantly cheaper than storing electric power to make

cooling [4]. In the building sector, sensible and latent storage methods are widely used [5]. Sensible storage materials have low thermal storage density which leads to large storage volume. To overcome this low thermal storage density, phase change materials (PCM) have enjoyed renewed popularity as they enable to absorb large energy amounts in a tiny volume [6]. Different types of PCM (organic and inorganic PCM, hydrated salts, microencapsulated PCM, shape stabilized PCM) with a large panel of temperatures in various containers have been extensively studied recently.

One of the interesting applications for phase change materials is in buildings by incorporating them in conventional construction [5-7]. By including PCM into wall construction, the through-wall heat transfer can be reasonably controlled with the absorption and release of latent heat [8-9]. The choice of phase change temperatures is a key parameter in the design of PCM building materials since they indicate their suitability by defining the storage capacity, size and application limit. This temperature has been investigated previously by different researchers [10-13]. Neepser [14] considered that the transition temperature of the PCM should be close to the indoor temperature to minimize the building thermal load. The melting temperature of 22°C, which is 2 °C higher than the indoor comfort temperature, is adopted by Heim and Clarke [15]. Zhang et al. [6] highlighted that the melting temperature of the PCM must be close the indoor temperature as a general rule. The common point by all these research works is PCM melting temperature, for an optimal use, depends strongly on the average room temperature, that in turn, fluctuates for many reasons from building to building and from season to season.

It is important to note that the characterization of the phase change process is an important issue for design and optimization of PCMs. Storage density and phase change temperatures are very important parameters since they decide the storage system capacity, size and

application range. Moreover, accurate estimation of PCM enthalpy variation in the working temperature range is essential for correct mathematical modeling of the storage system.

In this paper, a numerical model has been developed to investigate the thermal behavior of microencapsulated phase change materials incorporated in building material and to enable more accurate interpretation of the measured data provided by the fluxmeter instrument.

## 2. Physical model

A building material integrating phase change material is introduced in a rectangular mould. Both lateral sides of the studied sample are insulated. Each face of the sample is subjected to a temporal linear surface temperature:

$$T_{B,int} = T_{B,out} = T_p = \beta \cdot t + T_{ini} \quad (1)$$

where  $\beta$  is the heating/cooling rate.

At  $t = 0$  the initial conditions are  $T_{B,int} = T_{B,out} = T_{ini}$

The utilization of such linear temperature permits to easily notice any deviation on the temperature inside the sample. The building material and the PCM possess different thermal and physical properties, thereby the interaction between the two phases will surely impact the overall thermal behavior. The mathematical model must represent the two discretized domains. The main assumptions of the model are listed below:

- The PCM is pure, homogeneous and isotropic,
- Melting and solidification processes are isothermal,
- The PCM is supposed to be encapsulated in spherical capsules,

- The thermophysical properties of the PCM and of the building material do not depend on the temperature
- Supercooling during freezing is neglected,
- Heat transfer is generated by conduction and is one-dimensional.

Based on these assumptions, the energy balance equations for the building material and the PCM can be formulated as [16]:

- **Building material**

$$(1-\varepsilon)(\rho c)_B \frac{\partial T_B}{\partial t} = \frac{\partial}{\partial x} \left( (1-\varepsilon)k_B \frac{\partial T_B}{\partial x} \right) + U a (T_{PCM} - T_B) \quad (2)$$

$\rho_B$  and  $c_B$  denote, respectively the density and the specific heat capacity of the building material,  $k_B$  is the effective thermal conductivity of the building material,  $U$  is the overall constant heat transfer coefficient, while  $\varepsilon$  is the volume fraction of the PCM in the building material.

The superficial capsule area per unit volume  $a$  can be written as a function of the PCM volume fraction in the building material  $\varepsilon$  and the capsule diameter  $d$ :

$$a = \frac{6\varepsilon}{d} \quad (3)$$

- **PCM**

It is necessary to consider the two following situations:

- During sensible heat storage when the PCM is fully solid or liquid:

$$\varepsilon(\rho c)_{PCM} \frac{\partial T_{PCM}}{\partial t} = \frac{\partial}{\partial x} \left( \varepsilon k_{PCM} \frac{\partial T_{PCM}}{\partial x} \right) + Ua(T_B - T_{PCM}) \quad (4)$$

- During latent-heat storage when the PCM undergoes phase change

$$\frac{\partial f}{\partial t} = \frac{aU}{\varepsilon \rho_{PCM} L_F} (T_B - T_m) + \frac{k_{PCM}}{\rho_{PCM} L_F} \frac{\partial^2 T_{PCM}}{\partial x^2} \quad (5)$$

where  $f$  represents the liquid fraction of PCM,  $k_{PCM}$  expresses its thermal conductivity,  $\rho_{PCM}$  its density and  $c_{PCM}$  its specific heat capacity.  $T_m$  is the melting temperature of the PCM and  $L_F$  is the latent heat of the PCM.

### 3. Numerical solution

The governing differential equation subjected to the initial and boundary conditions shown in **Eqs. (2) – (4) – (5)** has been solved numerically by using the volume finite method. The physical model is divided into contiguous control volumes, where the grid points are placed at the geometric centers of these control volumes. The differential equation is integrated over each control volume and over the time step. Piecewise profiles expressing the variation of the dependent variable between the nodal point and the neighboring grid points are used to evaluate the required integrals. The time derivatives have been approximated by using fully implicit time integration. The obtained discrete equations have been solved iteratively at each time step by employing the TDMA algorithm.

### 4. Results and discussion

#### 4.1 Thermal behavior

In this work, the outside surface of the PCM wallboard is subjected to a temporal linear surface temperature on both lateral sides of the sample. Initially, it is supposed that the building material (i.e. cement mortar) is filled with 20% of BASF's free microencapsulated PCM (Microcanal PCM DS 5001 X) in order to have the possibility of comparing the numerical results by the experiments given in [17-18]. The rectangular mould in which the building material containing the PCM has a dimension of  $25 \times 25 \times 4 \text{ cm}^3$  [17-18].

The thermophysical properties of cement mortar and PCM are provided in **Table 1-a and Table 1-b**. The mean micro-encapsulated PCM diameter is taken as  $100 \mu\text{m}$  [17-18]. Each side of the phase change material wallboard is exposed to a time dependent linear surface temperature ( $T_{B,out}$  and  $T_{B,int}$ ) which is varied between 11 and 40 °C.

**Fig.1** plots the temperature variation at the center of the building material together with the imposed linear temperature. This figure contains three stages of heating and cooling with a period of 4 hours. This allows the PCM building material to recuperate its state of thermal equilibrium at each step. It can be shown that the temperature at the center of the building material presents an inflection point due to the phase change process occurring inside the PCM. These points match with the PCM melting temperature.

The validity of the mathematical model is verified by comparing our numerical results with experimental heat fluxes reported in [17-18] during the melting and solidification processes on the left side of the sample (see Fig.2). We note a close concordance between the model results and the experimental data reported in [17]. Only a slight difference between the experimental and numerical curves can be remarked at the beginning of the melting process. These deviations can be interpreted by the fact that in the numerical simulation, the PCM is

supposed to be pure, isotropic and homogeneous with constant properties for liquid and solid phases. These assumptions may not be entirely true in the reality. For more accurate numerical results, it is therefore recommended to consider temperature dependent material properties. It should be noted also that the numerical results obtained by the model are similar to those reported by Hasse et al. [19] under the same conditions.

**Fig.3** represents the time variation of heat fluxes on both lateral sides of the sample during the heating and the cooling processes. During the first stage, sensible heat is stored by the sample. When the building material temperature reaches 26 °C, the solidification/melting process begins by releasing/absorbing latent heat. This phenomena are evidenced by the sudden increases/decreases in the heat fluxes. These results are similar to the experimental data given by Joulin et al. [18].

The mathematical model gives the possibility of determining the liquid fraction values of the PCM inside the building material which can serve for understanding the shape of the heat flux on the sides of the sample. The evolution of these parameters as a function of  $T_{B,out}$  during the melting and the freezing processes is presented in **Fig. 4**. The temperature  $T_{peak}$  refers to temperature of  $T_{B,out}$  which lead to the maximum value of the heat flux through the sample.  $T_{peak}$  is found to be 21 °C during the solidification process and 31 °C during the melting process.

To highlight the effect of the volume fraction of the PCM in the building material, different values of  $\mathcal{E}$  are considered in the simulation. The numerical results of the heat flux as a function of  $T_{B,out}$  are displayed in **Fig.5**. One can see that the melting process is strongly influenced by the value of  $\mathcal{E}$ . It is clearly seen that increasing the PCM volume fraction in the sample, generate an increase in the time needed for the phase transition process. It is also

possible observe that the peak temperatures range becomes larger and it moves to higher temperatures (see **Fig.6**).

**Fig.6** compares also the behavior of the building material with and without PCM. Without PCM, the building material stores only a sensible energy. Moreover, this figure describes the large ability of PCM to absorb and release the heat and reaching the aim of time shifting.

#### **4.2 Thermophysical properties of the building material containing PCM**

Before melting process of PCM within the building material is studied, it is interesting to find the relation between the heat flux and the thermophysical properties of the building material containing PCM such as the apparent specific heat capacity, the apparent thermal conductivity, and when the phase change occurs, the melting temperature and the latent heat of PCM.

##### **4.2.1. Apparent specific heat capacity**

Repeating the numerical simulation, with different heating/cooling rates between 11 and 40°C, gives results as shown in **Fig.7**. For all heating and cooling rates the first signal reading that appears between 11 and 14 °C during heating process and between 40 and 35°C during cooling process is associated with the stabilization of the sample, that is, a transient state. This signal corresponds to a change of state from an isothermal state to a transient state. After the system overcomes this initial transient state, a continuous steady regime (between 14 and

26°C during heating process and between 35 and 26°C during cooling process) of constant heating is achieved, and this is reflected in a stable baseline that will change only by varying the heat capacity of the studied sample or by changing the heating/or cooling rate.

From **Fig.7**, we can note that the heat flux (between 14 and 25 °C during heating process and between 35 and 25°C during cooling process) can be expressed by the following equation:

$$\phi = C \beta + F \quad (6)$$

where  $\phi$  is the heat flux,  $C$  is the slope of the straight-line and  $F$  is a constant.

The above equation shows how the total heat flux increases linearly with heating rate due to the heat capacity of the sample [20-21]. Notice that, from this equation, the specific heat capacity of the PCM in liquid or solid state can be easily calculated by the following expression:

$$c = \frac{C}{\rho \cdot e} \quad (7)$$

where  $e$  is the width of the sample and  $\rho$  is the density of the mortar containing PCM.

The values of the apparent specific heat of the building material when PCM is in liquid or in solid state are presented in **Table 2**. We note that the apparent specific heat of the building material is approximately similar when the PCM is in the solid or in the liquid state.

#### 4.2.2. Melting temperature of the PCM

From **Fig.7**, one can observe that the heating/cooling rate do not affect the onset of the peak of the heat flux during the melting/freezing process of PCM. Accordingly, peak onset can be employed to specify the melting temperature of the PCM. If we focus on the end of each peak, a clear tendency can be seen. When the heating rate increases, the peak changes toward greater temperatures. This result originates from the increase in the thermal gradient inside the sample. When the building material is heated, heat flows from the outside surfaces and is absorbed by the material. During the heating/cooling process there is constantly heat supplied to the sample, and an internal thermal gradient is created. This thermal gradient rises with respect to higher heating/cooling rates (see **Fig.8**).

#### 4.2.3. Latent heat of the PCM

The mathematical model is able to predict the density of the heat flux exchanged at the borders of the sample. At the beginning, the sample is isothermal and is gradually heated from the temperature  $T_i = 11^\circ\text{C}$  to  $T_e = 40^\circ\text{C}$ . The expression of the total stored energy can be written as follows:

$$Q = \int_{T_i}^{T_e} [|\varphi_{out}| + |\varphi_{int}|] S dt \quad (8)$$

The sum  $|\varphi_{out}| + |\varphi_{int}|$  represents the cumulated density of the heat flux flowing into the sample (see **Fig.9**).  $\varphi_{out}$  and  $\varphi_{int}$  denote the heat flux on the left-hand side and the heat flux

on the right-hand side of the sample, respectively.  $S$  is the lateral area of the sample. Another manner to express the quantity  $Q$  is given by the equation:

$$Q = m_{sample} C_{s,app} \Delta T_s + m_{PCM} L_F + m_{sample} C_{l,app} \Delta T_l \quad (9)$$

where  $C_{s,app}$  and  $C_{l,app}$  are, respectively, the apparent heat capacity of the sample when PCM is in the solid phase and in the liquid phase;  $\Delta T_s$  is the temperature difference between the melting point ( $26^\circ\text{C}$ ) and  $T_i$ ;  $\Delta T_l$  is the temperature difference between  $T_e$  and the melting temperature.

The latent heat of the PCM is obtained with the following expression where  $m_{sample}$  is the total mass of the sample and  $m_{PCM}$  is the PCM mass:

$$L_F = \frac{Q - m_{sample} C_s \Delta T_s - m_{sample} C_l \Delta T_l}{m_{PCM}} \quad (10)$$

Based on Eq. (10), the value of latent heat can be obtained for various heating rates and for a temperature field varying from  $11^\circ\text{C}$  to  $40^\circ\text{C}$ . The results are presented in **Table.3** in which it is clear that the value of the latent heat of melting is somewhat sensitive to the heating rate level. This is mainly due to the increase in the thermal gradient inside the sample as a result of increasing the heating rate. Generally, for a precise approximation of the latent heat, it is advisable to consider lower heating rates. Nevertheless, lower heating rates require longer measurement times which may be expensive. As a result, these issues should be balanced while carrying out the measure.

#### 4.2.4. Apparent thermal conductivity

The thermal conductivity of the mortar with PCM at solid or liquid state can be calculated using the following expression:

$$\lambda = \frac{(\phi_{out} + \phi_{int}) \cdot e}{2 \cdot (T_{B,out} - T_{B,int})} \quad (11)$$

Note that this expression must be used when the steady state is reached inside the sample. To be sure that the PCM inside the building material is at solid state or at its liquid state, simulations are performed between 15°C and 20°C for a solid PCM (see **Fig.10**) and between 35°C and 40°C for a liquid PCM (see **Fig.11**). When steady state is reached, the average value of the apparent thermal conductivity of the building material with PCM is calculated for a temperature difference between the plates of about 5°C (see **Table.4**). We note that the thermal conductivity of the building material is not really influenced by the PCM's state (liquid or solid).

## 5. Conclusion

In this article, a physical model was developed to understand and analyze the thermal behavior of a building material comprising PCM. The validity of the numerical code used is ascertained by comparing our results with previously published results. A parametric study was carried out to study the effect of various parameters such as the heating rate and the volume fraction of the PCM on the thermal behavior of these materials. It is found that the thermophysical properties of the studied building material can be easily determined by using heat flux curves on both sides of the building material. It is also found that the use of higher heating rates increases the temperature gradients within the studied sample. In order to describe with accuracy the thermal behavior of materials containing phase change materials, it is recommended to use lower heating rates.

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**Table 1-a:** Physical Properties of Mortar

Density	1400 kg.m <sup>-3</sup>
Thermal conductivity	0.65 W.m <sup>-1</sup> .°C <sup>-1</sup>
Specific heat capacity	925 J.kg <sup>-1</sup> °C <sup>-1</sup>

**Table 1-b:** Physical Properties of PCM

Density (solid/liquid)	995 kg.m <sup>-3</sup>
Thermal conductivity (solid)	0.2 W.m <sup>-1</sup> .°C <sup>-1</sup>
Thermal conductivity (liquid)	0.13 W.m <sup>-1</sup> .°C <sup>-1</sup>
Specific heat capacity (solid)	1700 J.kg <sup>-1</sup> °C <sup>-1</sup>
Specific heat capacity (liquid)	2153 J.kg <sup>-1</sup> °C <sup>-1</sup>
Latent heat of fusion	16674 J.kg <sup>-1</sup>
Melting temperature	26 °C

**Table 2:** Apparent specific heat of the building material with PCM

PCM at solid state	PCM at liquid state
1255 J.kg <sup>-1</sup> .K <sup>-1</sup>	1261 J.kg <sup>-1</sup> .K <sup>-1</sup>

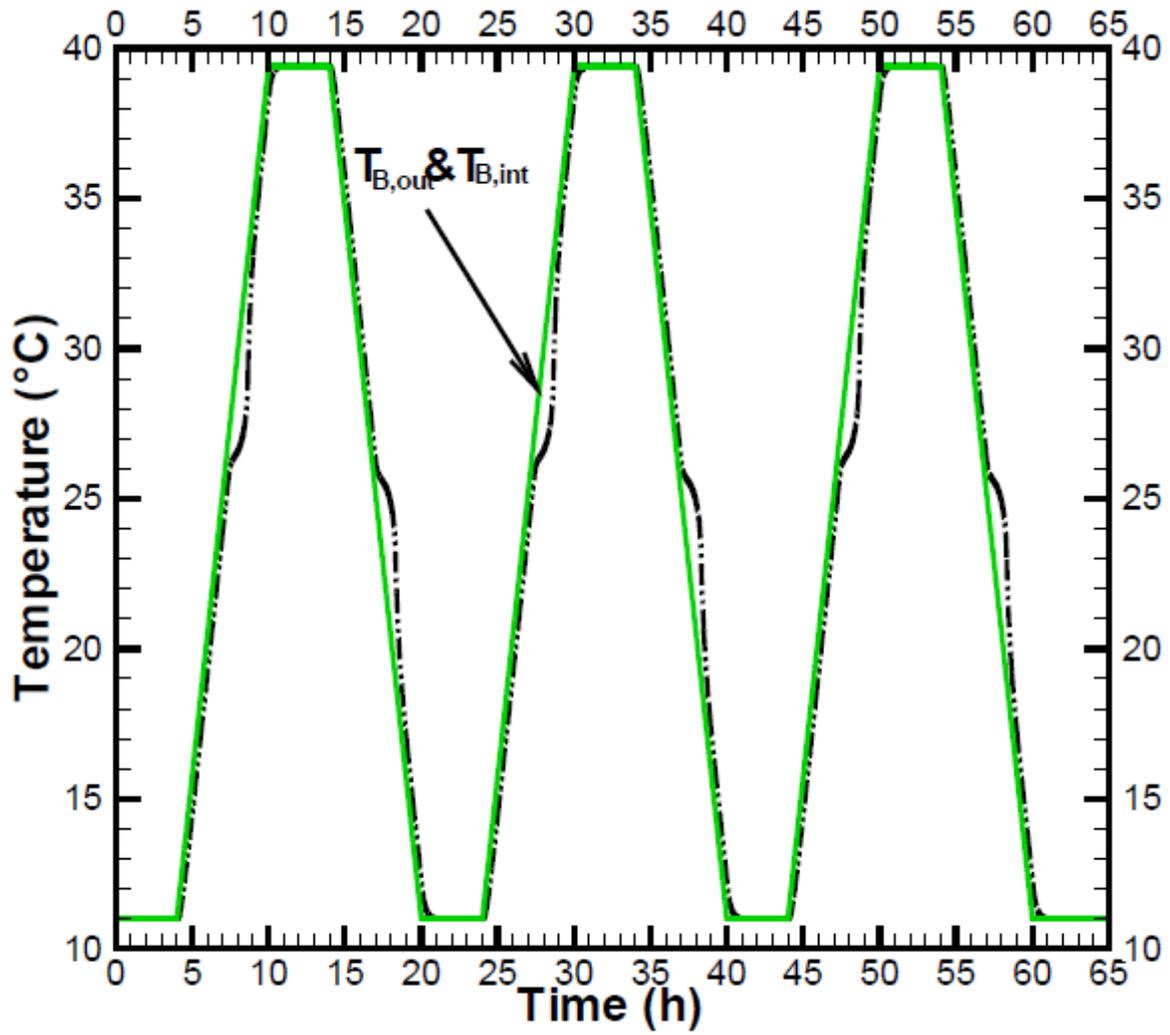
**Table 3:** Latent heat for different values of  $\beta$  for  $\varepsilon = 0.20$ 

Heating rate (°C/min)	Latent heat (J/kg)
0.04	166751.3
0.06	166759.2
0.08	166764.5
0.1	166772.7

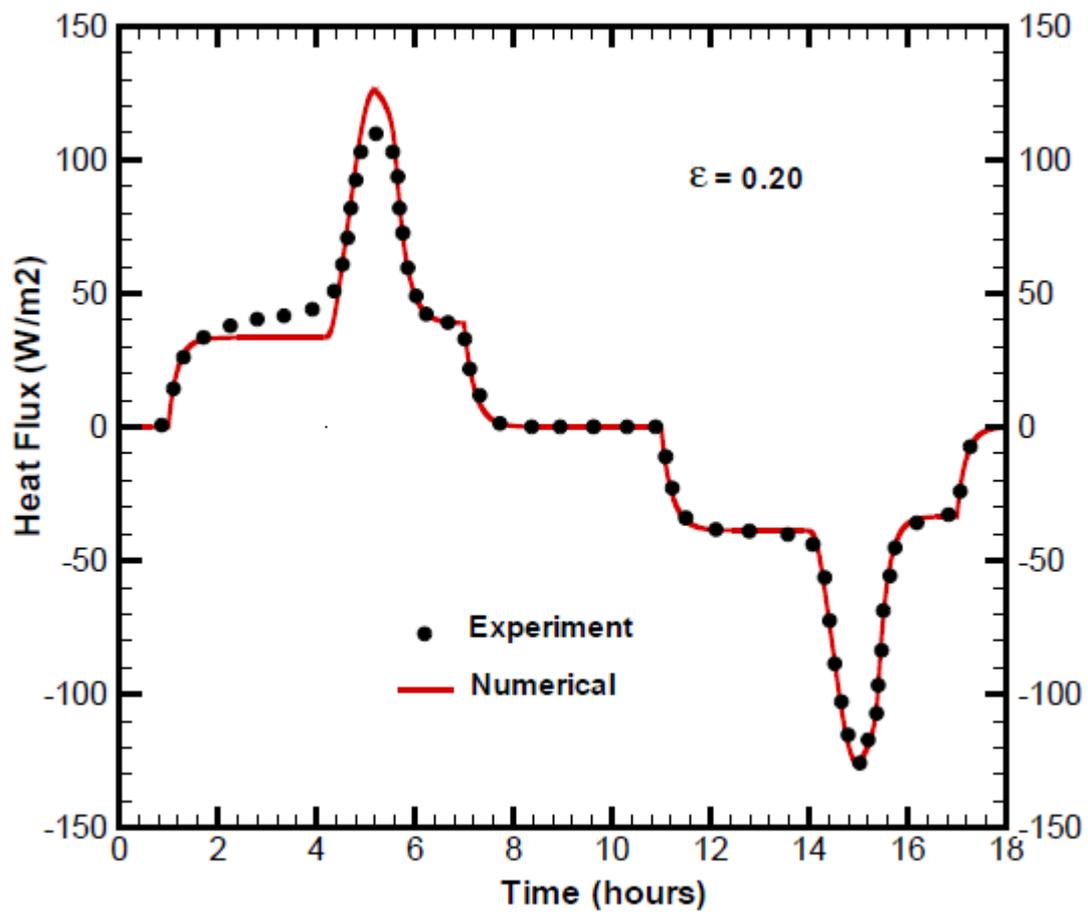
**Table 4:** Thermal conductivity of the building material with PCM

PCM at solid state	PCM at liquid state
0.365 W.m <sup>-1</sup> .K <sup>-1</sup>	0.368 W.m <sup>-1</sup> .K <sup>-1</sup>

**Fig.1:** Mortar temperature variation with time during melting and solidification processes



**Fig.2:** Numerical and experimental heat flux [17-18] during heating and cooling processes at the front side of the sample.



**Fig.3:** Numerical heat flux versus time during heating and cooling processes at the front sides of the sample.

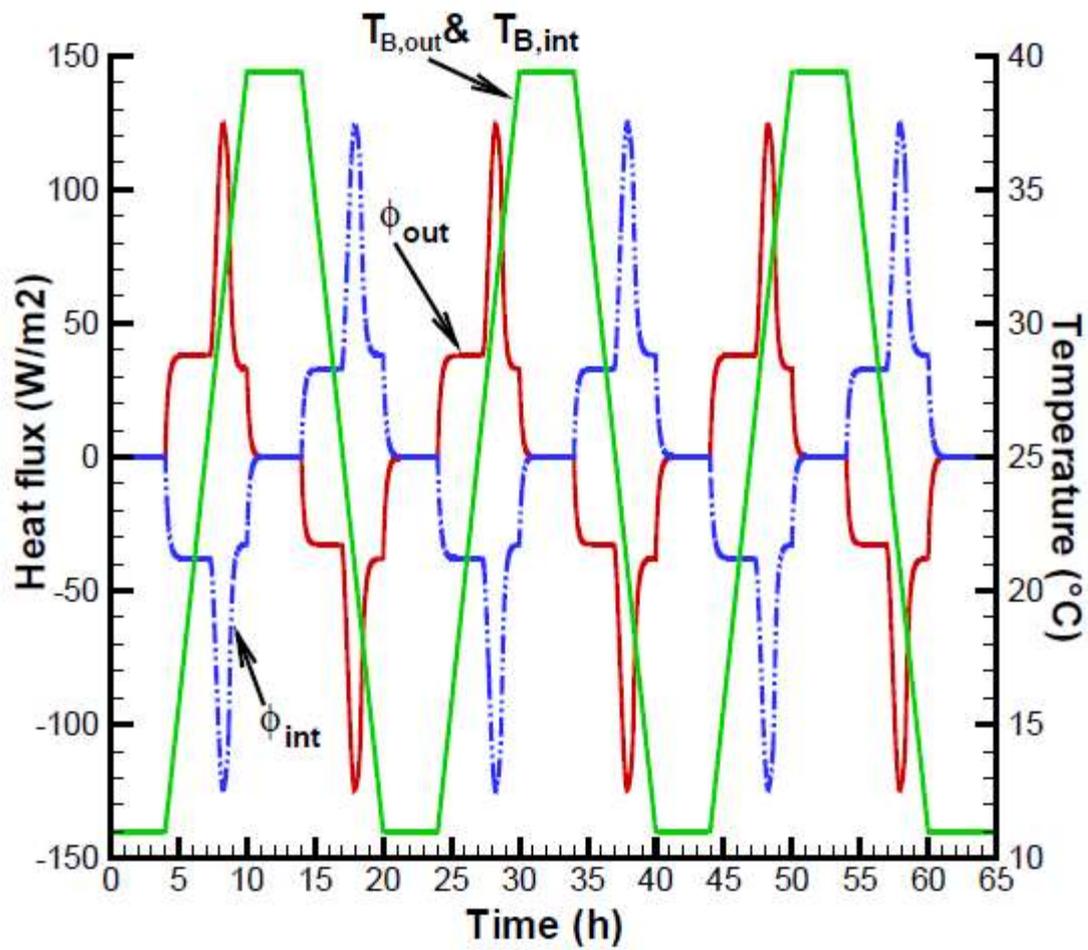


Fig.4: Numerical heat flux  $\phi_{out}$  versus  $T_{B,out}$  during heating and cooling processes

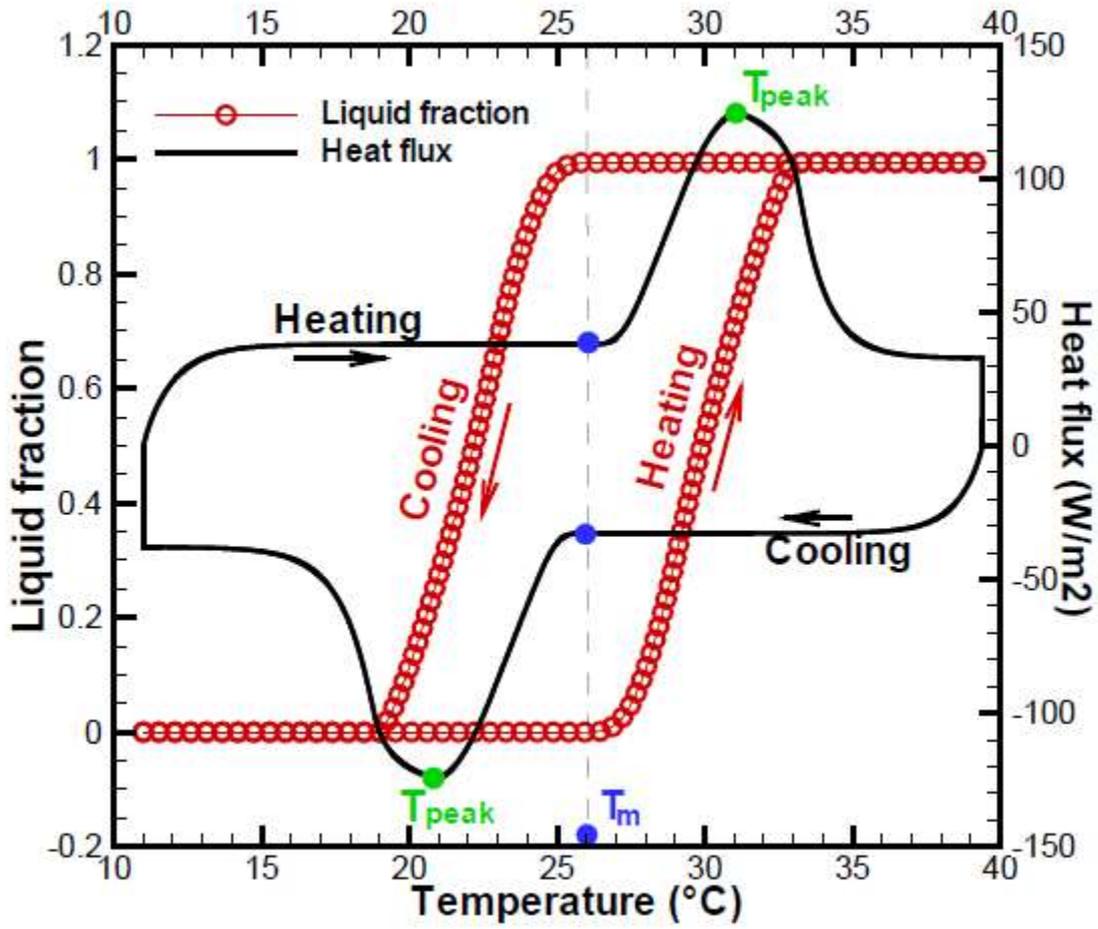


Fig.5: Numerical heat flux versus time during heating and cooling at the front sides of the sample for various  $\varepsilon$

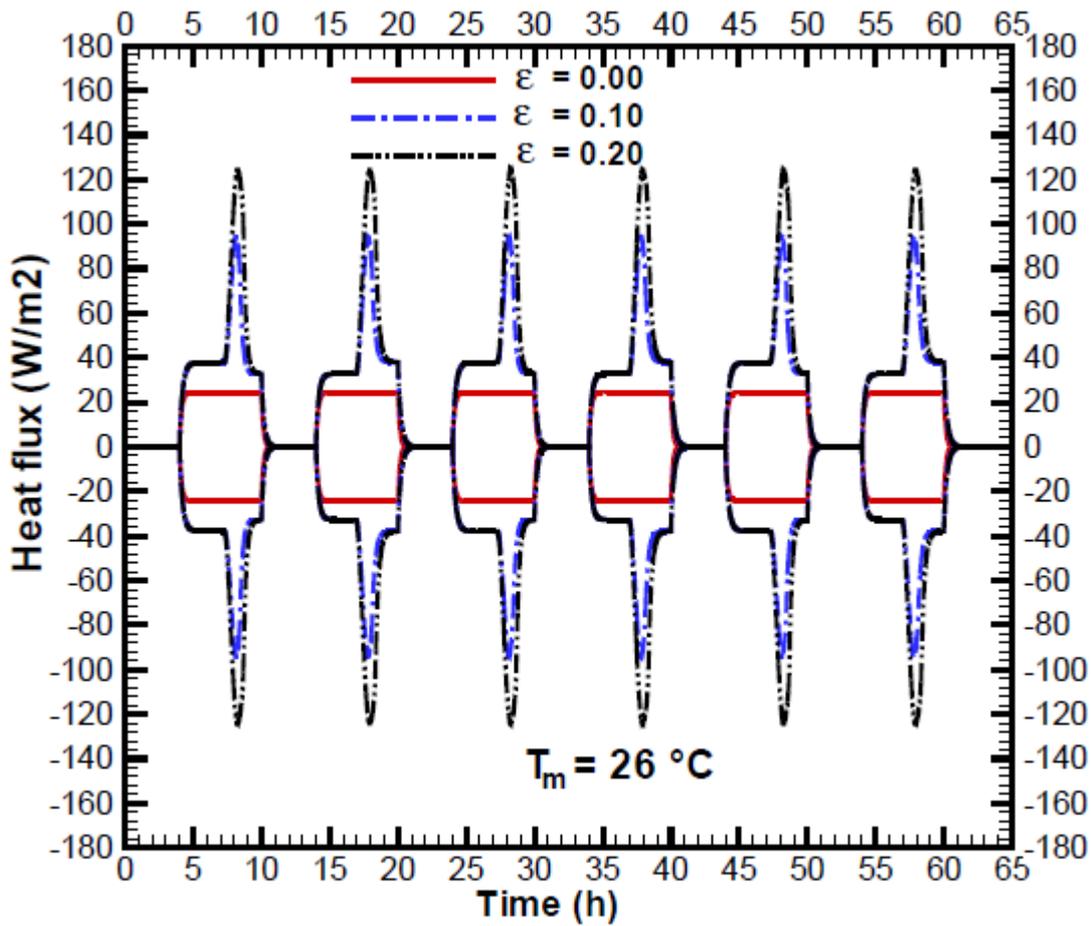
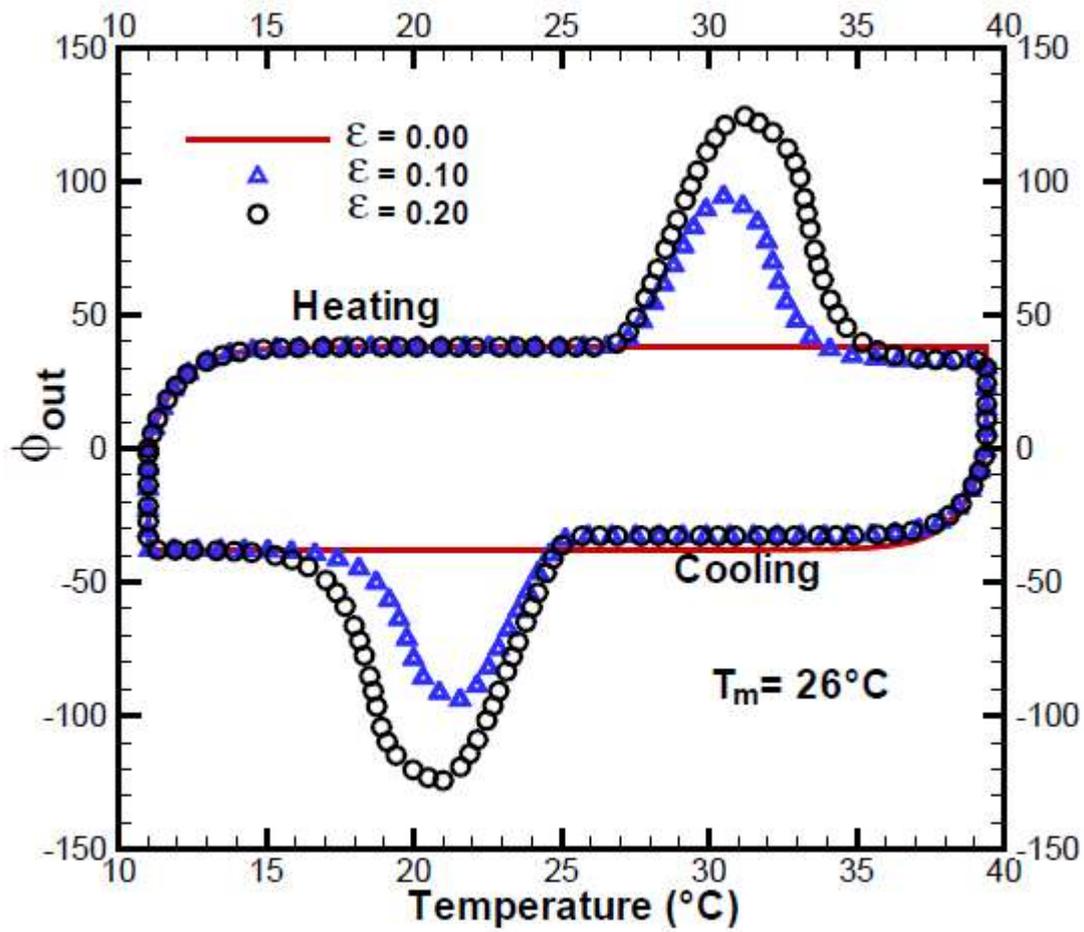
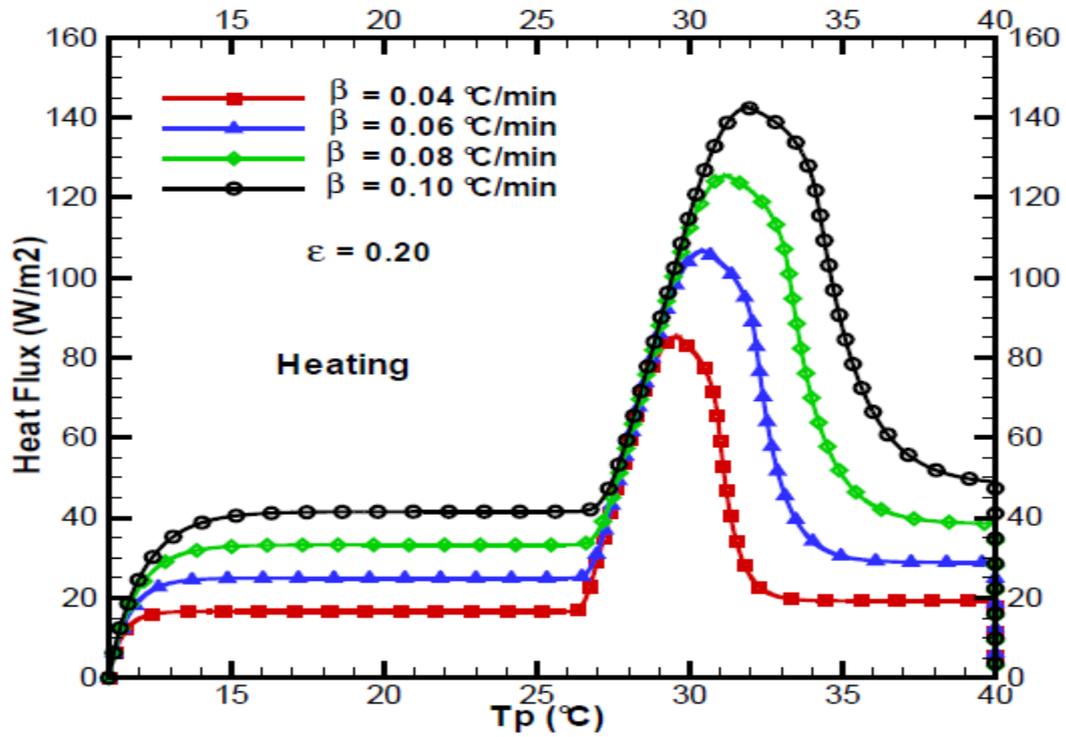
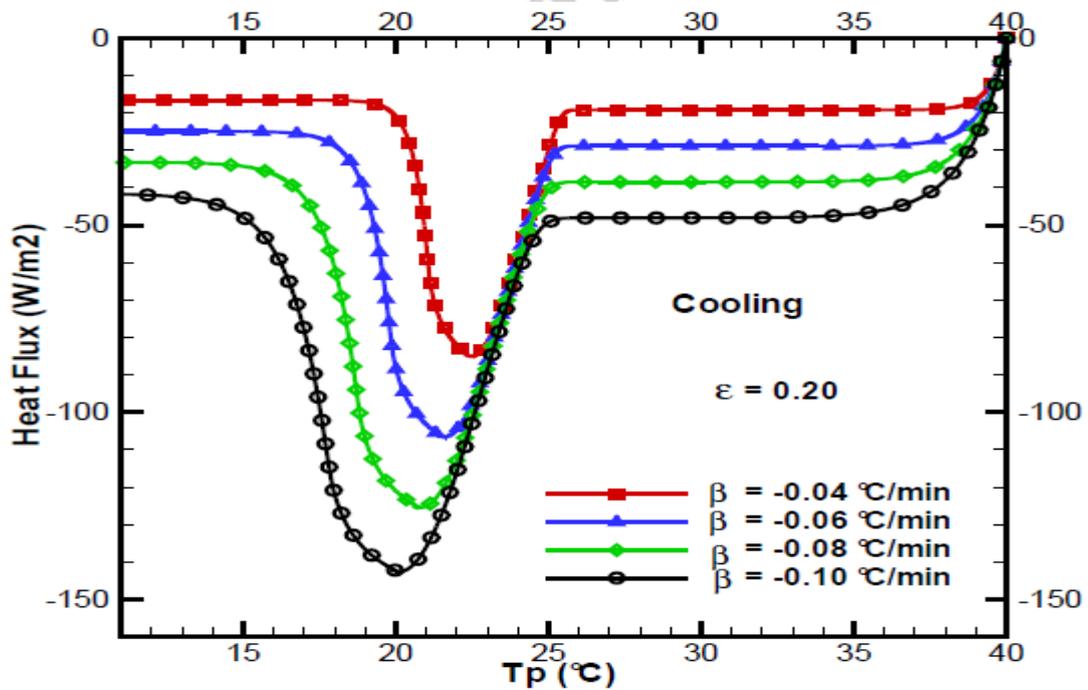


Fig.6: Numerical heat flux  $\phi_{out}$  versus  $T_{B,out}$  during heating and cooling for various  $\varepsilon$

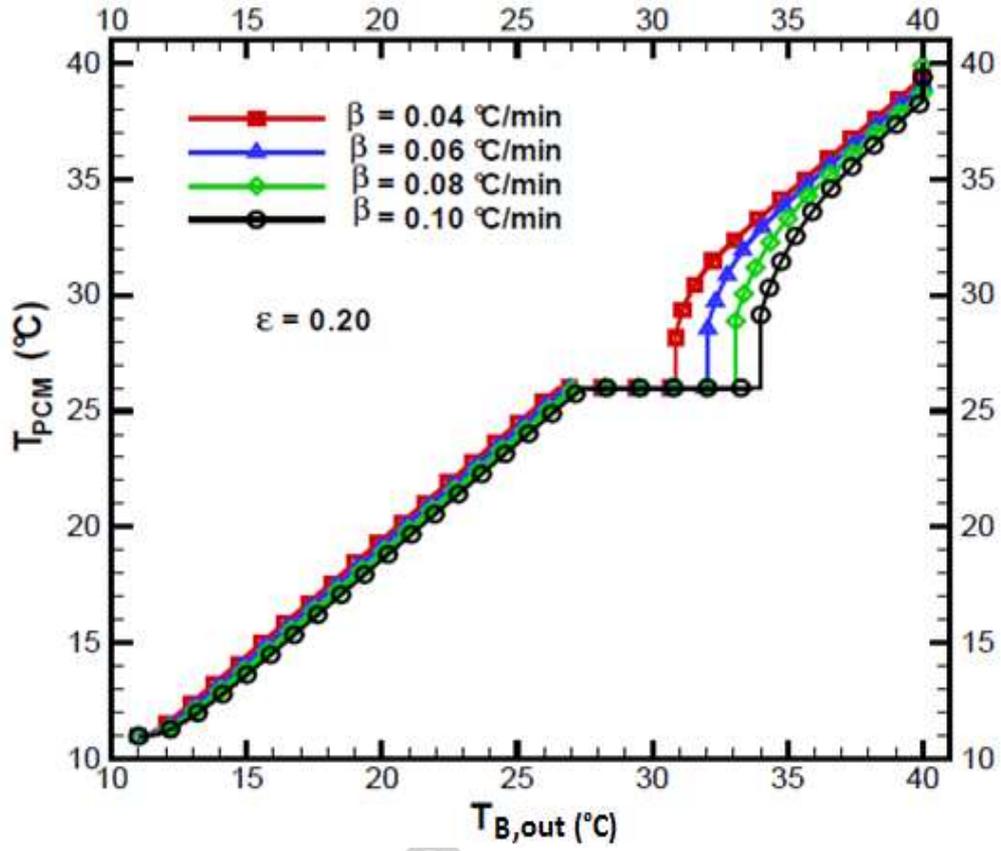


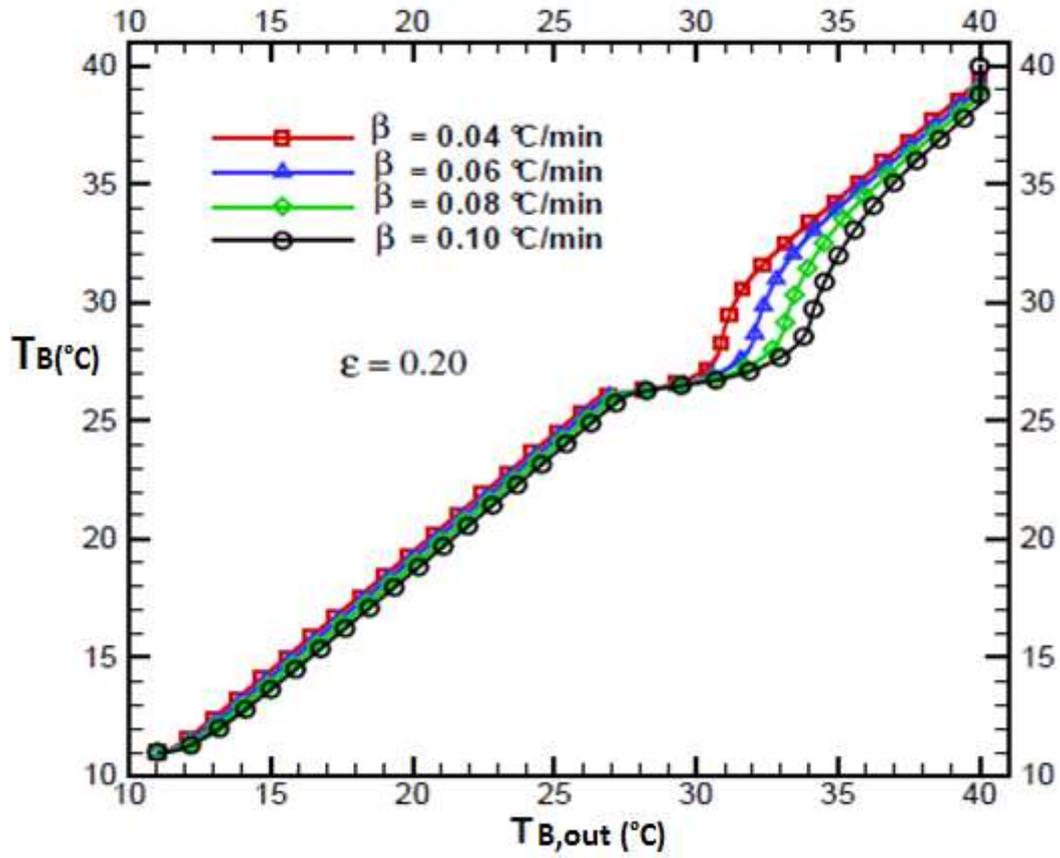
**Fig.7:** Numerical heat flux for different heating and cooling processes

(a) Heating process

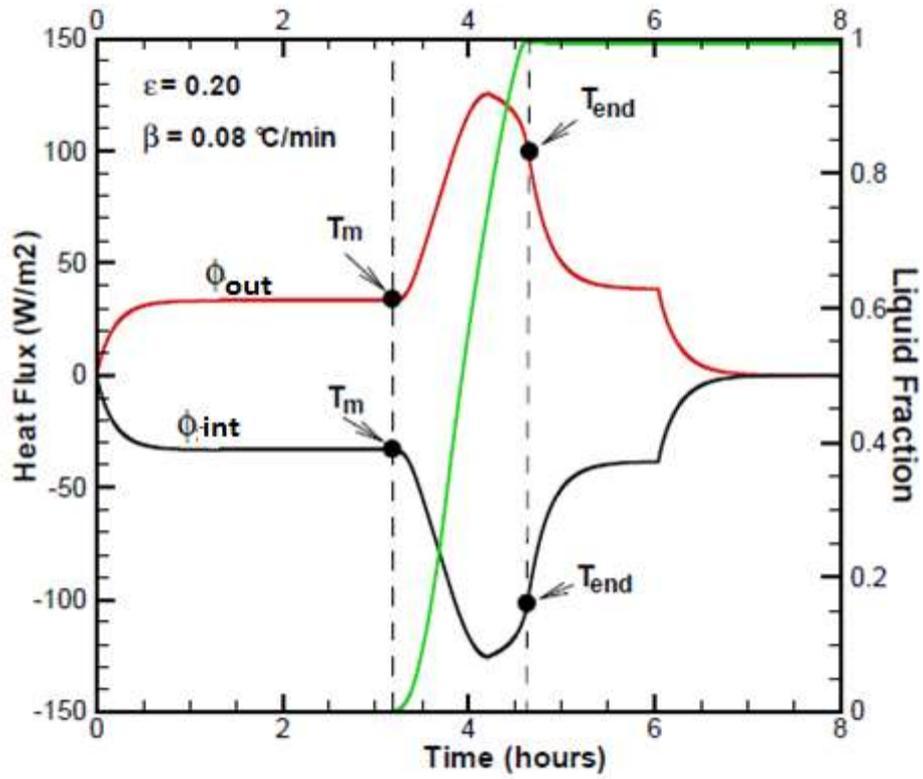


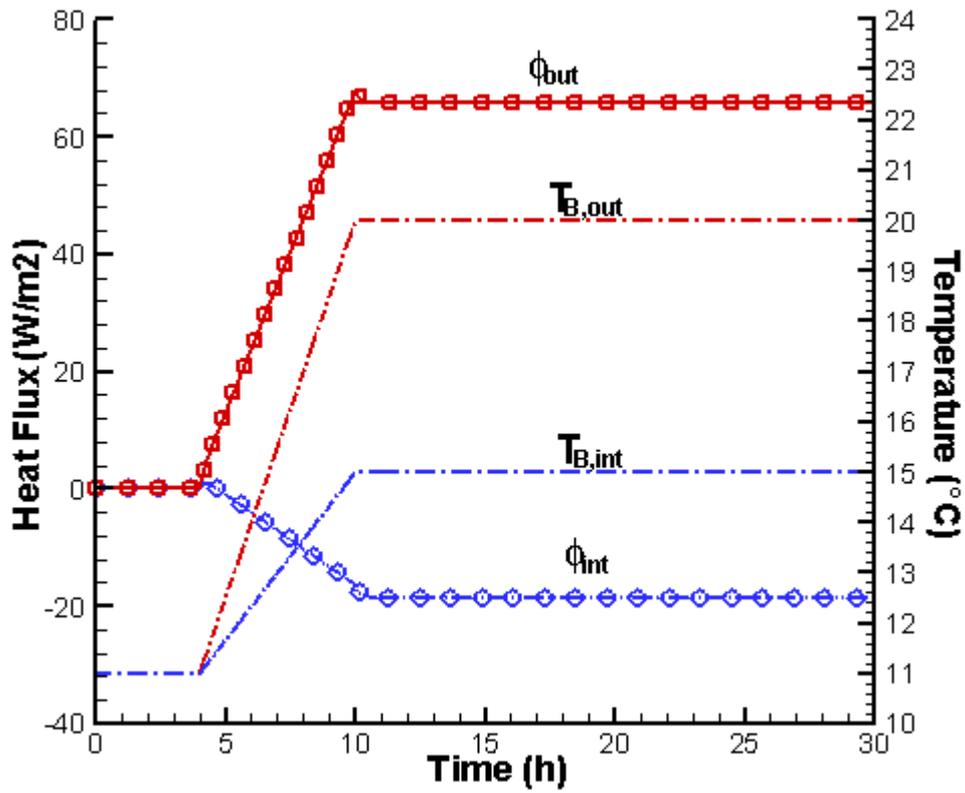
(b) Cooling process

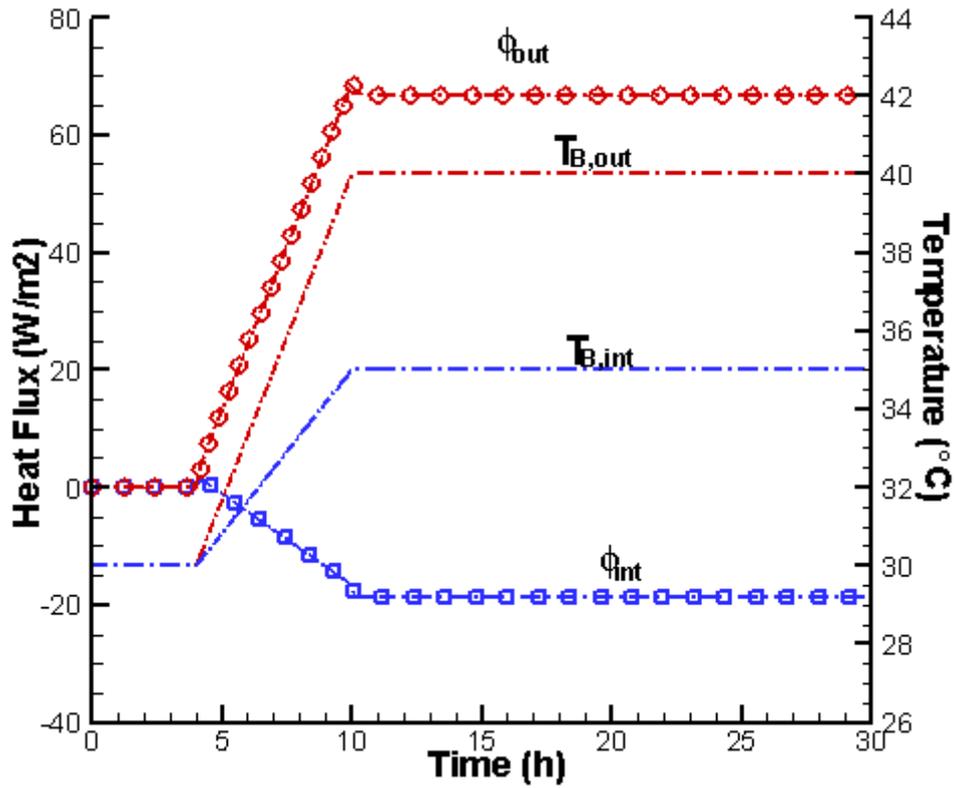
**Fig.8-a:** Numerical mortar temperature at the center of the sample versus  $T_{B,out}$ 

**Fig.8-b:** Numerical PCM temperature at the center of the sample versus  $T_{B,out}$ 

**Fig.9:** Numerical heat flux during melting process versus time at each side of the sample.



**Fig.10:** Numerical heat flux when PCM is at solid state

**Fig.11:** Numerical heat flux when PCM is at liquid state

## Highlight

- Thermal behavior of micro-encapsulated PCM wallboard.
- Effect of heating rate and volume fraction of PCM on the thermal behavior of PCM wallboard.
- Numerical approach to determine the thermophysical properties of PCM.