# Numerical modeling of thermal performance of a building envelope incorporating solid-solid phase change material

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**Abstract.** This research focuses on the study of the thermal performance of a building envelope structure incorporating a patented solid-solid phase change material (S-S PCM), designated as PUX-1500-20, a cross-linked polyurethane. This S-S PCM is capable of storing and releasing thermal energy via phase transitions within the human comfort temperature range, facilitating the temporal and spatial transfer of solar energy for optimizing energy efficiency. The primary aim of this work is to study numerically the thermal behavior of the building envelope (hollow brick) filled with the PCMs. The numerical simulations use Matlab software based on the method of the heat equation. In comparison with the thermal behavior of the building envelopes (hollow brick) without PCMs, the results presented herein provide convincing evidence of the important thermal inertia of these structures incorporating the PCMs, revealing their significant potential in contributing to the reduction of energy consumption of building.

**Keywords:** Patented phase change material, solid-solid transition, latent heat storage, cross-linked polyurethane, building integrated, passive thermal storage system, numerical simulation.

## 1. Introduction

With the rapid growth of the global population, the aggravation of climate change and the rising demand for thermal comfort in buildings, the sector of construction and building has become the largest consumer of energy in recent decades, accounting for approximately 40% of the world's annual energy consumption [12]. Over 27% of this amount comes from the household energy consumption, primarily for heating, ventilation, and air conditioning (HVAC) systems [345]. Due to these excessive energy demands, this sector is also a significant contributor to global carbon emission [67]. To reduce the high energy consumption of building operation and the associated carbon emissions, one of the main challenges for future buildings is the rational design of building envelopes. This involves

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insulation improvements as well as using renewable energy (e.g. solar energy). Developingpassive systems for thermal energy storage can also contribute to reducing the energy demand for cooling and heating while maintaining a thermally comfortable indoor environment. A proposed solution is to integrate smart materials into building envelopes.

Phase change materials (PCMs) are considered one of the most promising smart materials due to their ability to exchange (absorbing and delivering) thermal energy with the surrounding environment through phase transitions [8910]. This property enhances the thermal inertia of buildings optimizing the thermal comfort of building occupants, reduces indoor temperature fluctuations, improves energy efficiency which allows downsizing cooling and heating systems. These benefits contribute to lowering greenhouse gas emission and therefore mitigating global warming [11].

PUX-1500-20 is a cross-linked polyurethane developed and patented by T. Harlé et al. (2017). It is an organic solid-solid phase change material (S-S PCM) suitable for building application [12]. This material presents significant advantages: i) phase change temperature within the human comfort range ($T_{fusion}$ =38°C, $T_{crystallization}$ = 22.3°C); ii) high latent heat ($\Delta H_{fusion}$ = 91J/g, $\Delta H_{crystallization}$ = 89J/g); iii) no risk of leakage and minimal volume expansion rate due to the solid-solid phase change; iv) non-toxic and non-corrosive; v) high hardness (shore D: 30 ± 1); and vi) long term durability (thermal and chemical stability).

The objective of this work is to study the thermal performance of a building envelope (hollow brick) filled with the S-S PCM PUX-1500-20 through numerical simulations with Matlab software [13] based on the method of the heat equation. The analysis results show that the hollow brick integrating PUX-1500-20 can significantly increase thermal inertia of the building structures.

## 2. Experimental section

### 3.1 Materials

#### *3.1.1 MCPs*

The PUX-1500-20 used in this work was synthesized with Polyethylene glycol (PEG-1500: Mn = 1500g·mol$^{-1}$), hexamethylene diisocyanate (HMDI) and cross-linking agent glycerol according to Harlé et al. [12]. The molar ratio of isocyanate group/hydroxyl group ([NCO]/[OH]) was fixed at 1, and the molar ratio of hydroxyl group for glycerol and PEG-1500 is 1:5 [12].

The thermo-physical properties of PUX-1500-20 [12] are summarized in **Table 1**.

**Table 1:** Thermo-properties of the PCM PUX-1500-20.

| Property | value |
|---|---|
| Density ($kg/m^3$) | 1140 |
| Thermal conductivity (W/(m·K)) | |
| Semi-crystalline phase | 0.231 |
| Amorphous phase | 0.231 |
| Melting point (°C) | 38 |
| Freezing point (°C) | 22.3 |
| Specific heat capacity (J/(g·K)) | |
| Semi-crystalline phase | 1.31 |
| Amorphous phase | 1.51 |
| Latent heat (J/g) | |
| Fusion | 91 |
| Crystallization | 89 |

### *3.1.2 Testing materials*

In this study, the PCMs are emplaced inside the hollow bricks of which the shell thickness is 0.5cm, and the thickness of the cavity (PCMs or air) is 4cm, according to commercial bricks used in building envelopes. The model is illustrated in **Figure 1**, and the thermo-physical properties of the mediums are given in **Table 2**.

**Table 2:** Thermo-properties of the brick and air.

| Material | Thermal conductivity (W/(m·K)) | Density ($kg/m^3$) | Specific heat capacity (kJ/(kg·K)) |
|---|---|---|---|
| Brick | 1.15 | 2300 | 0.92 |
| Air | 0.03 | 1.20 | 1.00 |

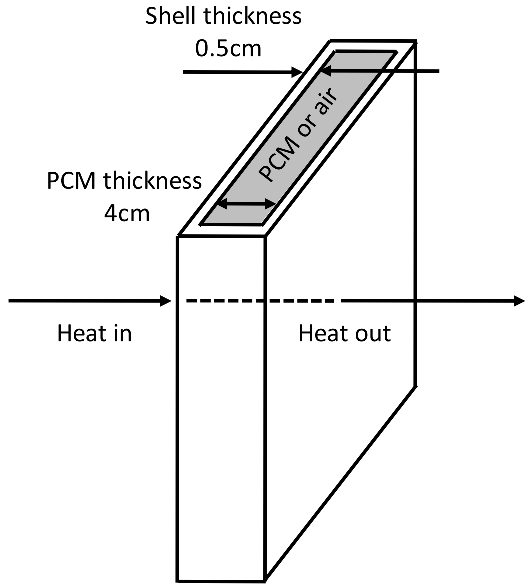


**Figure 1:** Schematic representation of the hallow brick and the brick incorporating PCMs.

### 3.2 Numerical simulation

As described in **Figure 1**, the heat transfer is considered to be one-dimensional in the direction of thickness of the bricks (from outdoor to indoor). The simulation results depend on the thicknesses of the bricks and of the PCMs. The height and width of the bricks have no influence on the simulation.

To study the system, the following assumptions are made to analyze the latent heat storage system:

- The PCM is thermal homogeneous and isotropic;
- The PCM is initially in solid semi-crystalline phase;
- Heat transfer through the materials is one-dimension in unsteady regime;
- Only conduction and phase change heat transfers are considered, convection and radiation heat transfers, etc. are neglected;
- Thermo-physical properties of the PCMs and other materials are independent of temperature.

The general energy transfer equation used in the software Matlab is the partial differential equation as follows [14]:

$$\frac{1}{\alpha}\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}T\right) \quad [1]$$

where $T$ is temperature (K), $t$ the time (s), $x$ the distance (m) and $\alpha$ the thermal diffusivity ($m^2/s$). The thermal diffusivity describes the ability of a material to transfer and store heat, and is given by:

$$\alpha = \frac{\lambda}{\rho C_p} \quad [2]$$

where $\lambda$ is thermal conductivity (W/(m.K)), $\rho$ volumetric mass ($kg/m^3$) and $C_p$ specific heat capacity (kJ/(kg.K)).

The resolution of this partial differential heat equation enables the investigation of the evolution of temperature in space and time $T(x,t)$.

In this study, a simulation analysis in the following two specific cases was realized:

1) A constant temperature of 50°C is applied on the outboard of the brick with/without the PCM to evaluate the temperature variation on the inboard of the brick;
2) The imposed temperature on the outboard of the brick with/without the PCM is a sinusoidal approximation between 15°C and 50°C during 24h (a day) to simulate the hottest days of summer in reality, which represents the peak of summer discomfort for residents.

## 3. Results and discussion

### 3.1 Thermal behaviors of the brick with/without PCMs with a constant temperature of 50°C applied on the outboard

In the case of imposing a temperature of 50°C on the outboard of hallow brick incorporating the PCMs, the temperature of the inboard surface of the brick remains almost constant for the first 1000s: varying from 15°C to 15.2°C, and then rises very slowly, while the temperature of the inboard surface of the hollow brick only reaches 24.2°C after 3600s (1h). The evolution of internal and inboard temperatures of the hollow brick over time is shown in **Figure 2** and **Figure 3**, respectively.

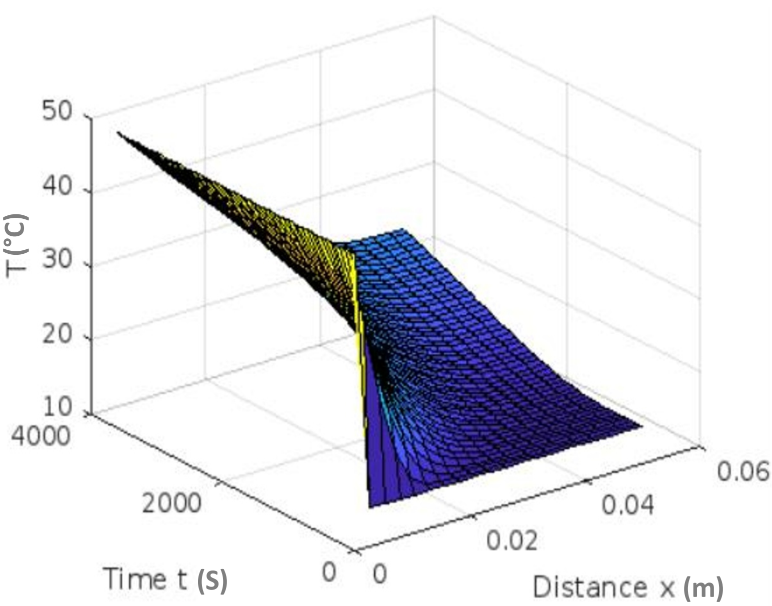


**Fig.2:** Evolution of the internal temperature of hollow brick with the PCMs in space and time under heating at 50°C on the outboard of the hollow brick.

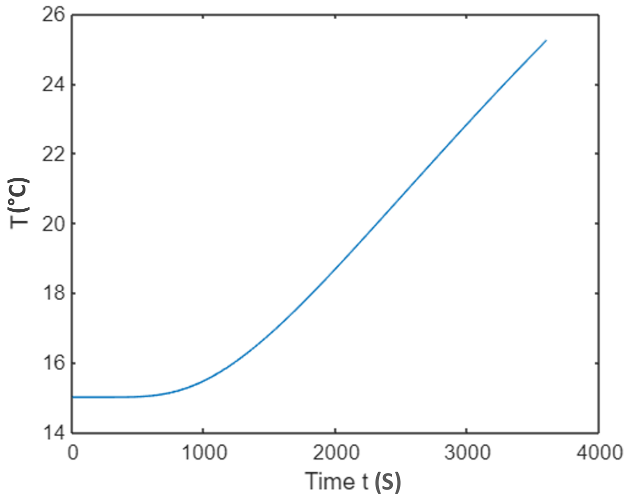


**Fig.3:** Evolution of the inboard temperature of hollow brick with the PCMs over time under heating at 50°C on the outboard of the hollow brick.

However, in the case of imposing the same temperature of 50°C on the outboard of hollow brick without the PCMs, the temperature of the inboard surface of the brick rises rapidly within the first 1000s: from 15°C to 47°C. At t = 1500s, the temperature of the inboard surface of the hollow brick reaches 50°C, which is the same as the outboard heating temperature. The evolution of internal and inboard temperatures of the hollow brick over time is shown in **Figure 4** and **Figure 5**, respectively.

In these two cases, it can be noted that there is a significant difference in the internal and inboard temperature evolution between the hollow bricks filled with the PCMs and those without PCMs. This difference proves the ability of the PCMs PUX-1500-20 to increase the thermal inertia of the building structure.

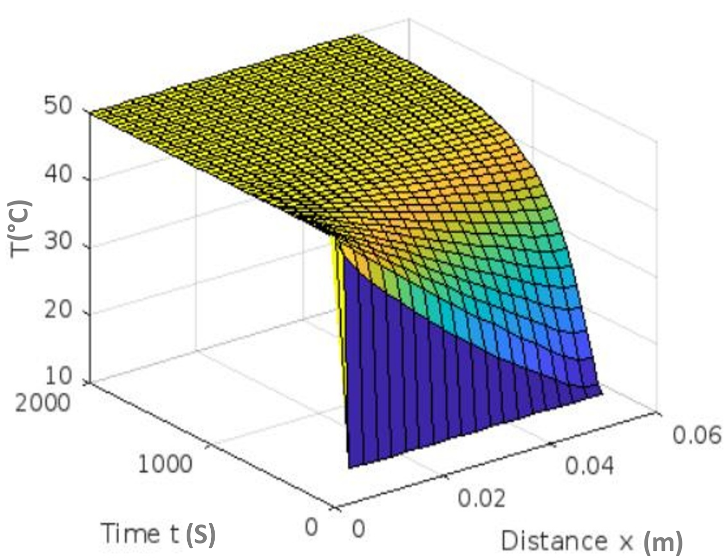


**Fig.4:** Evolution of the internal temperature of hollow brick without the PCMs in space and time under heating at 50°C on the outboard of the hollow brick.

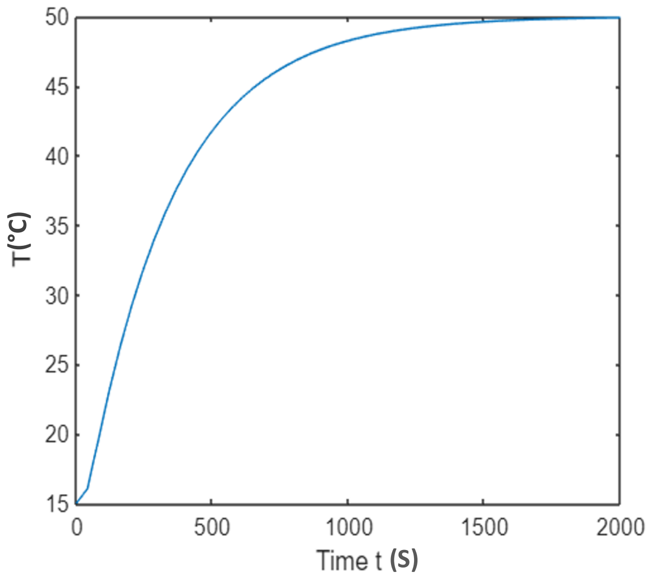


**Fig.5:** Evolution of the inboard temperature of hollow brick without the PCMs over time under heating at 50°C on the outboard of the hollow brick.

### 3.2 Thermal performance of the hollow brick with/without the PCMs with a sinusoidal temperature between 15°C and 50°C applied on the outboard)

**Figure 6** illustrates the evolution of the outboard and inboard temperatures of the hollow brick, both with and without PCMs, when a sinusoidal temperature variation ranging from 15°C to 50°C is applied to the outboard surface over a 48h period. This temperature variation is designed to simulate real summer environmental conditions. A phase shift of 2.45h between the two temperature evolution curves of the brick with the PCMs was observed, and there is a drop of about 1.57°C in the inboard temperature of the brick relative to the outboard temperature. The decrement factor, another important parameter that characterizes the thermal inertial of material, is determined by using the following formula: $f = (T_{imax} - T_{imin})/(T_{omax} - T_{omin})$, where i represents inboard; o represents outboard; max means the maximum value and min is the minimum value. The calculated value 0.91 (see **Figure 6**) shows the PCM has a decrement factor relatively high due to the weak specific heat capacity (see **Table 1**).

Different from the above results of the hollow brick filled with the PCMs, the curves of the evolution of the outboard and the inboard temperature of the hollow brick without PCMs almost overlap, only a gap of 0.21s was observed (see the inset in **Figure 6**). This means that the phase shift and the decrement factor are negligible, and that the hollow brick of building alone have very small even negligible thermal inertia.

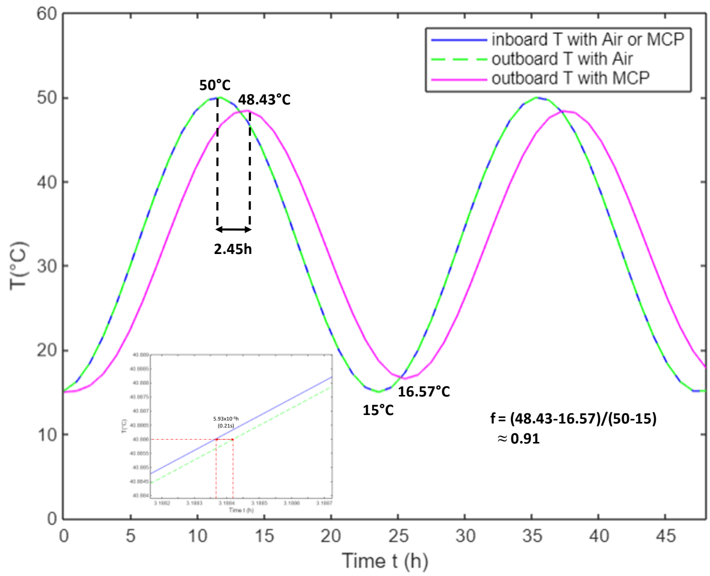


**Fig.6:** Evolution of the outboard and inboard temperature of hollow brick with/without the PCMs over time with application of a sinusoidal temperature between 15°C and 50°C on the outboard of the hollow brick.

## 4. Conclusion

To summarize, this paper presents preliminary results of a numerical study of the one-dimension heat transfer through three-layer surfaces of the building envelope with and without the S-S PCM PUX-1500-20. The aim of this work is to investigate the thermal performance of the building envelope incorporating this patented s-s PCM and estimate their potential in reducing energy consumption.

The hollow brick incorporating the patented S-S PCMs shows a very different thermal behavior compared to the hollow brick without PCMs. The former presents a phase shift of 2.45h and a decrement factor of about 0.91, while the latter has negligible phase shift and decrement factor. These results reveal a remarkable ability of the PCMs to smooth and reduce the inboard (indoor) temperature of building. Specifically, the patented S-S PCM exhibits significant potential in terms of enhancing the thermal inertia of building envelopes, improving occupant thermal comfort, and contributing to energy consumption reduction.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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