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Investigation of phase change materials (PCMs) on the heat transfer performance of building systems

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Abstract. The energy use of building systems contributes to a large percentage of total energy consumption, which requires consideration. Solutions of improvement to save energy are crucial. Phase change materials have been proved to be good candidates to be used in building envelopes for energy save. In this paper, an extended Explicit Finite Element Method (ex-FEM), which has been previously introduced and improved, is taken for simulation of temperatures and heat transfer in simplified multilayer wall constructions, consisting of PCM and insulation. The method has been validated against experimental data measured in a so-called Hot-Box. Temperature data are measured at different positions in a number of simplified multilayer walls. Our results show a reasonable good agreement between the simulations and the experiments, at both heating and cooling considering the temperature hysteresis effect in the PCM. The temperature stabilization ability of the PCM is clear, in both the simulations and the experiments, and particularly in the data when the transition range of the PCM is fully activated and matching the temperature variation in the wall at that particular PCM position. Our ex-FEM tool has here been proved to be able to predict the thermal performance of simplified wall constructions of multiple layers with PCMs incorporated.

1. Introduction

The thermal comfort of buildings is a crucial factor to be considered in construction. Nowadays, when people spent more than 90% of their time indoors, this issue is more acute [1]. How to improve the thermal comfort of buildings has attracted more and more interest. The incorporation of phase change materials (PCMs) into building systems has recently attracted widespread attention as they can bridge the mismatch between energy supply and demand [2], as well as decrease the temperature variation, through their large energy storage capacity. Cabeza et al. [3] experimentally scrutinised the thermal performance of PCM applied to concrete walls by constructing two identical concrete cubicles in the city of Lleida, Spain. According to the results obtained, the utilisation of PCM helped to achieve the maximum temperature reduction of 1 °C. Additionally, the peak indoor temperature was shifted by 2 h. Rathore and Shukla [4] evaluated the thermal performance of macro encapsulated PCM applied to the building located in the tropical climate. The authors studied the thermal performance inside two cubicles constructed for the experiment through the maximum temperature reduction, thermal amplitude reduction, and peak temperature shift. The results showed that the maximum temperature and thermal amplitude were decreased by up to 9.18 and 59.79%, respectively, and the time delay was by up to 120 min. Mahdaoui et al. [5] studied the thermal performance of building bricks impregnated by PCMs numerically. Their method is validated by experimental data obtained by other researchers. They found that the external heat transfer coefficient has less effect on the inner surface temperature variation than the internal coefficient. They also concluded that the integration of PCM in brick improves the storage ability and the insulation power of the building element in the way of a significant reduction in the temperature amplitude and considerable phase shift.

Besides the advantage of using PCMs, there are still some challenges left. Location of the PCMs in the building envelopes, for example, is a controversial topic. For example, Jin et al. [6] concluded there...
is a specific and optimized distance to the temperature variation (external) side for the PCM layer. Based on experiments Gounni and Alami [7] concluded that the PCM layer should be located next to the temperature variation side, so a complete transition can be assured. Similar conclusions were found, from simulations, by Heim and Wierprzkozwicz [8], who concluded that the PCM layer should be located at the external wall. Contrary results were found by Zhu et al. [9], who drew the conclusion that the PCM layer should be located nearest to the internal wall, where it is far from the temperature variation side.

In this study, phase change materials (PCMs) have been used as part of simplified wall configurations. The location of the PCM layer has been varied and optimized, in order to investigate the influence of PCMs on the thermal performance of the system, which is one purpose of this study. Both heating and cooling processes have been performed to study the melting and solidification mechanism of PCMs. In addition, an explicit finite element method that has been developed in a previous study [10] has been further validated by the experimental data purchased in this study, which is the other purpose of this study.

2. Experimental set-up and materials

A hot-box is used for experimental investigation, as shown in Figure 1. The details about the set-up can be found in Zhou et al. [10]. The phase change materials used in the study is Climsel28, which are purchased from Climator Sweden AB, with a phase change temperature around 28 °C. The latent heat of Climsel28 is about 170 kJ/kg.

The installation of the wall layers in the hot-box is shown in Figure 1. The three side walls of the hot box are covered by 1-layer glass, two-layer glass, and wood, respectively. The other side wall is fitted with extruded polystyrene (XPS) wall board (Figure 1c) or PCM bags (Figure 1b) for the purpose of the study. The same PCM bags were used in all experiments. Before and during the hot-box experiments the PCM bags were subjected to several repeated heating and cooling sequences. The properties of the XPS and PCMs are shown in table 1.

![Figure 1](image_url)

Figure 1. a) hot-box with heating source and temperature sensors attached to the wall; b) PCM bags that are packed by a net to make a simplified PCM wall layer; c) XPS board.
Table 1. Thermal properties of XPS (from Sundolitt AB) and PCM (from Climator Sweden AB).

|                  | XPS       | PCM              |
|------------------|-----------|------------------|
| Thermal conductivity (k)/W/(m·K) | 0.033     | 0.98 (solid)/0.72 (liquid) |
| Density (ρ)/kg/m³ | 34        | 1500             |
| Specific heat (c_p)/J/(kg·K)  | 1250      | See Fig.2        |

The specific heat of PCM as Eq. (1) (in [kJ/(kg·K)]) is derived based on the data provided by Climator Sweden AB:

\[
c_p = 3.2 + (a - b)d k^{d-1} \exp[-(kT)^d]
\]  

(1)

For heating process: a=176.6311, b=8.32946, d=17.59206, k=0.03406.

For cooling process: a=156.9963, b=10.43071, d=25.94152, k=0.0377.

T in Equation (1) is in unit K.

Figure 2. a) Enthalpy change of Climsel 28 (PCM) during the heating and cooling process from Climator AB; b) Specific heat change of Climsel 28 (PCM) derived from the enthalpy curves shown in a).

The inside temperature of the hot-box is controlled by a heating source, giving a temperature up to 60 °C. The hot-box is located in an office, where the temperature during the measurement is kept almost constant (around 23 °C with a variation within ±1°C).

Type-T thermocouples are used for the temperature measurement. The sensors are calibrated in an ice-water bath before the experiments were done. The accuracy of the sensors is within ±0.5 °C. Temperature sensors are used to measure temperatures in different locations, as shown in Figure 3. A small fan is used to increase the convection and equalize the vertical temperature gradient inside of the Hot-Box. The air temperatures inside and outside the hot-box (box and room) are measured and collected using a data logger.
Figure 3. Wall layer specifications with temperature measurement points indicated: a) one layer- XPS 1cm; b) two layers with PCM inside, 1 cm for each; c) three layers, with PCM in between, 1 cm each.

As indicated in Figure 3, the left side of the wall stands for the inside of the hot-box; the right side stands for the room where hot-box is located.

3. Simulation description

The heat transfer across the wall layer of the hot-box is taken as one-dimensional heat conduction, which is described by Equation (2)

\[ \frac{k}{\Delta x^2} \frac{\partial^2 T}{\partial x^2} = \rho c_p \frac{\partial T}{\partial t} \]  (2)

Where \( k \) is the thermal conductivity, \( \rho \) is the density, \( c_p \) is the specific heat of the corresponding materials mentioned in Table 1. \( T \) is the temperature in °C; \( t \) is time in second; \( x \) is the distance to the internal surface of the layers in unit m.

To solve Equation (1), an explicit finite element method making use of energy balance is used, with boundary equations for internal and external surface as Equation (3) and Equation (4).

\[
\begin{align*}
    k \frac{T_{i}^{t+1} - T_{i}^{t}}{\Delta x} + h_i (T_{in}^{t} - T_{i}^{t}) &= \rho c_p \frac{\Delta x}{2} (\frac{T_{i}^{t+1} - T_{i}^{t}}{\Delta t}) \\
    k \frac{T_{N}^{t+1} - T_{N}^{t}}{\Delta x} + h_o (T_{out}^{t} - T_{N}^{t}) &= \rho c_p \frac{\Delta x}{2} (\frac{T_{N}^{t+1} - T_{N}^{t}}{\Delta t})
\end{align*}
\]  (3, 4)

For in-between elements

\[
\begin{align*}
    k \frac{T_{m}^{t+1} - T_{m}^{t}}{\Delta x} + k \frac{T_{m+1}^{t} - T_{m}^{t}}{\Delta x} &= \rho c_p \Delta x (\frac{T_{m}^{t+1} - T_{m}^{t}}{\Delta t}) \\
\end{align*}
\]  (5)

Where \( N \) is the total element number for thickness. \( h_i \) and \( h_o \) are the heat transfer coefficient in the hot-box and room side, with unit \( W/(m^2 K) \).

For calculation, the mesh size is selected as 1 mm, time step is 0.001 seconds.

4. Results

4.1 one-layer XPS
The one-layer XPS experiment (Figure.3a) is firstly conducted for the adjustment of the inside and outside heat transfer coefficient \((h_i \text{ and } h_o)\). The internal and external (points 2 and 3 shown in Figure.3a) temperatures are compared from both simulation and experiment. Figure.4a, with XPS layer thickness as 1cm, is derived with \(h_i=18 \text{ W/m}^2\text{K}, h_o=5.5 \text{ W/m}^2\text{K}\), which indicating a good match for both internal surface temperature and external surface temperature. With the same values of \(h_i \text{ and } h_o\), for Figure.4b, where the thickness of XPS is 2 cm, there is a slight difference between the internal surface temperature from simulation and experiment. The root mean square error (RMSE) of the difference between the data sets has been calculated by Equation. (6), with a RMSE of 0.17°C and 0.21°C for the two temperature differences, at the internal and external surface respectively, which indicates a good agreement between our model and the experimental results.

\[
RMSE = \sqrt{\frac{\sum_{i=1}^{N}(T_{exp} - T_{sim})^2}{N}}
\]  

(6)

Figure 4. a) temperature profile across 1cm XPS layer; b) temperature profile across 2cm XPS layer. Note: internal surface stands for point 2; external surface stands for point 3 in Figure.3a.

4.2 two layers PCM/XPS

The temperature profile across the wall of two layers (Figure.3b) is shown in Figure.5. As derived from [9], only when PCM layer is next to the temperature variation side, the temperature of the PCM layer can pass the phase transition temperature, which means PCM can be activated. Otherwise, the PCM layer only works as an insulation layer, therefore, in the study, the wall configuration as PCM/XPS is only taken into consideration. The results are derived with a \(h_i\) of 50 W/m²K and \(h_o\) of 13 W/m²K, to give a best match between experimental and simulated results. In the matching procedure, a good fit at temperatures above transition is selected. A higher \(h_i\) is plausible that the uneven and irregular surface of PCM bags give a higher heat transfer than the smooth surface of XPS.

Figure.5 shows a fast increase of the air temperature inside the hot-box in the first 4 hours. Then, the air temperature increased slowly to a temperature of about 40 °C and then smooth increased to 41 °C, before the cooling process started at about 23 hours. In the cooling process, the air temperature dropped fast to 24°C within 7 hours, followed by a smoothly decrease to 23°C in the end of 48 hours.

The internal surface temperature (IST) and contact surface temperature (CST) increased due to the increase of air temperature from both simulation and experiment. From about 3 hours, the experimental value of IST shows a lower increase, and it ends at about 6 hours, indicating a phase transition during the period. The solid PCMs absorb the heat transferred in and change into a liquid. Then it’s followed by a sharp increase of temperature, because the specific heat of liquid PCMs is rather lower than that of the solid PCMs. When the system arrives a stable condition at about 10 hours, the experimental results give an IST temperature of about 37.5 °C, and a slightly change before cooling started. The IST and
CST curves from the simulation also shows a phase transition period, but the starting and ending point is not exactly the same with experimental data. Also, the maximum IST value from the simulation is about 39.5 °C, higher than the experimental value. This is possible because of the surface of PCM and XPS is different. After phase transition, the morphology of PCM changed to be much more uneven. The experimental value also shows a big difference between EST-3 and IST-4, which is caused by an air-gap between the two contact surfaces, which is getting bigger after phase transition.

For the cooling process, there is a good match during the beginning of the cooling until about 30 hours, where there is a sharp temperature rise shown in the experimental IST-2, EST-3 and IST-4, which didn’t show in the simulation. This phenomenon is caused by sub-cooling, which is not considered in simulation. The sub-cooling degree ($\Delta T_{sub}$) for the PCM used in this study is about 3 °C.

In the end of the cooling process the air temperature inside the hot-box AT-1 and the external surface temperatures EST-5 in the experimental and simulated cases, all decreased to 23°C. The temperature for the other positions at the experiment also reached to 23°C. However, the IST-2-simulated and CST-simulated decreased to about 25°C during this running time period. This temperature difference is due to the ongoing transition and heat release in the PCM. According to Figure 2b, on cooling the transition ends at about 22°C.

**Figure 5.** Temperature profile across the wall with configuration Figure 3b. IST: internal surface temperature; CST: contact surface temperature; EST: external surface temperature; AT: air temperature; number 1 to 5 are the locations indicated in Figure 3b.

4.3 three layers XPS/PCM/XPS

Figure 6 shows the results for wall specification as shown in Figure 3c. The temperature inside the hot-box is first heated to a maximum of about 42 °C, then kept at that temperature for about 40 hours, and after that the cooling sequence is started.

For the heating sequence, the experimental data show a clear phase transition period, from about 5 hours to 25 hours, as indicated by the curves of CST-3, CST-4, CST-5 and CST-6. Then, the temperature at those positions increased quickly for a short time (5 hours), followed by a linear increase until the cooling process was started. The simulation results also show a clear phase transition, but started at about 3 hours and ended at about 20 hours. In comparison with the experimental temperature data, the phase change in the simulation both started and ended somewhat earlier. A contributing reason for this shift towards longer times in the experimental data, may be due to larger and not so easy to predict...
thermal resistances in the experimental set-up between the PCM and the XPS layers, than those used in the simulation.

![Figure 6](image-url)  
Figure 6. Temperature profile across the wall with configuration Figure 3c. IST: internal surface temperature; CST: contact surface temperature; EST: external surface temperature; AT: air temperature; number 1 to 7 are the locations indicated in Figure 3c.

The cooling process started from about 45 hours, the air temperature inside the hot-box decreased rapidly to about 23 °C in about 5 hours, then slightly decreased to about 22 °C. The internal surface IST-2 and contact surface temperatures CST-3,4,5,6 from the experiment decreased firstly to about 25 °C, followed by a sharp increase to about 28 °C, and then decreased again smoothly to the final temperature of 23°C. This is the same as what is shown in Figure 5 for two layers case which is because of the sub-cooling of the PCM. The final temperature of the CST-5,6 and EST-7 from the simulation is for the same reason explained above for two layers study.

4.4 discussion
The heat transfer coefficient is affected by the material’s surface morphology, which needs to be adjusted when the surface is changeable due to phase change.

An extra air layer can appear after phase transition, which adds extra thermal resistance. This needs to be considered for the numerical method improvement in further study.

A sub-cooling phenomenon is noticed in the cooling process with PCMs incorporated in the wall layer, which also needs to be taken into account for the simulation.

When the PCMs is not close to the temperature variation side, the actual temperature variation at the PCM layer might then be out or partly out of the transition range of the PCM. This will then reduce the effect of the PCM. Therefore, the distance of PCMs to the temperature variation side is important and needs to be optimized before incorporating PCMs into building wall systems.

5. Conclusions
Phase Change Materials (PCMs) can be used to store energy only if they are activated during the process. Therefore, the distance of PCMs to the temperature required side should be carefully considered before installation.
The melting and solidification process of PCMs can change their surface morphology. Therefore, the filling method of PCM into wall board needs to be taken into account when they are considered for application.

The numerical method to predict the thermal performance of building systems with PCMs needs to be improved and validated in a further way.

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