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ABSTRACT

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Influence of building parameters on thermal mass modification with phase-change materials: numerical study based on design of experiments

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Abstract. Phase-change materials (PCM) offer new opportunities to modify thermal mass. The energy savings due to thermal mass modification, with or without PCM, may significantly vary between the studies reported in the literature. This has shown the interest to systematically study the effect of enhanced thermal mass on different buildings. This study investigates the influence of eight building parameters on the benefits of using three different PCM-panels, by simulating a test-cell based on an office building in a temperate climate. Our results showed that the building parameters strongly influenced the energy savings through use of PCM. The main building parameters influencing the potential benefits were the initial thermal mass and the parameters related to solar heat gain.

1. Introduction

Recently, researchers have shown an increased interest in phase-change materials (PCM) to modify thermal mass in the building sector (see the review articles of Soares et al. (2013) and Kalnæs et al. (2015)). PCM offer indeed an opportunity to increase the thermal mass effect on a given temperature range.

The potential benefits of PCM-enhanced building components can be affected by their properties, by the climate and by the building under investigation. Comparisons between studies have not always been straightforward due to different uses of key performance indicators (KPI), the parameters concerning thermal mass modification and the building under study (Verbeke et al. (2018) and Saffari et al. (2017)). More specifically, for the use of PCM in Cfb climates, Soares et al. (2014) obtained annual energy savings for cooling and heating needs of about 16 kWh/m² and Alam et al. (2014) 20 kWh/m². Saffari et al. (2017), considering the HVAC system efficiency of a typical office building and with less PCM quantity, achieved savings of less than 1 kWh/m². In a previous study (Baudoin et al., 2018), we also obtained relatively low gains of about 2 kWh/m². Could the different buildings under investigation explain the difference of energy savings? To the best of our knowledge, the influence of building parameters on the potential benefits of thermal mass modification with PCM has never been systematically studied.

This study aims to quantify the effect of the building parameters on the potential benefits of modifying thermal mass with PCM. Annual cooling and heating energy needs were used as KPI for the Belgian climate. Starting from a previous study (Baudoin et al., 2018), the effect of eight building parameters were tested on the use of three different PCM-panels. PCM\textsubscript{cool} was a panel specifically designed to minimise cooling energy needs, PCM\textsubscript{heat} to minimise heating energy needs and PCM\textsubscript{tot} was a non-specific one. The eight building parameters investigated were wall insulation (WI), window insulation (WDI), solar heat gain coefficient (SHGC), heat recovery percentage (HR), free-cooling rate (AFR), air leakage (ALE), orientation (OR) and initial thermal mass (TM).
The results of this study showed that the building parameters strongly influenced the energy savings resulting of PCM use. For the PCM-panel based on $\text{PCM}_{\text{tot}}$, the energy savings for cooling varied from zero to 16.40 kWh/m². The energy savings for heating varied from a negative effect of -0.41 to a positive effect of 3.96 kWh/m². The main building parameters influencing the potential benefits were the initial thermal mass (TM) and the parameters linked to solar heat gain, i.e. the solar heat gain coefficient (SHGC) and the orientation (OR). Interestingly, higher energy savings could be achieved using $\text{PCM}_{\text{tot}}$ instead of $\text{PCM}_{\text{cool}}$ or $\text{PCM}_{\text{heat}}$. This suggested that the optimum combination of PCM parameters to minimise the energy needs for cooling or heating would depend on the studied parameters of the building.

This study gave new insight to understand the discrepancies between authors. Knowing the effect of the building parameters on the potential benefits also allowed (i) to identify the building for which it is the most beneficial to modify thermal mass and (ii) to identify the boundaries of the potential benefits of modifying thermal mass with PCM.

2. Method

Annual dynamic building simulations were done for a simplified test-cell based on an office building, using EnergyPlus 8.8.0. For 50 combinations of building parameters, a case with and without phase-change material properties were compared to obtain the potential gains of using PCM on energy needs for cooling $\Delta E_{\text{cool}}$ and heating $\Delta E_{\text{heat}}$. The 50 combinations of building system parameters were selected based on design of experiments and one metamodel was constructed for $\Delta E_{\text{cool}}$ and one for $\Delta E_{\text{heat}}$. The metamodel linked the energy savings with the eight building parameters in the form of a second order polynomial function. Three different PCM-panels were tested: $\text{PCM}_{\text{cool}}$, a panel specifically designed to minimise cooling energy needs, $\text{PCM}_{\text{heat}}$, to minimise heating energy needs and $\text{PCM}_{\text{tot}}$, a non-specific one. For pre- and post-processing with EnergyPlus, python jupyter notebook was used with the eppy package (Figure 1). The JMP Pro 14.1.0 software was used as support for the design of experiment part and to build the metamodel.

Figure 1: Computational workflow.
2.1 Test-cell

The test-cell dimensions were based on the model specified in ASHRAE (2007) 140 standard (Figure 2.a), as previously used in similar studies. Annual cooling and heating energy needs $E_{\text{cool}}$ and $E_{\text{heat}}$ were used as KPI for the Belgian climate. The surface with the windows had outdoor boundary condition and the other surfaces were defined as internal surfaces with an adiabatic boundary condition. The surface compositions are given in Table 1, in which two compositions are given for the internal floor/ceiling: one for the lightweight case and one for the heavyweight. The selection of one composition was based on the building parameter TM. More details about envelope composition and test-cell loads can be found in the appendix of Baudoin et al. (2018).

Heat recovery system, diurnal and nocturnal free cooling were implemented in a simplified way using the Ideal-LoadsAirSystem object in EnergyPlus. The free cooling was based on difference in air-dry bulb temperature and the outside airflow was allowed to increase up to the number of air changes per hour defined by the building parameter AFR. For night cooling, the temperature was allowed to decrease up to 20.0°C.

Table 1: Test-cell envelope composition. The thickness of the Fiberglass quilts-1 varied between the simulations. The internal floor/ceiling was either the heavy one or the light one depending on the thermal mass parameter.

<table>
<thead>
<tr>
<th>Surface Type</th>
<th>Thickness [m]</th>
<th>$\lambda$ [W/mK]</th>
<th>Density [kg/m³]</th>
<th>Specific heat [kJ/kgK]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Internal floor/ceiling (heavy)</td>
<td>0.008</td>
<td>0.06</td>
<td>200</td>
<td>1300</td>
</tr>
<tr>
<td></td>
<td>0.06</td>
<td>0.93</td>
<td>1900</td>
<td>1000</td>
</tr>
<tr>
<td></td>
<td>0.04</td>
<td>1.7</td>
<td>2400</td>
<td>1000</td>
</tr>
<tr>
<td></td>
<td>0.16</td>
<td>1.23</td>
<td>1870</td>
<td>1000</td>
</tr>
<tr>
<td></td>
<td>0.01</td>
<td>0.52</td>
<td>1300</td>
<td>1000</td>
</tr>
<tr>
<td>Internal floor/ceiling (light)</td>
<td>0.014</td>
<td>0.13</td>
<td>525.0</td>
<td>1880.0</td>
</tr>
<tr>
<td></td>
<td>0.015</td>
<td>0.15</td>
<td>600.0</td>
<td>1880.0</td>
</tr>
<tr>
<td></td>
<td>0.230</td>
<td>0.05</td>
<td>125.0</td>
<td>1048.0</td>
</tr>
<tr>
<td></td>
<td>0.012</td>
<td>0.25</td>
<td>800.0</td>
<td>840.0</td>
</tr>
<tr>
<td>External wall</td>
<td>0.012</td>
<td>0.35</td>
<td>900</td>
<td>1000</td>
</tr>
<tr>
<td></td>
<td>0.06</td>
<td>0.05</td>
<td>35</td>
<td>1030</td>
</tr>
<tr>
<td></td>
<td>0.012</td>
<td>0.35</td>
<td>900</td>
<td>1000</td>
</tr>
<tr>
<td>External wall</td>
<td>0.009</td>
<td>0.14</td>
<td>530</td>
<td>900</td>
</tr>
<tr>
<td></td>
<td>0.16</td>
<td>0.04</td>
<td>12</td>
<td>840</td>
</tr>
<tr>
<td></td>
<td>0.012</td>
<td>0.16</td>
<td>950</td>
<td>840</td>
</tr>
</tbody>
</table>
The set point temperature $T_{th}$ was based on the operative temperature $T_{op}$ and set to 20.0 °C for heating and 26.0 °C for cooling. The weather data used came from the International Weather for Energy Calculation (IWEC) data file, which is a typical weather file for building energy simulation for Uccle in Belgium.

For the set of parameters corresponding to the base case studied in Baudoin et al. (2018), the annual heating energy need was 5.11 kWh/m² and the annual cooling energy need was 3.35 kWh/m². For this base case, the distribution of power loads varied between heating and cooling (Figure 2.b). By using $\text{PCM}_{\text{heat}}$, the saving in term of $E_{\text{heat}}$ was 1.13 kWh/m² and by using $\text{PCM}_{\text{cool}}$, the saving in term of $E_{\text{cool}}$ was 1.45 kWh/m².

### 2.2 PCM simulation

A 2 cm thick PCM-panel with an exchange surface of 1 m²/m²floor was added as an internal mass object in the test-cell. This approach allowed to consider the addition of PCM properties regardless of its position in the test-cell. The PCM-panel was directly in contact with the inside environment. For the base case, no phase-change properties were used for this panel. It allowed to separate the sensible contribution of the panel from its latent contribution on the energy savings.

The properties of the PCM-panel were based on DuPont Energain PCM. This product comes as an aluminium-laminated panel, containing a copolymer and paraffin wax compound. The latent heat is 110 kJ/kg, the density 855 kg/m³ and the specific heat 2500 J/kgK. In this study, the thermal conductivity value was assumed not to vary between the solid and liquid phase, and was set to 0.16 W/mK.

![PCM properties](image)

Figure 3: (a) PCM properties in the Enthalpy/Temperature curve and the associated heat capacity. Ideal behaviour (green) and quasi-ideal behaviour (red dotted line). (b) Conceptual comparison of the three PCM used in this study: $\text{PCM}_{\text{tot}}$, $\text{PCM}_{\text{cool}}$ and $\text{PCM}_{\text{heat}}$.

The PCM behaviour was considered as quasi-ideal, i.e. no hysteresis, nor sub-cooling effects were included. The main properties of a quasi-ideal PCM are the melting-peak temperature $T_{mp}$, the melting temperature range $\Delta T_m$ and the latent heat $E_l$ (Figure 3.a). An ideal solid-liquid PCM would melt and solidify at $T_{mp}$ and the latent heat would be stored and released at this temperature. The three different PCM studied only differed in their melting-peak temperature $T_{mp}$ and their melting temperature range $\Delta T_m$ (Figure 3.b). $\text{PCM}_{\text{cool}}$ was a panel designed to minimise cooling energy needs, $\text{PCM}_{\text{heat}}$, to minimise heating energy needs and $\text{PCM}_{\text{tot}}$ was a non-specific one. The sensible heat of the PCM-panel was about 21 kJ/Km² and the additional thermal energy storage due to the PCM latent heat was about 940 kJ/m² (261 Wh/m²).
2.3 Experimental design

Design of experiments was used to select the various combinations of building parameters (Table 2). The following parameters were investigated as continuous variable: wall insulation (WI), window insulation (WDI), solar heat gain coefficient (SHGC), heat recovery percentage (HR), free-cooling rate (AFR) and air leakage (ALE). The values of the parameters were directly changed in the EnergyPlus file by using the eppy python package in a python jupyter notebook. For the wall insulation, the thickness of the insulation layer was changed to match the given wall insulation. The two following parameters were investigated as categorical variable with two levels: the orientation (OR) and the thermal mass (TM). The orientation could be either south or north and the thermal mass was characterised as heavy or light. The heavy case had a ceiling/floor described as heavy in Table 1, and the light case had the light ceiling/floor.

Table 2: List of parameters and their simulated value boundaries: low and high values with a comparison of a set of value from a previous case study.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Low value</th>
<th>High value</th>
<th>Case study value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wall insulation (W/m²K)</td>
<td>WI</td>
<td>0.15</td>
<td>2.00</td>
<td>0.25</td>
</tr>
<tr>
<td>Window insulation (W/m²K)</td>
<td>WDI</td>
<td>0.80</td>
<td>3.00</td>
<td>1.50</td>
</tr>
<tr>
<td>Solar heat gain coefficient</td>
<td>SHGC</td>
<td>0.20</td>
<td>0.70</td>
<td>0.62</td>
</tr>
<tr>
<td>Heat recovery percentage (%)</td>
<td>HR</td>
<td>0</td>
<td>100</td>
<td>79</td>
</tr>
<tr>
<td>Free-cooling rate (ACH)</td>
<td>AFR</td>
<td>0</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>Air leakage rate (ACH)</td>
<td>ALE</td>
<td>0.03</td>
<td>0.50</td>
<td>0.03</td>
</tr>
<tr>
<td>Orientation</td>
<td>OR</td>
<td>north</td>
<td>south</td>
<td>north</td>
</tr>
<tr>
<td>Thermal mass</td>
<td>TM</td>
<td>heavy</td>
<td>light</td>
<td>heavy</td>
</tr>
</tbody>
</table>

The JMP Pro 14.1.0 software was used as support for the design of experiment part and to build the metamodel. Based on a D-optimal criterion, 50 combinations of building system parameters were selected with a custom design. Compared to classical design, the custom design allowed to avoid specific features related to no deterministic experiences. For example, a classical design would produce a number of repetition of the same set of building parameters. The D-optimal criterion allowed to get the best approximation of the coefficients of the building parameters in the metamodel.

For these 50 combinations of building system parameters, a case with and without phase-change material properties were compared to assess the influence of using PCM on energy needs for cooling $\Delta E_{\text{cool}}$ and heating $\Delta E_{\text{heat}}$. Based on these data, a metamodel was built to link the energy savings with the eight building parameters in the form of a second order polynomial function:

$$ Y = c_0 + \sum_{i=1}^{N} c_i X_i + \sum_{i=1}^{N} c_{ii} X_i^2 + \sum_{i=1, j=i+1}^{N} c_{ij} X_i X_j $$

where $Y$ represents the output value ($\Delta E_{\text{cool}}$ or $\Delta E_{\text{heat}}$) and $X$ represents the $N$ building parameters considered. The interaction term $X_i X_j$ of the two categorical variables OR*TM was not considered. The c’s are the coefficients of terms in the polynomial function.
3. Results and discussion

3.1 PCM\textsubscript{tot} case

For the 50 combinations of building system parameters, the values of $\Delta E_{\text{cool}}$ and $\Delta E_{\text{heat}}$ were calculated for the PCM-panel based on PCM\textsubscript{tot}. Depending on the set of building system parameters, the energy savings for cooling varied from zero up to 16.40 kWh/m$^2$. The energy savings for heating varied from a negative effect of -0.41 to a positive effect of 3.96 kWh/m$^2$.

These results confirmed that the potential benefits which could be achieved were generally higher for cooling than for heating. In our previous study, the potential energy needs for heating and cooling were of the same order of magnitude by using PCM\textsubscript{heat} 1.13 kWh/m$^2$ and PCM\textsubscript{cool} 1.45 kWh/m$^2$. It is worth noting that the same order of magnitudes than Soares et al. (2014) and Alam et al. (2014) could be achieved only by changing the building parameters, with the same PCM-panel properties and the same weather data file.

The calculated values were compared to the predicted values by the metamodel (Figure 4). The $R^2$ was of 0.98 for the function of $\Delta E_{\text{cool}}$ and 0.94 for the function of $\Delta E_{\text{heat}}$. The solar heat gain coefficient (SHGC), the thermal mass (TM) and the orientation (OR) played a major role on the potential benefits of using PCM on energy needs (Figure 5). The table shows the minimum p-value among the p-values for that effect on $\Delta E_{\text{cool}}$ and $\Delta E_{\text{heat}}$. The p-value was linked to the effect test, which tested the null hypothesis that the coefficient $c$ associated to the effect is zero. The associated coefficients for the metamodel for $\Delta E_{\text{heat}}$ were estimated to $-1.27$ for TM (heavy to light case), $-0.88$ for OR (north to south case) and $-1.70$ for SHGC. For the $\Delta E_{\text{cool}}$ metamodel, the associated coefficient were $-3.01$ for TM (heavy to light case), $-2.77$ for OR (north to south case) and $-7.63$ for SHGC.
Figure 5: Effect tests of the coefficients associated with the main and second order effect of the eight building parameters for the PCM\textsubscript{tot} case.

### 3.2 PCM\textsubscript{cool} and PCM\textsubscript{heat} cases

The same sets of calculation were conducted for the PCM-panel with PCM\textsubscript{cool} and PCM\textsubscript{heat}. Interestingly, higher savings of energy needs could be achieved using PCM\textsubscript{tot} instead of PCM\textsubscript{cool} (11.89 kWh/m\textsuperscript{2} of achievable savings for $\Delta E_{\text{cool}}$) or PCM\textsubscript{heat} (3.61 kWh/m\textsuperscript{2} of achievable savings for $\Delta E_{\text{heat}}$). In addition to the parameters related to solar gains and the thermal mass, the heat recovery percentage (HR) had a role to play in the case of PCM\textsubscript{heat} (Figure 6). The associated coefficient was -1.08. This means that, assuming no interactions and no second order effect, $\Delta E_{\text{heat}}$ would unexpectedly increase by -1.08 from a case without heat recovery (0\%) to a case with an ideal heat recovery system (100\%).

Figure 6: Effect tests of the coefficients associated with the main and second order effect of the eight building parameters for the PCM\textsubscript{cool} case on $\Delta E_{\text{cool}}$ (left) and for the PCM\textsubscript{heat} case on $\Delta E_{\text{heat}}$ (right).

### 3.3 Limitations of the model

The two categorical variables seemed to have a major influence on the energy needs. However, due to their categorical properties and the two levels studied, the influence of these parameters could not be analysed in details (Figure 7). It would be interesting to know intermediate values between the two extremes ones. For the thermal mass, the categorical variable could be turned into a continuous one. This could be done by considering the energy capacity of the thermal mass and the speed of (un)loading.
The model had limitations for accurate predictions. For example, considering PCM\textsubscript{heat} with the same set of parameter as in our previous study, a saving in term of $\Delta E_{\text{heat}}$ of 0.73 kWh/m$^2$ was calculated with the metamodel instead of 1.13 kWh/m$^2$. The experimental design was chosen with a D-optimal criterion, which optimises the approximation of the coefficients of the building parameters, instead of an I-optimal criterion, which optimises the predictions of the metamodel. Further studies should also consider using other metamodels than the polynomial one (Van Gelder et al., 2014) and using other experimental designs, more appropriated to computer experiments such as the space-filling design (Simpson et al., 2001).

Some parameters seemed to have no or small effects compared to what could have been expected. In a previous study, but with another key performance indicator, Evola et al. (2013) showed that the free-cooling rate (AFR) has a positive influence on the potential benefits for cooling. In our model, AFR determined the maximum rate for diurnal free cooling and nocturnal free cooling. For further investigations, the diurnal and nocturnal free cooling could be studied separately. In addition, a non-linear effect of the free-cooling rate was observed to have a potential negative influence. It could be explained by the low cooling energy with high AFR, which could affect the validity of the built metamodel.

4. Conclusion

This study investigated the influence of eight building parameters on the energy needs savings for cooling and heating. The case study was a test-cell based on an office building in the Belgian climate. The three main results of this study were:

1. The building parameters strongly influenced the energy savings due to PCM use. For the PCM-panel based on PCM\textsubscript{low}, the energy savings for cooling varied from zero up to 16.40 kWh/m$^2$.

2. The achievable savings could be higher for cooling than for heating. The energy savings for heating varied from a negative effect of -0.41 to a positive effect of 3.96 kWh/m$^2$. 

Figure 7: Influence of the two categorical variables on $\Delta E_{\text{cool}}$ for a given set of the six continuous variables.
3. The main building parameters influencing the potential benefits were the initial thermal mass (TM) and the parameters linked to solar heat gain, i.e. the solar heat gain coefficient (SHGC) and the orientation (OR).

Interestingly, it was also observed that higher savings of energy needs could be achieved with $\text{PCM}_{\text{tot}}$ instead of using $\text{PCM}_{\text{cool}}$ or $\text{PCM}_{\text{heat}}$. This suggested that the optimum combination of PCM parameters to minimise the energy needs for cooling or heating would depend on the studied parameters of the building.

These results gave new insight (i) to identify the building for which it is the most beneficial to modify thermal mass and (ii) to identify the boundaries of the potential benefits of modifying thermal mass with PCM.

The findings presented here provide a starting point for further examination of the influence of building parameters on thermal mass modification with PCM. The further studies could investigate in more details the influence of the initial thermal mass by changing it from a categorical variable to a continuous one. In addition to the energy capacity of the thermal mass, the loading and unloading speed could also be taken into consideration. This could be done by considering the exchange surface with the internal environment. The impact of the free-cooling rate (AFR) could also be studied in more details. In this study, the same parameter defined the maximum rate for diurnal and nocturnal free cooling. The two effects could be studied separately. Other building parameters could be added to the study: the occupation pattern (e.g. residential) and the set point temperature. Concerning the design of experiments method, the use of experimental designs, better adapted to computer experiments (e.g. space-filling design), could be studied in more details. The metamodel could also be built by using more complex form than the second order polynomial function.

Acknowledgement

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