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/m^2 and Alam et al. (2014) 20 kWh/m^2. 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/m^2. In a previous study (Baudoin et al., 2018), we also obtained relatively low gains of about 2 kWh/m^2. 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_{cool} was a panel specifically designed to minimise cooling energy needs, PCM_{heat} to minimise heating energy needs and PCM_{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 PCM_{tot}, the energy savings for cooling varied from zero 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. 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 PCM_{tot} instead of PCM_{cool} or PCM_{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 ΔE_{cool} and heating ΔE_{heat}. The 50 combinations of building system parameters were selected based on design of experiments and one metamodel was constructed for ΔE_{cool} and one for ΔE_{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: PCM_{cool}, a panel specifically designed to minimise cooling energy needs, PCM_{heat}, to minimise heating energy needs and PCM_{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.
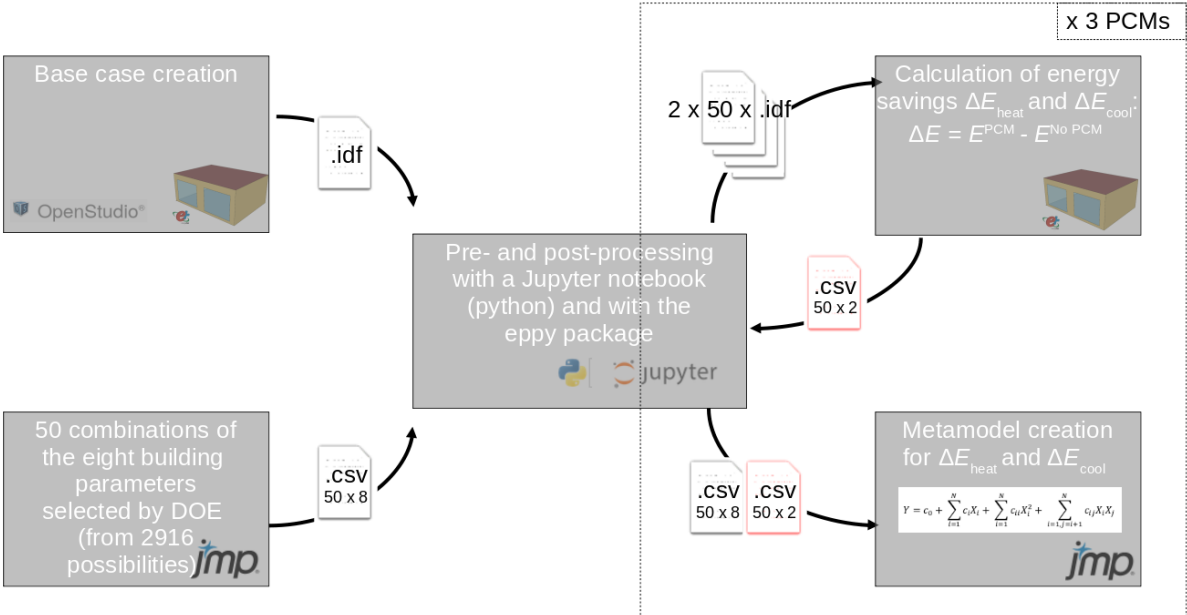

Figure 1: Computational workflow.

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_{cool} and E_{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).
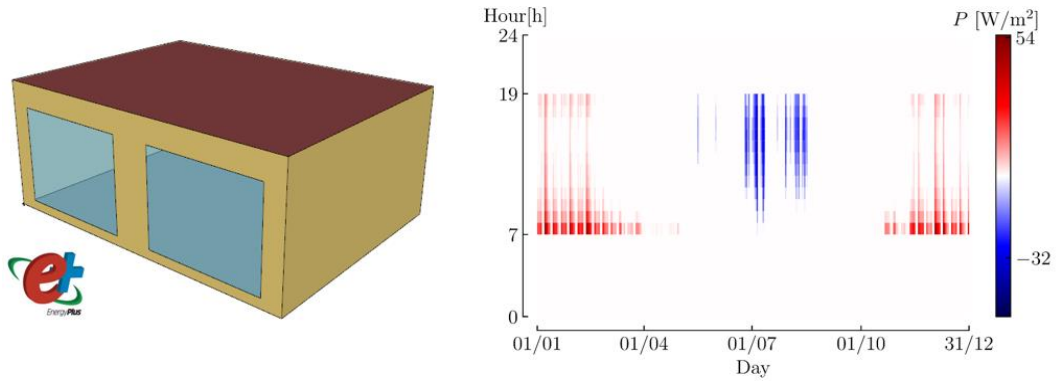

Figure 2: (a) Test-cell based on ASHRAE Standard 140. (b) Hourly energy needs for the base case with the ideal HVAC system.

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.

		Thickness [m]	λ [W/mK]	Density [kg/m^3]	Specific heat [kJ/kgK]
Internal floor/ceiling (heavy)	Carpet	0.008	0.06	200	1300
	Cement screed	0.06	0.93	1900	1000
	Reinforced concrete	0.04	1.7	2400	1000
	Precast concrete slab	0.16	1.23	1870	1000
	Plaster	0.01	0.52	1300	1000
Internal floor/ceiling (light)	Wooden floor	0.014	0.13	525.0	1880.0
	OSB	0.015	0.15	600.0	1880.0
	Wood and mineral wool	0.230	0.05	125.0	1048.0
	Plaster 2	0.012	0.25	800.0	840.0
Internal wall	Plasterboard	0.012	0.35	900	1000
	Mineral wool	0.06	0.05	35	1030
	Plasterboard	0.012	0.35	900	1000
External wall	Wood siding-1	0.009	0.14	530	900
	Fiberglass quilt-1	0.16	0.04	12	840
	Plasterboard-1	0.012	0.16	950	840

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/m^2 and the annual cooling energy need was 3.35 kWh/m^2. For this base case, the distribution of power loads varied between heating and cooling (Figure 2.b). By using PCM$_{heat}$, the saving in term of E_{heat} was 1.13 kWh/m^2 and by using PCM$_{cool}$, the saving in term of E_{cool} was 1.45 kWh/m^2.

2.2 PCM simulation

A 2 cm thick PCM-panel with an exchange surface of 1 m^2 /m$^2_{floor}$ 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/m^3 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.
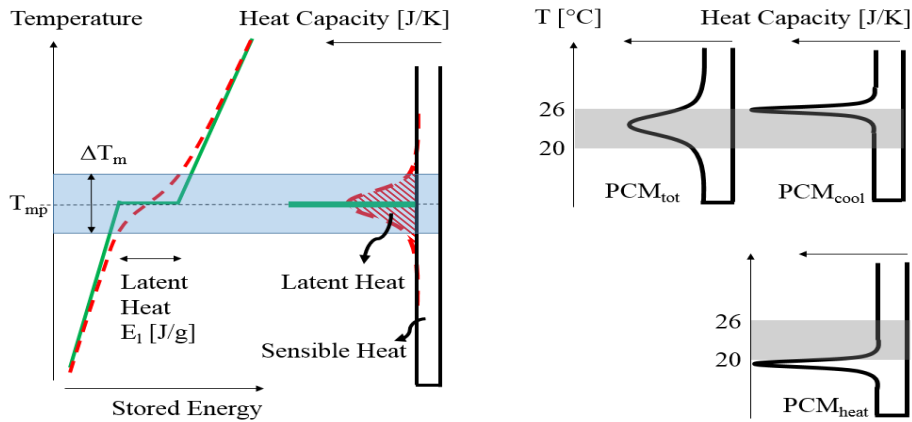

Figure 3: (a) PCM properties in the Enthalpy/Temperature curve and the associated heat capacity. Ideal behaviour (green) and quasi-ideal behaviour (red dotted line). (b) Conceptual comparison of the three PCM used in this study: PCM$_{tot}$, PCM$_{cool}$ and PCM$_{heat}$.

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 ΔT_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 ΔT_m (Figure 3.b). PCM$_{cool}$ was a panel designed to minimise cooling energy needs, PCM$_{heat}$, to minimise heating energy needs and PCM$_{tot}$ was a non-specific one. The sensible heat of the PCM-panel was about 21 kJ/Km^2 and the additional thermal energy storage due to the PCM latent heat was about 940 kJ/m² (261 Wh/m^2).

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.

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

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 ΔE_{cool} and heating ΔE_{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 (ΔE_{cool} or ΔE_{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$_{tot}$ case

For the 50 combinations of building system parameters, the values of ΔE_{cool} and ΔE_{heat} were calculated for the PCM-panel based on PCM$_{tot}$. 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$_{heat}$ 1.13 kWh/m^2 and PCM$_{cool}$ 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.
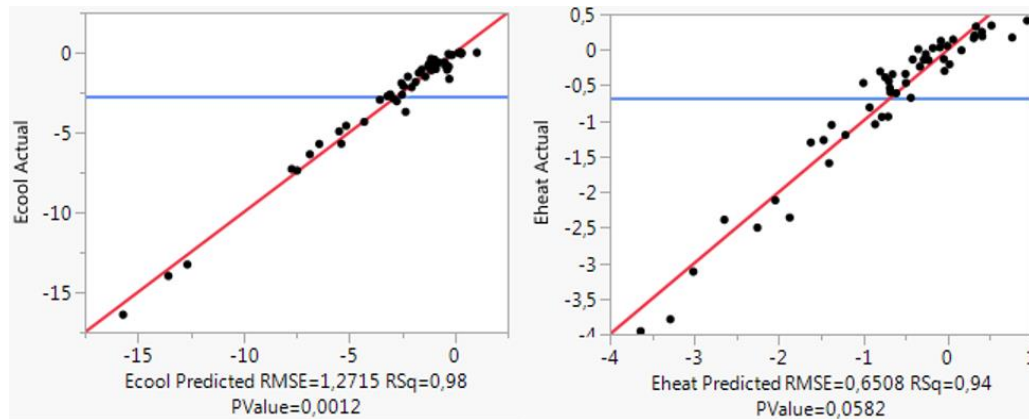

Figure 4: Comparison of the calculated values with EnergyPlus and the predicted values with the metamodel for ΔE_{cool} (left) and ΔE_{heat} (right). The blue line corresponds to the mean.

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 ΔE_{cool} and 0.94 for the function of ΔE_{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 ΔE_{cool} and ΔE_{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 ΔE_{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 ΔE_{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.

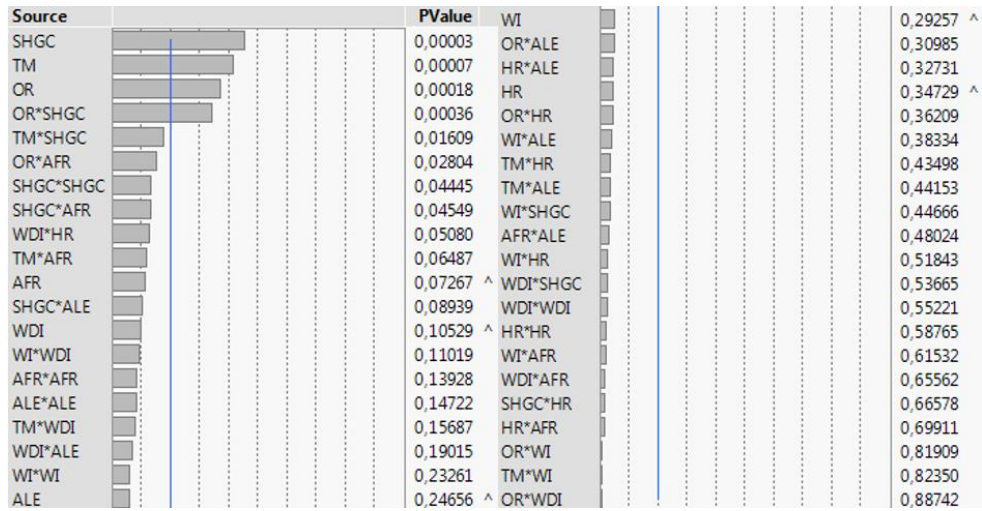| Source	PValue	Source	PValue
SHGC	0,00003	WI	0,29257 ^
TM	0,00007	OR*ALE	0,30985
OR	0,00018	HR*ALE	0,32731
OR*SHGC	0,00036	HR	0,34729 ^
TM*SHGC	0,01609	OR*HR	0,36209
OR*AFR	0,02804	WI*ALE	0,38334
SHGC*SHGC	0,04445	TM*HR	0,43498
SHGC*AFR	0,04549	TM*ALE	0,44153
WDI*HR	0,05080	WI*SHGC	0,44666
TM*AFR	0,06487	AFR*ALE	0,48024
AFR	0,07267 ^	WI*HR	0,51843
SHGC*ALE	0,08939	WDI*SHGC	0,53665
WDI	0,10529 ^	WDI*WDI	0,55221
WI*WDI	0,11019	HR*HR	0,58765
AFR*AFR	0,13928	WI*AFR	0,61532
ALE*ALE	0,14722	WDI*AFR	0,65562
TM*WDI	0,15687	SHGC*HR	0,66578
WDI*ALE	0,19015	HR*AFR	0,69911
WI*WI	0,23261	OR*WI	0,81909
ALE	0,24656 ^	TM*WI	0,82350
		OR*WDI	0,88742

Figure 5: Effect tests of the coefficients associated with the main and second order effect of the eight building parameters for the PCM_{tot} case.

3.2 PCM_{cool} and PCM_{heat} cases

The same sets of calculation were conducted for the PCM-panel with PCM_{cool} and PCM_{heat}. Interestingly, higher savings of energy needs could be achieved using PCM_{tot} instead of PCM_{cool} (11.89 kWh/m^2 of achievable savings for ΔE_{cool}) or PCM_{heat} (3.61 kWh/m^2 of achievable savings for ΔE_{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_{heat} (Figure 6). The associated coefficient was -1.08. This means that, assuming no interactions and no second order effect, ΔE_{heat} would unexpectedly increase by -1.08 from a case without heat recovery (0%) to a case with an ideal heat recovery system (100%).

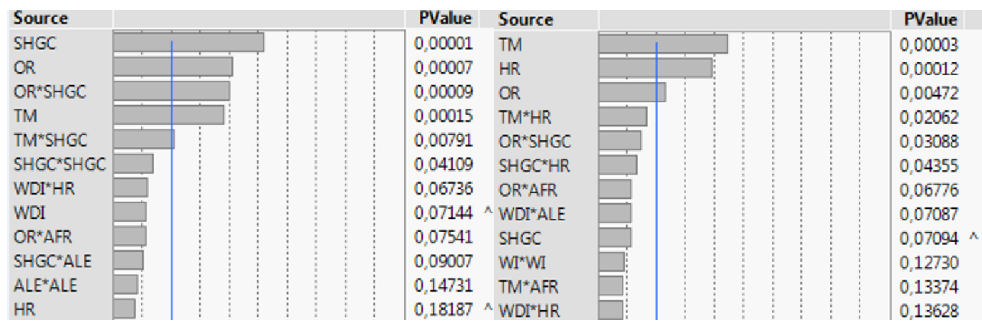| Source	PValue	Source	PValue
SHGC	0,00001	TM	0,00003
OR	0,00007	HR	0,00012
OR*SHGC	0,00009	OR	0,00472
TM	0,00015	TM*HR	0,02062
TM*SHGC	0,00791	OR*SHGC	0,03088
SHGC*SHGC	0,04109	SHGC*HR	0,04355
WDI*HR	0,06736	OR*AFR	0,06776
WDI	0,07144 ^	WDI*ALE	0,07087
OR*AFR	0,07541	SHGC	0,07094 ^
SHGC*ALE	0,09007	WI*WI	0,12730
ALE*ALE	0,14731	TM*AFR	0,13374
HR	0,18187 ^	WDI*HR	0,13628

Figure 6: Effect tests of the coefficients associated with the main and second order effect of the eight building parameters for the PCM_{cool} case on ΔE_{cool} (left) and for the PCM_{heat} case on ΔE_{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.
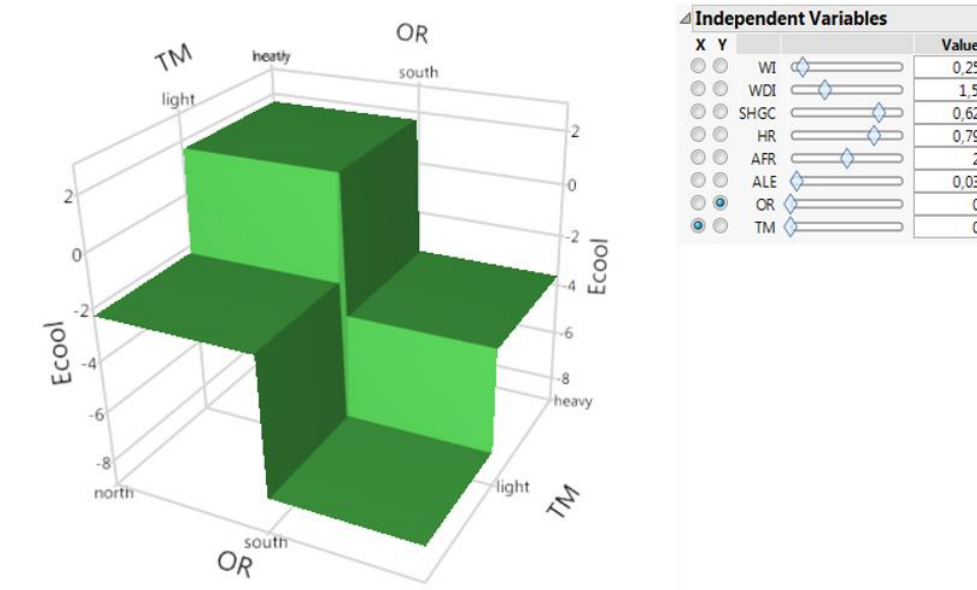
Figure 7: Influence of the two categorical variables on ΔE_{cool} for a given set of the six continuous variables.

The model had limitations for accurate predictions. For example, considering PCM$_{\text{heat}}$ with the same set of parameter as in our previous study, a saving in term of ΔE_{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$_{\text{tot}}$, the energy savings for cooling varied from zero up to 16.40 kWh/m2.

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/m2.

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 PCM_{tot} instead of using PCM_{cool} or PCM_{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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