Evaluation of modelling conditions imposed for simulation of building-integrated phase change materials

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Abstract

Phase change materials (PCMs) are a high energy density thermal storage option that, when integrated into buildings, store midday solar energy via solid-liquid phase change to shift the time a solar load is introduced into a space thus decreasing peak cooling and overnight heating loads. However, further research is required to minimize conditioning loads with PCMs, and therefore it is critical that the assumptions imposed by simulation software are carefully assessed. The objective of this research was to evaluate assumptions involved in modelling the characteristics of PCMs, such the treatment of solar radiation upon PCM surfaces. An experimentally validated single-room EnergyPlus model was developed, and scenarios were simulated while assessing the impact of selected modelling conditions. It was found that window geometry has a negligible impact on the room, and that peak room temperatures are greater when internal gains are introduced in place of the equivalent solar gains.

Introduction

Buildings, which are responsible for over 40% of the energy consumed within Canada (Statistics Canada, 2016), have the potential to be a key player in achieving national and international climate and emissions goals. Through implementing elements with high thermal capacity into buildings, energy can be stored in walls to reduce midday peak space cooling loads, and the stored energy can be later released to reduce overnight heating loads simultaneously. Phase change materials (PCMs) are high energy density materials that store energy via a solid-liquid phase change. They can be incorporated into materials such as drywall, paint, or concrete such that there would be no perceivable difference between PCM-integrated components and their traditional counterparts. In the building design phase, however, the thermal characteristics of PCMs must be carefully considered which can be done through simulations of building energy with PCMs.

In modelling the integration of PCMs within the built environment, it is of the utmost importance to maintain accuracy of the physical system and therefore to recognize the physical factors that have the largest effects within a model. For example, Zhou et al (2014) conducted a numerical analysis and found that thermal conductivity has a low impact on the wall surface temperatures. Accurate prediction of the wall temperatures is imperative, as it is closely linked to PCM responses: PCMs increases the convective mixing within a space and decreases wall surface temperatures (Kuznik & Virgone, 2009).

Thermal gains have a significant impact on wall temperatures within a space and thus knowledge of the corresponding assumptions associated with modelling thermal gains is of the utmost importance, particularly in rooms with thermal storage such as PCMs. If gains are introduced to a space via an auxiliary source (i.e. electric heater), heat is transferred directly from the source to the air, increasing the space temperature, resulting in the heat being transferred to the room surfaces to reach temperature equilibrium. Alternatively, if gains are introduced via solar radiation through a window, the gains first reach the floor of the space and a portion is then reflected to the walls and ceiling, directly heating these surfaces, prior to being convectively introduced to air within the space. Furthermore, if the window placement is varied, one would be likely to observe variations in localized temperature distributions across room surfaces. However, it is commonly assumed in building simulation that surface temperatures are uniform. As such, it may be expected that PCMs would perform differently depending on the introduction of a load to a space and location of a window. The capacity of building software to assess these factors may introduce simulation error; it is critical to understand the impacts associated with these modelling assumptions.

The objective of this study was to analyse the effects of windows in the modelling of PCMs using EnergyPlus. Two major factors are the treatment of thermal loads within the space and differences between solar and internal gains with PCMs, and window location and orientation. Improved knowledge on the effects of factors such as these within PCM models is imperative to accurately predict their thermal response, and the corresponding impact to building energy loads.

Methods

In this study, a single-room EnergyPlus model was created and validated against an experimental study (Kuznik & Virgone, 2009) prior to its use for examining two major simulation assumptions. These assumptions for the modelling of PCMs were the treatment of thermal gains in the space – comparing solar gains with electrical loads, and the window location within the wall. It is imperative to have detailed knowledge of the effects of these conditions on PCM behaviour in order to optimize the utilization of PCMs within any climate.

The results of the validation case for the developed model are shown in Figure 1. Due to the agreement between the experimental results and simulations for the parameters such as temperatures both with and without PCM, the model was deemed suitable for use within this study.

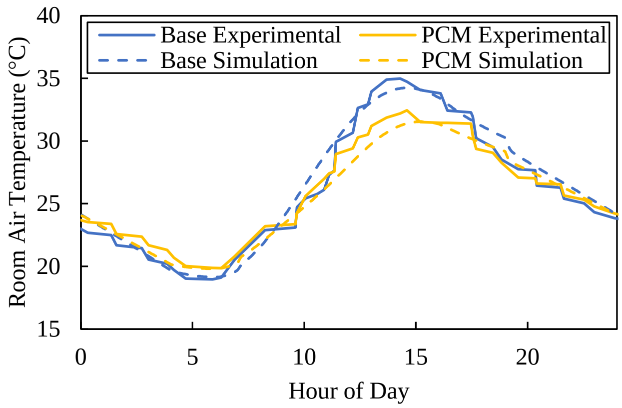

Figure 1: Model validation sample for room air temperature with and without PCM.

The model was developed as follows, while additional details about the parameters used within the validation case can be found in Kuznik and Virgone (2009). The developed model consisted of a 3.1 m by 3.1 m by 2.5 m height room. The room had a 1 m^2 window placed on the south facing wall with a solar heat gain coefficient (SHGC) of 0.775 and a U-factor of 0.618 W/m^2 K. The wall, floor, and roof constructions are shown in Table 1. The corresponding thickness (t), thermal conductivity (k), density (ρ), and specific heat capacity (C_P) of the materials used are shown in Table 2.

Table 1: Room construction (from outside to inside).

Wall	Floor	Ceiling
OSB	OSB	OSB
XPS	XPS	XPS
Insulation	Plaster	Insulation
Plaster	-	Plaster
PCM	-	-

Table 2: Properties of building materials used to model the building.

	t (m)	k (W/mK)	ρ (kg/m^3)	C_P (J/kgK)
OSB	0.018	0.13	650	1700
XPS	0.04	0.034	35	1400
Insulation	0.1	0.456	95	837
Plaster	0.01	0.35	817	1620
PCM	0.005	0.22	900	1200

The developed room was designed to represent one room of a house, and as such, a 20ºC boundary condition was imposed on the exterior of all building surfaces with the exception of the south facing wall. A constant air infiltration rate to the zone of 1 ach was imposed throughout all simulations. It was assumed that the room was unoccupied and there were no gains due to lights or electrical sources, unless otherwise noted, to maintain consistency between the test cases.

The ground reflectance was set at 0.7 for winter months of November through March to represent snow conditions, while for all other months, it was 0.2.

The PCM properties selected for this study were applied using the MaterialProperties: PhaseChangeHysteresis object. The latent heat capacity of the melting and solidifying processes was 160 J/g. The PCM was said to melt over a range of 14ºC temperature range that peaked at the stated melting temperature and solidify over a range of 10ºC that peaked at the solidifying temperature. The solidification temperature was said to be 6ºC below the stated melting temperature, thus showing some subcooling (cooling in the liquid phase below the melting temperature prior to solidifying).

In terms of the HVAC within the simulated room, an ideal load air system was used to temper the space. The heating setpoint was 18ºC and the cooling setpoint was 25ºC. The model was run using a conduction finite difference simulation approach to capture the PCM behaviour, using 3-minute timesteps. Weather conditions were imposed using Canadian Weather year for Energy Calculation (CWEC) for Ottawa, Ontario. The results of the simulation test cases were compared in terms of annual heating and cooling loads for the space. In addition, a sunny day in winter (March 6) and summer (July 2) were assessed to highlight daily trends in indoor and wall temperatures, imposed thermal loads, and heat fluxes.

Simulation Test Cases

Two sets of simulations were conducted within this study to evaluate the effects of different assumptions employed to model the effects of windows on PCMs within EnergyPlus. The base cases either had PCM melting temperatures of 18ºC or 24ºC PCM, with a window that was a 1m by 1 m square centred across the south facing wall and beginning at a height of 1 m up the wall (origin coordinates of (1, 0, 1)). These dimensions are width, depth, height of a point on the south facing wall, assuming the bottom left corner of said wall to an outside observer is (0, 0, 0). The base cases were used for comparison within both sets of simulations.

The first of the assumptions (A1) was the treatment of thermal gains within the space to evaluate effects of solar gains and equivalent electrical loads on PCM performance within a space. This was examined by running two cases: one with the window in place to allow in solar gains (A1-

W), and one without the window but with hourly electrical loads equal to those that entered the space due to solar gains when the window was in place (A1-E). For this set of simulations, melting temperatures of 18ºC, 21ºC, and 24ºC were analysed. It should be noted that the defined base case is equivalent to the A1-W cases for the corresponding PCM melting temperatures.

To obtain the electrical load profile, the solar simulation was first conducted, outputting the thermal load entering the space via the window, which was then read into EnergyPlus and implemented as an identical electrical load. The equal solar and electrical loads for a sample of sunny summer and winter days are shown in Figure 2.

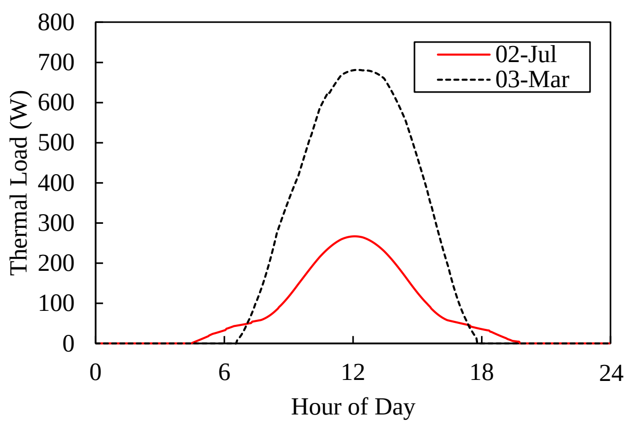

Figure 2: Thermal load profile used for solar and electrical loads on sunny summer and winter days.

The second assumption (A2) was the window location on the south facing wall. In a real-world experimental scenario, it may be expected that different window locations even with the same window area within the same wall would have some effect on the room temperatures and loads. This may be true particularly with PCM walls whose thermal response rely heavily upon wall temperatures. This set of simulations was run to examine the impact of window locations on PCM performance within the software. In all scenarios, the 1 m^2 window area from the base case was maintained, as were the window properties. One case examined a 2 m wide window that was 0.5 m tall (A2-W), with its origin at (0.5, 0, 1), and the other case was a 0.5 m wide and 2 m tall window (A2-T) with its origin at (1, 0, 0.5).

Figure 3 provides a summary of all assumptions-cases-melting temperatures assessed throughout this study.

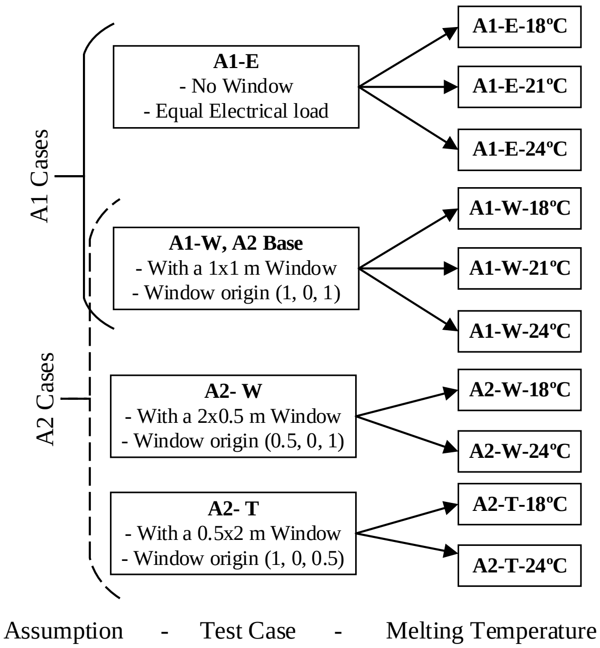

Figure 3: Assumptions and test cases used throughout the study.

In all cases examined for both assumptions, several parameters such as the annual heating and cooling loads, room and wall temperatures, wall heat storage and release rates, and wall heat fluxes were assessed. Through comparing these parameters to the base case scenarios, the impact and importance of the assumptions studied can be evaluated.

Results and Discussion

The two modelling assumptions assessed within this study both revolved around the imposition of thermal loads: a comparison of electrical and solar loads, and a comparison of window locations within a wall. This is critical to support advances in the integration of PCMs into the built environment with a focus on two new strategies. The first is concentrating the PCMs placement within the building with the greatest impact in the targeted loads (either heating or cooling). The second strategy consists of tuning of different melting points in different locations within the room to target either the heating or cooling loads based on the solar geometries present during either the summer or winter months.

Assumption 1: Window Versus Electrical Gains

The simulations of window solar gains and electrical gains were conducted to assess the corresponding impacts on air temperatures, conditioning loads, and overall PCM performance. The air temperature throughout each a sunny winter and summer day are shown in Figure 4 and Figure 5, respectively, where, for example, E24 indicates the electrical thermal load with a PCM melting temperature of 24ºC.

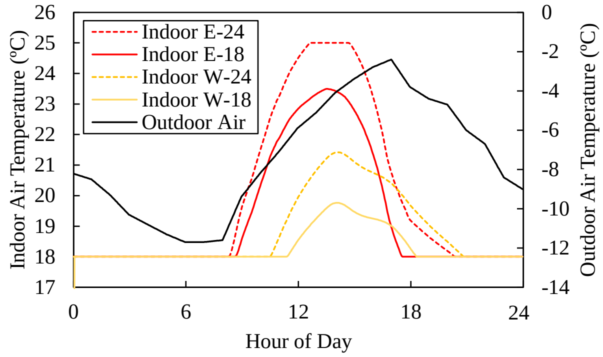

Figure 4: Air temperature trend for window and electrical thermal loads within the room on March 6th – a sunny winter day.

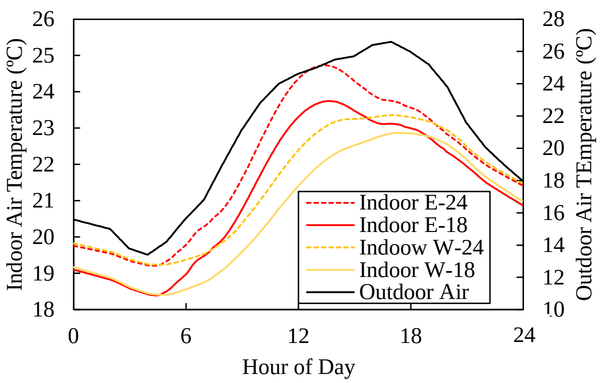

Figure 5: Air temperature trend for window and electrical thermal loads within the room on July 2nd – a sunny summer day.

It can be seen that PCMs with lower melting temperatures were associated with lower peak room temperatures throughout the day due to their greater latent heat capacity at these lower temperatures. In situations where there were limited solar gains, such as cloudy days, the benefits due to the PCMs were limited in both cases because the midday temperature peak was insignificant. In addition, the room exhibits greater air temperature fluctuation throughout a day and an earlier peak in room temperature when an electrical load is implemented than with equal solar gains. This is because the electrical system directly heats the air, while solar gains are reflected and absorbed by the room surfaces, before the energy is transferred to the room air, increasing its temperature. This trend is further illustrated through examining the energy storage and temperature distribution of the walls (Figure 6).

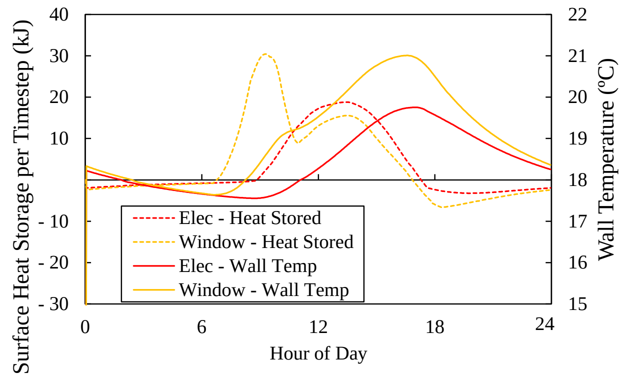

Figure 6: Temperature and heat storage of west wall with 18ºC PCM on March 6th.

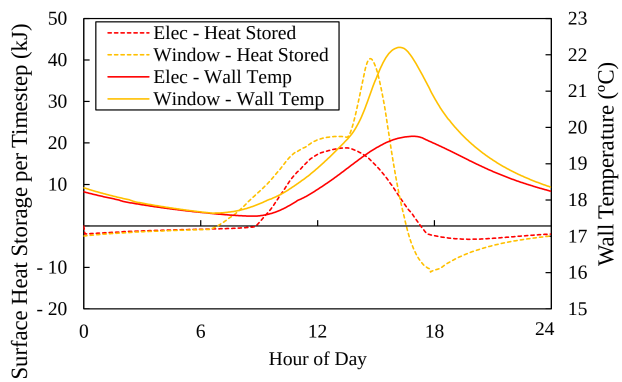

Figure 7: Temperature and heat storage of east wall with 18ºC PCM on March 6th.

On a sunny winter day when the sun is low in the sky, large solar gains are absorbed by the west wall in the morning, while large solar gains are absorbed by the east wall in the evening, as shown in Figure 6 and Figure 7, respectively. The solar gains absorbed by the walls are nearly twice that of the peak electrical gains for either wall. This leads to warmer peak wall temperatures for the window cases than the electrical load cases in which the walls do not receive direct thermal gains, but instead receive thermal energy from the room air. The trends for energy stored within the walls for the window and electrical load scenarios with 18ºC and 24ºC melting temperature PCMs are shown in Table 3. These values are the energy into the walls and as such does not include heat loss.

Table 3: Energy storage rate into walls on March 6th for the various thermal load and PCM scenarios.

	West Wall (MJ)	**North Wall (MJ)**	**East Wall (MJ)**
W-18ºC	2.722	2.596	3.282
W-24ºC	1.944	1.896	2.710
E-18ºC	1.992	1.992	1.992
E-24ºC	1.527	1.527	1.527

Two major trends can be observed with Table 3. The first is that the energy stored across all walls were equal for each of the electrical load scenarios. This is because the walls were the same size and were exposed to the identical thermal load, caused by the EnergyPlus assumption that room and wall temperatures are each uniform. The second major trend is that the east wall was found to absorb the most energy throughout the day; this was the case for the sunny summer day scenario, as well. With a window, the east wall can store the greatest amount of energy because it stores energy gradually throughout the day, and then stores a significant amount of energy later in the day when solar gains are directly striking it, while the room air temperature is also at its highest point. As such, there are higher peak temperatures and higher peak surface storage rates than can be seen for the west wall, as illustrated when comparing Figure 6 and Figure 7. This suggests that it may be advantageous to place a PCM with a higher melting temperature, or a greater quantity of PCM in the east wall than in the west wall, because of the greater capacity of the east wall to store energy, and at higher temperatures.

Despite the difference in stored energy within the walls, the time of the peak wall temperature differed by only a few minutes between the cases. This is due to the fact that, although the loads were applied differently, the load profile and corresponding decrease to zero was equal, thus a rapid peak in wall and room temperatures was observed at nearly the same time of day.

Table 4 illustrates the effects of these trends on the annual heating and cooling loads for both cases with different PCM melting temperatures.

Table 4: Annual heating and cooling loads for A1 cases.

	Annual Heating Load (GJ)	**Annual Cooling Load (GJ)**
E-24ºC	1.69	0.16
E-21ºC	2.14	0.06
E-18ºC	2.44	0.1
W-24ºC	1.81	0.01
W-21ºC	2.43	0.01
W-18ºC	2.82	0.04

It was found that the electrical load cases minimized the heating load. This is a consequence of the electrical load being applied directly to the air and thus limiting the time during which the supplementary heating system was called. In contrast, the cooling load was found to be minimized with the solar gains. Solar gains directly heated room surfaces which stored some of the thermal energy prior to introducing it to the air, thus limiting the cooling load.

It can be observed that the 24ºC melting temperature PCM led to the lowest heating load regardless of the window or electrical load scenario. This is caused by the assumed solidification temperature of the PCM that exhibited subcooling. The 24ºC PCM solidified at 18ºC, while the 18ºC PCM solidified at 12ºC. Thus, there were no instances in which the 18ºC melting temperature PCM could fully solidify and release its stored thermal energy. In contrast, the 24ºC PCM was able to fully melt during the day due to the gains and solidify overnight due to the 18ºC room temperature setpoint.

A designer could use the results illustrated in Table 4 to select a melting temperature that would minimize one space conditioning load, or if it was desired to minimize the total conditioning load, the annual heating and cooling loads could be summed to select the melting temperature with the lowest total load. Alternatively, designers may choose to select two PCMs – one better suited for heating loads and one for cooling loads to implement into a space to achieve conditioning load benefits during both seasons.

When additional simulations were conducted without PCM in the walls, it was found that the heating loads were 2.43 and 2.30 GJ and the cooling loads were 0.17 and 0.42 GJ for the window and electrical load cases, respectively. Thus, PCM did decrease these loads when it was able to fully melt and solidify, as was the case with 24ºC PCM. However, this also illustrates the importance of proper PCM selection and design within PCM systems. If the solidifying temperature is too low, the PCM will remain in the liquid state, having the effect of increasing heating loads due to the additional thermal storage and limited release of energy to the space.

It is likely that changes to the PCM properties would modify the space conditioning results for the A1 cases. If the PCM phase change range were smaller, increased PCM benefits on conditioning loads would be expected when the PCM melting temperature is closer to the room temperature setpoint. Similarly, if the melting and solidifying temperatures for a given PCM were closer together or equal, there may be additional conditioning benefits of lower melting temperature PCMs; they would then be able to solidify without requiring cooling to well below room temperature, and thus would achieve additional space conditioning benefit due to better facilitated thermal storage and release.

Assumption 2: Window Location

The second scenario that was examined was the impact of window geometry on the overall performance of the modelled space, as well as the modelled behaviour of the individual surfaces within the room. This is important to determine how the changes in the geometry of the solar radiation passing through the window, as a result of the changing window geometry, impacts the storage and release of energy within each wall. Detailed knowledge of the impacts of window geometries are critical to fully assess these PCM optimization strategies.

To study the impact of the window geometry, three geometries were modelled, each with a total area of 1 m^2, but three distinct shapes. The first was the base case, used to examine the window and electrical load comparison, in which a 1 m x 1 m window was modelled, followed by a window 2 m x 0.5 m and finally 0.5 m x 2 m (width and height). For each case, like previous cases studied, the model was run under an annual simulation, utilizing 18℃ and 24℃ melting point PCMs, and sunny cold and warm days were assessed – March 6th (heating loads) and July 2nd (cooling loads). A comparison of the overall outputs for the complete room were first examined, followed by specific performance metrics for the west, east and north wall of the space.

The first parameter examined was the total heating and cooling energy required to meet the annual loads for the modelled space, to determine the impact of window geometry, as shown in Table 5.

Table 5:Comparison of loads by window geometry.

Window Size (mxm)	PCM Melting Temperature (℃)	Heating Load (GJ)	Cooling Load (GJ
1x1	18	2.82	0.04
	24	1.81	0.01
2x0.5	18	2.81	0.04
	24	1.81	0.01
0.5x2	18	2.82	0.04
	24	1.81	0.01

These results show that no matter the window geometry, as long as the window area remains constant, there is almost no change in the required heating or cooling load. It also shows that there in no case does the full PCM melt or solidify, as the energy storage within the wall was never utilized to its full potential. To complete the analysis of the full space, the air temperature was compared across each modelled case as shown in Figure 8 for March 6th using the 18℃ PCM, with trends being observed for both PCM melting points and for both modelled days.

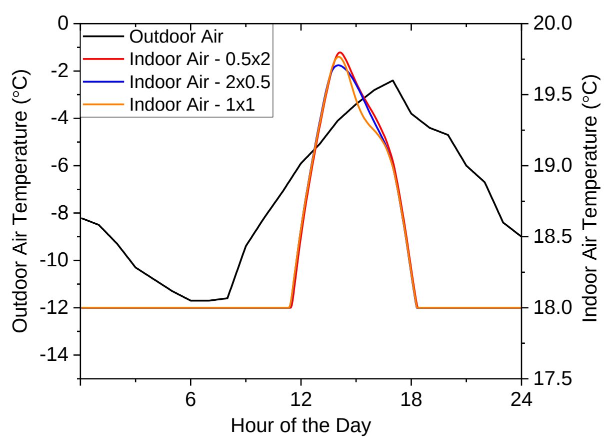

Figure 8: Air Temperature in the modelled space with the three different window sizes for 18℃ PCM on March 6th.

Based on these results, it can be seen that the interior air temperature within the space is predicted to follow almost identical trends, with only small variations in temperature during peak solar periods in the early afternoon. This confirms the initial conclusion that the geometry of the window, as long as the total area of the window remains constant, has limited impact on the air temperature and energy consumption within the space. Once the window geometry's impact on the macro conditions within the space were determined to be negligible, the impact on specific surfaces were examined.

When modelling the room, the surface temperatures for each of the five interior surfaces, and net energy storage within the wall assembly (predominantly stored within the PCM layer as a result of the phase change) were determined and compared. For simplicity and to clearly show the trends, only the 2 m x 0.5 m and 0.5 m x 2 m windows are included, with the 1 m x 1 m wall falling in between these two extremes. Figure 9 shows the comparison of the storage rates for the east and west walls within the modelled room.

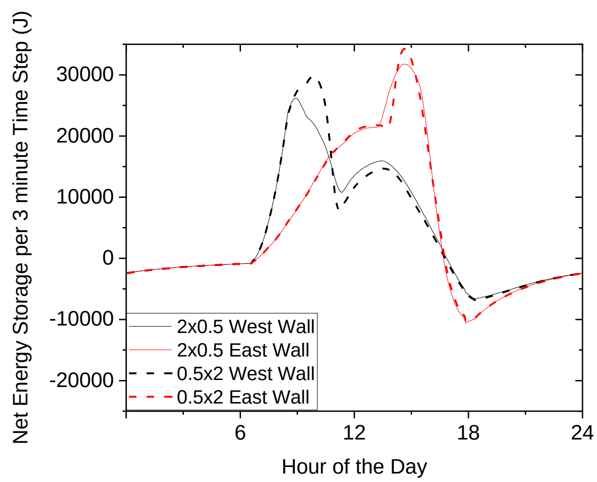

Figure 9: Comparison of the east and west wall net storage rates for the two window sizes.

This comparison shows that the energy storage for each wall follows the proper solar geometry, with solar energy originating in the east in the morning, entering the window and striking the west wall. This is represented with the early peak in energy storage on the west wall, where both window geometry cause an identical rise in storage, however the wider, less tall window begins to provide solar radiation on the west wall earlier then the tall narrow window that continues to provide all radiation on the west wall for longer period of time, resulting in a greater storage in the west wall. This is then repeated later in the day. When moving from the east and west wall to the north wall, Figure *10* shows the surface temperature and net energy storage over the course of the modelled day using the 18℃ PCM.

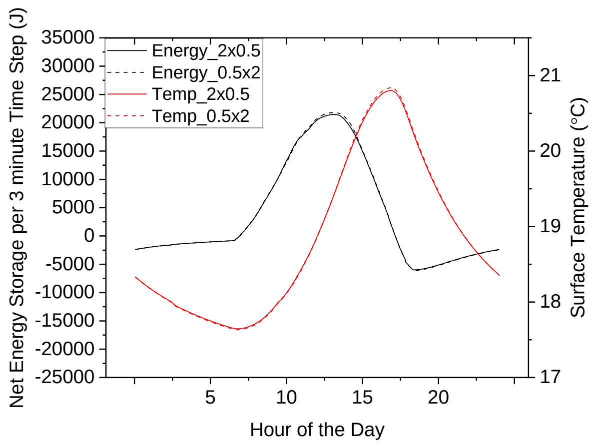

Figure 10: Comparison of surface temperature and net heat stored on the north wall.

These results that show the wide window leads slightly in both the surface temperature and energy stored, as it allows solar radiation to strike the north wall earlier, but the overall trend sees minimal impact on the north wall between the two window geometries. Finally, when the total energy stored within all of the surfaces within the building using the two window geometries is examined, it can be seen in Figure 11 that the total energy storage is basically identical throughout the day. This shows that the although different surfaces have different storage rates based on the window and solar geometry, the total storage is unaffected by the these factors.

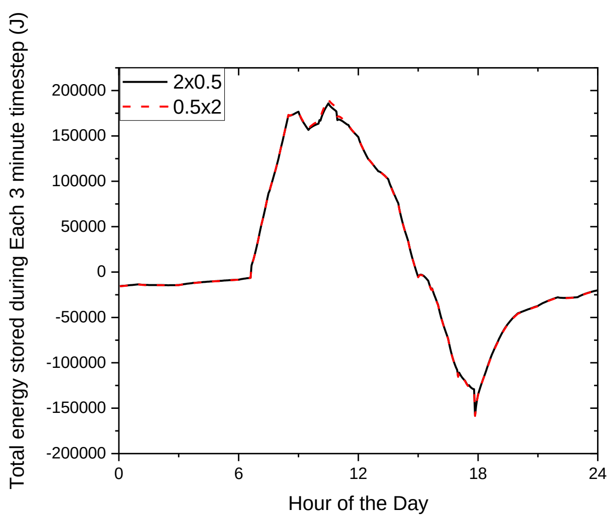

Figure 11: Total energy stored through the day on March 6th for the two window geometries.

These graphs are shown for the model with the 18°C PCM and for March 6th, but the same trend was observed for each scenario using different melting points for the PCM and during both the heating and cooling scenarios.

These modelling results show that the EnergyPlus model is able to account for the solar geometry and accounts for the solar radiation entering the space and the surface on which it strikes. Although, this occurs, a number of assumptions and simplifications remain, in that the entire surface is treated as uniform body, with a uniform surface temperature and uniform melting and solidification of the integrated PCM. These assumptions would become prohibitive when the non-uniform distribution of PCM type and quantity within the space is desired. To model these situations, a much more refined discretization of the space would be required, to model the surface temperatures, but not impacting the air flow/temperature within the space.

Summary of Key Findings

When analysing A1 comparing electrical and solar loads within a space and their impact on PCMs, it was found that annual heating loads were minimized with the former, while cooling loads with the latter. When solar gains enter a space, they are first absorbed and reflected by the room surfaces, followed by convective heat transfer to air in the space. Alternatively, electrical gains directly heat the air. As such, increased air temperatures in the electrical scenario prevented the heating system from operating as much in the winter and increased operation of the cooling system within the summer. If a full system approach was taken, considering the possibility of using solar energy within active systems as well as passively storing with PCMs, these trends could be utilized to provide insight into the instances in which it may be better to rely on passive gains versus active systems. Furthermore, it was found that the east wall stored greater quantities of energy throughout the day and exhibited greater peak temperatures than the west or north walls. As such, it may be the case that the PCM melting temperature should be greater in the east wall than the west wall to maximize useful solar gains and further reduce conditioning loads.

In terms of A2 on window geometries, it was found that there were minimal differences between conditioning loads and wall temperatures with the constant window area in different shapes. The greatest difference observed for the window geometries was for the east and west walls. With the wide and short window, solar energy began to strike the west and later east walls earlier than the tall and narrow geometry. However, the latter geometry provided a greater peak energy storage rate per timestep due to the greater concentration of solar energy striking the wall for a given timeframe. These trends can be further expanded in optimization of PCM systems: if it is desirable to store a greater quantity of energy within the wall at a given time, taller windows help achieve this, while if a slightly more uniform storage profile throughout the day is desired, shorter windows may be selected.

It is important to note that this study was done with a specific set of PCM properties that include hysteresis, subcooling, and a relatively large melting temperature range. In addition, all simulations were conducted for Ottawa, Ontario. Although it may be expected that some trends described within this study would hold true with other PCM characteristics in other geographical locations, further simulation should be conducted to verify whether this is the case.

Conclusions

In this modelling study, a single room model was used to analyse the effects of two major modelling assumptions and their effects on PCM simulation. it is imperative to understand the effects of factors such as window implementation on PCMs in order to develop an optimized PCM. This study aimed to provide insight into these factors.

The first assumption studied was the implementation of thermal loads within the space – be it solar gains or an equivalent electrical load. It was found that peak room air temperatures and cooling loads were greater with the electrical load scenario, while peak wall temperatures and heating loads were greater with the solar gain window scenario. This is caused because solar gains strike the walls while electrical loads directly heat the air. In addition, it was found that the east wall had greater peak temperatures and thermal storage than the west wall. The implication of this is that if a system with multiple PCMs of different melting temperatures is used to maximize potential gains, it may be beneficial to implement a PCM with a higher melting temperature into the east wall than the west or north walls.

The second assumption was the window geometry. It was observed that although there was a negligible difference in conditioning loads with different window geometries and the same window area, the peak quantity of energy into the walls for a given timestep was greater for a tall, skinny window. This implies that if creating a more uniform energy input to the wall is desired, a wide, short window may be a better choice, if window area is restricted.

The major conclusion of this study is that it is imperative to understand the impacts of all design decisions when modelling details such as PCMs due to the variations in their response to variations in thermal loads. This study provides insight into trends relating to window considerations within PCM systems, however significant research is suggested to facilitate the development of accurate PCM models in the future.

Suggested Future Work

In the future, experiments should be conducted to examine the real-world impacts of the assumptions in comparison to the simulation-based results from this study. Furthermore, experiments should be conducted to quantify the impact of the software-imposed assumption that wall temperatures are uniform on each surface. It may be observed, particularly within PCM walls, that there are non-negligible errors introduced due to this assumption because of varying solar insolation upon single surfaces.

The findings within this study that suggest advantages to installing PCM as a function of building layout should be expanded upon in the future. This should include a detailed analysis of different PCM options within different surfaces of the room, to determine whether there are consistent trends observed in performance that can be translated into guidelines for building design in the future.

In addition, in situations where the PCM distribution within the walls is non uniform, current EnergyPlus models will be limited due to the assumption that wall temperatures are uniform. More detailed discretized models would be necessary in these instances, thus indicating the importance of fully understanding the modelling assumptions for scenarios that are desired.

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