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ABSTRACT

Phase change materials (PCMs) can be implemented into building practice to enhance thermal storage performance, reduce indoor temperature fluctuations and improve the thermal comfort of occupants. As building energy simulation is taking an ever larger role in the design and analysis of energy efficient buildings, it is important to understand the capabilities and performance of these tools. A popular and powerful building simulation program is ESP-r which is capable of incorporating the use of PCM into the thermal simulation. An effect of using multiple layers of PCM versus using a single layer was investigated. It was found that in general the application of PCM can significantly affect the thermal performance of the building. It was also shown that multilayered PCM demonstrated more realistic thermal benefit than single layer PCM in some cases.

1. INTRODUCTION

Building energy consumption and its resulting greenhouse gas emissions can be substantially reduced if solar energy is adequately utilized. Storage of thermal energy in buildings has gained prominence in the past two decades due to a strong need to reduce the total thermal energy requirement (both heating and cooling) in buildings (Zalba *et al.*, 2003). The integration of phase change materials into building fabrics can accumulate the gain from solar radiation during the day and release the stored energy at night. Therefore, the energy requirement at peak hours can be reduced and pre-cooling or heating becomes possible. Furthermore, the implementation of PCMs can reduce the indoor temperature fluctuations and improve the thermal comfort of occupants.

Phase change material has been implemented in building simulations using TRNSYS and ESP-r. Stritih and Medved (1994) and Ahmad *et al*. (2006) used a finite element approach to model PCM in TRNSYS. Kuznik *et al*. (2010) developed a TRNSYS module that applies the effective heat capacity method with a finite difference scheme. Heim and Clark (2004) used the built in special material facility in ESP-r to model a house with PCM-gypsum walls.

The most popular PCMs available currently are the solid-liquid type (SLPCMs), which undergoes liquid-to-solid (freezing) or solid-to-liquid (melting) phase change. These PCMs can suffer from inefficient energy recovery and reduction in overall thermal performance during the solid-liquid phase transition (Farid *et al.*, 2004). Considering the ever increasing application of PCMs in building practice, PCMs in the liquid state affect the structural integrity and cause undesirable "wetness" in the walls. The aforementioned difficulties could be avoided if solid-solid PCMs (SSPCMs) are employed. In the current study, a type of SSPCM was used in a house modeled in ESP-r.

In order to understand the heat transfer process in SSPCMs, mathematical models for SLPCMs are briefly reviewed here. The governing equations for the heat transfer in the solid-liquid PCMs are composed of the Navier-Stokes (momentum) equation, the mass conservation equation, and the energy conservation equation. From a mathematical point of view, the momentum and mass conservation equations can be neglected for the SSPCMs because there is no convective term in the PCMs (Zhang *et al.*, 2007). This conclusion significantly simplifies the numerical analysis. Therefore, the energy equation is the only governing equation for the analysis of SSPCMs, and can be expressed as follows,

$$\rho C_p \left(\frac{\partial T}{\partial t} \right) = \nabla \left(k \nabla T \right) \tag{1}$$

where ρ, C_p and k are the density, specific heat and thermal conductivity of PCMs, respectively. There are two types of numerical methods, namely enthalpy method and effective heat capacity method.

The enthalpy method enables the governing equations to be applied over the entire domain of interest rather than on the phase change interface. The total energy required for the phase change, i.e. the overall sensible heat and latent heat, can be determined by the enthalpy function $H(T)$. For the SSPCM, the enthalpy term for the energy equation (Eq. 1) can be expressed as follows

$$\rho \frac{\partial H(T)}{\partial t} = \nabla(k \nabla T) \tag{2}$$

An alternate way of solving the non-isothermal phase transition in PCM is the effective heat capacity method. The effective heat capacity of the material (C_{eff}) is a linear function of the latent heat of fusion on both the heating and cooling processes. It is inversely proportional to the temperature difference between the onset and the end of the phase transition. The effective heat capacity of the PCM during the phase change is given as,

$$C_{\text{eff}} = \frac{L}{T_e - T_o} + C_p \tag{3}$$

where L is the latent heat of fusion, T_o is the onset temperature of phase transition happens and T_e is the temperature when the phase transition completely finishes. Thus, the governing equation (Eq.1) for the binary solid state PCM can be expressed as

$$\rho C_p(T)\left(\frac{\partial T}{\partial t}\right) = \nabla(k \nabla T) \tag{4}$$

$$C_p(T) = \begin{cases} C_p & T < T_o \\ \dfrac{L}{T_e - T_o} + C_{p@T_o} & T_o \leq T \leq T_e \\ C_p & T > T_e \end{cases} \tag{5}$$

2. PROBLEM DEFINITION

2.1 ESP-r
ESP-r is an advanced building energy simulation tool which allows for detailed thermal and optical description of buildings. The software discretizes the problem domain in a control volume scheme and solves the corresponding conservation equations for mass, momentum, energy, etc. ESP-r can integrate the effect of a variety of factors including, weather, external shading, occupancy gains, HVAC systems, and many others. For the current simplified simulation, no ventilation and no HVAC system was used. The simulation period is from June 1st to June 14th, using Toronto climate data.

2.2 Building Model Definition
In order to illustrate the effect of multilayered PCMs, a simple single zoned house was modeled in ESP-r, as shown in Figure 1. The house has dimensions of 3 m by 3 m and a height of 2.7 m. There is a single south facing window which uses 40% of the south facing wall. ESP-r has a predefined database of materials and construction layers that can be used directly or modified. A standard floor construction is used which is made up of four layers consisting of marble, concrete, gravel and earth. PCM was placed in the interior surface all four walls and the ceiling. The walls are based on the database materials consisting of five layers made up with PCM, an air gap, concrete, wool, and brick. The ceiling is also based on a standard database material made up of four layers of PCM, an air gap, concrete, and roofing felt. These constitute the one layer PCM model. However, for the multilayered PCM model, the single layer PCM was replaced with four layers of PCM with the total thickness remaining the same.
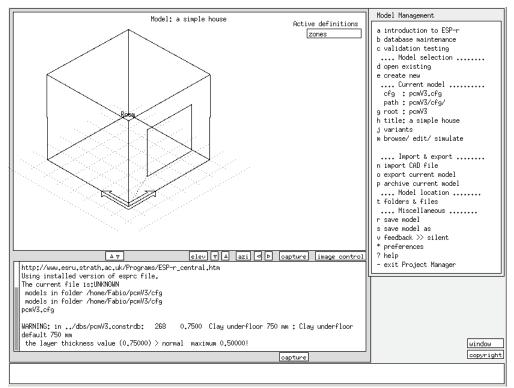
Figure 1: A typical ESP-r session running the PCM building model

2.2 PCM Definition

A typical phase change material is of the liquid-solid type, where energy is stored as latent heat during the phase change of the material. In the present study a new solid-to-solid phase change material called Dal HSM is used and analyzed. Since the material stays in solid state, the thermal conductivity remains constant. The phase change temperature range is from 20°C to 22°C and the latent heat of fusion is 80000J/kg. The physical properties are summarized in Table 1.

Table 1: Properties of Dal HSM

Property	Value
Density [$kg \cdot m^{-3}$]	800
Thermal conductivity [$W \cdot m^{-1} \cdot K^{-1}$]	0.3
Specific heat [$J \cdot g^{-1} \cdot K^{-1}$]	1.6
Phase change temperature range [°C]	20~22
Latent heat of fusion [$J \cdot kg^{-1}$]	80000

3. NUMERICAL RESULTS

To ensure that all cases start the simulation with the same initial conditions, no pre-simultion start up days was chosen. The simulation was run with a time step of one minute. ESP-r has a built-in capability to take into account the effect of phase change material. This is done through ESP-r active material module where the label of phase change is assigned to a material layer. From there ESP-r will incorporate the effected of phase change by determining the effective specifc heat, thermal conductivity, and energy stored in the material. The simulation was done for six different cases by considering: with and without PCM, 8 mm versus 40 mm of PCM, single layer versus four layers of PCM. The different cases are summarized in Table 2.

Table 2: Summary of numerical test cases

Case number	Total PCM thickness [mm]	Number of layers	Presence of PCM
1	8	-	No
2	40	-	No
3	8	1	Yes
4	8	4	Yes
5	40	1	Yes
6	40	4	Yes

3.1 Effect of PCM on Room and Surface Temperatures

First the effect of phase change material on room and surface temperatures is studied. The effect of PCM (single later) on the room temperature is shown in Figure 2 and it is compared with the no-PCM case. In order to reduce as many factors as possible, the non-PCM material has the same material properties as the PCM but with no latent heat of fusion. Here each peak represents the mid aftertoon corresponding to peak daytime temperature. Thus each peak can be viewed as a 24-hour cycle. What is displayed is a 14-day period. In the first seven days, a significant difference in room temperature between the PCM case and no PCM case can be observed. The PCM case have a reduced room peak temperature. However for the last seven days there is little to no difference between the two cases.

In order to understand what has happened, it is necessary to look at the surface temperature of the PCM in Figure 3. Here, the surface temperature is the interior surface temperature of the north wall (the wall opposite the window). Again the PCM has a significant effect on surface temperature for the first seven days than little to no difference for the last seven days. It is on the seventh day that the surface temperature of the PCM goes above 22°C and is no longer discharging latent energy over night. It is therefore behaving as a regular material with no latent heat storage. Thus as long as the phase change material can go through the charge-and-discharge cycle of its latent heat, then, there will be a noticetable effect on room temperature. In the current model no HVAC system is in place, so the room temperature is allowed to increase. However in a realistic situation, the operation of an air-conditioning system would 'cap' the peak daytime temperatures and thus allow the PCM to discharge its latent heat over night.
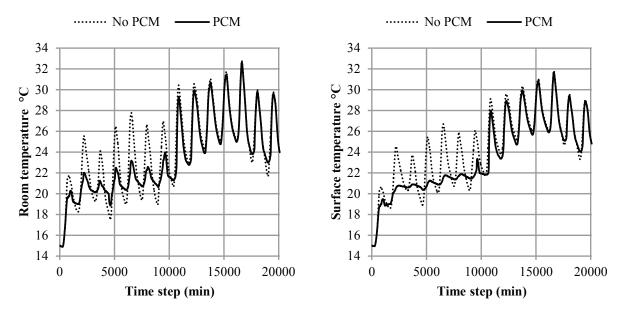

Figure 3: Room temperature with and without PCM (8mm case)

Figure 2: Surface temperature with and without PCM (8mm case)

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For comparison a thicker PCM layer (40 mm) is considered and its effect on room temperature is shown in Figure 4. Now with a larger potential of latent heat storage there is an even greater affect of PCM on the room temperature. While in this case the weather conditions are the same, due to the larger latent heat storage, the peak temperature remains significantly lower throughout the 14 days. This is due to the fact that the PCM is never fully charged and is always within the phase change range at some point throughout the day. So the PCM goes through a charge-and-discharge cycle within every 24 hour cycle.
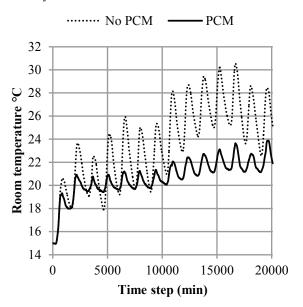

Figure 4: Room temperature with and without PCM (40 mm case)

3.2 Comparison of One- and Four-Layer PCM Models

Figure 5 illustrates the effect of using four layers versus one layer for the 8-mm PCM case. As it can be seen, there is little to no difference. During the phase change range on day 6 and 7 (the 6th and 7th peaks) there are small differences that can be seen where the peak temperature is about 1°C higher in the four-layer case than the one-layer case. For the other days the two sets of data are practically the same.

Figure 6 compares the room temperature of the four-layer and one-layer models for the 40-mm case. There is no difference initially between the two models until day 6 with the difference increasing with each subsequent day. During the entire simulation, the four-layer model is always at a higher room temperature than the one-layer model. For a given 24-hour cycle the difference is largest during the daytime hours and smallest over night. The room temperature difference is as much as 2°C in the last 3 days of the simulation.

In order to better understand this discrepancy between the two models, the north-wall interior surface temperatures of the one- and four-layer models for the 40-mm case are shown in Figure 7. In this figure it is easier to see the deviation propagating from day 6 to day 14. Also it can be seen why the four-layer model has the largest discrepancy on the last 3 days. On the 11th day the PCM is now above the phase change temperature range and thus it no longer goes through the charge-and-discharge cycle. While in the one-layer model the PCM is still discharging over night and thus is still absorbing energy as latent heat in daytime. As mentioned previously, the current simulation does not employ some temperature control scheme which would essentially force the PCM into a charge-and-discharge cycle and thus would reduce this deviation of the one-layer and four- layer models.
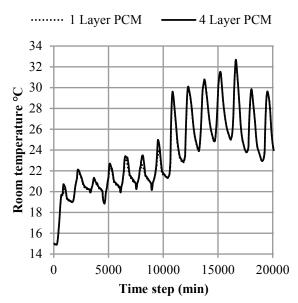
Figure 5: Comparison of room temperature using one and
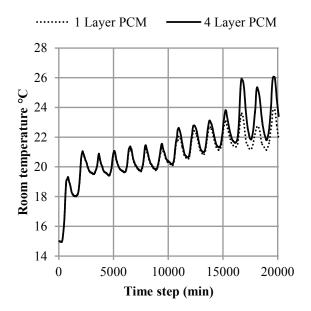four layers (8mm case)

Figure 6: Comparison of room temperature using one and
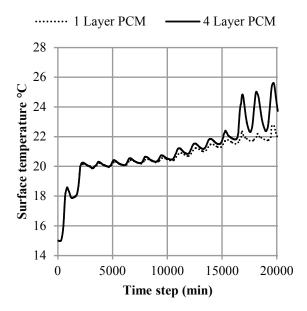four layers (40 mm case)

Figure 7: Comparison of surface temperature using one
and four layers (40 mm case)

3.3 Comparison of Temperature Profiles for One- and Four-Layer PCM Models

One way to understand the difference between one-layer and four-layer models is to examine the temperature profiles in the PCM layer. Figure 8 shows the temperature profiles for the 40-mm case and Figure 9 shows the temperature profiles for the 8-mm case. All of these are taken at the same snapshot in time, specifically 11am on June 14th (Toronto, Canada). This snapshot was chosen to illustrate the differences between one- and four-layer models. From Figure 8 one can see that the four-layer case deviates greatly from a hypothetical linear temperature profile (one-dimensional steady state conduction) and at its peak it deviates by 54%. While the one-layer case deviates from the linear temperature profile by as much as 26%. For the 40-mm one can see that the one- layer and four-layer have difference temperature profiles. For the 8-mm case one can see that the four- layer and one-layer give more or less the same temperature profiles. Thus for the 8-mm case the two models give the same results, while the 40-mm case it gives different results. In ESP-r each construction layer is made up of one interior node and one surface node on each surface with one-dimensional heat conduction. Since the temperature of each control volume is represented by one node, this effectively implies that the one interior node has a larger control volume than the one with multi-interior nodes, and hence its temperature changes more slowly due to its larger thermal capacitance especially for a PCM layer. Therefore, for a thicker layer (40 mm) of PCM with only one interior node, it would respond thermally sluggish, as compared to a thinner layer (8 mm) of PCM with only one interior node. Obviously the one-layer model for the 8-mm PCM layer is "small" enough with respect to its effective thermal capacitance, and hence, leading to similar response as the four-layer model for the 8-mm PCM layer.
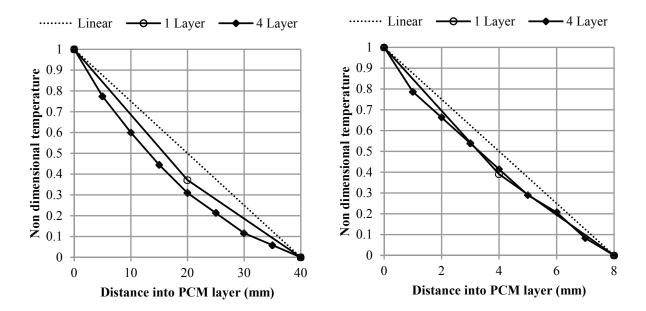

Figure 8: Temperature profiles for one and four layer (40 mm case)

Figure 9: Temperature profiles for one and four layer (8 mm case)

While a deviation of four layer and one layer is only seen for a few days (when a charge-and-discharge cycle is occuring), this deviation would be of greater importance in more 'realistic' house. A deviation is only seen when the PCM goes through a charge-and-discharge cycle. If an air-conditioning system was employed, then that would put an upper limit to the room temperature and the PCM would continue to go through this cycle.

4. CONCLUSIONS

The use of a novel multilayered approach to model the effect of phase change material in building energy simulation was investigated. It was found that the presence of PCM can have a significant effect on the room temperature. Also a comparison of a four layered PCM with a more typical one layer PCM was made. For a thin 8-mm PCM layer there was little to no difference between the one-layer and four-layer models. For a thick 40-mm PCM layer there was a significant difference between the one-layer and four-layer models in both the room and surface temperatures. Looking into the temperature profiles in the PCM layer, it was shown that the thin PCM layer is "small" enough with respect to its effective thermal capacitance and thus it can be approximated as a single layer. While the thick PCM layer has to be treated with multiple layers in order to have each "small" layer responding adequately. The results shown here represent a preliminary investigation into the effect of multilayered PCM modeling. A parametric study would be required (and is ongoing) in order to better quantify this affect. Also a validation, either through experiments or a rigorous model, would be beneficial in order to understand the underlying phenomenon.

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