An Enhanced Simulation Model for Building Envelopes with Phase Change Materials

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ABSTRACT

Utilizing Phase Change Materials (PCMs) in building envelopes as a measure for reducing energy use has been studied and practiced over the last four decades. In the context of whole building Energy simulation, building envelopes are typically modeled using a simplified one dimensional finite difference approach. PCMs can be included in such models if the models handle property variation. Simplified models generally do not capture detailed physical phenomena of PCMs such as hysteresis and sub-cooling. This paper presents the enhancements to the simulation model for Phase Change Materials in a modern whole building energy simulation program, EnergyPlus. The EnergyPlus PCM model was modified to an equation based model and the new model was validated. Demonstration of construction of temperature enthalpy curve from the properties of PCM available from experiments and manufacturers is also presented in this paper. Wallboards with experimental property data and manufacturers' catalog data were studied. In both cases, a similar behavior of the material is observed under same simulation conditions.

INTRODUCTION

Use of PCMs in building envelopes has proved to be a promising technique for reducing building peak load demands and fluctuations in the zone temperatures especially in places with extreme climates (Kosny et al. 2009; Kosny et al. 2009 a). The design of low energy building requires simulation studies using a building simulation tool such as EnergyPlus, TRNSYS and ESP-r, etc. Energy simulation tools use a heat balance method to assess the building loads and surface temperatures at a particular geographical location. Modeling PCMs requires taking into account the latent heat storage of the material. EnergyPlus (Crawley et al. 2000) is one such tool that has PCM modeling capability. The Conduction Transfer Function (CTF) model of calculating the temperatures of building surfaces has been used in building simulation, including EnergyPlus, for a long time due to its advantages in simplicity, linearity and use of a single equation. However, the CTF method assumes constant material properties and PCMs have properties that are temperature dependent. Hence EnergyPlus was equipped with a Finite Difference (FD) algorithm that models property variation including phase change simulations (Pedersen 2007) was included in the whole energy simulation program, EnergyPlus (Crawley et al. 2000). However this model (referred to hereafter as the current model) cannot simulate the natural behavior of PCMs viz:

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hysteresis and sub-cooling. The current phase change model is improved (referred to hereafter as new model) in this work to accommodate hysteresis which is mostly neglected while modeling PCMs.

MODEL DEVELOPMENT

Experiments (Kuznik and Virgone 2009, Bony and Citherlet 2007) have revealed that the behavior of a PCM when it is melting is different from that when it is freezing (i.e.) different enthalpy-temperature curves are followed during melting and freezing. This phenomenon is known as hysteresis. When the material cools below its phase change temperature it begins to solidify. However in some cases the solidification process is initiated at a temperature known as the nucleation or crystallization temperature which is below the phase change temperature. This phenomenon is called sub-cooling. The phenomena of hysteresis and sub-cooling may be significant when designing a building as the storage properties of the PCM are highly dependent on the sub-cooling amount which in turn influences building design (Gunther et al. 2007)

To model PCMs accurately, the current EnergyPlus model uses detailed enthalpy (*h*) and temperature (*T*) data to define the phase change region. This data is not generally provided for commercially available wallboards with PCM. Hence it is necessary to construct the *h-T* curve from catalog data when simulating a building with commercially available PCM wallboards. The new model uses properties (referred to as critical properties) of PCMs such as latent heat storage capacity, melting temperature and specific heats which are available from experiments and manufacturer. Hysteresis phenomenon of the PCM is also incorporated which is not available in the current model.

Construction of Enthalpy-Temperature Curve from properties of PCM

Pure crystalline and eutectics show discontinuity at the melting temperature (Figure 1 Curve A) and enthalpy is not a unique function of temperature, while materials such as paraffin show enthalpy as a continuous function of temperature (Figure 1 Curve B). This results in a 'mushy' (phase change) region between solid and liquid regions. It is appropriate to use polynomial fitting curves to describe the properties of PCM in agreement with the Ginzburg-Landau theory of phase transitions Egolf and Manz (1994).

Egolf and Manz (1994) provide explicit equations for the enthalpy of a PCM as a function of temperature for a melting process. The equations developed by Egolf and Manz (1994) are:

$$h(T) = c_{p,1}T + \eta_1 \quad \text{, for} \quad T \leq T_m \tag{1}$$

$$h(T) = c_{p,1}T_m + (h_2 - h_1) + c_{p,2}(T - T_m) - \eta_2 \quad \text{, for } T > T_m \tag{2}$$

where:

$$\eta_n = \left(\frac{h_2 - h_1}{2}\right) e^{\frac{-2|T-T_m|}{\tau_n}}$$

Equations (1) and (2) are applicable to PCMs that show different widths of melting region and different specific heats in the solid and liquid phases. Performance of the curve depends on the width of the melting region. For a narrow melting range, the curve is steep (Figure 1 Curve A) and includes minimal characteristic rounding above and below the melting region. As τ increases, the transition of the PCM from solid state to liquid state is smoother (Figure 1 Curve B).

The specific heat is independent of temperature in the solid and liquid regions and has a functional relationship with temperature in the phase change region. For materials that show symmetry in specific heat at the melting temperature, Feustel (1995) provides a correlation which is a simplification of that given by Egolf and Manz (1994). The advantage of the Feustel (1995) correlation is that enthalpy is a single hyperbolic tangent function of temperature.

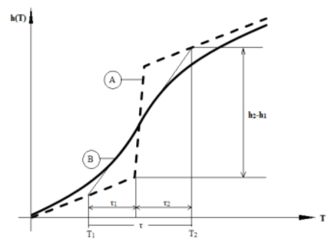

Figure 1 Discontinuous (A) and continuous (B) functions for enthalpy (Adapted from Egolf and Manz 1994)

Studies (Kuznik and Virgone 2009, Bony and Citherlet 2007, Dolado et al. 2011 and Tabares-Velasco et al. 2012) have shown that hysteresis is necessary for accurate modeling of PCMs. The current EnergyPlus model is based on tabulated *h-T* data which is not readily available for commercially available wallboards. The new model is based on equations (1) and (2) (Egolf and Manz 1994). The new approach requires only the critical properties of the PCM as input instead of detailed enthalpy-temperature data. The new model also captures transition of the material from solid to liquid or vice-versa in the two-phase region which is explained in the later section of the paper.

Evaluation of the equation for a melting process

The equation from Egolf and Manz (1994) is validated against experimental data obtained from Shrestha et al. (2011) for a pure PCM. The PCM has a melting point of 33°C (91.4°F) with latent heat storage capacity of 170.6 J/g (73.3 Btu/lbm). The experimental *h-T* data for the material is shown in Figure 2(b). From this data, specific heat is plotted as a function of temperature and shown in Figure 2(a). The melting region of the PCM is estimated from this graph. τ_1 is the difference between the melting temperature and the temperature at which the specific heat curve shows steep raise. τ_2 is the difference between the temperature at which specific heat curve begins to show a flat trend and the melting temperature. The properties of the PCM are listed in Table 1. The correlation results are compared with the experimental data (Shrestha et al. 2011) as shown in Figure 2(b). The results are in good agreement with errors between the experimental and model lying within 10% as specified by Gunther et al. (2009).

Table 1. Critical Properties of PCM Tested for Melting

Property	Value
T_m	33°C (91.4°F)
Δh_m	170.6 J/g (73.3 Btu/lbm)
$C_{p,1}$	1.82 J/g-C (0.435 Btu/lbm-F)
$C_{p,2}$	1.84 J/g-C (0.439 Btu/lbm-F)
τ_1	5°C (9°F)
τ_2	2.5 (4.5°F)

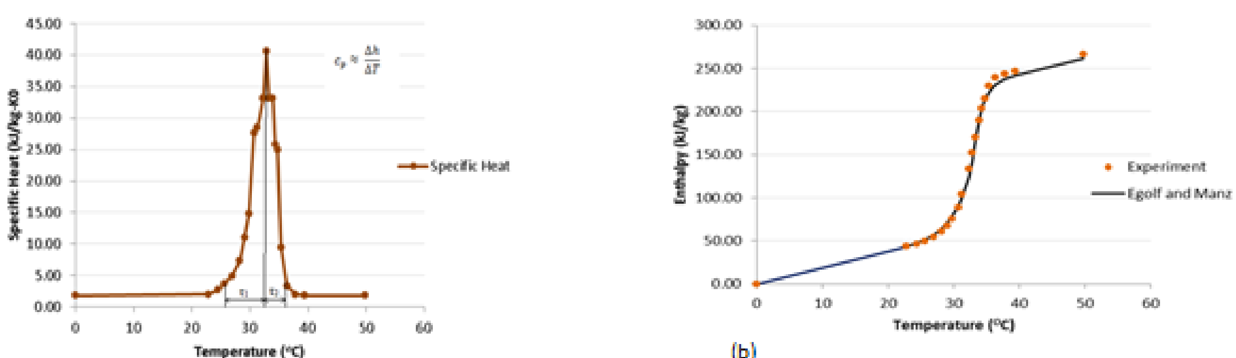

Figure 2 (a) Specific heat as a function of temperature (b) Validation of the equation for melting of PCM

Evaluation of the equation for a freezing

The functional relation for enthalpy and temperature is defined for a melting of PCM but there is no such explicit relation defined in literature for the freezing of PCM. Hence the application of the same equation (1 and 2) with critical parameters defined for the freezing process was tested. Kuznik and Virgone (2009) tested a new commercial wallboard for its critical properties. The wallboard consists of 60% microencapsulated PCM in a copolymer with a latent heat capacity of 71.0 J/g (30.52 Btu/lbm) during freezing. The work also provides the *h-T* curve for the wallboard that clearly showed hysteresis exhibited by the PCM. The critical properties of PCM tested are shown in Table 2. One important parameter that needs to be determined is the freezing region of the PCM which is not usually provided in many literatures and by the manufacturers. Kuznik and Virgone (2009) also provides a graph between specific heat and temperature of the PCM over the entire temperature range. From the specific heat graph the freezing regions viz: τ_1 and τ_2 of the PCM are determined as described in the previous section. The correlation is compared against the experimental data as shown in Figure 3. The correlation predicts values within 10% of the experimental results as specified by Gunther et al. (2009). Thus using the procedure previously prepared for melting as a freezing model proved successful. The physical transition from either region to the other can be captured successfully with this simplified model. As such, it is used to simulate both the melting and freezing effects in the new model.

Table 2. Critical properties of PCM board tested for freezing

Property	Value
T_f	17.8°C (64.04°F)
$\Delta h_{freezing}$	71.0 J/g (30.52 Btu/lbm)
$C_{p,1}$	3.38 J/g-C (0.807 Btu/lbm-F)
$C_{p,1}$	2.3J/g-C (0.549 Btu/lbm-F)
τ_1	6.23°C(11.21°F)
τ_2	6.23°C(11.21°F)

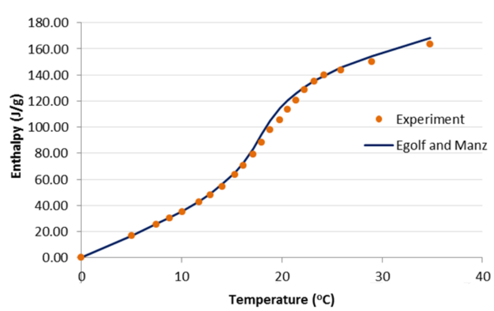

Figure 3 Validation of the equation for freezing of PCM

Modeling transition between freezing and melting in the phase change region

Modeling PCMs with hysteresis requires special attention to the process encountered in the transition region between phases. The transition region is between the melting and freezing curves in the phase change region as shown in Figure 4(a). This phenomenon is not well documented in the literature and is a topic of current research. There are two approaches supported by the new model. In Bony and Citherlet (2007) model, a material that shows hysteresis, which initially is cooling in the phase change region, on the freezing curve, then has to follow a transition phase to reach the melting curve if the temperature of the material is increased (referred as transition model in this paper). This transition occurs similarly when switching from the melting to the freezing curve. The transition process is shown in Figure 4(a). The transition process is modeled as a straight line of the form $y = mx + c$ between the two curves. The transition process implemented in EnergyPlus is defined by (3).

$$h = c_{p,T}.T + (h_r - c_{p,T}.T_r) \qquad (3)$$

In (3), the term $(h_r - c_{p,T}.T_r)$ is the y-intercept of the line. The transition specific heat $c_{p,T}$ is taken as the average of solid and liquid specific heats. However recent research indicates that some materials may follow the same curve (referred as non-transition model in this paper) during melting and freezing in the phase change region as shown in Figure 4(b). Hysteresis for such materials is seen only when it cools from a complete liquid state.

The current state of PCM simulation is based upon the temperature of the material sampled at a previous time. If the temperature shows an increase the model assumes melting curve, whereas if it decreases, the model assumes freezing curve. In transition model, the transition process is assumed as a straight line when the increasing temperature starts decreasing or vice-versa and the process continues until hitting the adjacent curve.

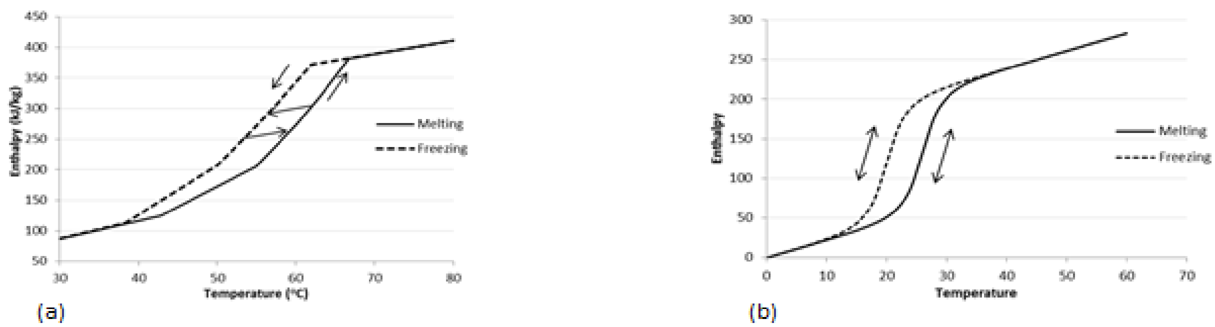

Figure 4 (a) Transition model (Adapted from Bony and Citherlet 2007) (b) One curve model

MODEL EVALUATION

Validation of the model

The PCM solver is tested for a real PCM wallboard containing 40% microencapsulated PCM. The latent heat storage capacity of the material is 41J/g (17.63 Btu/lbm) with the melting and freezing temperature being 10°C (50°F) and 5°C (41°F) respectively. The material is assumed to have a phase change range of 20°C (36°F) in both melting and freezing processes. The solid and liquid specific heats of the material are 0.7J/g-C (0.167 Btu/lbm-F). The wallboard is used in a single story single zone building simulation model composed of six surfaces. The zone has a total floor area is 37 m^2 (398 ft^2). The construction includes PCM board in all the four vertical wall surfaces of the building. The building has a window on the north wall. The building includes a total internal heat gain of 2.9 kW (9895 Btu/hr) by the equipment and three occupants. There are no lighting loads and no infiltration.

The result for the new solver with the transition model is demonstrated in Figure 5. The simulation was performed for a day in April with the zone located in Chicago, IL. Figure 5 shows the temperature-enthalpy relation of the PCM over a particular time interval for the day during which the material shows heating and cooling in the melting, transition and freezing curve regions respectively. The material melts with increase in temperature (a-b) following its melting curve. This is followed by a decrease in temperature (b-c) in the transition region. Before the process could reach the freezing curve an increase in temperature of PCM was observed (c-b). When the temperature/enthalpy path approaches the melting curve, the process shifts to pure melting and the material starts to follow the melting curve (b-d). As the temperature drops, the material cools down through the transition region (d-e) eventually reaching the freezing curve. From Figures 5 it could be inferred that the new solver that accommodates the hysteresis of PCM along with the transition functions properly and the switch between the processes takes place at appropriate temperatures. This test is intended to only demonstrate proper operation, not validity of the model's ability to match experimental data, which is demonstrated in later sections.

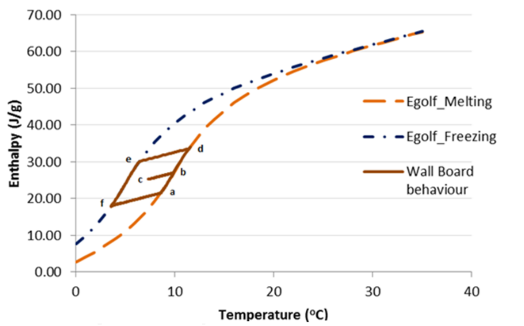

Figure 5 PCM showing a full cycle of all the processes

The new solver with the non-transition model is tested for the same material with results shown in Figure 6. Figure 6(a) shows for a day in December when the material follows the melting curve during both heating and cooling during the day. Figure 6(b) shows the working of the material model during an April day. It could be seen that the same material follows the freezing curve during the day for both heating and cooling. Thus in the non-transition model, it is the start condition of the material that decides which curve to follow.

Figure 6 (a) One curve (melting) model (b) One curve (freezing) model

Application of the model

This section of the paper is a demonstration of the PCM behavior using EnergyPlus in a building. Emphasis is given on generating the *h*-*T* curve from the property data available from experiments and manufacturers. This is demonstrated for a commercial board whose catalog data is available from manufacturers.

EnergyPlus simulation from Experimental Data

The new model is tested for a phase change material for which the property data was made available through experiment. The product is a PCM board used for suspended ceiling applications. A Digital Scanning Calorimeter (DSC) test was conducted by the manufacturer to determine the PCM critical properties. The DSC graphs are shown in Figure 7. From Figure 7(a) it could be observed that the material exhibits hysteresis as the melting and freezing peaks occur at different temperatures. This is also true from Figure 7(b) which shows specific heat peak values occurring at different temperatures. Experiment also revealed that the latent heat values of the material during melting and freezing are also not equal. The specific heats of the material in its solid and liquid states are determined from Figure 7(b) as the flat lines of the curve in the respective regions. From Figure 7(b) the melting and freezing regions are also estimated. τ_1 is the difference between the melting temperature and the temperature at which the specific heat curve (for melting) begins to show a steep rise. τ_2 is the difference between the temperature at which the specific heat curve begins to show a flat trend and the melting temperature. τ_1' and τ_2' for the freezing curve are also estimated in a similar way. The critical properties of the PCM are summarized in tabular form in Table 3.

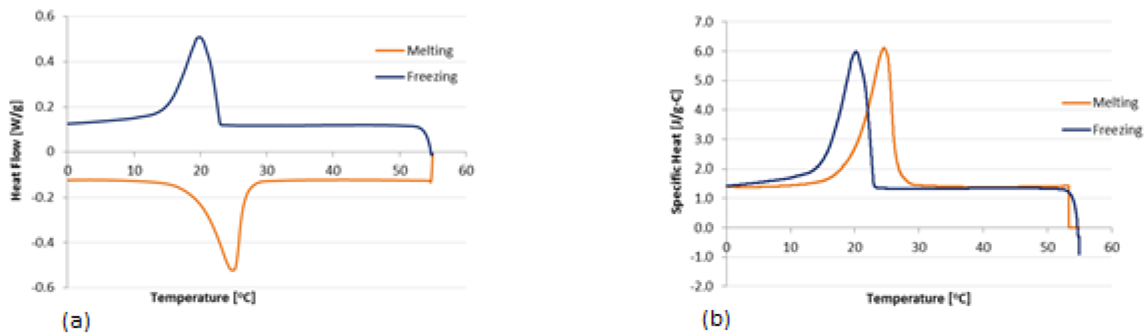

Figure 7 (a) Heat flow vs. temperature (b) Specific heat vs. temperature
Courtesy: Armstrong World Industries Inc.

Table 3. Experimental Critical Properties of the Commercial PCM Board

Property	Value
T_m	24.54°C (76.17°F)
T_f	20.24°C (68.43°F)
$C_{p,1}$	1.404 J/g-C (0.336 Btu/lbm-F)
$C_{p,2}$	1.33 J/g-C (0.317 Btu/lbm-F)
Δh_m	24.26 J/g (10.43 Btu/lb)
Δh_f	23.65 J/g (10.17 Btu/lb)
τ_1	11.22°C (20.2°F)
τ_2	8.81°C (15.86°F)
τ_1'	8.98°C (16.16°F)
τ_2'	5.56°C (10°F)

The PCM board is simulated in EnergyPlus for the same building and construction type described earlier for a day in May in Chicago. The simulation result is shown in Figure 8. The melting and freezing curves in the figure are generated using equation (1) and (2) from the data shown in Table 3. From Figure 8 it could be seen that the material shows a complete cycle for freezing (a-b), transition (b-c), melting (c-d) and again freezing (d-a) during the day.

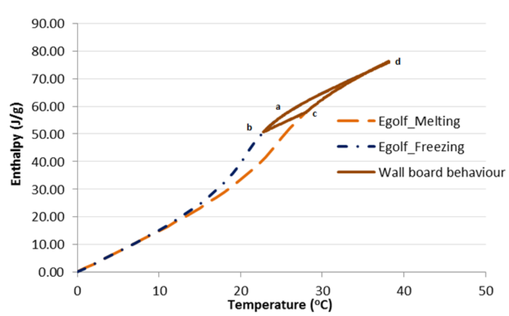

Figure 8 Simulation result for the commercial PCM board

EnergyPlus simulation for a commercial PCM board

The PCM board selected is a commercially available board used as a suspended ceiling for passive climate control in buildings. The technical data provided by the manufacturer is shown in Table 4. The material is assumed to have a total melting and freezing range of 6°C (10.8°F). The simulation is carried out for the same building described earlier but situated in Phoenix, AZ. The behavior of PCM is studied for a day in April. From the simulation results it was observed that the material shows a cycle of freezing, transition and melting and finally freezing in order, during the day.

Table 4. Catalog Data for Commercial PCM Board

Property	Value
Basic Ingredient	Salt Hydrate
Melting Temperature	22-28°C (71.6-82.4 °F)
Crystallization Temperature	22 °C (71.6°F)
Cooling Capacity	25-40 W/m² (7.9-12.68 Btu/hr-ft²)
Melting Energy	158 J/g
Density (Solid/Liquid)	1.6/1.5 (kg/m³)
Thermal Capacity (Solid/Liquid)	2.7/2.2 J/g-C (Btu/lbm-F)
Thermal Conductivity (Soild/Liquid)	1.12/1.56 W/m-K (0.647-0.901 Btu/hr-ft°F))
Max Service Capacity	60°C (140°F)
Weight	Dependent on energy capacity
Dimensions	300x600 mm (11.8x23.6”)

Comparison of Energy Use

An annual simulation was performed to study the energy use in the same building situated in Phoenix, AZ. The building consists of a PCM wallboard on all the four vertical walls as an inside layer exposed directly to the zone environment. Comparison of average annual building energy use with and without PCM showed a 22% decrease. The PCM wall case also showed a 15% decrease in peak heating load but the peak cooling load showed negligible variation from the dry wall case. The annual building energy consumption with and without hysteresis were also analyzed. It was observed that the decrease in total annual energy in the hysteresis model was less than 1%. Furthermore, no shift in the peak loads was observed with hysteresis. However, with increase in the degree of hysteresis (difference between the melting and freezing temperatures) of up to 6°C (10.8°F), there was a decrease in the peak heating load by 5.5% from the non-hysteresis model value of 2841 W (9694 Btu/hr). But the peak cooling load showed negligible difference from the non-hysteresis model value of 7522 W (25659 Btu/hr).

The hourly surface temperature with and without PCM was compared for a day in May and is shown in Figure 9(a). It could be clearly seen that the surface temperature fluctuation is higher in drywalls than the PCM wall. This alteration in surface temperature profile is often considered a justification for the application of PCM in building materials (Pedersen 2007). An interesting aspect was observed with hysteresis for the chosen day. The fluctuation in the surface temperature showed a decrease in the hysteresis model when compared to the non-hysteresis model. A closer observation was made to quantify the temperature variation. The fluctuation in the surface temperature with hysteresis was 2°C (3.6°F) lesser than that without hysteresis. The zone temperature was also found to be show more stable values with hysteresis. The hourly cooling load comparison between the models for a day in May is shown in Figure 9(b). The maximum decrease in cooling load observed with hysteresis compared to the dry wall case was close to 10%. This difference however did not affect the cooling coil loads.

Figure 9 (a) Hourly inside surface temperature comparison (b) Hourly cooling loads comparison

Hence hysteresis is insignificant to the equipment sizing for the building. Thus, hysteresis behavior of PCM in the wallboard has showed only a small effect on building energy consumption under the tested conditions but has resulted in a more stabilized zone and surface temperatures.

A similar study was conducted with the transition and non-transition hysteresis models. The difference between the total annual energy values from both the models was again less than 1%. Also with increase in degree of hysteresis by 6^{o}C (10.8^{o}F), the peak heating load decreased by 3.2% negligible change in peak cooling load was observed. Coil loads in the non-transition hysteresis model increased by 1.5% which is insignificant to the overall equipment sizing. Thus from the two energy analyses it could be inferred that the hysteresis phenomenon does not have significant effect on annual building energy performance and size of heating and cooling equipment for the tested case.

SUMMARY AND CONCLUSION

The phase change material solver in EnergyPlus has been modified to simulate the real behavior of the material viz: hysteresis and to simulate commercially available PCM materials using manufacturers' data which was difficult in the current version of EnergyPlus. The current version uses tabulated property data that is not generally available, while the new PCM model is based on a formulation by Egolf and Manz (1994). This reduces the input requirements down to the critical parameters of PCM which are available both from experiments and manufacturers. The solver has been validated for correct working and proper transitions of processes.

The new model implementation has been demonstrated for two materials. One, , a PCM board for which Digital Scanning Calorimeter experimental data (non-published) was provided and other, a commercially available ceiling board for which catalog data is available from the manufacturers. The EnergyPlus simulation showed that using PCM wall instead of a dry wall had impact on energy use of the building. The simulation for the commercial board also showed that the impact of hysteresis on the total annual building energy was less than 1%. Also the hysteresis did not have significant effect on equipment sizing for the building. However, hysteresis had impact on the surface and zone temperature. The surface temperature oscillation was observed for a day in January which showed reduction in the surface temperature variation by 2^{o}C (3.6^{o}F) than that without hysteresis. Zone temperature also showed stability in the hysteresis model compared to the non-hysteresis model. The reduction in zone temperature fluctuation was 1.25^{o}C (2.25^{o}F) compared to that without hysteresis. From the results it could be concluded that for energy analysis single curve model of the PCM could be used with good accuracy. But when studying surface heat transfer, hysteresis needs to be considered to model the surface accurately. However, the results presented in this study are preliminary. PCMs need to be characterized further to better study the building energy performance which is a subject of future research.

ACKNOWLEDGEMENT

The authors would like to thank Armstrong World Industries Inc. for providing the DSC data needed for the demonstration of the model functioning. The authors would also like to thank the reviewers for valuable suggestions.

NOMENCLATURE

c_p = specific heat
$c_{p,T}$ = specific heat during transition
h = specific enthalpy
τ = width of melting/freezing zone melting zone
T = temperature
T_m = melting temperature
T_r = process reversal temperature
h_r = enthalpy at T_r
y = ordinate
x = abscissa
m = slope
c = y-intercept

Subscripts

1 = solid phase
2 = liquid phase

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