NUMERICAL THERMAL PERFORMANCE ANALYSIS OF PCMS INTEGRATED WITH RESIDENTIAL ATTICS

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ABSTRACT

During the last decade, following a rapid growth of low-energy building projects, building components using phase change materials (PCMs) have become more popular in North America. As the focus has slowly begun to shift to a new generation of salt hydrates and bio-based PCMs, it is critical to develop new energy models that can describe the true behavior of these PCMs.

While thermodynamic models are essential to analyze the impact at different conditions and using different control strategies of building structures which integrate PCMs, there are few whole-building simulation tools containing sufficient numerical algorithms of the detailed physics, which are necessary to provide accurate simulations of the thermodynamic behavior of these structures.

In this paper, a whole-building energy modelling program, ESP-r, based on a finite difference method, is utilized to simulate the thermal behavior of different PCM configurations within an attic space of a ranch-style house. This numerical tool is capable of predicting temperature profiles and heat fluxes within different configurations of PCM applications. In order to evaluate the accuracy of the PCM model in ESP-r, the model is first validated with experiments.

INTRODUCTION

Continued improvements in building envelope technologies suggest that residences soon will be routinely constructed with low heating and cooling loads. The use of novel building materials containing active thermal components (e.g., phase change materials) would be an ultimate step in achieving significant heating and cooling energy savings using technological building envelope improvements (Kissock et al. 1998, Feustel 1995, Tomlinson 1992, Kosny 2001). PCMs have been tested as a thermal mass component in buildings for at least 40 years, and most studies have found that PCMs enhance building energy performance. However, problems such as high initial cost, loss of phase-change capability over time, corrosion, and PCM leaking have hampered widespread adoption (Balcomb 1983, Salyer et Sircar. 1989).

Today, paraffins dominate the PCM market for building applications for several reasons: they are non-toxic, abundant in supply, and easy to microencapsulate. Other attractive features include relatively small sub-cooling, chemical inertness and good recyclability. However, the high cost of paraffin chemicals along with the low phase-change enthalpies and flammability issues are proving to be major barriers to a widespread acceptance of these PCMs. Inorganic salt hydrates and bio-based PCMs with lower chemical cost and higher enthalpies not only hold a great potential to substitute paraffins in the future (see Table 1), but compete with the existing energy efficient building materials and technology as well. In fact, inorganic salts such as Glauber's salt were the first PCMs to be applied in building applications (Kubiszweski 2007).

Until now, in whole-building energy simulations, PCM modeling efforts have primarily been focused on idealized PCM models, which do not incoprate subcooling effects. When modeling such PCMs for building applications, one single enthalpy curve has been commonly used for both the melting and solidification processes. The results obtained for a simple application of the PCM-gypsum board were found to be in relatively good agreement with the experimental data (Heim et al. 2004; Kissock et al. 1998). However, as more complex PCM systems are examined, it is critical to develop new energy models that can describe the true behavior of these PCMs. For example, figure 1 shows heat capacity data that we obtained using a heat flow meter apparatus (HFMA) for an insulation sample containing a bio-based PCM (Kosny et al 2008, 2010). A large sub-cooling of ~8 °C is observed. In addition, the shape and magnitude (area under the specific heat-temperature curve) are very different for melting and solidification processes. This example underlines the pressing need to design models that consider separate enthalpy curves for melting and solidification cycles to account for the effect of sub-cooling and different magnitudes of enthalpies for these cycles.

In this work, we propose to use separate enthalpy curves to investigate the behavior of one such PCM sample. We use ESP-r – the whole-building energy simulation program - for the modeling and analysis. We validate our model with experimental data and present one case study to analyze the placement of the PCM in the attic location to maximize the energy efficiency.

Table 1: Comparison of some key features of paraffin and salt hydrate

PCM type	Paraffins	Salt Hydrate
Latent heat ($MJ/m^3 \cdot K$)	150–200	250–550
Cost	Expensive	Cheap
Inflammability	High	Low
Toxicity	Mid	Mid-High
Encapsulation	Easy	Difficult

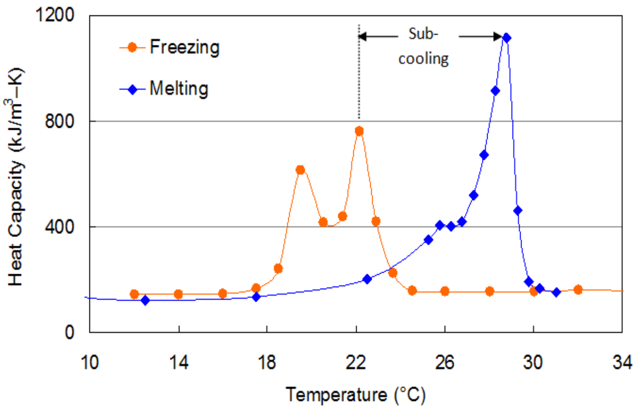


Figure 1: Heat capacity as a function of temperature for an insulation sample that contains bio-based PCM. A heat flow meter apparatus (HFMA) is used to measure enthalpies. Large jumps in the heat capacity represent the latent heat released/absorbed during melting/freezing. A significant amount of sub-cooling (~8 °C) is present.

EXAMPLES OF PAST APPLICATIONS OF PCM IN BUILDING ENVELOPES

PCMs have been used in buildings for at least 40 years. Many potential PCMs have been tested for building applications, including inorganic salt hydrates, organic fatty acids and eutectic mixtures, fatty alcohols, neopentyl glycol, and paraffinic hydrocarbons. There were several moderately successful attempts in the 1970s and 1980s to use different types of organic and inorganic PCMs to reduce peak loads and heating and cooling energy consumption (Balcomb 1983). Historically, performance investigations focused on impregnating concrete, gypsum, or ceramic masonry with salt hydrates or paraffinic hydrocarbons. Most of these studies found that PCMs improved building energy performance by reducing peak-hour cooling loads and by shifting peak-demand time.

The capability of PCMs to reduce peak loads is well documented. For example, Zhang, Medina, and King (2005) found peak cooling load reductions of 35 to 40% in side-by-side testing of conditioned small houses with and without paraffinic PCM inside the walls. Similarly, Kissock et al. (1998) measured peak temperature reductions of up to 10°C (18°F) in side-by-side testing of unconditioned experimental houses with and without paraffinic PCM wallboard. Kosny (2006) reported that PCM-enhanced cellulose insulation can reduce wall-generated peak-hour cooling loads of magnitude between 1 to 2.5 (Btu/ft^2) by about 40%.

Other studies (Feustel 1995, Tomlinson 1992, Kosny 2001) demonstrate that the use of thermal mass can generate heating and cooling energy savings of up to 25% in U.S. well-insulated residential buildings.

NUMERICAL MODELING OF PCM

An important factor to predict the behavior of PCMs in numerical models is the calculation of corresponding thermal properties at each time step (specific heat Cp, or enthalpy H). Since the dependency of specific heat on temperature is highly non-linear during phase changes, it becomes critical for the numerical model to take into account accurate temperature-dependent specific heat. In addition to temperature dependency, specific heat is also dependent on whether the PCM is melting or solidifying (crystallizing); for example if the PCM temperature rises and exceeds its melting point, its specific heat profile would be different from the case when the temperature drops and goes below the melting point. This temperature difference in between the two specific heat profiles is called the sub-cooling effect (see figure 1). In other words, for PCMs to solidify, their temperature needs to drop below the melting point temperature for the crystallization to start.

In some PCMs, the sub-cooling temperature range is relatively small, and it is reasonable to define temperature-dependent specific heat with a single curve for simple systems (i.e. PCM-gypsum board facing unconditioned space) . However, in the case of more complex PCM applications (i.e. PCM blends with insulations, or arrays of PCM containers), ignoring the sub-cooling may lead to major errors in predicting PCM thermal behavior. Therefore, in these applications, there is a need to have two separate curves to define temperature-dependent specific heat.

In search for a whole building energy software with a built-in capability to model PCM sub-cooling effects with two different specific heat profiles (during melting and solidification), ESP-r was chosen.

ESP-r is an advanced whole-building energy modeling software, extensively used by researchers to model multi-zone thermal, air, HVAC and other building-domain related phenomena. It allows a detailed parametric study of the factors which influence the energy and environmental performance of buildings. It uses a finite-difference central solver, discretizing the problem domain in a controlled volume scheme, and solves the corresponding conservation equations for mass, momentum, energy, etc.

Within ESP-r, PCMs are modeled using the concept of special materials (Kelly 1998). Special materials were introduced to ESP-r as a means of modeling active building elements that have the ability to change their thermo-physical properties in response to some external influence. The special material functions of ESP-r may be applied to a particular node within a multi-layer construction. Any node defined as a special material is then subjected to a time variation in its basic thermo-physical properties.

ESP-r assumes one-dimensional heat transfer across the PCM layer(s). As reported by Heim and Clarke (2004), the differential equation of transient heat conduction with variable thermo-physical properties is:

$$\frac{\partial}{\partial t}\rho(T)\ h(T) = \nabla \cdot [k(T)\nabla \mathrm{T}(\vec{r},t)] + q(\vec{r},t)$$

where T is the temperature, ρ the density, h the enthalpy, k the conductivity and q the heat generation rate.

ESP-r uses special material files SPMCMP53 through SPMCMP56 to simulate PCM's thermal behavior, ranging in resolution. The SPMCMP56 model developed by Geissler, A. (Geissler 2008) based on the Hoffmann, S. (2006) numerical model, is an enhanced model capable of taking into account the sub-cooling effect. In addition to density, conductivity and phase change temperatures, this model also uses the temperature-dependent specific heat of PCMs both during melting and solidification to describe in a mathematical way the material properties within the phase change temperature limits. In this method, the stored/released latent heat, *LH(T)*, during phase change is calculated from:

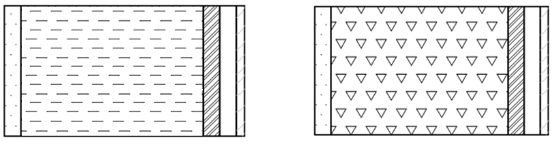
$$LH(T) = \int_{T_1}^{T_2} T^f \left(\frac{a + cT + dT^2}{1 + b + eT^2}\right)\ dt$$

where *a*, *b*, *c*, *d*, *e* and *f* are curve-fitting parameters approximating specific heat capacity of the PCM as a function of temperature during phase change. T_1 is the onset melting/solidification temperature, and T_2 is the temperature where melting/solidification ends. Outside those two limits (T_1 & T_2), the PCM stores/releases energy only in the form of sensible heat. Within the limits, the heat capacity of the PCM is a function of temperature.

NUMERICAL MODEL VALIDATION WITH MEASURED DATA

In order to evaluate the accuracy of the enhanced PCM model in ESP-r (SPMCMP56), a base case wall assembly was validated against experimental field data obtained from the Oak Ridge National Lab. testing facility located in Charleston, South Carolina.

In May and June 2006, in the Charleston testing facility (Figure 2), two wood stud walls were used for testing (Kosny et al. 2008, 2009, 2011). The total size of the test wall was 8 × 8 ft (2.4 × 2.4 m). These walls were constructed with 2 × 6in. (60 × 152 mm) wood framing installed 24 in. (610 mm) on center (o.c.). One wall cavity was insulated with conventional cellulose with a density of about 2.6 lb/ft^3 (42 kg/m^3). The other wall cavitiy was insulated with a cellulose-PCM blend with a density of about 2.6 lb/ft^3 (42 kg/m^3) and containing approximately 22% PCM by weight.



a) b)

Figure 2: Wall assemblies at the ORNL testing facility in Charleston.

a) Interior air (left), ½" gypsum board, 5 ½" cellulose insulation in 2 x 6 studs cavity; 24 in o.c., ½" OSB, ½" air, ¼" wood cladding, exterior air (right)

b) Interior air (left), ½" gypsum board, 5 ½" PCM-enhanced cellulose insulation in 2 x 6 studs cavity; 24 in o.c., ½" OSB, ½" air, ¼" wood cladding, exterior air (right)

It is estimated that about 38 lb (17 kg) of PCM-enhanced cellulose insulation containing 8 lb (3.6 kg) of PCM was used for this dynamic experiment. The air temperature inside the building was kept at about 69°F (20°C)—about 10° F below the level of the theoretical melting point of PCM. In this paper, the measured heat flux across the walls and the measured exterior wall surface temperatures were used to validate the PCM model SPMCMP56 in ESP-r. The measured heatflux across the walls with and without PCMs in the Charlston testing facility is shown in figure 3.

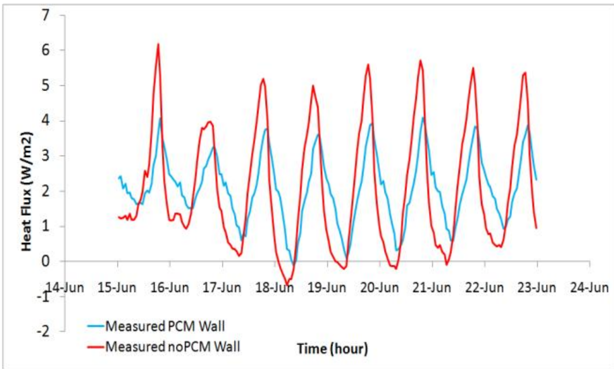


Figure 3: Comparison of measured data for PCM and non-PCM walls at the ORNL testing facility in Charlseton

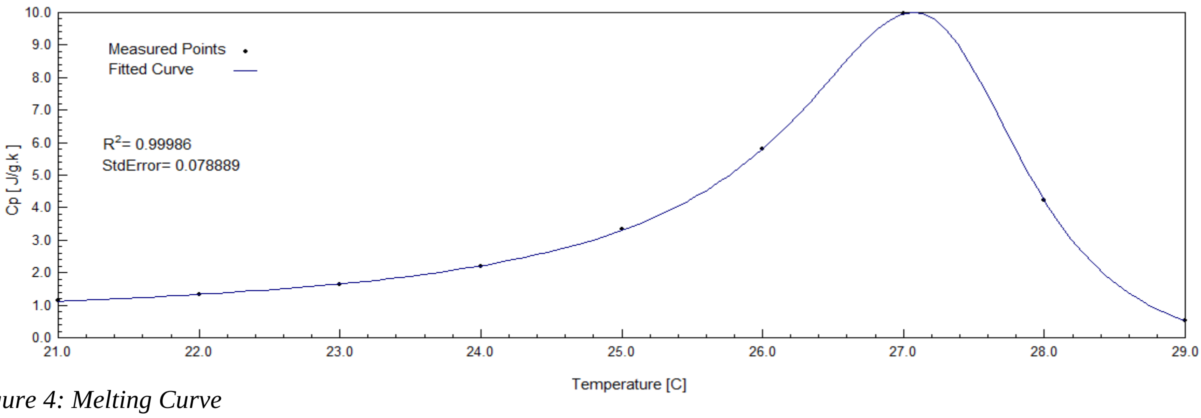


Figure 4: Melting Curve

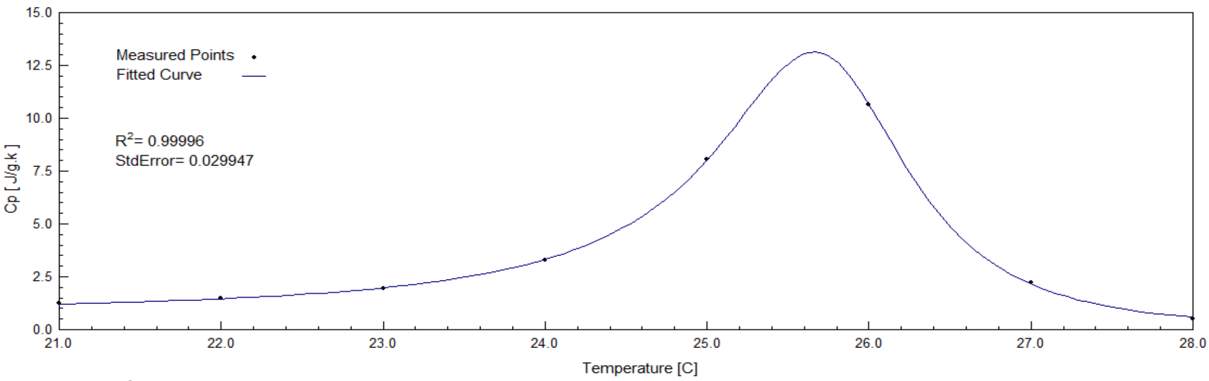


Figure 5: Solidification Curve

In the Charleston testing facility, parafinic phase-change microcapsules mixed with cellulose were used in the wall assembly.

The PCM-enhanced cellulose ceiling is manufactured using PCM mixed with cellulose during the cellulose manufacturing process, where the maximum uniformity of PCM distribution through the cellulose can be achieved. Phase-change microcapsules used in this experiment are plastic pellets filled with a wax that absorb and release energy by melting and solidifying. The melting and solidification curves are illustrated in figures 4 & 5.

In former applications mostly overseas, the chosen locations for building board or tile products cotaining flammable paraffinic PCMs were the interior surfaces of the wall, ceiling, or floor. In this work, the PCM-enhanced materials were positioned inside the wall cavity or installed as a part of the attic insulation system. Placement in these locations is expected to significantly reduce flammability issues that were common in earlier applications of the technology.

Also, detailed optimizations performed for PCM applications showed a significant material and fabrication cost reduction potential combined with improvements in energy performance. This was corresponding with reductions in payback times for PCM applications (Kosny et al. 2012). To model the PCM's thermal behavior in ESP-r, two theoretical chambers with the same characteristics as those of the testing facility were modeled: one chamber for the case without PCM walls as a baseline and one for the case with PCM walls. The measured boundary conditions of the walls in the testing facility were imposed on the ESP-r models, i.e., exterior surface temperatures and interior chamber air temperature. Then, to evaluate the accuracy of the PCM model SPMCMP56, the modeled heat fluxes across the walls in ESP-r were compared with measured heat fluxes from the Charleston testing facility.

To perform the verification of modeled and measured parameters, first the base case chamber model was developed without PCM walls (figure 2-a) and was compared with the measured data from the Charleston testing facility. The modeling results from this base case showed there is a good agreement between modeled and measured heat flux across the wall (figure 6).

In this case, the discrepancy between the simulated and measured total heat flux was around 4.4%. This also proves that the modeled base case chamber is predicting the thermal behavior of the testing facility fairly well (figure 8).

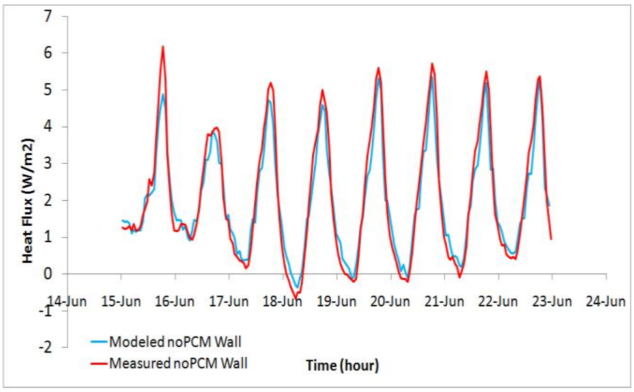


Figure 6: Comparison of modeled and measured heat flux across the wall assembly for the base case without PCM wall

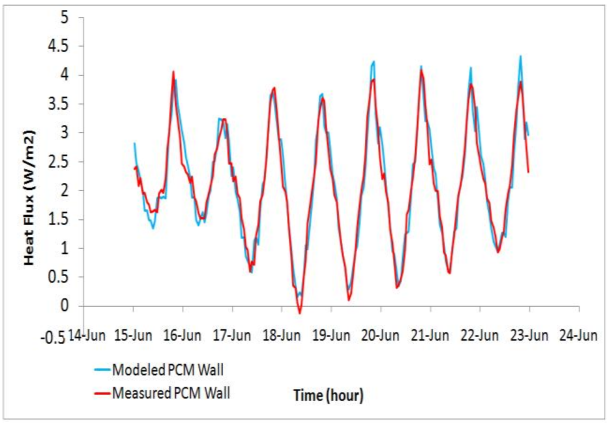


Figure 7: Comparison of modeled and measured heat flux across the wall assembly for the case with PCM wall

Then to evaluate the accuracy of the PCM model SPMCMP56 in predicting thermal behavior of PCMs, the wall in the already developed base case configuration was replaced with a PCM wall assembly (figure 2-b). After running the model, the simulation results showed that the modeled heat flux across the wall as shown in figure 7 coincides well with the measured heat flux and the total heat gain discrepancy between measured and modeled cases are about 0.6%. This indicates the PCM model SPMCMP56 is capable of good predictions of PCM thermal behavior.

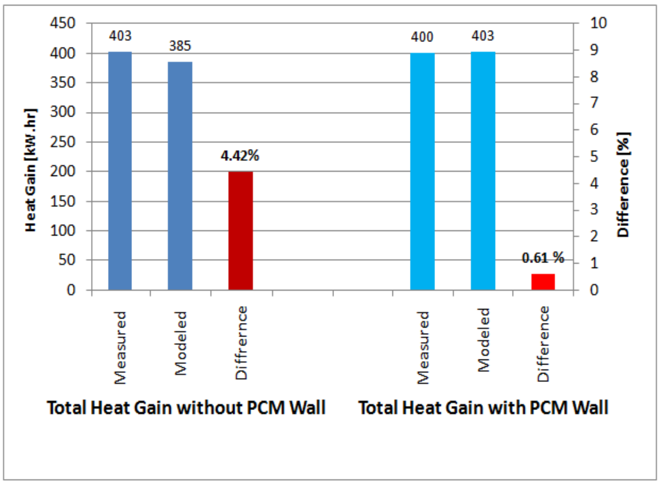


Figure 8: Comparison of modeled and measured total heat gains inside the testing facility with and without PCM walls. PCM model SPMCMP56 in ESP-r used for modeling. The heat gain is over the course of June-15 to June 22.

MODELING CASE STUDY:

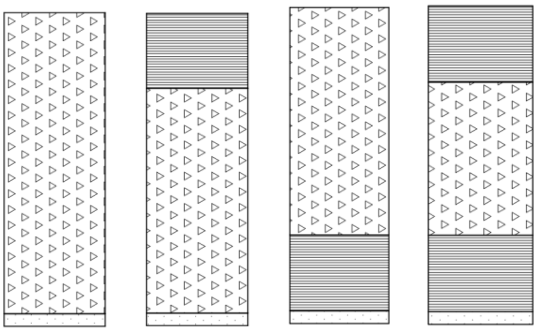
Since residential attics are subjected to greater temperature extremes than any other component of the building envelope, increasing the thermal capacitance of the attic can reduce diurnal temperature swings and, in turn, reduce both the total energy use and peak demand characteristics in moderate and cooling-dominant climates.

As a case study and to demonstrate a practical application of the PCM model SPMCMP56, a residential ranch-style house in a hot climate with PCM-enhanced cellulose ceilings was modeled and the energy savings were compared with the conventional cellulose insulation ceiling. As depicted in figure 9, parametric analysis of four configurations of the attic floor insulation blended with 25% by weight of microencapsulated PCM was performed. Nominal enthaphy of the microencapsulated PCM was about 110 kJ/kg (~50 Btu/lb).

The analyzed house is a lightweight residential building of approximately 143 m^2 (1540 ft^2) floor area and conventional attic located in Phoenix, AZ. The geometry is shown in figure 10. The house was modeled as two separate zones: one zone for the living areas and one for the attic. The living areas are conditioned during cooling season with a set point of 22°C (72°F).

The ranch house was simulated with the Phoenix, AZ climate over the course of one year. As the simulation results show, PCM-enhanced cellulose yields whole-building cooling load energy savings from 3.6% to 5.7% depending on PCM configuration (figure 12). Twelve inch PCM-enhanced cellulose insulation yields the highest savings of 5.6%. Placing 9” PCM on top of the attic insulation yields 5% savings, while placing it on the bottom yields 4.7% savings. This is due to the fact that when PCM is located on top of the attic insulation, it is exposed to the higher temperature fluctuations of the attic as opposed to the constant room temperature.

As a result of being exposed to variable temperatures, the PCM goes through the full cycles of melting and solidification. Placing PCM between two layers of cellulose insulation reduces the overall heat storage capacity of PCM and makes a thinner part of the PCM undergoe full melting and solidification cycles. This yields the lowest savings of 3.6%. This highlights the importance of accurate placement of PCMs and the accurate prediction of PCM cycles and temperature gradients across the assembly during the design stage.



a) b) c) d)

Figure 9: Ceiling assemblies with PCM-enhanced cellulose.

a) Living space room air (bottom); ½” gypsum board; 12” PCM-enhanced cellulose; attic air (top)

b) Living space room air (bottom); ½” gypsum board; 9” PCM-enhanced cellulose; 3” cellulose insulation; attic air (top)

c) Living space room air (bottom); ½” gypsum board; 3” cellulose insulation; 9” PCM-enhanced cellulose; attic air (top)

d) Living space room air (bottom); ½” gypsum board; 3” cellulose insulation; 6” PCM-enhanced cellulose; 3” cellulose insulation; attic air (top)

If we assume 12% to 15% of the whole building cooling load is due to heat gains through the ceiling (Huang et al. 1987, 1996), then savings from 38.0% to 47.5% in ceiling-generated cooling loads can be achieved.

Note that the above improved energy performance is due to reducing peak-hour cooling loads. Energy cost savings can be also obtained by PCM-enhanced cellulose insulation due to shifting peak-demand time.

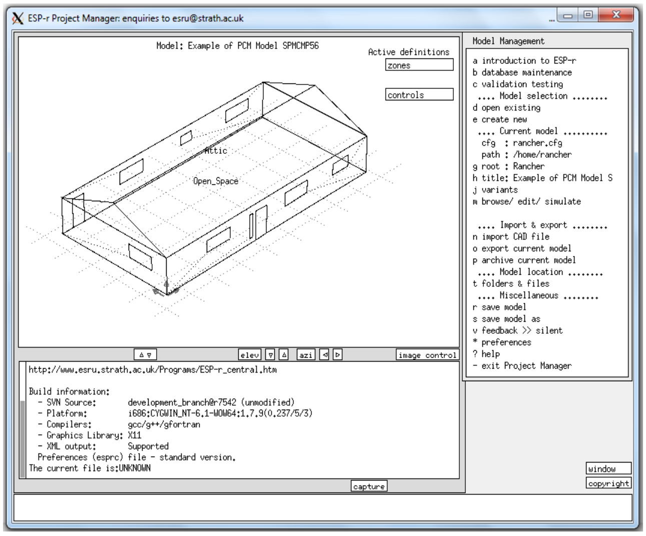


Figure 10: Ranch style house geometry modeled in ESP-r program

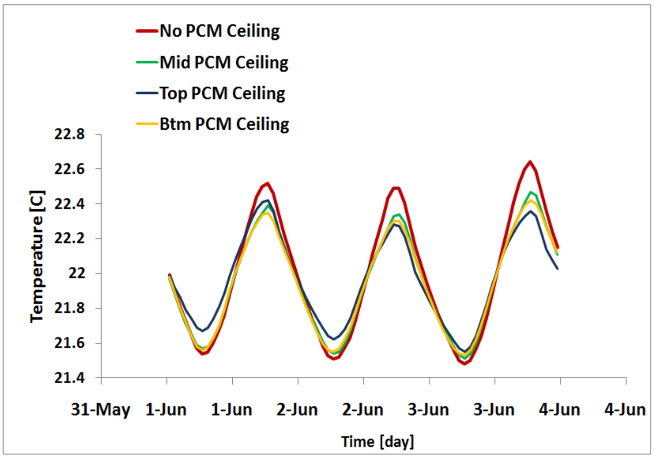


Figure 11: Surface Temperature of underside of the ceiling for different PCM configurations. Mid PCM refers to configuration d), Top PCM to configuration b), Btm PCM to configuration c).

Detailed modeled energy parameters of the house were accessible through the ESP-r central interface.

Figure 11 illustrates the temperature profile of the ceiling surface exposed to the living areas as simulated for the IWEC June climatic conditions. The "No PCM" configuration has the highest surface temperature fluctuations, while the "Top PCM" configuration was the lowest.

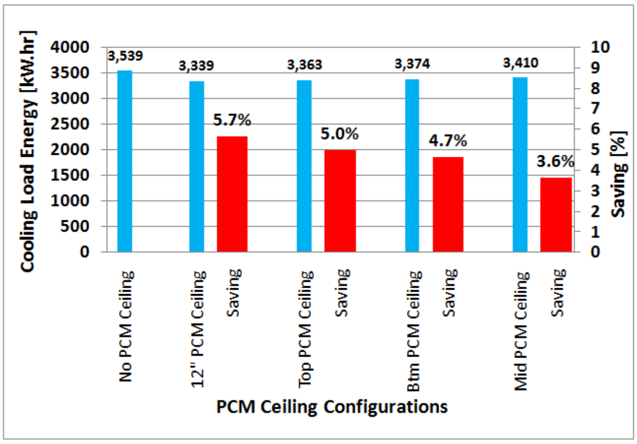


Figure 12: Modeled annual cooling load energy of the ranch style house with different PCM-enhanced ceiling configurations. The base of comparison for the savings is a base case ranch style house with no PCM ceiling.

CONCLUSION

During the last few decades, simple PCM applications like PCM-gypsum boards have dominated the thermal storage market for building envelope applications. Today the focus has slowly begun to shift to more complex PCM applications (i.e. PCM blends with insulations, PCM containers, etc.). Therefore,it is critical to develop new energy models that can describe the true behavior of PCMs used in these applications.

In this work, we propose to use separate enthalpy curves to investigate the behavior of one such PCM sample. We used the ESP-r program for the modeling and analysis. We validated our model with experimental data and presented one case study to analyze the placement of the PCM in the attic floor location to maximize energy efficiency. Simulation results showed PCM-enhanced cellulose yields whole-building cooling load energy saving from 3.6% to 5.7%, depending on the PCM configuration for the

Phoenix, AZ climate. The savings corresponds to approximately a 38.0% to 47.5% reduction in the attic-generated cooling loads.

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NOMENCLATURE

T – temperature [°C]
ρ – density [kg/m^3]
h – enthalpy [J/kg]
k – conductivity [W/m K]
Cp – effective heat capacity [J/kg °C]
q – heat generation rate [W]
LH – latent heat [J/g]
a,b,c,d,e & f – curve fitting parameters [-]
t – time [s]

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