COMSOL Modeling of Temperature Changes in Building Materials Incorporating Phase Change Materials

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Abstract: The usage of Phase Change Materials (PCMs) in structural materials shows promise as a practical means of reducing HVAC energy consumption in buildings. However, to find the optimum percentage of PCM for different climates and buildings, the changes in the interior temperature of buildings should be analyzed when real temperature profiles are applied. Since laboratory experiments are expensive, time-consuming, and not always practical, a COMSOL model has been generated to simulate temperature changes in structural elements incorporating PCMs. The results show that a COMSOL model can accurately calculate temperature changes in buildings and precisely take the effects of the PCM's phase changes into account. Results of the model indicate that the incorporation of PCMs in building materials increases occupant comfort and brings down energy consumption by HVAC system.

Key Words: COMSOL Software, Temperature Changes in Buildings, Occupant Comfort, Porous Media, Phase Change Materials

1. Introduction

Improving the energy efficiency of buildings by cutting down on energy consumption has attracted significant research [1-3]. In buildings, most energy is lost through the building envelope (the walls, floors, roof, etc.). While most of the methods proposed for reducing energy consumption have the potential to be implemented on a large scale, the idea of using Phase Change Materials (PCMs) in building components is one of the most viable [4].

Phase Change Materials (PCMs) have a high latent heat of fusion and absorb heat energy from the surroundings during the day, when the temperature is above their melting point, and release it back to the surroundings during the night, when the ambient temperature drops below melting point [5]. Incorporation of PCM in structural materials such as wall panels, roofing, and flooring help make a building more energy efficient by lowering the use of HVAC systems [6-9]. This leads to both a reduction in the consumption of electric power and a decline in the emissions of greenhouse gases produced by the use of non-renewable energy [10-12].

The amount of PCM used could be varied in a given system until the optimum conditions are reached, i.e., until the desired energy efficiency levels are attained. This analysis should be done when the buildings' walls are subjected to realistic temperature profiles. To conduct such analysis, laboratory experiments may be expensive, time consuming, and impractical. Therefore a COMSOL model was developed to simulate the temperature changes of a wall model under the temperature profiles representative of different cities. The wall was modeled under "Heat Transfer in Porous Media" and the incorporated PCM was modeled under "Heat Transfer with Phase Change."

2. COMSOL Multiphysics® Modeling

2-1- Governing equations

To simulate the temperature changes in building walls under different temperature profiles, a 2D heat transfer model was generated using the COMSOL Multiphysics® software package. The involved physics were heat transfer by conduction, convection, and radiation. The conduction heat transfer equation for a system without a heat source inside it is described by [13]:

$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right)=\rho C_p\frac{\partial T}{\partial t} \qquad (1)$$

where λ is the thermal conductivity of the material (W/m · K), T is temperature (K), ρ is the density of the material (kg/m^3), and C_p is the specific heat of the material (J/kg · K). Because of the constant thermal conductivities of the materials, the equation will be reduced to:

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}=\frac{\rho C_p}{\lambda}\frac{\partial T}{\partial t} \qquad (2)$$

Initially, a model was generated to compare the results of the simulation with the results of a laboratory experiment. The set up involved a 5.08 cm (2 inch) mortar cube between two pyroceram meter bars in turn placed in between two insulations. This comparison was done to validate the accuracy of the COMSOL models (Figure 1). Equation 2 is second order in the spatial coordinates in the x and y directions, and first order in time, therefore two boundary conditions in each direction and one initial condition need to be specified. The first boundary condition in the y-direction was the heat load that was applied to the bottom layer of the model:

$$T(y=0,t)=T_{input} \tag{3}$$

The other three boundary conditions were based on the conservation of thermal energy at the sides of the model:

$$-\lambda\frac{\partial T}{\partial x}=h[T_\infty-T_s]\,,-\lambda\frac{\partial T}{\partial y}=h[T_\infty-T_s] \tag{4}$$

where λ is the thermal conductivity of the material (W/m · K), T is temperature (K), h is the heat transfer coefficient (assumed to be 5 W/m^2 · K for free air [13]), T_∞ is the ambient temperature (assumed to be room temperature, i.e., 296.15 K), and T_s is the temperature of the material surface (K).

For the initial condition, the entire system was assumed to be at room temperature before the heat load was applied. Therefore:

$$T(x,t=0)=T_R \tag{5}$$

where T_R is the room temperature and assumed to be 296.15 K. The surface radiation of the sides is described by [13]:

$$\begin{aligned}\lambda\frac{\partial T}{\partial x}&=\varepsilon\sigma(T_\infty^4-T_s^4)\\ \lambda\frac{\partial T}{\partial y}&=\varepsilon\sigma(T_\infty^4-T_s^4)\end{aligned} \tag{6}$$

where ε is the surface emissivity and σ is the Stefan-Boltzmann constant. Other properties of the material are provided in Table 1.

Equation 2 describes heat transfer in solid media, but for a model with a porous media template incorporating PCM, more equations must be involved. Mortar that is a mix of sand, cement, and water was the main material in the media. The volume fraction of mortar was defined as Θ_m and thus the volume fraction of the porosity (the volume fraction filled with PCM) was equal to $(1-\Theta_m)$. Therefore, the effective thermal conductivity of the media was defined as:

$$\lambda_{eff}=\lambda_m\Theta_m+\lambda_{PCM}(1-\Theta_m) \tag{7}$$

The subscript *m* stands for mortar.

Similarly:

$$(\rho C_p)_{eff}=\rho_m C_{p,m}\Theta_m+\rho_{PCM}C_{p,PCM}(1-\Theta_m) \tag{8}$$

The PCM was modeled as “Heat Transfer with Phase Change”, with β as the volume fraction of PCM at phase 1. Therefore, the effective density of PCM was equal to:

$$\rho_{PCM}=\rho_{phase1}\beta+\rho_{phase2}(1-\beta) \tag{9}$$

Similarly:

$$\lambda_{PCM}=\lambda_{phase1}\beta+\lambda_{phase2}(1-\beta) \tag{10}$$

$$\begin{aligned}C_{p,PCM}&=\frac{1}{\rho_{PCM}}(\rho_{phase1}C_{p,phase1}\beta\\ &+\rho_{phase2}C_{p,phase2}(1-\beta))+L\frac{\partial\alpha_m}{\partial T}\end{aligned} \tag{11}$$

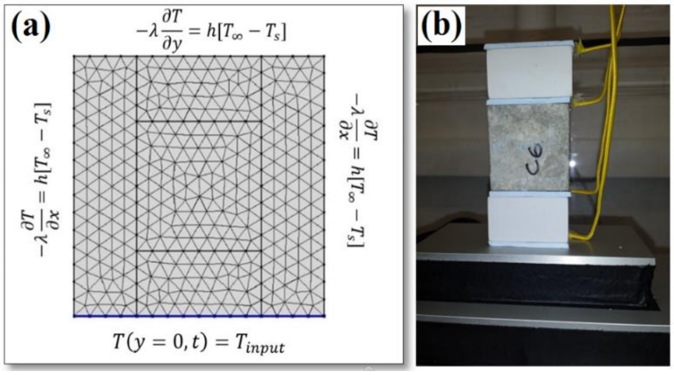


Figure 1. a) COMSOL heat transfer model geometry, mesh, and boundary conditions. b) Laboratory set up (Insulations are not shown in this picture)

Table 1: COMSOL material properties inputs

Material	Density (kg/m^3)	Heat Capacity (J/kg . K)	Thermal Conductivity (W/m . K)	Surface Emissivity
Mortar	2200	750	1.78	--
Pyroceram	2600	From COMSOL Material Browser		0.85
Insulation	1050	1300	0.0285	0.95

where C_p is the specific heat (J/kg · K), L is the latent heat of fusion (J/kg), and α_m is:

$$\alpha_m = \frac{1}{2}\frac{\rho_{phase2}(1-\beta) - \rho_{phase1}\beta}{\rho_{phase1}\beta + \rho_{phase2}(1-\beta)} \qquad (12)$$

The transition interval between phase 1 and phase 2 of the PCM was selected to be 3 °C (5.4 °F). This number was selected based on the results of Differential Scanning Calorimetry (DSC) tests in another study [9]. Modeling of the porosity of the mortar and of the phase transition of water and PCM was done under "Heat Transfer with Porous Media" and "Heat Transfer with Phase Change." Comparing the results of the simulation with the results of the laboratory experiment and validating accuracy of the COMSOL model to simulate the changes in temperature through the sample and the phase transition in the PCM was discussed in another study [14].

2-2- Different Models

2-2-1- Walls with different PCM percentages under sine temperature profiles

Time Lag (ϕ) and Decrement Factor (f) are two important thermal properties of a wall. By definition, time lag is the difference between the times that the peak temperature occurs inside and outside of the wall. Also, the decrement factor can be calculated by [15]:

$$f = \frac{A_{x=0}}{A_{sa}} \qquad (13)$$

where $A_{x=0}$ is the difference between the maximum and the minimum temperature of the inside of the wall and A_{sa} is the same difference in temperatures but for the outside of the wall. To study the effect of PCM incorporation on the Time Lag and the Decrement Factor of a simulated wall, four models with different percentages of PCM were generated. For that, a 25 cm (9.84 inch) thick wall was modeled and four different percentages (0 vol.%, 10 vol.%, 30 vol.%, and 50 vol.%) of its gypsum board were replaced by PCM (Figure 2). The gypsum board, with the thickness of 2.5 cm (0.98 inch), was placed in the inside of the wall and the incorporated PCM was uniformly distributed through it. Three sine temperature profiles (T10, T20, and T30) with the amplitudes of 10 °C (18 °F), 20 °C (36 °F) and 30 °C (54 °F), respectively, a period of 24 hours, and a duration of 48 hours were applied to all the models.

In addition to the Time Lag and Decrement Factor, two more parameters were taken into account to evaluate the efficiency of PCM to modify the temperature changes in buildings. The first one was the time duration for which the inside temperature was in the occupant comfort zone. For that, two comfort levels were introduced; for level 1, the comfort zone was the reference temperature ± 1.5 °C (± 2.7 °F), and for level 2, the comfort zone was the reference temperature ± 3.0 °C (± 5.4 °F). The melting temperature of the PCM was equal to the reference temperature and the specific heat and heat of fusion of the PCM were selected to be equal to 2.11 J/g.K (0.50 BTU/lb.°F) and 161 J/g (69 BTU/lb), respectively, which are equal to that of a common PCM used in previous studies [9].

The second parameter was the energy required by an HVAC system to keep the room temperature in the comfort zone. The inside of the wall is in contact with the room air, therefore the heat energy can be transferred from the wall to the air by convection [13]:

$$\frac{dQ}{dt} = hA(T_R - T_s) \rightarrow \qquad (14)$$

$$Q = hA\int_{t_1}^{t_2}(T_R - T_s)dt$$

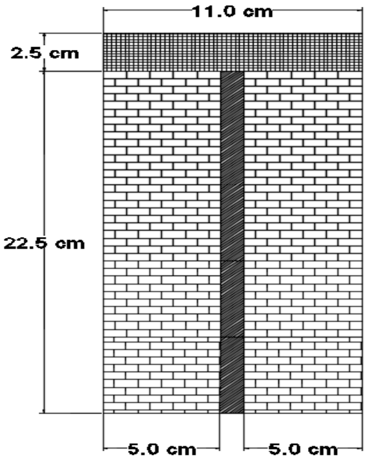


Figure 2. Wall's cross section

where Q is the heat energy (J), h is the heat transfer coefficient (assumed to be 5 $W/m^2 \cdot K$ for free air [13]), A is the area of the wall in contact with the air (m^2), T_R is the room temperature, and T_s is the temperature of the inside of the wall (K). The integral in Equation 14 represents the area under the Temperature-Time curve. If the room temperature is in the occupant comfort zone, the HVAC system is not required to work. But if the room temperature falls outside this zone, the HVAC system needs to employ energy to adjust the temperature. Therefore, the mentioned area is directly related to the energy that is used by the HVAC system to bring the room temperature back to the comfort zone. This area was calculated by Simpson's trapezoidal integration method.

2-2-2- Walls with different percentages under real temperature profiles

For this set of simulations, the 25 cm (9.84 inch) thick wall was studied under real temperature profiles. Typical Meteorological Year (TMY3) data was used to extract the real temperature profiles of six different cities, which are located in different parts of the U.S., as the input files for the COMSOL model. TMY is a collection of selected weather data for a specific location and for a specific period of time, provided by the National Renewable Energy Laboratory for 1,020 locations in the US. The weather data includes the hourly temperature history of each cite. The occupant comfort zone for this set of models was selected to be between 22 °C (71.6 °F) and 26 °C (78.8 °F) [16]. Therefore, the PCM had a melting temperature of 24 °C (75.2 °F) and the same heat of fusion as the early test. One-week duration temperature profiles for each city was selected and therefore each input profile had 10080 data points. The time intervals and the relative tolerance were selected to be 1 second and 0.01 seconds, respectively.

3. Results

3-1- Walls with different PCM percentages under sine temperature profiles

Three sine temperature profiles (T10, T20, and T30) were applied to the 25 cm (9.84 inch) thick wall when different percentages of the volume of its gypsum board were replaced by PCM. The melting point of the PCM was 22 °C (71.6 °F) and its latent heat of fusion was equal to 161 J/g (69 BTU/lb) [9]. The output results of the COMSOL simulation was a text file that included the temperature of the inside of the wall at different times.

As the results show, for all the three temperature inputs, when the outside temperature goes up, the PCM absorbs the applied heat energy and turns to liquid, thus reducing the inside peak temperature (Figure 3). When the applied temperature drops below the melting point, the PCM releases the heat energy that was absorbed in the first place, thereby increasing the temperature. These results show how PCM can effectively make the temperature changes smoother. This efficiency increases by incorporating more PCM in walls. However, PCMs have a limited latent heat of fusion and therefore they cannot completely eliminate changes in temperature.

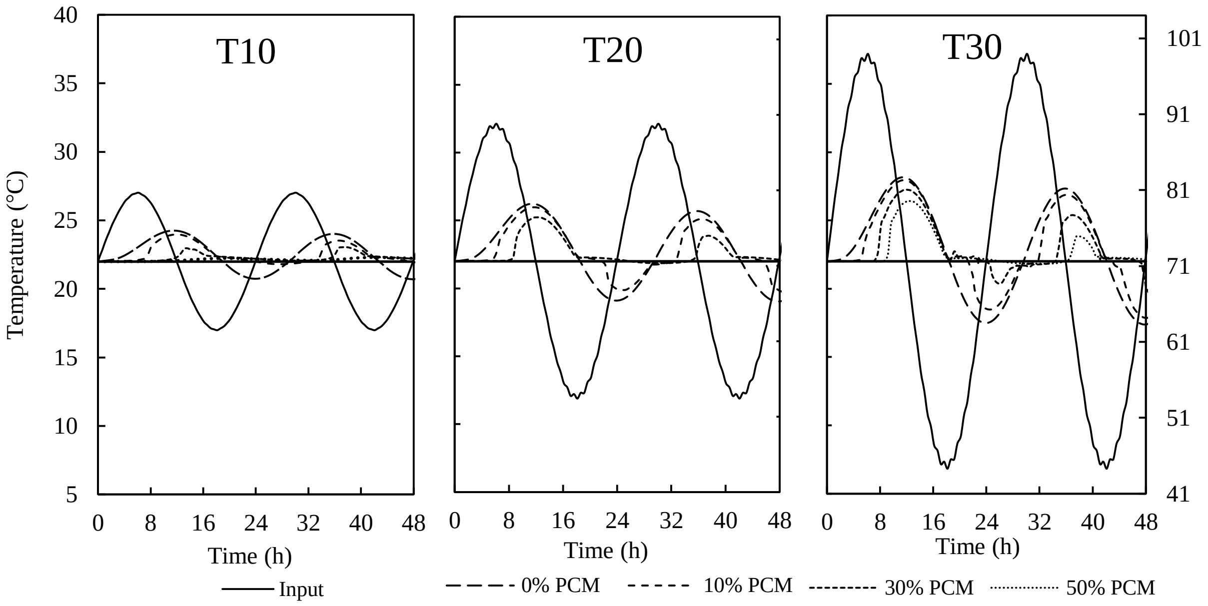


Figure 3. Temperature changes in walls with different PCM percentages under sine function temperature profiles

The effects of different percentages of PCM on the Time Lag and Decrement Factor were also calculated (Figure 4). By increasing the PCM percentage, the time lag increases. This increase is bigger when the applied temperature has a smaller amplitude. This is because of the limited latent heat of fusion of the PCM. Additionally, the decrement factor decreases with increasing PCM percentage. When 50% of the gypsum board volume is replaced with PCM and a temperature profile with an amplitude of 10 °C (18 °F) is applied, this factor can be as low as 8% which means more than 90% of the peak temperature is damped by the PCM (Figure 4).

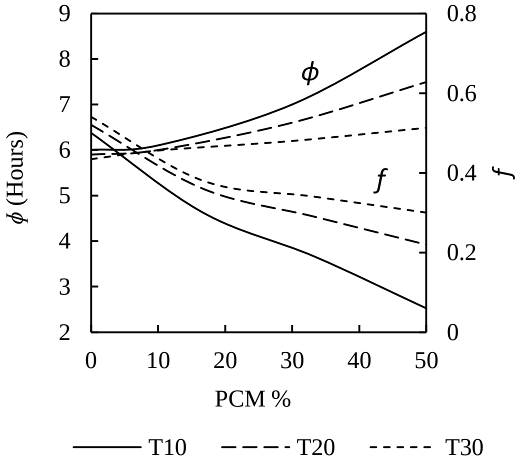


Figure 4. Time Lag and Decrement Factors for 25 cm (9.84 inch) wall with different PCM percentages in its gypsum board and under sine temperature profiles with different amplitudes

The efficiency of incorporating PCM in increasing the time duration of the inside temperature to stay in the comfort zone was also evaluated. Two different levels of comfort zone were introduced: level 1 with reference temperature ± 1.5 °C (2.7 °F) and level 2 with reference temperature ± 3.0 °C (5.4 °F). By increasing the PCM percentage, this duration increased for all the three input temperature profiles (Table 2). For T10 and for the first comfort level, 30% of PCM was enough to ensure that the inside temperature stays in the comfort zone for the entire duration. For the second comfort level, no PCM was required to ensure that the entire graph fells inside the comfort zone; therefore, using PCM does not increase the comfort duration. These results show that the optimum PCM percentage is related to the input temperature.

For all the input temperature profiles, the efficiency of PCM to increase the comfort duration is higher for the first level of comfort, because when the temperature tolerance is bigger, even when PCM is not used, a big portion of the inside temperature stays inside the comfort zone. This suggests that PCMs are more efficient when a narrower range for comfort zone is desired.

The efficiency of PCM to decrease the energy required by HVAC systems to keep the inside temperature within the comfort zone was evaluated by using Equation 14. The decrease in the area of the temperature profile that is outside of the comfort zone shows the decrease in the energy required for the HVAC system. By increasing the PCM percentage, this area decreases (Table 2). As the latent heat of fusion of the PCM is limited, by increasing the amplitude of the input temperature, the efficiency of PCM reduces.

Table 2: The effect of PCM on the comfort duration and the area out of the comfort zone for sine functions

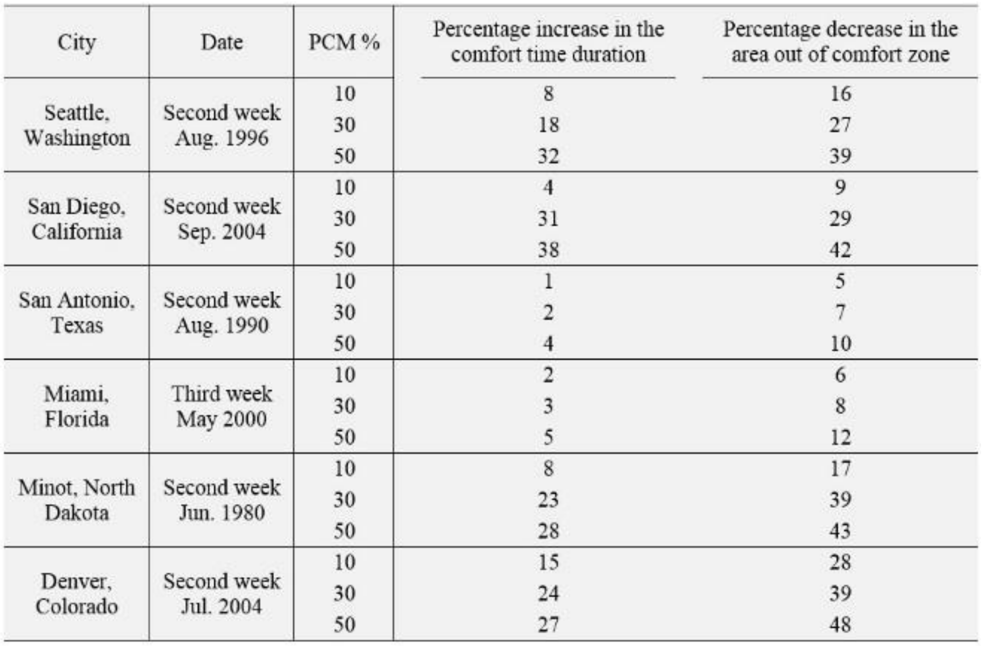
Input	PCM %	Percentage increase in the comfort time duration		Percentage decrease in the area out of comfort zone	
		22 ± 1.5 °C	22 ± 3.0 °C	22 ± 1.5 °C	22 ± 3.0 °C
T10	10	29	0	82	100
	30	41	0	100	100
	50	41	0	100	100
T20	10	69	18	43	63
	30	181	29	88	95
	50	202	33	98	100
T30	10	75	26	26	35
	30	208	97	73	84
	50	323	118	92	93

3-2- Walls with different PCM percentages under real temperature profiles

To evaluate the efficiency of PCM to increase the comfort duration and decrease the energy required by HVAC systems for building walls under real temperature inputs, the temperature of six cities with different climates was applied to the model. For each city, a single week was selected. The occupant comfort zone for this set of models was selected to be between 22 °C (71.6 °F) and 26 °C (78.8 °F) [16]. The melting temperature of the PCM was selected to be equal to 24 °C (75.2 °F).

By increasing the PCM percentage, the duration of being in the comfort zone increases, but this increase is not linear (Table 3). For the case of San Diego, this duration can be increased by up to 40% when 50% of the gypsum board volume is replaced by PCM, but with the same amount of PCM in the case of San Antonio, this increase is as low as 4%. This shows that the efficiency of PCM is completely dependent to the location of the building or in simple words the outside temperature. A similar pattern was observed for the decrease in the area out of the comfort zone.

Table 3: The effect of PCM on the comfort duration and the area out of the comfort zone for real temperature profiles



City	Date	PCM %	Percentage increase in the comfort time duration	Percentage decrease in the area out of comfort zone
Seattle, Washington	Second week Aug. 1996	10	8	16
		30	18	27
		50	32	39
San Diego, California	Second week Sep. 2004	10	4	9
		30	31	29
		50	38	42
San Antonio, Texas	Second week Aug. 1990	10	1	5
		30	2	7
		50	4	10
Miami, Florida	Third week May 2000	10	2	6
		30	3	8
		50	5	12
Minot, North Dakota	Second week Jun. 1980	10	8	17
		30	23	39
		50	28	43
Denver, Colorado	Second week Jul. 2004	10	15	28
		30	24	39
		50	27	48

4. Conclusions

A 2D computational finite element model using COMSOL Multiphysics® software was developed to simulate the temperature changes in structural elements when Phase Change Materials (PCMs) were incorporated in their elements. Sine functions with different amplitudes as well as real temperature profiles of six different cities that were taken from the TMY3 data were applied to the models as thermal loads. The following findings were obtained:

- COMSOL Multiphysics® software can accurately simulate changes in temperature in porous media, such as gypsum boards, and can accurately take the effects of phase transition of PCMs into account.
- Under sine function inputs, depending on the percentage of the PCM, the inside peak temperature can be delayed by up to 7 hours and be decremented by up to 80%. Also, the energy consumption by the HVAC system can also be drastically reduced.
- The efficiency of PCM to modify the changes in the inside temperature of a building depends on the outside temperature profiles. When 50 vol.% of the wall's gypsum board was replaced by PCM, for some of the cases, the comfort duration was increased by up to 40% and almost half of the energy required by HVAC systems was reduced.

More studies should be conducted to find the optimum percentage and melting temperature of PCM for different cities. Furthermore, cost analysis should also be conducted to compare the efficiency of PCMs to alternative methods.

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