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Using COMSOL modeling to investigate the efficiency of PCMs at modifying temperature changes in cementitious materials – Case study

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HIGHLIGHTS

- COMSOL software was used to simulate temperature changes in structural elements.
- The accuracy of the model was validated by GLCC experiments.
- TMY2 and TMY3 temperature profiles were applied to models as thermal load.
- The duration of being in the comfort zone in a building increased when PCM was used.
- The number of freeze/thaw cycles experienced by the pavement decreased when PCM was used.

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ABSTRACT

In recent decades, much research has investigated the efficiency of Phase Change Materials (PCMs) in improving the thermal properties of concrete. In buildings, increasing the thermal inertia of structural elements by incorporating PCMs decreases the energy required to keep the inside temperature in the comfort range. In concrete pavements, using PCMs decreases the number of freeze/thaw cycles experienced by the pavement and thus increases service life. In this study, COMSOL multi-physic modeling software was used to make a computational model of a concrete specimen containing PCM in order to simulate the temperature changes of a structural element under typical meteorological year (TMY2 and TMY3) data. Guarded Longitudinal Comparative Calorimetry (GLCC) tests were conducted to verify the accuracy of the COMSOL model. The results show that using a PCM with a melting point near the occupant comfort zone makes the inside temperature profile smoother and increases the length of time during which the temperature is in the comfort zone. In the cases of PCMs with melting temperatures close to the freezing point of water in concrete, the number of times that the core temperature of a simulated concrete pavement dropped below the freezing point decreased, thus reducing the number of freeze/thaw cycles experienced by the pavement.

1. Introduction

Energy consumption in buildings has been increasing significantly during the last two decades [1,2]. As an example, the energy consumption of Chinese buildings doubled between 1998 and 2009 [3]. Decreasing the energy consumption of buildings by increasing their energy efficiency has therefore been the topic of many research efforts [1–4]. Different methods have been introduced to reduce the energy lost through the walls, floors, and roofs of buildings. These methods also address changes in the interior temperature of structures and suggest different methods for keeping that temperature in the comfort range and reducing HVAC energy consumption [5,6].

The incorporation of Phase Change Materials (PCMs) in structural materials has been proposed as one method of increasing the energy efficiency of buildings and improving occupant comfort [3,7–11]. PCMs are substances with relatively high latent heats of fusion. When the ambient temperature rises above its melting point, a given PCM absorbs heat and liquefies while remaining at an almost constant temperature. When the ambient temperature falls below the melting point, the PCM begins to release heat and solidify, again remaining at an almost constant temperature [12]. Thus PCMs work as passive heat storage agents

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Nomenclature

q	heat flow per unit area (W/m^2)	λ	thermal conductivity (W/m K)
T	temperature (K, °C, and °F)	ε	surface emissivity
ΔQ	change in heat flow (W)	Θ and β	volume fractions
h	heat transfer coefficient (W/m^2 K)	ρ	density of the solid material (kg/m^3)
Cp	specific heat at constant pressure (J/kg K)	σ	Stefan–Boltzmann constant (W/m^2 K^4)
L	latent heat of fusion (J/kg)		

that can increase the thermal inertia of structures. Using PCMs in buildings increases occupant comfort by preventing rapid changes in the inside temperature and decreases energy consumption [13–16]. Both laboratory tests and computational modeling suggest that using PCM in construction materials increases the heat storage capacity and improves the thermal performance of buildings [17–19]. As an example, the inclusion of 5% PCM in a concrete mix can save up to 12% of the energy consumption in a structure [20].

Extreme changes in temperature not only cause occupant inconvenience and increase energy consumption in buildings, but also cause quality and performance problems in pavements. Both very low and very high temperatures can cause cracking [21,22]. Cyclic changes in temperature can also cause fatigue failure in concrete pavements after a period of time [23]. Finally, freeze/thaw cycles can cause cracks in concrete due to the solidification and expansion of pore solution [22,24], In 2011, the U.S. federal government and state departments of transportation spent over $100 billion on maintaining and improving core highways, roads, and bridges [25,26]. Despite this, the American Society of Civil Engineers gave a grade of D to American roads in 2013, and reported that an estimated $100 billion is needed annually to maintain the current roadway conditions, while an additional $79 billion annually is needed to improve the quality of the roadways [27]. PCMs can be used as an additive to increase the service life of concrete pavements and therefore reduce the waste of money and materials [28–30].

PCMs cannot be added to cementitious materials directly, because they interfere with the hydration reactions between calcium silicates and water and thus affect the mechanical, physical, and chemical properties of the mortar or concrete [31,32]. Therefore different carrier agents such as high-density polyethylene balls [18,33], Lightweight Aggregate (LWA) [28,34,35], and rectangular steel pipes [36] have been introduced to indirectly incorporate PCM in the media. These methods each face their own particular challenges, which are not within the scope of this research. Here, it is assumed that PCM can be added to the media without significant deterioration of properties through an appropriate containment method.

Although the efficiency of PCMs to decrease the energy usage in buildings and to increase the service life of pavements has been shown by different studies, few studies have investigated the changes in temperature of a structural element under specific, realistic temperature profiles. Therefore a COMSOL model was developed to simulate temperature changes of a concrete specimen when the real temperature profiles of different cities and for different periods of time are applied. The modeled samples contained different percentages of PCMs with different melting temperatures (depending on the application of PCM). To validate the accuracy of the COMSOL model, a laboratory setup was used to apply simple temperature profiles to samples, and the results of the tests were compared to the results of the computational modeling.

3. Materials and methods

2.1. Materials[1]

Samples were prepared using commercially available ASTM C150 type I Portland cement, local sand, and water. Lightweight Aggregate (LWA) was selected as the carrier agent to incorporate either additional water or PCMs. Solite LWA with a specific gravity of 1.5 g/cm^3 (96.3 lb/ft^3) and a water absorption capacity of 17.5% by mass was used. For the laboratory tests, three different samples were prepared. In one, LWA was presoaked in water. In the other two, LWA was presoaked in two different types of PCM (PCM 28 and PCM 6) with different melting temperatures and different specific latent heats of fusion. The PCMs were produced by Microtek Laboratories and their properties are described in Table 1.

2.2. Mixture proportioning

A water/cement ratio of 0.4 by mass and an aggregate/mortar ratio of 0.55 by volume were used. The volume of PCM, when used, was arbitrarily set at 6% of the total mortar volume. When LWA was used, it replaced sand on a volumetric basis; as such, the aggregate sizes distributions were maintained the same in specimens with and without LWA. To add PCM to the mix, LWA was presoaked in the PCM for 24 h and then added to the mix. The same process was used for presoaking LWA in water. It should be mentioned that as PCM 28 is solid at room temperature, the presoaking procedure was conducted in an oven at a temperature of 40 °C (104 °F).

During the mixing process, the cement, water, and aggregates were mixed for 3 min. If the elements were not properly mixed, the mix was manually manipulated and the mixing continued for another 30 s. After all the elements were confirmed to be properly mixed, the mix was placed into molds that were then placed inside plastic bags and placed in a curing room for 24 h. The specimens were then removed from the molds and placed back in the curing room without the bag until their specified testing date. The proportions for each mix of a 1000 cm^3 (61 in^3) batch are shown in Table 2.

2.3. Guarded Longitudinal Comparative Calorimetry (GLCC)

A Guarded Longitudinal Comparative Calorimeter (GLCC) based on ASTM standard methods D5470-06 and E1225-09 was used to determine the specimen thermal properties. The GLCC consists of a cold plate, thermal insulation, thermocouples, two standard meter bars of known thermal properties (Pyroceram 9606), and thermal contact media (Fig. 1). The specifications of the GLCC setup are explained in detail elsewhere [37,38]. By placing the mortar specimen between meter bars, the thermal properties of the mortar specimen can be determined over the course of a thermal cycle using:

$$q_{\text{standard}} = \lambda_{\text{standard}} \cdot \frac{T_{\text{top of standard}} - T_{\text{bottom of standard}}}{depth_{\text{standard}}} \quad (1)$$

in which q is heat flow per unit area (W/m^2), λ is thermal conductivity of Pyroceram 9606 (W/m K), T is temperature in (K), and depth is measured in meters. The thermal conductivity of Pyroceram 9606 is calculated by Eq. (2)[39]:

$$\lambda = -0.0061(T) + 4.2013 \quad (2)$$

where λ is thermal conductivity of Pyroceram 9606 (W/m K) and T is temperature (°C). The average unit heat flow and total heat flow through the specimen was calculated with:

$$q_{\text{Specimen}} = \frac{q_{\text{Top standard}} + q_{\text{bottom standard}}}{2} \quad (3)$$

[1] Certain commercial equipment, instruments, or materials are identified in this report in order to specify the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

Table 1
PCM properties [35].

PCM type	Melting point	Specific heat	Heat of fusion
PCM 6	6 °C (43 °F)	2.08 J/g K (0.50 BTU/lb °F)	160 J/g (69 BTU/lb)
PCM 28	28 °C (82 °F)	2.11 J/g K (0.50 BTU/lb °F)	150 J/g (64 BTU/lb)

$$\Delta Q_{\text{Sample}} = (q_{\text{Bottom standard}} - q_{\text{top standard}}) * A \tag{4}$$

in which ΔQ is the change in heat flow through the specimen (W) and A is the cross section area (m^2). Finally, the average temperature of the sample was the arithmetic average:

$$T_{avg} = \frac{(T_{\text{bottom of concrete}} + T_{\text{top of concrete}})}{2} \tag{5}$$

2.4. COMSOL multi-physic modeling

A 2D heat transfer model was generated using the COMSOL multi-physic software package to simulate the temperature changes in structural elements under real temperature profiles. The COMSOL model represents the GLCC setup, with a 50.8 mm × 50.8 mm (2″ × 2″) mortar sample placed between two pyroceram standards and surrounded by insulation (Fig. 2). Pyroceram 9606 was taken from the material browser within the COMSOL program and used as the standard material. The specimen material was a user-defined material to simulate C_p a cement mortar saturated with impregnated water and PCM.

The general form of the heat transfer equation in Cartesian coordinates for a system without a heat source inside it is described by [40]:

$$\frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda \frac{\partial T}{\partial y}\right) = \rho C_p \frac{\partial T}{\partial t} \tag{6}$$

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 is the specific heat of the material (J/kg K). Since the thermal conductivity stays constant through the sample, and the system is isolated in the horizontal directions, the equation will be reduced to a 1D heat transfer equation:

$$\frac{\partial^2 T}{\partial x^2} = \frac{\rho C_p}{\lambda} \frac{\partial T}{\partial t} \tag{7}$$

Because the heat equation is second order in the spatial coordinates, two boundary conditions must be expressed for each coordinate needed to describe the system, and because the equation is first order in time, one initial condition must be specified. The entire system before applying the heat load was at room temperature, therefore the initial condition for the system is:

$$T(x, t = 0) = T_R \tag{8}$$

where T_R is the room temperature and is assumed to be 23 °C (73.4 °F).

The first boundary condition was the temperature that was applied to the bottom layer of the sample stack:

$$T(x = 0, t) = T_{input} \tag{9}$$

The second boundary condition is based on the conservation of thermal energy at the top layer of the sample stack:

$$-\lambda \frac{\partial T}{\partial x} = h[T_\infty - T_s] \tag{10}$$

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 [40]), T_∞ is the ambient temperature which is assumed to be room temperature (296.15 K), and T_S is the temperature of the material surface (K). The surface radiation of the top layer is described by:

$$\lambda \frac{\partial T}{\partial x} = \varepsilon\sigma\left(T_\infty^4 - T_s^4\right) \tag{11}$$

where ε is the surface emissivity (Table 3), and σ is the Stefan–Boltzmann constant.

The mortar specimen was modeled using the "Heat Transfer with Porous Media" template and the PCM was incorporated into the porosity of the mortar. The volume fraction of mortar was defined as θ_m and thus the volume fraction of PCM was equal to $(1 - \theta_m)$. Therefore, the effective thermal conductivity of the media assuming a parallel configuration is:

$$\lambda_{eff} = \lambda_m \theta_m + \lambda_{\text{PCM}}(1 - \theta_m) \tag{12}$$

The subscript m stands for mortar. Similarly:

$$(\rho C_p)_{eff} = \rho_m C_{p,m} \theta_m + \rho_{\text{PCM}} C_{p,\text{PCM}}(1 - \theta_m) \tag{13}$$

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

$$\rho_{PCM} = \rho_{\text{phase 1}}\beta + \rho_{\text{phase 2}}(1 - \beta) \tag{14}$$

Similarly:

$$\lambda_{\text{PCM}} = \lambda_{\text{phase 1}}\beta + \lambda_{\text{phase 2}}(1 - \beta) \tag{15}$$

$$C_{p,\text{PCM}} = \frac{1}{\rho_{\text{PCM}}}(\rho_{\text{phase 1}} C_{p,\text{phase 1}}\beta + \rho_{\text{phase 2}} C_{p,\text{phase 2}}(1 - \beta)) + L\frac{\partial \alpha_m}{\partial T} \tag{16}$$

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

$$\alpha_m = \frac{1}{2}\frac{\rho_{\text{phase 2}}(1 - \beta) - \rho_{\text{phase 1}}\beta}{\rho_{\text{phase 1}}\beta + \rho_{\text{phase 2}}(1 - \beta)} \tag{17}$$

For the simulation, the software requires a transition interval between phase 1 and phase 2. To have an accurate temperature range in which the phase change takes place, results of Differential Scanning Calorimetry (DSC) tests were used [35]. For both of the PCMs, the main portion of phase transition takes place over a range of 3 °C (5.4 °F) (Fig. 3). The COMSOL material inputs are presented in Table 3.

Before applying the real temperature profiles, the accuracy of the COMSOL model needed to be validated, and thus, the results of the COMSOL models were compared to the results of laboratory experiments. To have a quantitative criterion, Coefficient of Determination (R^2) was calculated for different cases. This number indicates how well the model's results fit the experiment's results [41]. Coefficient of Determination can be calculated by:

$$R^2 = 1 - \frac{\sum (T_i - f_i)^2}{\sum (T_i - \bar{T})^2} \tag{18}$$

where for each temperature profile, T_i is the temperature at each time step obtained from laboratory experiment, $\bar{T}$ is the laboratory average temperature, and f_i is the temperature at each time step calculated by COMSOL model. An R^2 of one indicates that the COMSOL temperature profile perfectly fits the temperature profile obtained from the laboratory experiment, while an R^2 of zero indicates that the two sets of temperature profiles do not fit at all.

Finally, typical meteorological year (TMY) data was used to extract the real temperature changes of different cities as the input file for the COMSOL model. TMY is a collection of selected weather data for a specific location and for a specific period of time. The National Renewable Energy Laboratory's latest TMY collection (TMY3) was based on data for 1020 locations in the U.S. between the years of 1991 and 2005 [42]. TMY2 provides the same set of data for fewer locations from 1961 to 1990 [43]. These two different TMY datasets were used to have a wider range of temperatures available for the simulations.

3. Results

3.1. Verifying the validity of the COMSOL model

The goal of this project was to apply the real temperature profiles of different cities to structural elements in order to investigate the ability of PCMs to modify the inside temperature of buildings and the core temperature of concrete pavements using a COMSOL model in place of GLCC experiments. The use of the model is both more rapid and more accurate than the use of the GLCC, as the cold plate can be programmed with only 8 set points, compared to the 168 datapoints in a week and 1440 datapoints in two months of weather data.

Two temperature profiles were applied to the samples in the GLCC and the results were compared to those of the model. This

Table 2
Mix proportioning for 1000 cm^3 (61 in^3) of mortar.

Mix specification (LWA presoaked in)	Mass, g (lb)				
	Presoaked Water	Presoaked PCM	Sand	Cement	Water
Water	60 (0.13)	–	1059.7 (2.34)	585.4 (1.29)	234.2 (0.52)
PCM	–	45.8 (0.10)	1059.7 (2.34)	585.4 (1.29)	234.2 (0.52)

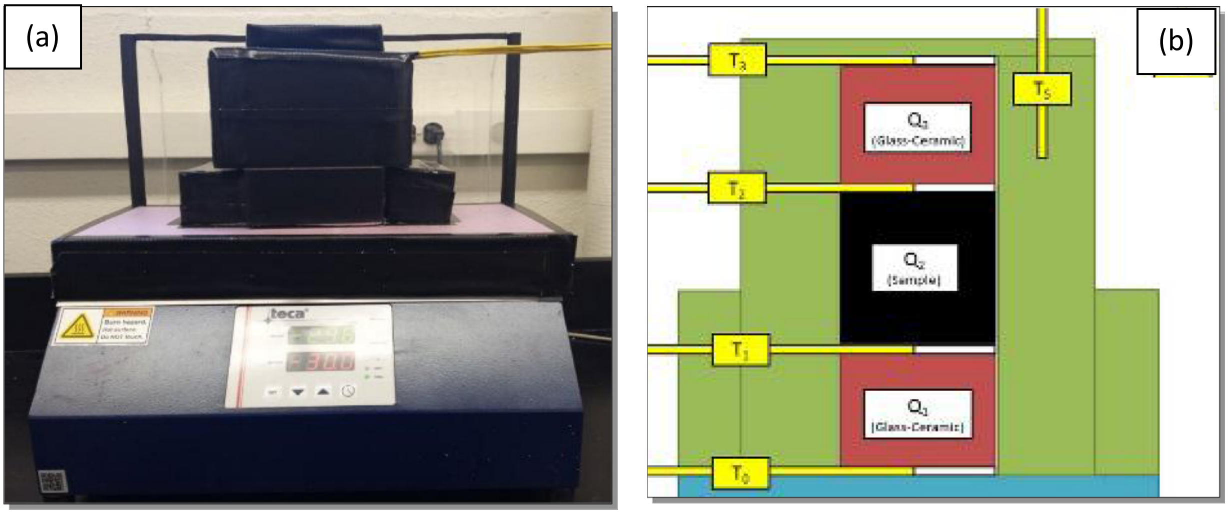

Fig. 1. Guarded longitudinal comparative calorimeter. (a) Laboratory setup including the cold plate. (b) Meter bar/sample/meter bar stack, insulation, and thermocouples.

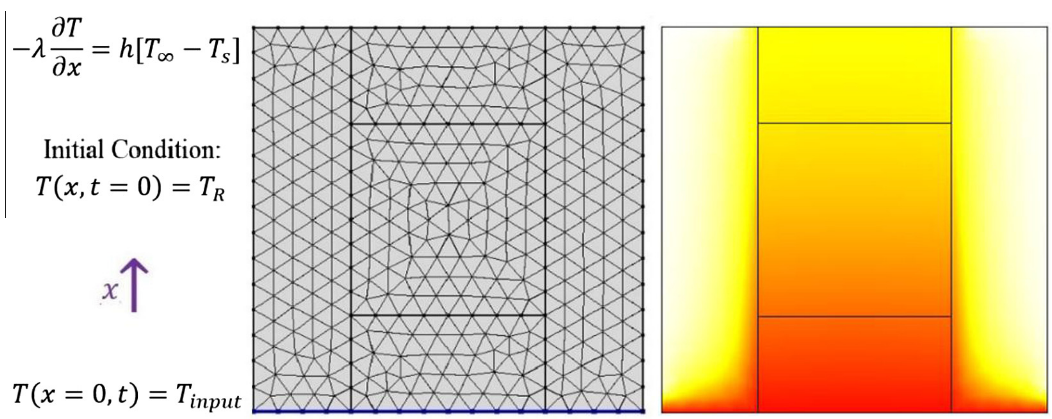

Fig. 2. COMSOL heat transfer model geometry, mesh, and boundary conditions.

Table 3
COMSOL material properties inputs.

Material	Density (kg/m^3)	Heat capacity at constant pressure (J/kg K)	Thermal conductivity (W/m K)	Ratio of Specific Heats	Latent heat of fusion (J/kg)	Surface emissivity
Cement Mortar	2200	750	1.78	–	–	–
Water	997	4179	0.613	1	4179	–
Ice	918	2052	2.31	1		–
Pyroceram	2600	From COMSOL material browser	Equation (2)	–	–	0.85
Insulation	1050	1300	0.0285	–	–	0.95

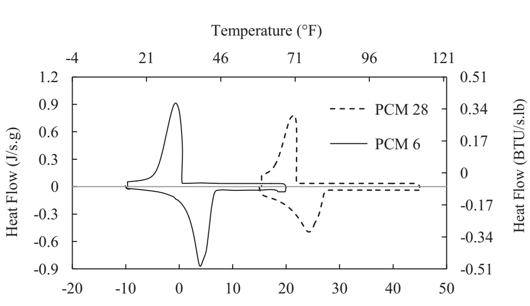

Fig. 3. Differential Scanning Calorimetry (DSC) test for PCM 6 and PCM 28 [35].

test was done for three samples; the first contained LWA presoaked in water and the other two contained LWA presoaked in either PCM 6 (with a melting point of 6 °C (42.8 °F)), or PCM 28 (with melting point of 28 °C (82.4 °F)). The first temperature profile varied between −25 °C (−13 °F) and 25 °C (77 °F) and was used for the samples incorporating water or PCM 6. The second temperature profile varied between −10 °C (14 °F) and 40 °C (104 °F) and was used for the sample incorporating PCM 28 (Fig. 4).

By applying the temperature profiles as thermal loads to the base of the sample stack, the temperature at the tops of the specimens changed gradually when the average temperature of the specimen was not close to the phase transition temperatures of water or PCM. When the average temperature approached the phase transition temperature, the slope of the temperature profile

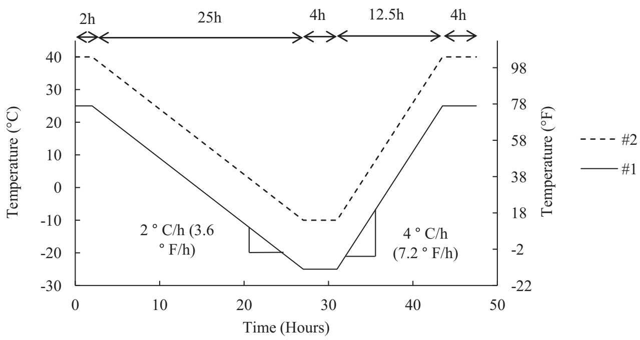

Fig. 4. The two temperature profiles applied to the samples as the thermal load. Profile #1 for samples presoaked in water and PCM 6, and Profile #2 for sample presoaked in PCM 28.

changed as a result of the latent heat of fusion of water or PCM. The COMSOL model was supposed to accurately calculate the gradual temperature changes in the specimen, and also correctly calculate the effect of the latent heat of fusion of the incorporated water and PCMs during the phase changing. The values that were assigned to the materials' parameters in the COMSOL model (physical properties, dimensions, etc.) matched the values that were used in the laboratory set up. Therefore, the results of the model should match with the results of the experiment.

For the sample incorporating LWA presoaked in water, the calculated gradual changes of temperature for both the declining temperature (at a rate of 2 °C/h (3.6 °F/h)) and the increasing temperature (at a rate of 4 °C/h (7.2 °F/h)) are in agreement with the results of the laboratory setup (Fig. 5a). The COMSOL model also accurately simulates the effects of the phase change of water when sample temperatures approach the freezing point. Same conclusions can be reached for the samples incorporating LWA presoaked in PCM 6 or PCM 28, Fig. 5b and c, respectively. Coefficient of Determination (R^2) for the samples with incorporating LWA presoaked in water, PCM 6, and PCM 28 was equal to 0.97, 0.97, and 0.96, respectively. This shows that the computational model can accurately calculate changes in temperature both due to the gradual temperature changes and the phase transition of water and PCM.

3.2. Using the model to simulate changing in temperature

3.2.1. Duration of occupant comfort in buildings

After validation of the COMSOL model, TMY datasets, which include hourly temperatures for various locations, were used as input files. These input files were applied as the temperature load to one side of an 203 mm × 203 mm (8″ × 8″) mortar sample and the change in temperature on the other side of the specimen was recorded as the inside temperature. To simulate the effects of PCM-impregnated concrete on the temperature changes of a building, the model was run using the data for the first day of Jul., 1992, in Worcester, Massachusetts. This temperature profile was applied to a concrete specimen containing 0%, 10%, or 30% PCM by volume (Fig. 6). The occupant comfort zone was defined as the range of 22.2 °C (72 °F) to 24.4 °C (76 °F) [44], and therefore a simulated PCM with a melting point of 23.3 °C (74 °F) was used. The heat of fusion of the simulated PCM was set to be equal to that of PCM 28, 150 J/g (64 BTU/lb) (Table 1). The results of the simulation demonstrate how including PCM in the concrete increases the thermal inertia of the media and thus makes the changes in the inside temperature smoother. Further, the duration for which the inside temperature stays within the occupant comfort range increases from 10 h for the sample without PCM to 13.5 h for the

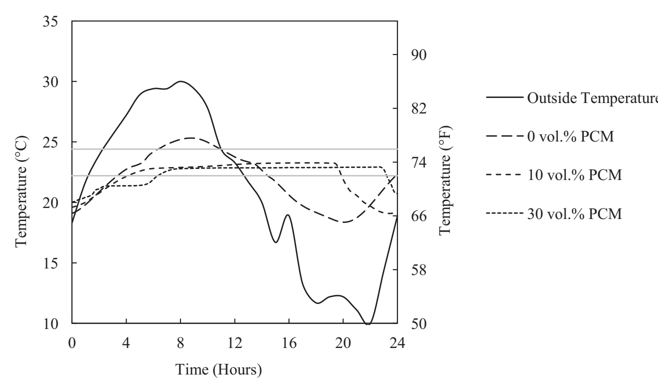

Fig. 6. First day of Jul. 1992 – Worcester (MA).

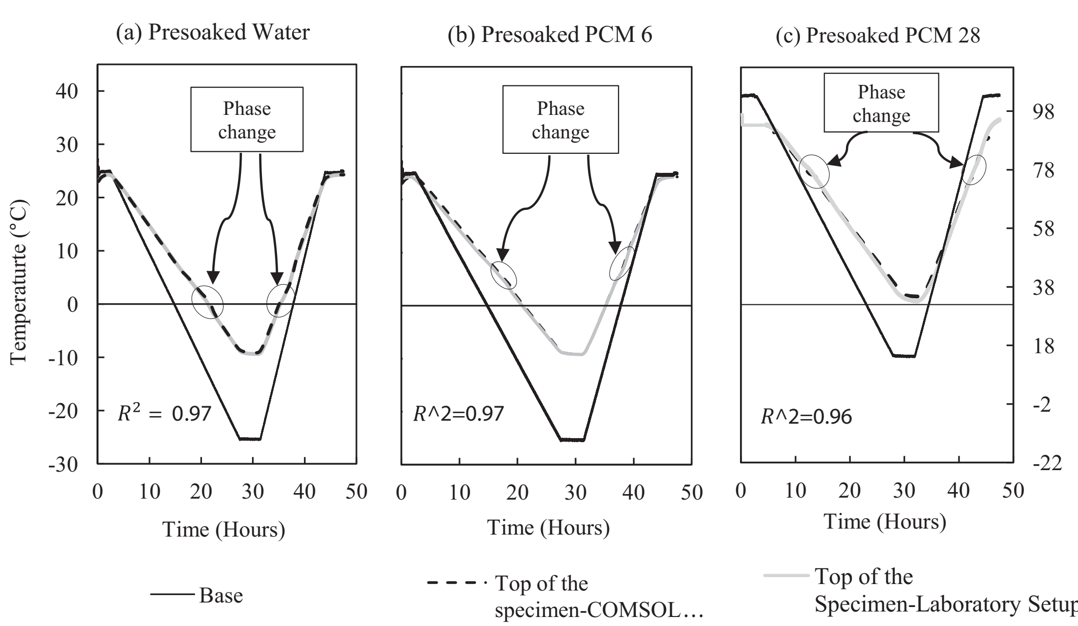

Fig. 5. Comparison between results of the laboratory experiments and results of the COMSOL models.

Table 4
Temperature properties of selected cities.

Category	City	Period of time (week of)	Temperature °C (°F)		
			Minimum	Average	Maximum
Hot climate	Austin (TX)	First/Jun. 2003	15.6 (60.1)	25.7 (78.3)	35 (95)
	Delta (UT)	Second/Jul. 2000	13.5 (56.3)	24.4 (75.9)	35 (95)
	Casa Granda (AZ)	Third/Jun. 2001	17.3 (63.1)	30.8 (87.4)	41 (105.8)
	Reno (NV)	Fourth/Aug. 1987	9.4 (48.9)	22.2 (72)	33.3 (91.9)
Moderate climate	Boston (MA)	Fourth/Jun. 2002	15.6 (60.1)	24 (75.2)	33 (91.4)
	Grand Forks (NV)	Third/Jun. 1998	11 (51.8)	18.1 (64.6)	28 (82.4)
	San Diego (CA)	First/Sep. 1990	18.9 (66)	22.6 (72.7)	28 (82.4)
	New York (NY)	First/Sep. 1979	20.6 (69.1)	24.8 (76.6)	28.9 (84)
Cold climate	Miles City (MT)	First/Jun. 2002	6.7 (44.1)	17.2 (63)	27.8 (82)
	Chicago (IL)	Second/May 2003	9 (48.2)	15 (59)	29 (84.2)
	Worcester (MA)	First/Jun. 1990	5.6 (42.1)	16.4 (61.5)	27.8 (82)
	Hulton (ME)	Fourth/Jul. 2004	5.6 (42.1)	17.9 (64.2)	27.8 (82)

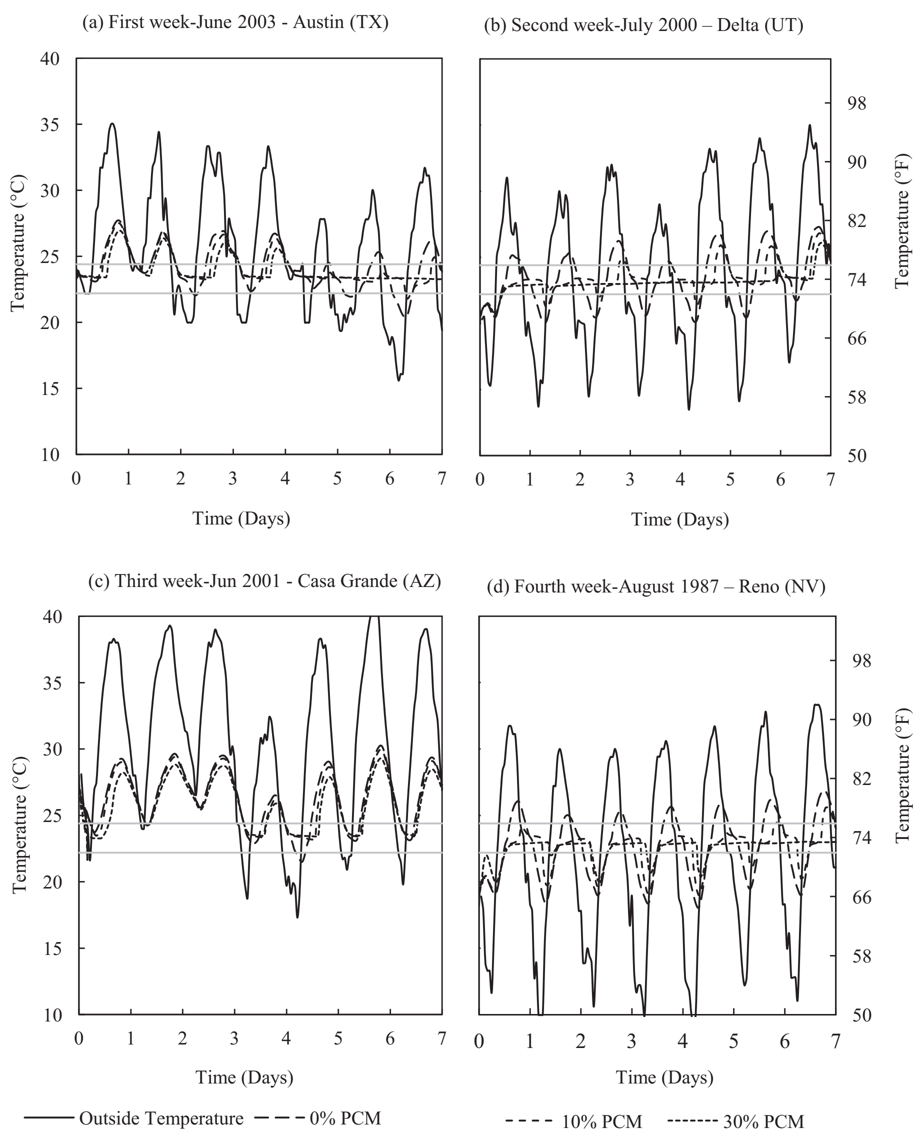

Fig. 7. Hot climate category – changes in temperature for one week duration.

sample with 10% by volume of PCM (a 35% increase) and to 16.5 h for the sample with 30% by volume of PCM (a 65% increase). This happens because when the outside temperature rises, the latent heat of fusion of PCM absorbs the applied heat load and prevents the temperature of the other side of the specimen to be changed drastically; and during the night when the outside temperature drops, the PCM releases the absorbed heat and keeps the inside warmer.

As a more comprehensive study, the temperature profiles of 12 U.S. cities were simulated in order to compare the lengths of time during which the inside temperature stays in the comfort zone for conventional and PCM-impregnated concrete. Depending on the maximum and minimum temperatures of these profiles, the cities were divided into three categories: cold, moderate, and hot (Table 4). The temperature profiles obtained from either TMY2 or TMY3 datasets were applied to specimens with 0%, 10%, and 30% by volume PCM with a melting point of 23.3 °C (74 °F).

The 'hot' category included Austin, Texas; Delta, Utah; Casa Grande, Arizona; and Reno, Nevada, with maximum temperatures of 35 °C (95 °F), 35 °C (95 °F), 41 °C (105.8 °F), and 33.3 °C (91.9 °F), respectively. For the first four days of the Austin simulation, the maximum temperature was above 32.2 °C (90 °F), which is significantly above the upper limit of the comfort zone and also the melting point of the PCM. Therefore the PCM cannot keep the inside temperature in the occupant comfort zone (Fig. 7a). But for the last three days of the simulation, the oscillation of temperature is close to the comfort zone and therefore the PCM can effectively increase the length of time for which the inside temperature is in the comfort zone.

The same conclusion can be reached for the other three cases that are in this category (Fig. 7b–d). Increasing the percentage of PCM from 10% to 30% increases the duration of time during which the inside temperature is in the comfort zone. When the variation in temperature for a single day is about 16.7 °C (30 °F), 30% PCM can effectively keep the inside temperature in the comfort zone. When the temperature difference is more than 20 °C (36 °F), the PCM cannot completely keep the temperature in the comfort zone, but instead delays the time at which the temperature becomes uncomfortable.

The 'moderate' temperature category contains Boston, Massachusetts; Grand Forks, Nevada; San Diego, California; and New York City, New York. The average temperatures of these locations are in the comfort zone. In Boston, the maximum temperature for the first day is 27.8 °C (82 °F), which is relatively close to the comfort zone (Fig. 8a). Therefore not all the incorporated PCM will turn to liquid and thus not enough heat energy will be stored in the PCM. When the minimum temperature of the following night falls to 15.6 °C (60.1 °F), the PCM cannot provide the required heat

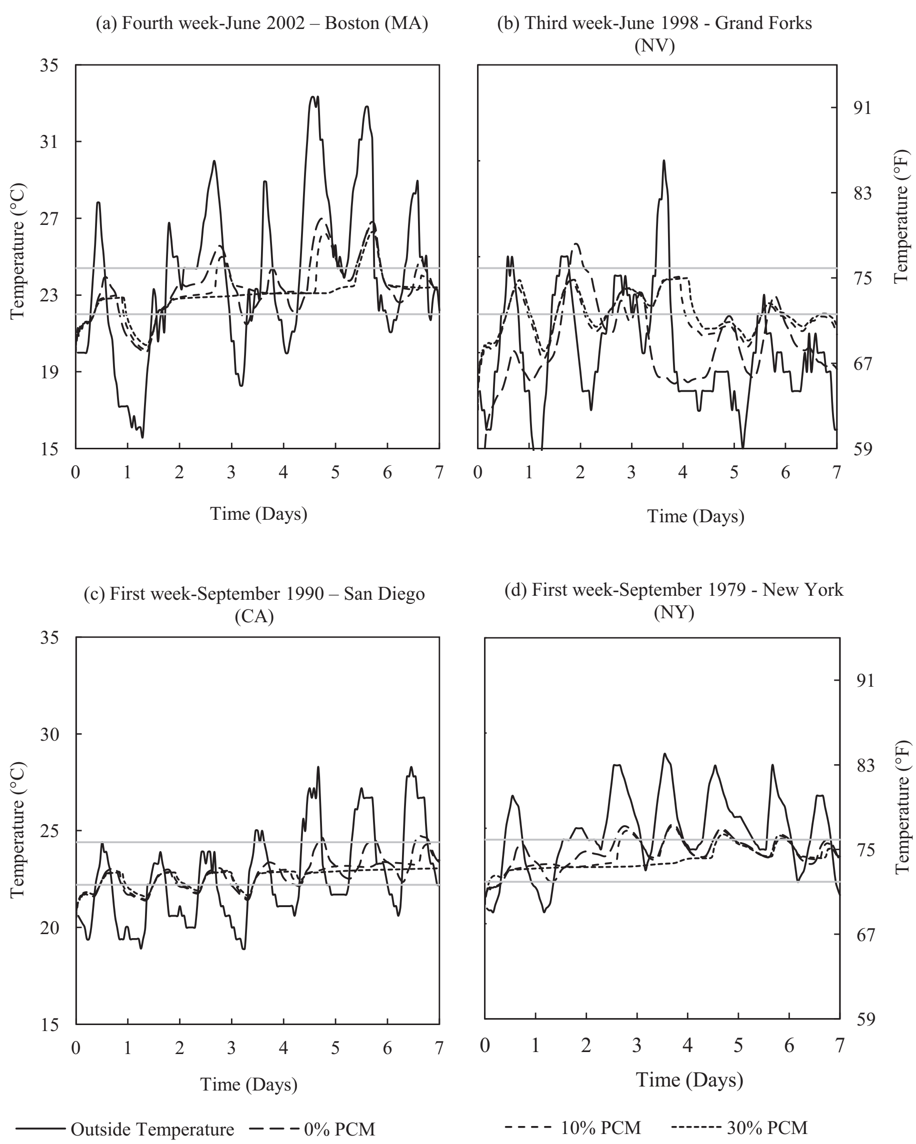

Fig. 8. Moderate climate category – changes in temperature for one week duration.

energy to keep the inside temperature in the comfort zone. But for the third day, the maximum temperature during the day is 30 °C (86 °F), therefore the PCM stores enough heat energy to make it possible to keep the inside temperature in the comfort zone for the following night. The same general behavior is observed for Grand Forks (Fig. 8b) and San Diego (Fig. 8c). The temperature oscillation of New York is very close to the comfort zone and the minimum temperature during the nights is only 1.1 °C (2 °F) less than the lower limit of the comfort zone. Therefore PCM, especially when 30% is used, can keep the inside temperature in the comfort zone almost for the entire week (Fig. 8d).

The 'cold' climate category includes Miles City, Montana; Chicago, Illinois; Worcester, Massachusetts; and Hulton, Maine. The minimum temperature of these cities is about 5.6 °C (42.1 °F). For the first three days of the Miles City temperature profile, the outside temperature is below the comfort zone during the nights and barely goes above the upper limit of comfort zone during the days (Fig. 9a). Therefore no heat energy is stored in the PCM and the inside temperature does not stay in the occupant comfort zone, even for the case that 30% PCM is used. But for the last three days of the week, as the temperature oscillates evenly above and below the comfort zone, PCM can effectively keep the inside temperature in the comfort zone. This shows that in addition to the percentage of the incorporated PCM, the temperature change range plays an important role in the effectiveness of the PCM. The same results can be reached for the other cities in this category (Fig. 9b–d).

The data generated from the computational model was used to calculate the percentage increase in the occupant comfort duration for different locations (Table 5). For each case, the number of hours that the inside temperature stays in the comfort zone is calculated for samples containing 0%, 10%, and 30% by volume PCM. For specimens containing 10% PCM, Delta, Utah saw the greatest increase, with the duration of being in the occupant comfort zone increased by 53.7%. For San Diego this increase was less than 22%. This shows that the efficiency of PCM to increase the occupant comfort is dependent on the profile temperature. The same conclusion can be reached for the cases that 30% PCM was used. In Chicago, the increase in being in the comfort zone was up to 78%. In San Diego this number was as low as 25%, which is even less than in some of the other cases where 10% PCM was used.

To investigate the effect of ambient temperature differences on the efficiency of PCM incorporation, the percentage increase in the duration of being in the comfort zone was graphed as a function of temperature difference between day and night (Fig. 10). When the

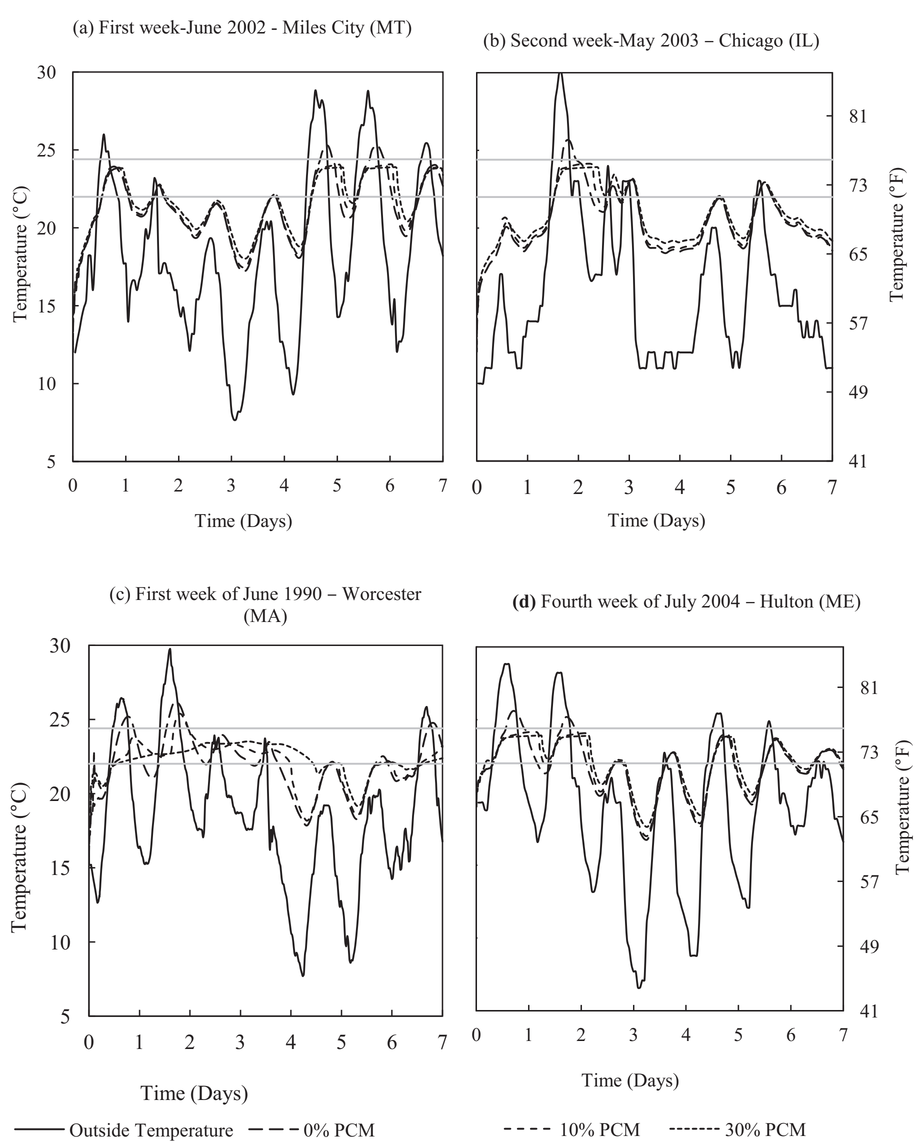

Fig. 9. Cold climate category – changes in temperature for one week duration.

Table 5
Increase in the occupant comfort duration.

Category	City	Duration of being in the comfort zone for one week (h)				
		0% PCM	10 vol.% PCM		30 vol.% PCM	
		Duration	Duration	Increase%	Duration	Increase%
Hot climate	Austin (TX)	92	118	28.3	130	41.3
	Delta (UT)	82	126	53.7	140	70.7
	Casa Granda (AZ)	38	50	31.6	62	63.2
	Reno (NV)	77	114	48.1	130	68.8
moderate climate	Grand Forks (ND)	47	66	40.4	70	48.9
	Boston (MA)	98	120	22.4	134	36.7
	San Diego (CA)	105	128	21.9	132	25.7
	New York (NY)	105	130	23.8	156	48.6
Cold climate	Miles City (MT)	44	64	45.5	72	63.6
	Chicago (IL)	28	40	42.9	50	78.6
	Worcester (MA)	72	96	33.3	114	58.3
	Hulton (ME)	70	94	34.3	102	45.7
Average of percentage increase ± standard deviation			35.5 ± 7.6%		51.2 ± 11.3%	

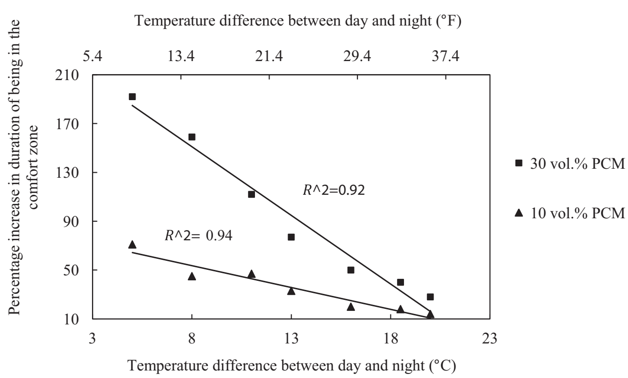

Fig. 10. Efficiency of PCM as a function of temperature difference.

temperature difference is as low as 5 °C (9 °F), the comfort duration can be almost doubled if 30% PCM is used. For the same temperature difference, the comfort duration can be increased by more than 50% when 10% PCM is used. These numbers are respectively about 90% and 40% when the temperature difference is 9 °C (16.2 °F) for 30% and 10% PCM. But when the temperature difference is as high as 20 °C (36 °F), the efficiency for both cases will be dropped to about 15%, which shows the PCM efficiency is highly dependent on the temperature difference.

3.2.2. Number of freeze/thaw cycles experienced by a concrete pavement

In addition to increasing occupant comfort in buildings, PCMs can be used to increase the service life of concrete pavements by decreasing the number of freeze/thaw cycles that they experience. It should be mentioned that freeze/thaw degradation is not a significant degradation mechanism in all locations because it only exists in certain environmental conditions. Only locations that have sufficiently wet climates, as the concrete must be saturated with water for damage to occur, and that reach freezing temperatures regularly are subject to significant freeze/thaw degradation. In the United States, locations that meet these criteria are parts of the Northwest including California, parts of the Southeast, most of the Midwest and Mid-Atlantic, and the entire Northeast. In this study, it was assumed that there is enough moisture available in the environment for all the case studies and therefore the temperature of the pavement is the only parameter that affects the number of freeze/thaw cycles. Further, although it is well known that the freezing point of pore solution in concrete is lower than that of water and depends on the exact chemistry of the pore solution, for comparative purposes 0 °C (32 °F) was chosen as the freezing point. Thus, the temperature at the depth of 203 mm (8″) was considered as the parameter to count for the number of freezing cycles.

To evaluate the effectiveness of PCMs to decrease the number of freeze/thaw cycles in pavements, the temperature profiles for two sequential months in six different cities were applied to models that contained 0%, 10%, and 30% by volume PCM with a melting point of 2 °C (35.6 °F) (Table 6). These cities are located in the northern and eastern parts of the United States where the temperature frequently drops to the freezing point during the cold seasons of the year. For each city, the selected two sequential months is the harshest period of time in the year in which the temperature drops to the freezing point with the highest number of times. When 10% PCM by volume was used, the reduction in the number of freeze/thaw cycles varied between 11.5% to 18.5% and on average, about one sixth of the freeze/thaw cycles were eliminated. When 30% PCM was used, the reduction percentage varies

Table 6
Percentage reduction in the number of freeze/thaw cycles experienced by the pavement.

City	Period of time	Number of freeze/thaw cycles				
		0% PCM	10 vol.% PCM		30 vol.% PCM	
		Number	Number	Reduction%	Number	Reduction%
Blacksburg (VA)	Jan.–Feb.	18	15	16.7	11	38.9
Lancaster (PA)	Jan.–Feb.	26	23	11.5	16	38.5
Montpelier (VT)	Mar.–Apr.	24	20	16.7	14	41.7
New York (NY)	Jan.–Feb.	17	14	17.6	12	29.4
Oxford (CT)	Feb.–Mar.	27	22	18.5	18	33.3
Silver Bay (MN)	Apr.–Jun.	33	28	15.2	20	39.4
Average of percentage reduction ± standard deviation			16.1 ± 2.5%		35.9 ± 4.1%	

between 29.4% and 41.7% depending on the temperature profile of the city, and on average, about one third of the cycles can be mitigated. The results match with the results presented in [28,29]. These results show that using PCMs in concrete pavements can effectively reduce the number of freeze/thaw cycles experienced by the pavement. More studies should be conducted to find the optimum percentage and melting temperature of the PCM.

4. Conclusions

A computational finite element model using COMSOL multiphysic software was developed to simulate the temperature changes in structural elements when Phase Change Materials were incorporated. The accuracy of the model was verified by Guarded Longitudinal Comparative Calorimetry tests and the real temperature profiles of different cities that were taken from TMY2 and TMY3 data were applied to the models as the thermal loads. The following findings were obtained:

– The duration of being in the occupant comfort zone in a building can be increased by up to 35% and 51% when 10% and 30% by volume PCM with a melting point of 23.3 °C (74 °F) is used, respectively.
– The efficiency of PCM to modify the changes in the inside temperature of a building depends on the temperature difference between day and night. As the latent heat of fusion of PCM is limited, this efficiency significantly drops when the temperature difference is high.
– The number of freeze/thaw cycles experienced by a concrete pavement during a period of two months can be decreased by up to 16% and 35% when 10% and 30% by volume PCM with a melting point of 2 °C (35.6 °F) is used, respectively.

These results show the efficiency of PCMs to improve the thermal performance of concrete, however more studies should be conducted to find the optimum percentage and melting temperature of PCM for different applications. Also, energy and cost analysis should be conducted to compare the efficiency and life cycle costs of PCMs to alternative methods.

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