Numerical Simulation of Thermal Performance of Micro-PCM Cement Mortar Composite Wall

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Abstract: In order to give full play to the effect of temperature regulation and energy saving of the phase change wall, the cement mortar mixed with phase change microcapsules was coated on the surface of the wall to form the phase change energy storage wall. Considering the thermal response of the temperature inside the wall, the heat transfer theoretical model of the phase change energy storage wall was established. The heat transfer process in the phase change energy storage wall and the temperature change inside the wall. The calculation results show that the content of phase change microcapsules in the phase change energy storage wall is one of the important factors affecting the temperature attenuation of the inner side of the wall. The peak time of the temperature change response curve on the inner side of the phase change wall is lagging behind that of the conventional wall, and the existence of the highest temperature is also lower, the peak temperature fluctuation is also lower, and the heat flow is reduced. It can be seen that the introduction of phase change microcapsules into the wall can achieve the purpose of reducing the temperature inside the wall and reducing the capacity of the air conditioning and refrigeration system of the building, which provides a good way to reduce the energy consumption and cost of building refrigeration.

Keywords: Phase Change Microcapsule; Phase Change Energy Storage Material; Numerical Simulation; Thermal Properties; Insulation Performance of Wall

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1 Introduction

The rapid growth of global energy has produced adverse effects on the environment, such as climate change caused by global warming [1, 2]. According to the International Energy Agency, between 1984 and 2004, primary energy consumption increased by 49% and carbon dioxide emissions by 43%, with average annual growth rates of 2% and 1.8% respectively [3]. The building and construction sector accounts for a large share of CO_2 emissions. The United Nations Environment Programme (UNEP) reported that the total energy consumption of the world's building sector in 2019 was little changed from the previous year, but CO_2 emissions continued to rise, accounting for 28% of the global total of relevant carbon emissions, and this proportion rises to 38% when the building sector is added [3-5]. Space heating and cooling account for more than one third of the total energy consumption of buildings. It is estimated that building cooling energy consumption will increase by 300% to 600% in developing countries by 2050 [6, 7]. Therefore, reducing space cooling is the best way to optimize building energy use patterns. One of the important factors affecting space refrigeration is the thermal physical

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characteristics of building envelope [8, 9]. Traditional building envelope materials are sensible heat energy storage, which has disadvantages such as low energy storage density and large volume ratio [10, 11]. To overcome these drawbacks of sensible heat storage, PCM are often integrated into building envelopes to improve heat storage capacity, thereby reducing energy consumption for space heating and cooling [12].

Phase change microcapsules (Micro-PCM) encapsulate PCM into spherical core-shell capsules with a diameter of 1-500 μm. The shell is usually composed of high polymer to prevent leakage of liquid phase PCM [13, 14]. In the published literature, different kinds of energy storage building materials have been developed. For example, Cao [15] integrated Micro-PCM into Portland cement concrete (PCC) and geopolymer concrete (GPC) respectively. The experimental results show that when the room temperature is stable at 23℃, PCC with 3.2wt% Micro-PCM can reduce the power consumption by 11%. GPC with 2.7wt% Micro-PCM can reduce power consumption by 15%. Kuznik [16] prepared a wall panel containing 60% Micro-PCM. The results show that the PCM with a thickness of about 1 cm strengthens the thermal inertia of the wall and stores energy during the day to prevent the room from overheating, while the energy released at night increases the minimum temperature. Lee and Medina [17] developed a numerical model to reduce the peak load of residential air conditioning. The results show that the energy consumption and space cooling load can be reduced by 7.2% and 10.4%, respectively, by using PCM in the wall. Therefore, the introduction of Micro-PCM into building materials will significantly improve the thermal properties of composites. However, the introduction of foreign particles can change the microstructure of concrete and thus affect the mechanical properties of concrete. Numerous studies have shown that the compressive strength is significantly reduced when Micro-PCM is added to concrete. For example, Djamai [18] and Lecompte [19] reported that the compressive strength of cement mortars containing 5wt% and 6.3wt% Micro-PCM was reduced by 34.1% and 50%, respectively. Figueirdo [20] found that integrating Micro-PCM into concrete reduced the compressive strength and flexural strength by about 66% and 52%, respectively. In order to overcome the above problems, Micro-PCM mixed with cement mortar is applied to the building envelope, which can not only avoid the loss of structural material strength, but also improve the thermal performance of the envelope. Therefore, this paper integrted Micro-PCM into cement mortar coated on the surface of the concrete wall, and then studied the cooling performance of the Micro-PCM wall. Then, based on the two-dimensional unsteady heat transfer theory of phase transformation process, the heat conduction model of phase transformation wall was established by using the energy equation of equivalent heat capacity method. The temperature and heat flow distribution of ordinary wall and Micro-PCM wall were numerically simulated by finite element software COMSOL. The effect of Micro-PCM volume fraction on the temperature amplitude and temperature delay of the wall surface is also studied.

2 Generation of Random Array of Micro-PCM

From the literature survey, it is known that Micro-PCM is randomly distributed in cement mortar, and the random distribution model of the Micro-PCM is established by Rand function in PFC software. The model is generated using the following algorithm:

(1) Input the number of Micro-PCM (n_P), the radius of Micro-PCM (r_P) and the size of the matrix material model ($a \times b$).

(2) The coordinates of the first Micro-PCM are randomly generated using the RAND function.

(3) The location of the i Micro-PCM is randomly generated by using the RAND function, and whether the location will intersect with the $i-1$ micro-PCMs that have been generated is judged. If not, the Micro-PCM model is generated, otherwise the model is regenerated.

(4) The above process is repeated until the specified number of micro-PCMs is generated.

In addition, the thickness and height of the cement mortar coating layer are set to $a = 20\text{mm}$ and $b = 300\text{mm}$ respectively, and the radius of Micro-PCM is set to $r = 1\text{mm}$ according to the actual situation. The number of Micro-PCM is calculated by the following equation.

$$f_P = \frac{n_P \times \frac{1}{2}\pi r_P^2}{a \times b} \quad (1)$$

where n_P is the number of Micro-PCM, r_P represents the diameter of Micro-PCM.

Following this rule above, the required 2D composite cubic unit cell models can be generated directly as shown in Figure 1.

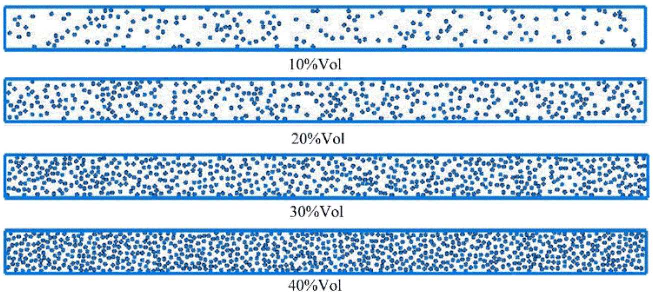

Figure 1 Flow chart of random distribution model of Micro-PCM particles in cement mortar

3 Heat Transfer in the Micro-PCM Wall

In this paper, the equivalent heat capacity method is used to theoretically model the melting and solidification phase transition process, and the governing equation is as follows.

$$\rho C_P \frac{\partial T}{\partial t} = k\nabla^2 T \tag{2}$$

Where ρ is the density of the PCM, C_p is the specific heat capacity of PCM, k is the thermal conductivity of PCM.

In the phase transition analysis, in order to ensure the stability of the calculation, it is assumed that the phase transition occurs in a small temperature interval $[T_s, T_l]$, where T_s and T_l are $T_m - \Delta T_m/2$ and $T_m + \Delta T_m/2$, respectively, and $T_m = T_l - T_s$ is a small temperature interval, i.e., 1K.

Obviously, in the melting process, the liquid volume fraction f is related to the temperature field T in the PCM and be defined by:

$$f = \begin{cases} 0 & T < T_s \\ \dfrac{T - T_s}{T_l - T_s} & T_s \leqslant T < T_l \\ 1 & T > T_l \end{cases} \tag{3}$$

Based on the definition of liquid volume fraction, the effective thermal conductivity k, the effective density ρ and the effective specific heat capacity C_P can respectively be given by the following mixture relations:

$$k = (1-f)k_s + fk_l \tag{4}$$

$$\rho = (1-f)\rho_s + f\rho_l \tag{5}$$

$$C_P = \frac{1}{\rho}[(1-f)\rho_s C_{p,s} + f\rho_l C_{p,l}] + L_m D(T) \tag{6}$$

Where the subscripts s represents the solid phase and the subscript l represents the liquid phase. $D(T)$ is the standard Gaussian function which is zero everywhere except the temperature interval ΔT. More importantly, its integral is equal to 1.

In order to simplify the calculation, the following assumptions are made for the problem studied:

(1) Micro-PCM is randomly distributed in cement mortar, and the volume change during phase transition is ignored.

(2) Wall, cement mortar and Micro-PCM isotropy, constant physical properties.

(3) Due to the small particle size of Micro-PCM, the influence of natural convection is ignored.

(4) The thickness of the wall is far less than the width and height, the temperature only changes along the thickness direction, and the heat transfer process is one-dimensional heat conduction process.

Based on the data of a typical meteorological year in a region of China, the dynamic thermal insulation of phase change wall is analyzed. The temperature of the hottest July 25~27 and solar radiation intensity were selected as the boundary conditions, and the expression of outdoor air comprehensive temperature on the western wall was as follows:

$$t_{25}(\tau) = 33.0+8.0\sin(\pi(\tau\text{-}8.28)/9.96)+273.15 \tag{7}$$

$$t_{26}(\tau) = 34.5+9.2\sin(\pi(\tau\text{-}8.12)/11.7)+273.15 \tag{8}$$

$$t_{27}(\tau) = 35.0+9.0\sin(\pi(\tau\text{-}9.32)/11.6)+273.15 \tag{9}$$

In order to facilitate analysis, for phase change microcapsule mortar coated on the outer surface of the wall, the fixed solution conditions set in this paper are as follows:

Initial conditions:

$$T(x,0) = T_0, \qquad x \in [0,120], \tau = 0 \tag{10}$$

Outdoor side boundary conditions:

$$-\lambda_b \frac{\partial T}{\partial x}\Big|_{x=0} = h_{in}(T_b - T_{in}) \tag{11}$$

Indoor side boundary conditions:

$$-\lambda_b \frac{\partial T}{\partial x}|_{x=120} = h_{out}(T_b - T_{out}) \quad (12)$$

The upper side of the wall is insulated:

$$-\lambda_b \frac{\partial T}{\partial y}|_{y=0} = 0 \quad (13)$$

The underside of the wall is insulated:

$$-\lambda_b \frac{\partial T}{\partial y}|_{y=300} = 0 \quad (14)$$

The Micro-PCM cement mortar was applied to the inner side of the concrete wall with a thickness of 100mm and a height of 30mm. The thermal physical parameters of the concrete wall were $\rho_w = 1800\text{kg/m}^3$, $k_w = 0.81\text{W/m/K}$, $C_{Pw} = 1.05\text{J/(kg·K)}$. The thermal physical parameters of the Micro-PCM were $\rho_{Micro-PCM} = 880\text{kg/m}^3$, $k_{Micro-PCM} = 0.232\text{W/m/K}$, $L_{Micro\text{-}PCM} = 175.39\text{J/g}$, $C_{PMicro-PCM} = 3.22\text{J/(kg·K)}$, $T_m = 26.44℃$. Moreover, the left side of the wall is the indoor environment, the right side is the outdoor environment, and the upper/lower surface is the adiabatic condition.

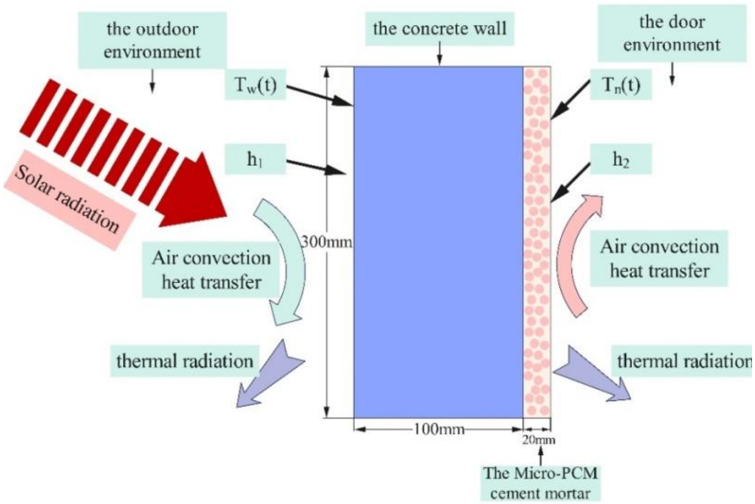

Figure 2 Computational modeling for Micro-PCM wall

A large general finite element software (COMSOL) was used to establish the finite element model, see Figure 3. In the finite element simulation of heat conduction, extremely fine triangular meshes and quadrilaterals are used to obtain mesh independent convergent solutions. In the simulation, the computation time step is set to 1s, and the PARDISO direct solver in COMSOL is used to solve the highly nonlinear multi-physics field coupling problem.

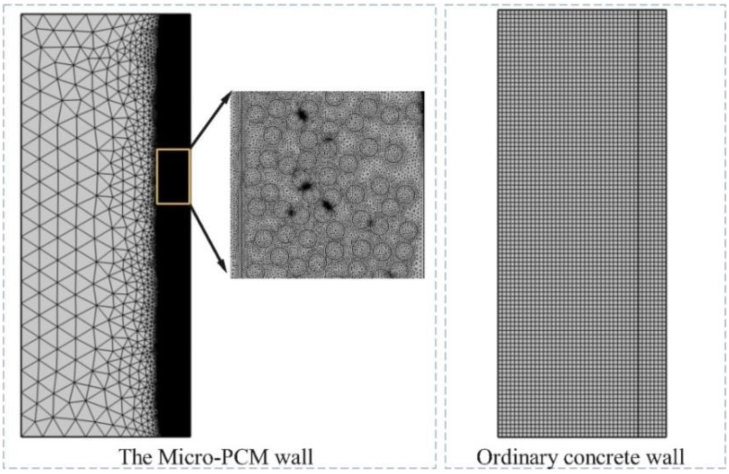

Figure 3 Meshing of Micro-PCM wall and ordinary wall finite element models (Micro-PCM, 40%vol)

Based on the above physical and mathematical models, COMSOL software is used to simulate and calculate the heat transfer process of ordinary wall and Micro-PCM wall. The temperature cloud image at 8h-65h is shown in Figure 4. It can be clearly seen from Figure 4 that under the same outdoor temperature boundary conditions, The heat transfer process of the ordinary wall is faster than that of the Micro-PCM wall, and the Micro-PCM wall all block the high temperature zone in the outer area of the wall, indicating that the phase change material enhances the thermal inertia of the wall.

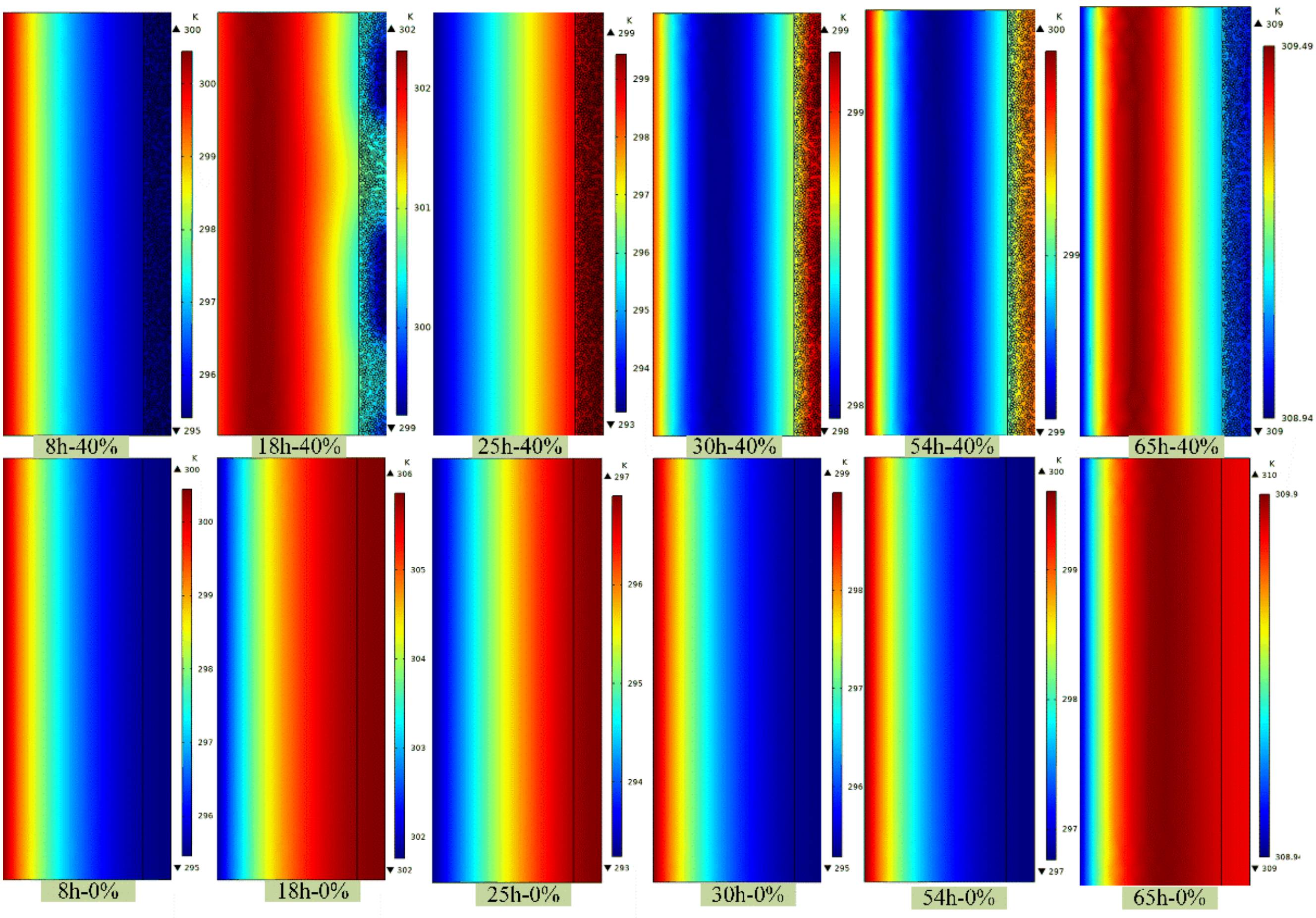

Figure 4 Cloud diagram of calculated temperature of Micro-PCM wall (top) and ordinary wall (bottom) (Micro-PCM, 40Vol%)

4 Results and Discussions

4.1 Internal Surface Temperature Analysis of Micro-PCM Wall

According to the staged heat transfer equations (7) to (9) of the phase transition process of Micro-PCM wall, the transient distribution curves of temperature and liquid fraction on the inner side of Micro-PCM wall under outdoor transient meteorological conditions can be obtained, as shown in Figure 6. From the liquid fraction curve and the temperature curve of the inner side of Micro-PCM wall in Figure 6, it can be seen that when the Micro-PCM-CM layer with a certain thickness is coated on the outer surface of the ordinary wall, the temperature of the inner surface of the ordinary wall is lower than that of the ordinary wall. The specific analysis is as follows:

(1) 0-11h: it means that the external surface temperature of Micro-PCM is lower than the phase change temperature, and the phase change material is solid. The heat transfer process of the phase change energy storage wall is the same as that of the ordinary wall, but the temperature is lower than that of the ordinary wall.

(2) 11h-26h: it means that the external surface temperature of Micro-PCM is higher than the phase transition temperature, and the phase change material starts to change from solid to liquid, and absorbs heat continuously in the form of latent heat, and the temperature at the solid-liquid interface remains unchanged at the phase transition temperature.

(3) 26h-33h: it means that after the solid-liquid phase transition, the phase change material is in liquid state and continues to transfer heat under the action of external temperature. The heat transfer process is the same as that of ordinary wall, but the temperature is lower than that of ordinary wall.

(4) 33h-41h: it means that the external surface temperature of Micro-PCM begins to be lower than the phase transition temperature, the phase change material begins to change from liquid to solid, and the heat is released continuously in the form of latent heat, and the temperature at the solid-liquid interface remains unchanged at the phase transition temperature.

(5) 41h-46h: it means that the external surface temperature of Micro-PCM is higher than the phase change temperature, part of the solid phase change material begins to melt and absorbs heat in the form of latent heat, and the temperature at the solid-liquid interface remains unchanged at the phase change temperature.

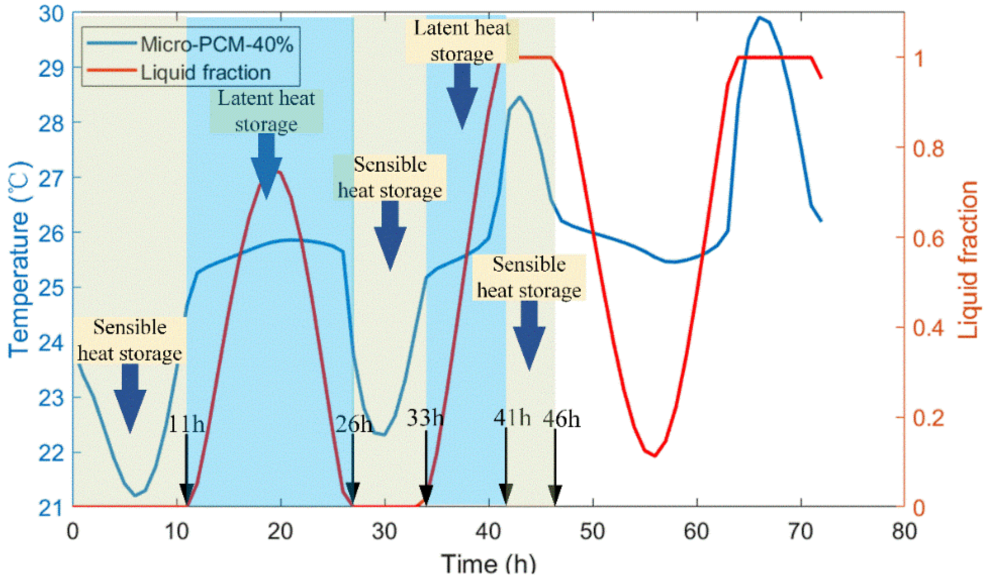

Figure 5 Temperature change inside the Micro-PCM wall and liquid fraction change inside the Micro-PCM wall (Micro-PCM, vol-40%)

4.2 Effect of Micro-PCM Content on Inner Wall Temperature

The temperature of the wall determines the indoor thermal environment. The relationship between the temperature of the inner wall and the ambient temperature of the outdoor air is shown in Figure 6. It can be seen from Figure 6 that the outdoor ambient temperature fluctuates in 3 cycles within 72 hours with a cycle of 24h, and the internal wall temperature of the nine types of walls also fluctuates in 3 cycles. Due to the thermal inertia of the wall, the internal wall temperature fluctuations of the nine types of walls delay the change of the external environment temperature, but the delay of the Micro-PCM wall is higher than that of the ordinary wall. And the higher the Micro-PCM content, the higher the delay. For example: In the first temperature fluctuation cycle, the ordinary wall reaches the maximum temperature of 29.48℃ at 16h, while the phase change energy storage wall with 40% volume content of Micro-PCM reaches the maximum temperature of 25.86℃ at 21h, the lag time is 5h, and the temperature reduction is 3.62℃. The maximum temperature, time, lag time, and temperature reduction of the nine types of walls are summarized in Table 1. Table 1 shows that the temperature peak lag time and temperature reduction of the micro-PCM-CMW wall are better than those of the ordinary wall, and the higher the Micro-PCM content, the greater the temperature peak lag time and temperature reduction of the wall.

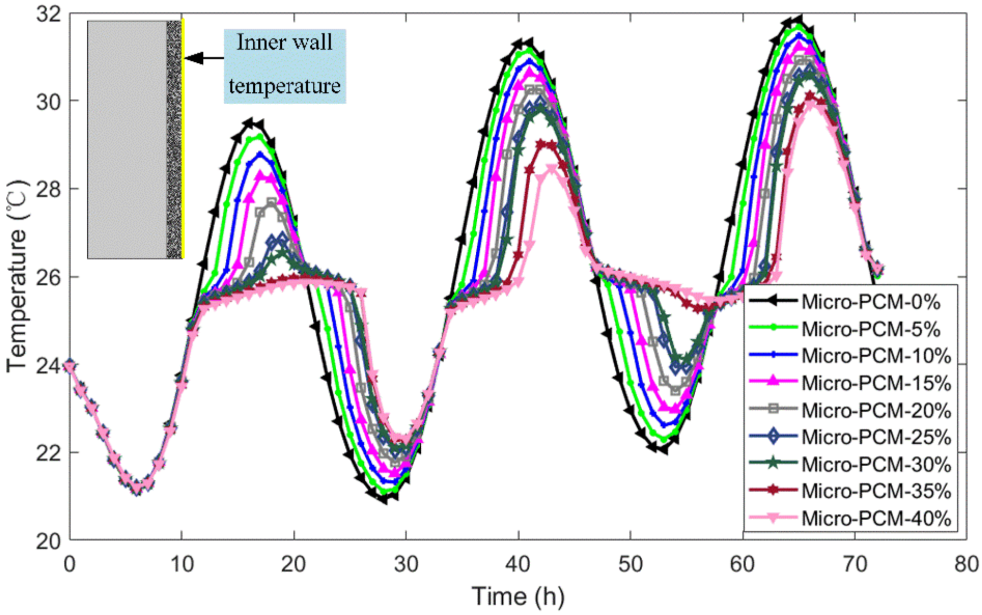

Figure 6 The inner temperature change of Micro-PCM-W wall under different Micro-PCM content

Table 1 Temperature peak lag time and temperature reduction under different volume contents of Micro-PCM

	Volume content (%)	**Maximum temperature (℃)**	**Time (h)**	**Lag time (h)**	**Temperature reduction (℃)**
First period	0	29.48	16	-	-
	5	29.17	17	1	0.31
	10	28.78	17	1	0.70
	15	27.28	17	1	2.20
	20	27.69	18	2	1.79
	25	26.78	18	2	2.70
	30	26.54	19	3	2.94
	35	25.96	20	4	3.52
	40	25.86	21	5	3.62

In the second wave period, the peak and trough difference of the temperature of the inner wall of the ordinary wall is 9.24℃. When the content of Micro-PCM is 5%~40%, the peak and trough difference of the temperature of the inner wall is 3.01℃~8.83℃, which is 0.18℃~2.84℃ lower than that of the ordinary wall (see Table 2). That is, the higher the Micro-PCM content is, the smaller the temperature fluctuation of the Micro-PCM wall indoor side is, that is, the phase change energy storage wall will provide a stable indoor thermal environment.

Table 2 Peak and trough difference and temperature reduction of Micro-PCM with different volume contents

	Volume content (%)	**Maximum temperature (℃)**	**Minimum temperature (℃)**	**Peak trough difference (℃)**	**Temperature reduction (℃)**
Second period	0	31.31	22.07	9.24	-
	5	31.13	22.30	8.83	0.18
	10	30.90	22.61	8.29	0.41
	15	30.62	22.97	7.65	0.69
	20	30.25	23.39	6.29	1.06
	25	29.93	23.96	5.97	1.38
	30	29.81	24.12	5.69	1.50
	35	29.01	25.27	3.74	2.30
	40	28.47	25.46	3.01	2.84

4.3 Effect of Micro-PCM Content on First Layer of Material Temperature

The inner temperature of the first layer of material in the micro-PCM wall is shown in Figure 7. During the heating process of three cycles, when the measured temperature of the first layer of material reaches about 26℃, the temperature rise rate of the micro-CPM wall begins to be lower than that of the ordinary wall, and the higher the content of Micro-PCM, the lower the rate of rise of temperature. This is because when outdoor air transfers heat to the inside of the wall, when the wall heats up to about 26℃, PCM begin to undergo phase change, and heat is stored in the form of latent heat, reducing the heat transferred to the inside of the wall. In the first period, the inner temperature of the first layer of materials with a volume content of 40% decreased by 3.13℃ compared with the ordinary wall, indicating that the latent heat storage effect of Micro-PCM did indeed reduce the temperature rise in the inner area of the wall. During the cooling process over three cycles, the initial temperature of the ordinary wall is higher than that of the micro-PCM wall, but the cooling rate is also higher because the heat stored in the form of latent heat in the Micro-PCM is released to the external environment as an internal heat source during cooling.

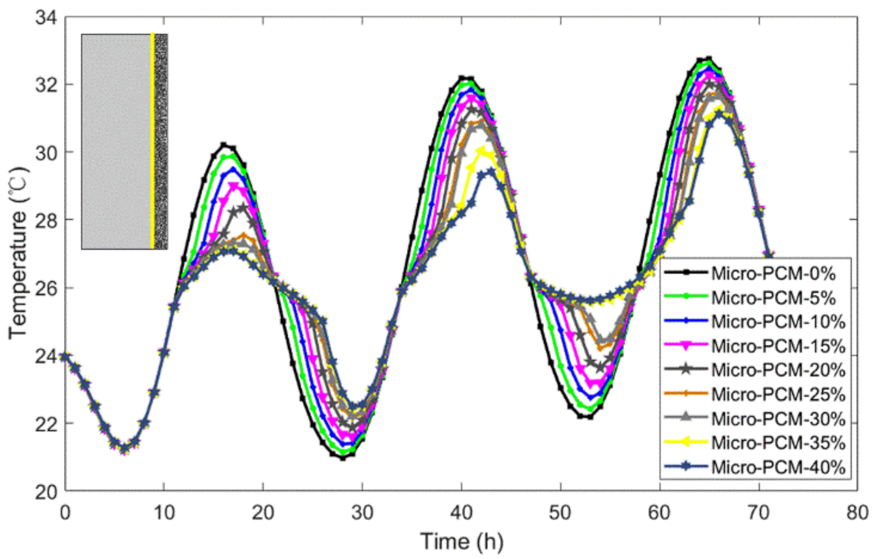

Figure 7 Temperature changes in the inner side of PCM mortar layer under different Micro-PCM contents

5 Conclusions

(1) In the process of external environment changes, the latent heat storage/energy release of PCM in Micro-PCM changes periodically, and the temperature at the solid-liquid interface remains unchanged at the phase change temperature, thus delaying or even reducing the indoor temperature peak.

(2) After the addition of Micro-PCM, the heat storage performance and temperature control performance of cement mortar composite wall are significantly improved. For example, the internal wall peak temperature of 40Vol% micro-PCM is reduced by 3.62℃, and the indoor peak temperature is delayed by 5h.

(3) The peak temperature fluctuation of the ordinary wall is 9.24℃, while the Micro-PCM integrated in the plaster layer of the wall can effectively reduce the indoor temperature fluctuation, among which the minimum peak temperature fluctuation is 3.01℃. Phase change material greatly reduces indoor temperature fluctuation and improves indoor thermal comfort.

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