Optimization of phase change material component and its application in buildings

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Abstract. Improving the thermal transfer performance of phase change material (PCM) component has attracted more and more attention in building the energy-saving field. This paper presented an optimized PCM component which is encapsulated in a metal container, to promote the thermal performance of the wall. Thermal transfer of PCM component is optimized by adding internal fin through numerical simulation software COMSOL Multiphysics. The simulation model was verified by data from publicly available published literature. The temperature difference of PCM component in front and back heating surface ($\Delta T$) was employed to obtain the optimal geometric parameters including spacing ($S_{fin}$) and length ($L_{fin}$) of the fin. Thermal performance of the wall with the optimized and non-optimized PCM component was compared under the summer typical climate. The wall with optimized PCM component has the best capacity for heat storage and release. The interior surface temperature reduction of the wall with optimized PCM component is lower by 2.1 ºC than reference wall.

1. Introduction
Taking advantage of latent heat into the building envelope, can significantly reduce the building energy consumption and improve the temperature regulation for the indoor thermal environment. Among the different combinations of PCM applied in building, macro-encapsulation is the simplest and most economical method. Package PCM in the container as a PCM component combined with building envelopes is considered a promising option in building energy conservation [1, 2]. The superiority of this technique embodied at various packaging shapes and size, are safe and avoid leakage of material. Sufficient thermal storage capacity and the function of the construction structure can be less affected [3]. However, unreasonable application and poor thermal conductivity would cause the regulating ability untimely and incomplete for the indoor thermal environment [4]. Metal fins are widely used to increase the thermal transfer areas of PCM component. This method could compensate PCM for low thermal conductivity and relatively easy to fabricate [5]. The fin type can be divided into partitioning fin and partial fin according to the objective application [6]. Many types of
research mainly focused on optimizing the thermal performance of fin number and geometry in PCM component. From the above, thermal transfer enhancement of PCM component with fin would promote the charging and discharging rate of PCM. Few pieces of research investigate this technology applied in building envelope and evaluate the application effects under the actual indoor and outdoor thermal environment. In the present work, the optimal geometric parameters of fin were obtained and the thermal performance of the composite wall with optimized PCM component was analyzed. The conclusion can provide references for PCM application in building.

2. Numerical simulation method

2.1. Physical model

The two-dimensional physical model of the multi-layer wall filled with PCM is shown in Fig. 1. The aerated concrete structure is selected, which is widely used in Southern China. The aerated concrete has good thermal insulation but poor thermal storage capacity. The wall consists of 20 mm thick plaster layer on the exterior and interior surface, and 200 mm aerated concrete layer inside. The dimension of the PCM component are as follows: the net depth, height, and thickness are 200 mm, 200 mm and 10 mm. Aluminum is selected as shell and fin material for good thermal conductivity. The thickness of the shell is set as 1 mm. The partial fin in the PCM component is added to the indoor side (right side), which can adjust the indoor thermal environment directly. The thermo-physical properties of PCM used in the simulation are shown in Table 1. The different spacings ($S_{\text{fin}}$) and lengths ($L_{\text{fin}}$) of the fin are employed to determine the optimal geometric parameters.

![Figure 1. Schematic diagram of wall with the optimized PCM component](image)

![Figure 2. Boundary conditions variation over the typical summer day in Shenzhen](image)

| Martials          | $k$ (W·m$^{-1}$·K$^{-1}$) | $\rho$ (kg·m$^{-3}$) | $c$ (kJ·kg$^{-1}$·℃$^{-1}$) | $L$ (kJ·kg$^{-1}$) | $T_{pc}$ (℃) |
|-------------------|--------------------------|----------------------|-----------------------------|-------------------|--------------|
| PCM               | 0.23/0.21                | 833.8/786.7          | 1.91/2.03                   | 122               | 33.7         |
| Aerated concrete  | 0.22                     | 700                  | 1050                        | /                 | /            |
| Plaster layer     | 0.93                     | 1800                 | 1050                        | /                 | /            |
| Fin and shell     | 211                      | 2675                 | 9.03                        | /                 | /            |

Note: $k$, $\rho$, and $c$ are solid/liquid phase of PCM at each property.

2.2. Governing equations
To perform multiple physical fields simulation, the thermal transfer module for solid, liquid and laminar flow physical fields are employed [7]. The assumptions are as following:

(1) One-dimensional thermal transfer is assumed. The boundary conditions of the top and bottom of the PCM component are set as adiabatic and the initial temperature is uniformly distributed.

(2) All the solid materials are homogenous.

(3) The liquid PCM is incompressible Newton fluid, and density change during the phase change process conforms to Boussinesq approximation.

Based on the above assumptions, the effective heat capacity method is used to simulate thermal transfer in the phase change process and the transient energy equations are as follows:

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) + \rho C_p u \nabla T = 0$$  \hspace{1cm} (1)

where $\rho$ is the density of materials; $C_p$ is specific heat of materials; $T$ is transient temperature; $k$ is thermal conductivity of materials; $u$ is a vector of the liquid PCM velocity field. The liquid fraction ($\theta$) of PCM can be defined with $T$:

$$\theta = \begin{cases} 
0 & T<T_m - \frac{\Delta T}{2} \\
\frac{T-T_m + \Delta T/2}{\Delta T} & T_m - \frac{\Delta T}{2} < T < T_m + \frac{\Delta T}{2} \\
1 & T>T_m + \frac{\Delta T}{2}
\end{cases}$$  \hspace{1cm} (2)

where $T_m$ is the melting point of PCM; $\Delta T$ is the phase change temperature range; $\theta$ varies linearly from 0 to 1 through the transition zone over $\Delta T$. Based on the definition of $\theta$, density ($\rho_{PCM}$), thermal conductivity ($k_{PCM}$) and specific heat ($C_{pcm}$) of PCM can be expressed as follows (Subscripts s and l are solid and liquid properties for PCM):

$$\rho_{PCM} = \theta \rho_s + (1-\theta) \rho_l$$  \hspace{1cm} (3)

$$k_{PCM} = \theta k_s + (1-\theta) k_l$$  \hspace{1cm} (4)

$$C_{pcm} = \frac{1}{\rho_{PCM}} (\rho_s C_{ps} \theta + \rho_l C_{pl} (1-\theta)) + \frac{L \partial \alpha_m}{\partial T}$$  \hspace{1cm} (5)

where $L$ is the latent heat of PCM; $\alpha_m$ is volume fraction in the phase change process:

$$\alpha_m = \frac{\rho_l (1-\theta) - \rho_s \theta}{2 \rho_s \theta + \rho_l (1-\theta)}$$  \hspace{1cm} (6)

The changes of $\rho$ in phase change drive buoyancy in liquid PCM. Based on the Navier-Stokes equation, the momentum conservation equation is as follows:

$$\rho_{PCM} (u \cdot \nabla) u = -\nabla p + \nabla \cdot \mu \nabla u + \nabla \Phi_{PCM} + \rho_{PCM} \beta \alpha_m (T - T_0)$$  \hspace{1cm} (8)

where $p$ is the fluid pressure of PCM; $g$ is gravity; $\mu$ is the dynamic viscosity of PCM.

2.3. Validation of the Model

Before proceeding further, the grid quantity and timesteps are checked. Simple linear free triangular elements are applied to generate a grid. Four grid quantities (39433, 49793, 72623 and 91396) and four timesteps (1, 0.5, 0.25 and 0.1 hours) are studied. Considering the simulation accuracy and computational resources, 72623 grid quantity and timestep of 0.25 h are chosen. The reliability of the model is validated based on the data of Huang et al [5]. The average temperature of the PCM component heating surface ($T_s$) and PCM ($T_{PCM}$) are selected for validation. The initial temperature and ambient environment temperature are set as 20 C. The front and back surface heat transfer coefficients of PCM are set as 10 W·m⁻²·C⁻¹ and 5 W·m⁻²·C⁻¹. The radiating surface is set as a constant value of 1000 W·m⁻². The top and bottom boundaries of the system are adiabatic. $T_s$ and $T_{PCM}$ are compared which are shown in Fig. 3. The maximum relative error of $T_s$ and $T_{PCM}$ are 4.58 % and 1.67 %, the average relative error of $T_s$ and $T_{PCM}$ are 0.51 % and 1.62 %. It indicates that the model is credible to investigate the thermal transfer of the PCM component.
2.4. Evaluation index of the composite wall with PCM

To avoid the influence of periodical temperature variation on the optimization of the fin, constant boundary conditions of the PCM component are employed to evaluate the PCM thermal behavior with different geometric parameters. The initial temperature is set as 20 °C, the heat transfer coefficient and temperature of the heating surface of the PCM component are set as 8.7 W/m²·K and 40 °C. The temperature difference in front and back heating surface of the PCM component in front and back heating surface (ΔT_i) at heat storage stage is used to assess the efficiency of the fin. The integer multiples of fins’ spacing (S_fin) and length (L_fin) are used as simulation cases. The values of S_fin are 20, 10, 5 and 4 mm, the values of L_fin are 8, 4, 6, and 2 mm.

The optimal quantity of PCM can fully achieve the heat storage capacity of the PCM composite wall. Latent heat utilization of PCM ($\varepsilon_{PCM}$) and interior surface coefficient of heat accumulation for the PCM composite wall ($Y_i$) are used to determine the optimal PCM thickness:

$$\varepsilon_{PCM} = f_{max} - f_{min}$$

$$Y_i = \frac{A_h}{A_d}$$

In Eq. (9), $f_{max}$ and $f_{min}$ are the maximum and minimum value of $\theta$. In Eq. (10), $A_h$ is the wave amplitude of interior surface heat flux and $A_d$ is the temperature amplitude of the interior surface.

As shown in Fig. 4, $Y_i$ and $\varepsilon_{PCM}$ are influenced by PCM thickness. $\varepsilon_{PCM}$ decreases with the increase of PCM thickness. $Y_i$ increases with PCM thickness from 2-10 mm, then tend to be stable with 0.6 of $\varepsilon_{PCM}$. The optimal thickness of PCM of the non-optimized PCM component is determined as 10 mm and the thickness of PCM in optimized PCM component is calculated as 10.3 mm.

3. Results and discussion

3.1. Optimization of fin-based on thermal behavior

Figure 5 presents the comparison of $\Delta T_i$ with different fins’ geometric parameters at heat storage stage. The lower value of $\Delta T_i$ means the better thermal behavior of the PCM component. From Fig. 5 (a) and (b), three stages of phase change process are observed: sensible heat of solid phase, latent heat of phase change process and sensible heat of liquid phase [8]. At the sensible heat of the solid phase, $\Delta T_i$ varies linearly from 0-10 min due to the thermal resistance of the PCM component. By comparing all cases, $L_{fin}$ has a significant impact on the sensible heat of the solid phase. At the latent heat of the phase change process, $\Delta T_i$ tends to be stable and natural convection becomes dominant in thermal transfer. Also, $L_{fin}$ has a significant impact on the latent heat of the phase change process. In addition,
\( \Delta T_s \) of the PCM component with no fin is higher than that with a fin. The PCM melting rate decreases due to the PCM is not melted completely. At the sensible heat of the liquid phase, \( \Delta T_s \) increases when the PCM melts completely. From the above, the optimized geometric parameters of the fin in the PCM component are determined: 5 mm of \( S_{\text{fin}} \) and 8 mm of \( L_{\text{fin}} \).

![Figure 5](image1.png)

(a) \( \Delta T_s \) comparison with different \( S_{\text{fin}} \), (b) \( \Delta T_s \) comparison with different \( L_{\text{fin}} \)

3.2. Thermal performance of the PCM composite wall

According to the optimization of the fin, a multi-layered wall without PCM component is defined as “Reference wall”. The wall with installed non-optimized PCM component and the wall with installed optimized PCM component is defined as “Wall with non-optimized PCM component” and “Wall with optimized PCM component”. To investigate the thermal performance of the PCM wall, interior surface temperature and interior surface heat flux of each wall are compared.

![Figure 6](image2.png)

Figure 6. Interior surface temperature comparison of different walls

![Figure 7](image3.png)

Figure 7. Interior surface heat flux comparison of different walls

Interior surface temperature is presented in Fig. 6. The results demonstrate that two types of PCM walls can regulate the peak interior surface temperature. Comparing with reference wall, the average lag time of the peak interior surface temperature is 2.5 h for the wall with non-optimized PCM component and 3 h for the wall with optimized PCM component. The interior surface temperatures reduction of two walls with non-optimized and optimized PCM component are lower by 1.7 °C and 2.1 °C than reference wall, respectively. These results indicate that the wall with the optimized PCM component has the best thermal stability.

Interior surface heat flux is shown in Fig. 7. When heat flux is greater than 0, it means the heat is transferring from interior surface to indoor (heat release at night). The heat is absorbing from indoor to
interior surface (heat storage in the daytime) when the heat flux is less than 0. The thermal storage/release capacity of the wall is reflected in two aspects: the duration and intensity. The duration of the reference wall is 10 h (7:00-17:00). The wall with the non-optimized PCM component and optimized PCM component are 12.25 h (8:00-20:15) and 13 h (8:15-21:00). The intensity of heat storage/release can be express by the fluctuation of heat flux. The peak value of the wall with non-optimized and optimized PCM component is 3.8 W·m\(^{-2}\) and 5.9 W·m\(^{-2}\), which are higher than the reference wall during the daytime. It means that the PCM component promotes the heat storage capacity of the wall and increases the heat storage capacity. Similarly, PCM component increases the heat release capacity at night. The peak heat flux of the wall with the non-optimized and optimized PCM component are higher by 4.4 W·m\(^{-2}\) and 8.5 W·m\(^{-2}\) than reference wall. According to the above analysis, the wall with optimized PCM component has the best capacity in terms of heat storage and release.

4. Conclusions

In present work, optimization of PCM component was conducted based on COMSOL Multiphysics considering the geometric parameters of the fin. The temperature difference in the front and back heating surface of the PCM component heating surface (\(\Delta T_s\)) was used to assess the fin efficiency. Suitable geometric parameters including spacing (\(S_{\text{fin}}\)) and length (\(L_{\text{fin}}\)) of the fin are a benefit for thermal transfer of PCM component. The optimal \(S_{\text{fin}}\) and \(L_{\text{fin}}\) of the fin are determined as 5 mm and 8 mm, respectively. In addition, the optimal thickness of PCM was determined with the actual indoor and outdoor environment. The thermal performance of the wall with the non-optimized and optimized PCM component was compared with the interior surface temperature and heat flux. The wall with optimized PCM component presents the best thermal stability. Results show that the interior surface temperature reduction of the wall with the optimized PCM component is lower by 0.4 °C than the wall with the non-optimized PCM component.

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