

Influence of Phase Change Material Physicochemical Properties on the Optimum Fin Structure in Charging Enhancement

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Orthogonal fins made of a vertical and a horizontal fin shorten total charging time and enhance average charging rate of lowly conductive phase change materials (PCMs) such as paraffin wax. An optimum dimension of orthogonal fins exists during charging of paraffin wax under top heating. The optimum dimension is represented by the optimum relative distance. The relative distance d/l_v is defined as the ratio of the distance between horizontal fin and bottom wall of enclosure to length of vertical fin. However, the physicochemical properties of PCMs are variant in practical. Their influences on this optimum relative distance of orthogonal fins are not conducted. In current investigation, the investigations on influence of PCMs' physicochemical properties on the optimum relative distance of orthogonal fins are numerically carried out. Influences of PCMs' physicochemical properties including thermal conductivity, thermal expansion coefficient and viscosity on the optimum relative distance of the orthogonal fins are analysed. Results demonstrate that these physicochemical properties significantly influence the optimum relative distances. The optimum relative distance decreases from ~ 0.1633 to ~ 0.1020 when thermal conductivity increases from $0.1 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ to $1.5 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$. When thermal expansion coefficient of PCM increases from 0.0001 K^{-1} to 0.005 K^{-1} , the corresponding optimum relative distance decreases from ~ 0.1877 to ~ 0.0816 . When viscosity of the liquid PCMs increases from $0.2 \text{ mPa}\cdot\text{s}$ to $80 \text{ mPa}\cdot\text{s}$, the optimum relative distance of orthogonal fins increases from ~ 0.1224 to ~ 0.2245 . The results supply an effective guideline to design an optimum orthogonally structured fins to enhance the average charging rate of organic PCMs with random physicochemical properties.

1. Introduction

Latent heat thermal energy storage systems (LHTES) seem effective to solve uneven spatial and temporal distributions of energy, it can also efficiently recover the waste energy (Mahdi et al., 2019) thus reduce energy consumption (Zheng, 2017). Phase change materials (PCMs) are the core components of LHTES and have been extensively applied in thermal management (Sandra and José, 2020) and energy storage (Faraj et al., 2020). The organic PCMs are significantly inhibited their extensive applications in industrial and civil utilization by their relatively low thermal conductivities (Peng et al., 2019). Investigators strive for efficient techniques to improve their equivalent thermal conductivity thus enhance charging performance of PCMs. Metal fins have attracted many researchers' attention because their incomparable advantages (Bazri et al., 2018).

Metal fins possess many advantages including simple fabrication, high thermal conductivity and relatively low specific heat capacity. Small amount of volumetric fraction can induce high improvement of charging performance. Although the capital cost is relatively high because their high density (Peng et al., 2019), the operation life is relatively long. Both simply (Pu et al., 2020) and complicated fins (Duan et al., 2020) have been applied to enhance the charging performances of PCMs. The influences of the fin numbers (Kamkari and Shokouhmand, 2014), fin arrangements (Nie et al., 2020), fin distributions (Yang et al., 2020), fin inclination angles (Kalapala and Devanuri, 2021), fin structures (De Césaró Oliveski et al., 2021), fin shapes (Yu et al., 2020) and heating conditions (Peng et al., 2020) on the charging characteristics have been conducted. The

optimum structures and inclination angles are obtained by simulations (Peng et al., 2021) and experiments (Kamkari and Groulx, 2018). These optimum fins are only suitable to promote charging performances of PCMs with assigned physicochemical properties (Peng et al., 2021). The influences of PCMs' physicochemical properties on the optimum dimensions of fins have not been deeply investigated.

In current study, the influences of PCMs' significant physicochemical properties including thermal conductivity, thermal expansion coefficient and viscosity of liquid PCMs on optimum relative distances of orthogonal fins that shorten total charging time and enhance average charging rate in a maximum content are numerically discussed and analysed by enthalpy-porosity method (Brent et al., 1988). The detailed results about the variation of the optimum relative distance of orthogonal fins with the change of PCMs' physicochemical properties are displayed clearly. The corresponding mechanism is also demonstrated semi-quantitatively. A rough guideline for predicting appropriate and optimum orthogonal fins to enhance the charging efficiency of organic PCMs with random physicochemical properties is proposed.

2. Problem presentation and simulation method

2.1 Problem presentation

The PCMs-based thermal energy storage system (TES) is simplified as a 2D rectangular enclosure. Both the length and width of the enclosure (made of copper) are 50 mm. A vertical fin and a horizontal fin made of copper compose the orthogonal fins. The length of the horizontal fin is 44 mm. The thickness is 3.0 mm. The length of the vertical fin is 49 mm. The thickness is also 3.0 mm. Aims to obtain the optimum relative distance of the orthogonal fins to enhance the average charging rate of PCMs with variant physicochemical properties in a maximum content, the distance between the horizontal fin and the bottom wall of enclosure ranges from 1.0 mm to 13.0 mm. The corresponding relative distance is 0.0204 to 0.2653. The vertical fin is installed at the middle of the enclosure. The schematic diagram of the orthogonal fins in the PCMs-based TES is displayed in Figure 1(a). The unstructured grid is applied to solve this problem for convenient, the grid generations are displayed in Figure 1(b). The orthogonal fins applied to shorten the total charging time and enhance the average charging rate of organic PCMs has been discussed (Peng et al., 2021). An optimum relative distance has been obtained for a given PCM. When the physicochemical properties of PCMs change, the variation of the optimum relative distance has not been analysed. According to the criterion which obtains the optimum relative distance (Peng et al., 2021), the physicochemical properties of PCMs such as thermal conductivity, thermal expansion coefficient and viscosity seem influence it. The current investigation focuses on the influences of above PCMs' physicochemical properties on the optimum relative distance.

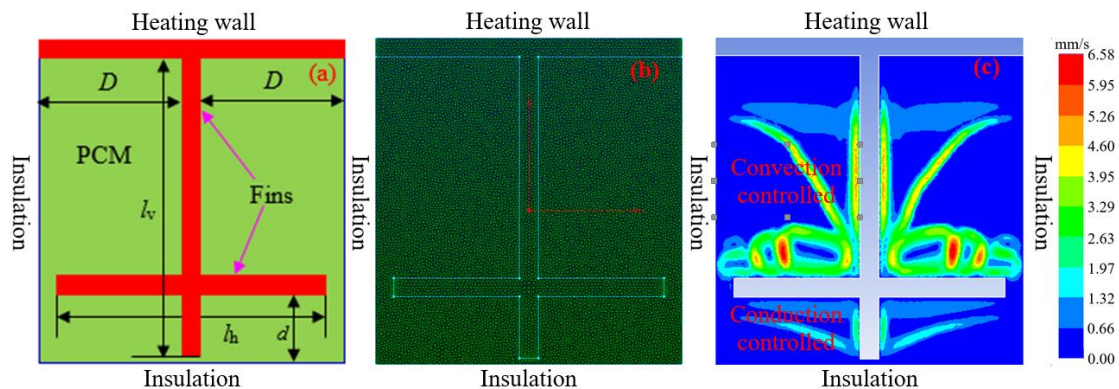


Figure 1: Schematic diagram of PCMs-based TES unit with orthogonal metal fins enhancement system and the grid generations ((a) schematic diagram of the PCMs-based TES, (b) grid generations, unstructured grid, (c) conduction controlled and convection controlled regions during charging)

2.2 Model description and simulation process

Model description

The enthalpy-porosity model (Brent et al., 1988) is applied to solve the charging or melting problem described above. This method has been extensively used to simulate and analyse the charging/discharging processes of PCMs-based TES. A mixed liquid-solid region is defined where the solid phase and the liquid phase are not clearly separable (liquid fraction ranges 0% to 100%) in this model. "Liquid fraction" is applied in this "pseudo" porous zone to instruct the interface. The governing equations include continuity, momentum and energy conservation. The Boussinesq approximation is applied to evaluate the effect of natural convection during the

charging. Total charging time and average charging rate are applied to represent the charging performances. The total charging time of PCMs is defined as the elapsed time that the PCMs are melted completely from the initial state. The average charging rate is defined as the ratio of total charging heat to total charging time. Constant temperature is adopted on heating wall and other walls of the enclosure are adiabatic. The temperature of the heating wall is 90°C. The initial temperature of the PCMs is 20°C. Non-slip boundary conditions are adopted for all the walls. The charging process is completed until all the solid PCMs transfer to liquid PCMs. The finite volume method is employed to solve the governing equations. The SIMPLE algorithm is adopted to calculate the coupling between the pressure and velocity, the scheme of PRESTO! is adopted for pressure correction equations. The momentum and energy equations are discrete by the second order upwind scheme. The residuals of governing equations are respectively 10^{-4} , 10^{-5} and 10^{-10} to check the convergence at every time step. The relaxation factors of pressure, velocity, density, body force and momentum update are respectively 0.3, 0.7, 0.3, 0.3 and 0.1 in simulation for rapid convergence. The detailed calculation procedures can be found in our previous study (Peng et al., 2021).

Model verifications

Grid size and time step independent verifications of above numerical method have been carried out in the previous study of the same authors (Peng et al., 2021). Grid number about 12000 and time step of 0.1 s are economic and efficient to deal with above problem. The model is also verified by comparing the experimental results in other studies (Kamkari and Shokouhmand, 2014) and can be found in the previous study of the same group (Peng et al., 2021). Therefore, the above model can effectively deal with the problem and clarify the influence of the PCMs' physicochemical properties on the optimum relative distance.

Table 1: Physicochemical properties of PCMs and fins in current study (25 °C except specifically explained)

| Properties | PCM | Copper |
|---|---------------|-----------------------|
| Melting point (°C) | 69~73 | 1,083.4 |
| Thermal conductivity ($W \cdot m^{-1} \cdot K^{-1}$) | 0.10~1.50 | 380 |
| Specific heat capacity ($J \cdot kg^{-1} \cdot K^{-1}$) | 2545 | 390 |
| Viscosity of liquid (mPa·s) | 0.2~80 | - |
| Density ($kg \cdot m^{-3}$) | ~900 | 8,960 |
| Latent heat of fusion ($kJ \cdot kg^{-1}$) | ~210 | ~205.2 |
| Thermal expansion coefficient (K^{-1}) | 0.0001~0.0050 | 1.75×10^{-5} |

3. Results and discussions

3.1 Influence of thermal conductivity

The charging process of PCMs-based TES with orthogonal fins under top heating is divided into two regions by the horizontal fin (Peng et al., 2021). Region above the horizontal fin is mainly controlled by convection. Region below the horizontal fin is mainly determined by conduction. The convection intensity is represented by velocity distributions and shown in Figure 1(c). The optimum relative distance is obtained by simultaneously complete the charging process of the two regions (Peng et al., 2021). Thermal conductivity of PCMs greatly affects the heat conduction efficiency in the PCMs and the natural convection intensity in liquid PCMs during charging process thus significantly influences the total charging rate of the two regions. The optimum relative distance of the orthogonal fins to enhance the average charging rate of PCMs-based TES in a maximum content depends on thermal conductivity inevitably. The results are displayed in Figure 2.

From Figure 2, it can be found that high thermal conductivity of PCMs induces short total charging time and high average charging rate because conduction heat transfer in charging is improved. The shortest total charging time is 879 s, the corresponding average charging rate is 839.36 W when the thermal conductivity is $1.50 W \cdot m^{-1} \cdot K^{-1}$. When thermal conductivity decreases to $0.10 W \cdot m^{-1} \cdot K^{-1}$, the shortest total charging time is 2435 s, the maximum average charging rate is only 308.94 W. The optimum relative distance of the orthogonal fins is variant when thermal conductivity changes. Higher thermal conductivity induces smaller optimum relative distance. The optimum relative distances are 0.1633, 0.1429, 0.1225 and 0.1020 when thermal conductivities are $0.10 W \cdot m^{-1} \cdot K^{-1}$, $0.50 W \cdot m^{-1} \cdot K^{-1}$, $0.65 W \cdot m^{-1} \cdot K^{-1}$ and $1.50 W \cdot m^{-1} \cdot K^{-1}$.

According to the criterion, regions divided by horizontal fin in PCMs-based TES are completely charged simultaneously, total charging time becomes shortest. For one thing, conduction heat transfer rate and thermal conductivity is considered as a linear relationship (marked as $q_{cond} \propto \lambda$). Charging rate of the conduction-controlled region is linearly enhanced. For another, thermal conductivity also strongly influences natural convection intensity in liquid PCMs in charging. Convection heat transfer rate increases as a power law (approximately $q_{conv} \propto \lambda^{2/3}$) with the increase of thermal conductivity (Incropera and DeWitt, 2002). Natural convection is intense in the upper region but that is insignificant in lower region. When thermal conductivity of

PCMs increases, the total heat transfer rate (consists of conduction and convection heat transfers) of the upper region increases more rapidly than that of lower region. The total charging time of the upper region is shortened more rapidly than that of the lower region. Charging process of the two regions becomes not simultaneously complete. The optimum relative distance of orthogonal fins becomes non-optimum. The area of the upper region needs to increase while that of the lower region needs to reduce. The relative distance needs to reduce to maintain orthogonal fins in optimum dimension.

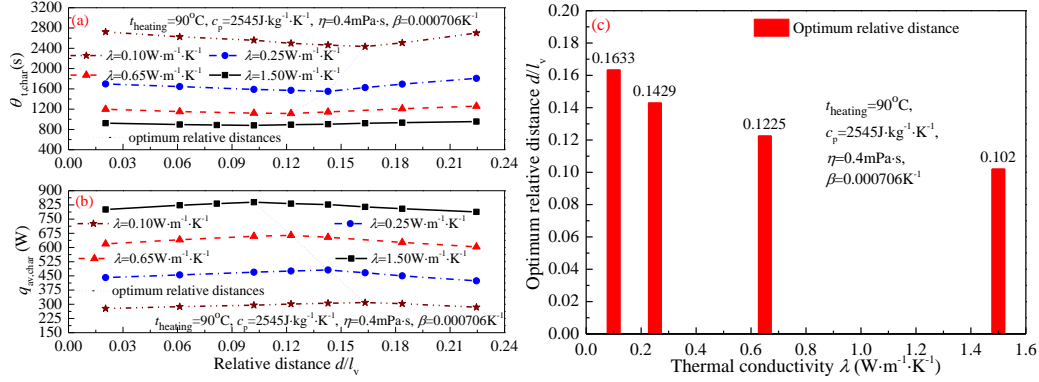


Figure 2: Influence of thermal conductivity on total charging time $\theta_{t,\text{char}}$ (a), average charging rate $q_{\text{av, char}}$ (b) and optimum relative distance d/l_v (c) in PCMs-based TES with orthogonal fins (other properties remain constant, the subscript in $q_{\text{av, char}}$ means average charging, that in $\theta_{t,\text{char}}$ means total charging)

3.2 Effect of thermal expansion coefficient

Thermal expansion coefficient of PCMs only affects the natural convection heat transfer rate in the liquid PCMs during charging but hardly influences the conduction heat transfer. The thermal expansion coefficient of PCMs affects the total charging time of the upper region determined by natural convection, the average charging rate and the optimum relative distance. The results are illustrated in Figure 3.

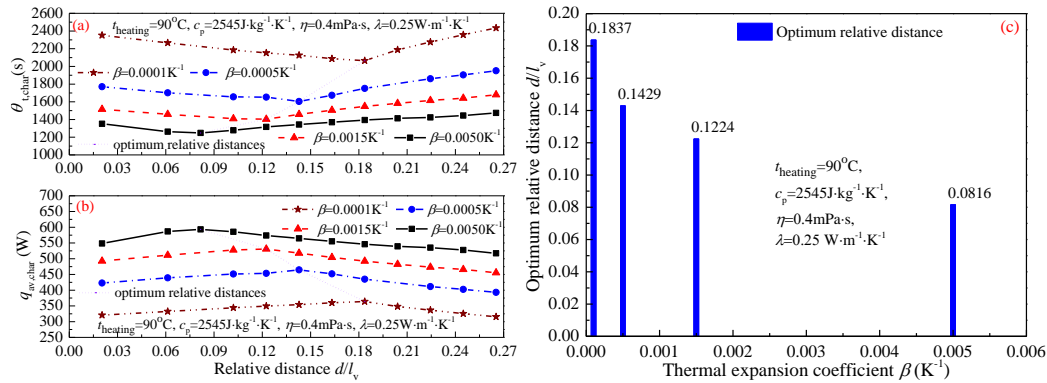


Figure 3: Effect of thermal expansion coefficient on total charging time (a), average charging rate (b) and the optimum relative distance (c) in PCMs-based TES with orthogonal fins (other properties are constant)

The results in Figure 3 demonstrate that when thermal expansion coefficient increases, total charging time of PCMs is shortened and average charging rate increases. The shortest total charging time decreases from 2065 s to 1248 s when thermal expansion coefficient increases from 0.0001K^{-1} to 0.0050K^{-1} , the maximum average charging rate increases from 364.06 W to 593.29 W. The optimum relative distance decreases from 0.1837 to 0.0816. Thermal expansion coefficient only affects natural convection heat transfer rate with a power law that is $q_{\text{conv}} \propto \beta^{1/3}$ (Incropera and DeWitt, 2002). When thermal expansion coefficient of PCMs increases, natural convection in liquid PCMs during charging becomes intense, total charging time of convection determined region becomes shorten while that determined by conduction is almost constant. The area of conduction-determined region (lower region) needs to reduce to simultaneously complete the charging of two regions, the optimum relative distance of orthogonal fins decreases.

3.3 Influence of viscosity

Viscosity instructs the intensity of the fluid flow thus influences the charging performance of PCMs and the optimum relative distance of the orthogonal fins. The results are illustrated in Figure 4.

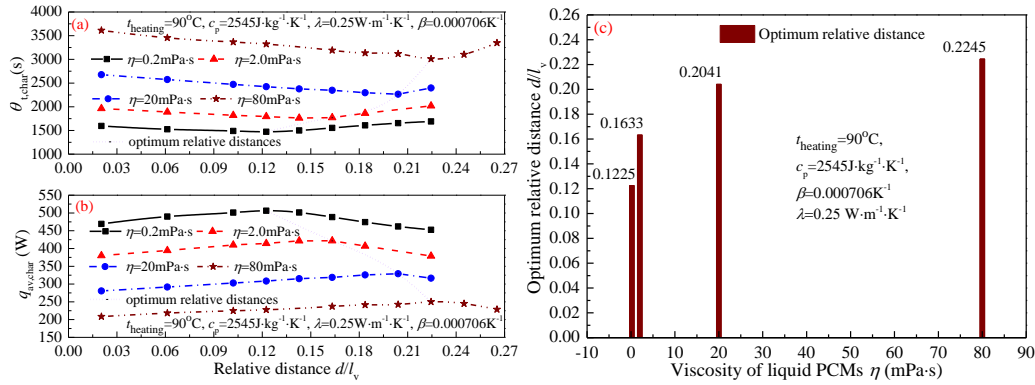


Figure 4: Influence of viscosity on total charging time $\theta_{t, char}$ (a), average charging rate $q_{av, char}$ (b) and optimum relative distance d/l_v (c) in PCMs-based TES with orthogonal fins (other properties are constant)

The results in Figure 4 demonstrate high viscosity prolongs total charging time and reduces average charging rate of PCMs. When the viscosity of liquid PCMs is 0.2 mPa·s, the shortest total charging time is 1472 s and average charging rate is 506.30 W. The shortest total charging time becomes 3009 s and average charging rate reduces to 250.05 W when viscosity of PCMs increases to 80 mPa·s. The optimum relative distance of orthogonal fins increases from 0.1225 to 0.2245. Although the increasing viscosity induces longer total charging time and lower average charging rate, optimization of orthogonal fins' dimensions is still necessary.

Natural convection heat transfer rate relates with viscosity as a power law that is $q_{conv} \propto \eta^{-1/3}$ (Incropera and DeWitt, 2002), the increasing viscosity induces obvious decrease of natural convection heat transfer rate, conduction heat transfer rate is hardly affected by viscosity. Total charging rate of upper region reduces more rapidly than that of lower region because the charging of upper region is determined by natural convection. The relative distance of orthogonal fins needs to increase to complete the charging of two regions simultaneously. As a result, when the viscosity of the liquid PCMs increases from 0.2 mPa·s to 80 mPa·s, the optimum relative distance increases from 0.1225 to 0.2245.

Other physicochemical properties of organic PCMs including specific heat capacity, density and latent heat of fusion also influence the optimum relative distance of orthogonal fins, will be conducted in future.

4. Conclusions

Physicochemical properties of PCMs affect average charging rate and the optimum relative distance of orthogonal fins system in the charging of PCMs-based TES unit. Their influences are analysed by enthalpy-porosity method. Results illustrate that higher thermal conductivity and thermal expansion coefficient of PCMs induce higher average charging rate. When viscosity of PCMs increases, average charging rate decreases. Higher thermal conductivity and thermal expansion coefficient induce smaller optimum relative distances. Higher viscosity induces higher optimum relative distances. Although other physicochemical properties of PCMs are not considered, the results supply an effective thinking to design the optimum orthogonal fins to enhance the average charging rate of PCMs with random physicochemical property in the maximum content.

Nomenclature

c_p – specific heat capacity, $\text{J}/(\text{kg}\cdot\text{K})$
 d, D – distance, m
 h – enthalpy, kJ/kg
 l, L – length, m
 q – heat transfer rate, W
 t – temperature, $^\circ\text{C}$

β – thermal expansion coefficient, $1/\text{K}$
 γ – liquid fraction
 δ – fin thickness, m
 η – viscosity, $\text{Pa}\cdot\text{s}$
 θ – time, s
 λ – thermal conductivity, $\text{W}/(\text{m}\cdot\text{K})$

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