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Optimization of filler distribution for organic phase change material composites: Numerical investigation and entropy analysis

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HIGHLIGHTS

- We numerically modeled heat transfer with phase change for organic PCM.
- Phase change time for PCM composite is affected by the filler distribution.
- A non-uniform distribution of filler may lead to a better performance.
- Optimal filler distribution can reduce the phase change time significantly.
- A shorter phase change time is correlated with a lower entropy generation rate.

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ABSTRACT

Organic phase change materials have been attracting great attentions for their promising potential in thermal energy storage applications. Due to their poor thermal conductivity and thermal diffusivity, thermally conductive fillers are often added to form composites to enhance the thermal performance. To achieve the optimized performance without sacrificing the thermal capacity, a novel numerical methodology has been developed to model the thermal behavior of phase change material composites, which has been validated by the experimental results for pure n-octadecane and n-octadecane/expanded graphite composites. Effects of different filler concentration distributions have been analyzed and compared. It is found that the phase change time is significantly affected by the filler distribution. An optimal polynomial filler distribution can reduce the phase change time by more than 50% with the same filling content, compared with the uniform distribution. Entropy analysis indicates that a shorter phase change time is correlated with a lower entropy generation rate.

1. Introduction

Thermal energy storage systems, particularly the systems based on phase change materials (PCMs), have attracted increasing attentions in recent decades for their unique energy transforming property. PCMs have shown great potential in numerous engineering applications, such as heat pump [1], solar engineering [1], and electrical device cooling system [2]. PCM wall is also believed suitable for green building and effective in shifting the heating and cooling load to off peak electricity periods [3–5]. However, PCMs, especially those widely used organic PCMs, generally have an extremely low thermal diffusivity and thermal conductivity [6,7], which significantly limit the performance of thermal energy storage. High thermal diffusivity is requested for PCM units to achieve a high charge and discharge efficiency. Many approaches to increase the thermal conductivity have been proposed in the last decade. External fin structures are often used to enhance the heat exchange efficiency between PCM units and the surrounding through enlarging surface area [8,9]. Adding highly thermally conductive fillers into PCMs to form shape-stabilized composites is widely recognized as an efficient solution. The most widely used fillers are carbon-based materials, such as carbon nanotube [10], carbon nanofiber [10,11], natural graphite, expanded graphite [12,13], nano-graphite [14] and exfoliated graphite [15], due to their high thermal conductivity and low density. Apparently, with more filler embedded, the thermal energy storage and release rate will be higher, but the overall thermal capacity and energy density will be reduced. For applications with rigorous constraints on volume and weight, such as vehicles and wall materials, less PCM content leads to less energy storage capacity. So it is desirable to achieve optimized thermal performance with the same filler

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content and fin structure. However, currently there are very few systematic optimization guidelines for the optimization of system design.

In order to optimize the thermal performance of latent heat storage system, it is necessary to develop a model that can accurately describe the thermal transport process in phase change materials. Phase change of a material is often described as a moving boundary problem for partial differential equations, where the phase interface can move with time. By considering a simple one-dimensional semi-infinite system [16], the so-called classic Stefan problem can be solved analytically. However, the assumption of a semi-infinite system is invalid for many real systems and the uncertainties introduced by this assumption are unclear. On the other hand, the solutions for the classic Stefan problem rely on the accurate determination of phase change temperature and many of them adopt a single-point phase change temperature for convenient calculation. This is reasonable for crystalline phase change materials. However, many widely used PCMs are semi-crystalline organic PCMs, which do not have a well-defined phase change point due to their entangled molecular chain structures. Therefore, an accurate model that can be applied to organic PCMs is demanded.

In this paper, we intend to optimize the energy efficiency of thermal storage system with a fixed amount of fillers and PCM. A comprehensive model designed for finite organic PCM systems will be firstly presented, which considers the phase transition temperature range of organic PCMs and material property changes accompanying with the temperature variation. Experiments on pure n-octadecane and n-octadecane/expanded graphite composites have been carried out and the obtained results show a good agreement with the theoretical predictions, confirming the accuracy of this model. Then this model is applied to analyze the effect of different filler distribution and the optimum distribution is then explored. To explain why different filler distributions affect the thermal performance of the latent heat systems, the entropy analysis is performed and the relationship between the entropy generation rate and the thermal performance of the latent heat system is discussed.

2. Numerical modeling of one-dimensional phase change in organic PCMs

The governing equation for one-dimensional heat transfer with phase change is shown as below,

$$\begin{cases} \dfrac{\partial^2 T}{\partial x^2} = \dfrac{1}{\alpha(x,T)}\dfrac{\partial T}{\partial t} \\ k(x)\left.\dfrac{\partial T}{\partial x}\right|_{x=0} = h(T_{sur}-T) \\ T(x,0) = T_i \end{cases}, \tag{1}$$

where T is the temperature, k is the thermal conductivity, α is the thermal diffusivity and is defined as $k/(\rho c)$ (ρ and c are the density and specific heat, respectively), h is the convective heat transfer coefficient, T_i is the initial temperature, T_{sur} is the surrounding temperature. The third class boundary condition is considered for general case. It can be easily converted to the first class boundary condition by changing h to infinity. This model has been widely used for crystalline materials. Enthalpy method [17] and effective capacity method [18] are widely applied in this model to specify the thermal properties during the one-dimensional phase change process. Although both methods can quantitatively describe the phase change for crystalline materials, they have drawbacks when applied to organic PCMs, since they assume the phase change only takes place at one specific temperature. The sectional description of material properties according to phase status also introduces difficulty in obtaining converged temperature result.

Currently most widely used PCMs are organic PCMs. In this study, n-octadecane is selected as an example without losing generality. Due to the semi-crystalline nature of n-octadecane, its phase change behavior is different from crystalline materials. As illustrated in Fig. 1, the semi-crystalline organic PCM has a much wider phase transition temperature range and therefore it is difficult to define a single-point phase change temperature. In the literatures, the onset temperature was often used as the phase change temperature to conduct the analysis [19]. According to the characteristic of organic PCMs shown in Fig. 1, a latent heat model has been constructed based on a Gaussian function, as shown in Eq. (2), where $C_{p,eff}$ is the effective heat capacity, C_{pcm} is the conventional specific heat L is the latent heat, T_m is the peak temperature, and τ is the temperature constant related to material microstructure. Specifically, the phase transition temperature range equals to 4τ, as shown in Fig. 1. Compared with the C_{pcm}, $C_{p,eff}$ is an overall evaluation for heat storage ability, considering extra heat storage during phase change over C_{pcm} because of latent heat.

$$C_{p,eff} = \frac{L}{\sqrt{2\pi}\tau} Exp\left(-\frac{(T-T_m)^2}{2\tau^2}\right) + C_{pcm} \tag{2}$$

The variation of density, thermal conductivity and specific heat with respect to the temperature also need to be modeled accordingly. The thermal properties of organic PCMs are assumed to follow the variation tendency shown in Eqs. (3) and (4) when the temperature is beyond the transition range, where Y can represent the density, the thermal conductivity or the specific heat. The subscripts s and l indicate the solid phase and liquid phase, respectively. $\mu(T)$ is a coefficient function which only changes linearly within the transition range in consistent with effective thermal capacity model, and the first derivative is continuous as well.

$$Y = Y_s + \mu(T)(Y_l - Y_s) \tag{3}$$

$$\mu(T) = \begin{cases} 1, & T \ll T_m - 2\tau \\ 0, & T \gg T_m + 2\tau \end{cases} \tag{4}$$

Given above analysis, a novel material model is then constructed by applying error function which is the integration of Gaussian function. So the thermal properties of pure PCM are described by Eqs. (5)–(7), in which the phase transition process is considered. Here k is the thermal conductivity, ρ is density, C is the specific heat, and τ is the temperature constant the same as shown in Eqs. (2) and (3).

$$k_{pcm} = k_s + \frac{k_l - k_s}{2}\left[1 + Erf\left(\frac{T-T_m}{\sqrt{2}\tau}\right)\right] \tag{5}$$

$$\rho_{pcm} = \rho_s + \frac{\rho_l - \rho_s}{2}\left[1 + Erf\left(\frac{T-T_m}{\sqrt{2}\tau}\right)\right] \tag{6}$$

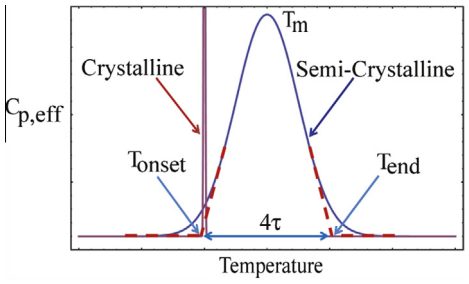

Fig. 1. Schematic of effective thermal capacity of crystalline and semi-crystalline PCMs.