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Phase-Field Modeling of Multiple Phase Change Materials (PCMs)

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Micro Abstract
A latent heat storage medium with various heat transfer enhancement techniques is being studied. The methods include using multiple immiscible PCM constituents with different melting temperatures and adding highly conductive fins. The system is modeled using the finite element method and the phase-field method is employed as a numerical approach to account for the phase change process. This method relies on specification of free energy density function and employs a phase-field variable that defines the state of the material, and it also allows for realistic simulations of dendritic growth (including anisotropy) and other solidification microstructures.

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Introduction

Energy storage is an important process for conserving available energy and improving its utilization. A well-designed energy storage system offers the advantages of increasing the efficiency, and reducing the energy costs, equipment size, pollutant emissions [1]. Latent energy storage with phase change materials (PCMs) is one of the most efficient ways of storing available energy because of its high energy storage density, compact storage space and isothermal nature of the storage process with small temperature variations [2].
Although PCMs are widely used in buildings, electronics, automobiles and solar systems [3], their low thermal conductivity is the main problem that limits their heat transfer rate. However, this problem may be overcome by the use of heat transfer enhancement techniques [4].
The problem of predicting the behavior of phase change systems is challenging due to its non-linear nature at moving interface and the different thermo-physical properties between the solid and liquid phases. The phase change formulation are classified into: sharp interface model (the Stefan problem), enthalpy method and phase field method. The phase-field method employs a phase-field variable, e.g., ϕ, which is a function of position and time, to describe whether the material is liquid or solid. It relies on specification of free energy density function which is the main driving force for the movement of the phase transition region [5]. It eliminates the heat flux or energy balance at the interface and allows a mushy zone (smooth interface) between the two phases [6]. Moreover, this approach is found to be very effective in obtaining realistic simulations of dendritic growth in super-cooled melts during solidification for isotropic and anisotropic cases [5, 7].
The present work aims to investigate the effect of various heat transfer enhancement techniques on the energy storage process. PCMs with multiple configurations and extended surfaces (fins) are simulated using the finite element method and employing the phase-field technique.

1 Heat transfer enhancement methods(Multiple PCMs and finned Surface)

The phase-field model is applied to study the heat transfer and melting process of different PCM configurations. The free energy functional is defined to guarantee local positive entropy

production [7]. The phase-field equation for pure isotropic material is given by:

$$\frac{1}{M}\frac{\partial \phi}{\partial t} = \operatorname{div}\left(\epsilon^2 \operatorname{grad}\phi\right) - W g'(\phi) + Q(T)\, p'(\phi)\,. \tag{1}$$

In this, $g(\phi) = \phi^2(1-\phi)^2$ is a double well function having local minimima at $\phi = 1$ (liquid) and $\phi = 0$ (solid), and $p(\phi) = \phi^3(6\phi^2 - 15\phi + 10)$ is an interpolating function. The parameters ϵ and W are related to the interface thickness δ and the surface tension of the material (σ) by $\epsilon = \sqrt{6\,\delta\,\sigma}$ and $W = 3\frac{\sigma}{\delta}$. The interface mobility M can be obtained through $M = \frac{\alpha\, T_m}{6\,\delta\, L}$, with L is the latent heat of fusion per unit volume, α is the kinetic coefficient at the ineterface and T_m is the melting temperature of the material. $Q(T)$ is the thermal driving force represented by $Q(T) = L\frac{(T-T_m)}{T_m}$ [7].
The continuity and momentum equations are used to simulate the behavior of the PCM in liquid phase, considering the effects of natural convection. The governing equations for the heat transfer melting process are represented by the mass conservation (eq. 2), momentum balance (eq. 3), energy conservation (eq. 4) and the phase-field equation (eq. 1) discussed above:

$$\operatorname{div}\mathbf{u} = 0\,, \tag{2}$$

$$\rho\Big(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\operatorname{grad}\mathbf{u}\Big) = \mu\operatorname{div}(\operatorname{grad}\mathbf{u}) - \operatorname{grad}p + A_s\,\mathbf{u} + \mathbf{k}\,F\,, \tag{3}$$

$$C_p\Big(\frac{\partial T}{\partial t} + \mathbf{u}\operatorname{grad}T\Big) = \operatorname{div}(K\operatorname{grad}T) - L\frac{\partial \phi}{\partial t}\,. \tag{4}$$

Herein, p is the pressure, ρ is the density, μ is the dynamic viscosity and $\mathbf{k}$ is a unit vector in a direction opposite to that of the acceleration of gravity. $F = g\rho\beta(T - T_m)$ is the buoyancy force with g is the gravitational acceleration and β is the thermal expansion coefficient. A_s is a step function that insures the velocities reduce gradually from a finite value in the liquid to zero in the solid over the computational cell that undergoes phase change [8, 9]. C_p is the volumetric specific heat capacity and K is the thermal conductivity.

1.1 Numerical results and discussion

The effect of heat transfer techniques (Multiple PCMs and extended surface) on the energy storage process is investigated in four cases: single PCM, 3-PCM composite slab, 2-PCM matrix slab and single PCM slab with highly conductive fins. The PCM chosen is isotropic and homogeneous (Praffin wax) and the melt flow is assumed laminar and incompressible. The PCMs in all configurations are initially in the solid state and are heated from the left wall. The other walls are kept insulated. For the single PCM slab the height and width of the domain are $L = H = 0.05\,m$. Figure 1 shows the solid-liquid interface with the effect of natural convection at $time = 600\,s$ and $time = 1200\,s$. It is clear that the interface is affected by the motion of the melted fluid, where the hot fluid moves to the top, replacing the colder fluid.
Following this, computations are performed for the 3-PCM and 2-PCM-matrix composite slabs. The melting temperatures are assigned such that their average equals the melting temperature of the single slab. All the composite slabs arrangements were simulated for a melting time of $time = 1200\,s$ (Figure 2) to compare the energy charged with that for the single slab. Table 1 presents the cumulative energy charged for the different configurations, where it is observed that the highest enhancement in the energy stored is found for the 3-PCM slab with series arrangement.
The last part of the simulation is to study the effect of adding highly conductive metal fins to the left wall of the single PCM slab. As shown in Figure 3 the addition of the fins played an important role in accelerating the melting process. The PCM in the region near the fins started

melting rapidly due to the presence of high amount of heat conducted through the fins. Using this method the PCM was completely melted by 1200 s, the thing that indicates that addition of fins or extended surface is the most effective among the methods detected in this study (Table 1).

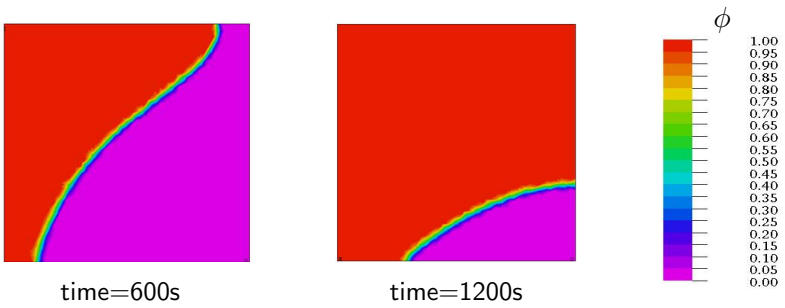

Figure 1. Solid-liquid interface progress

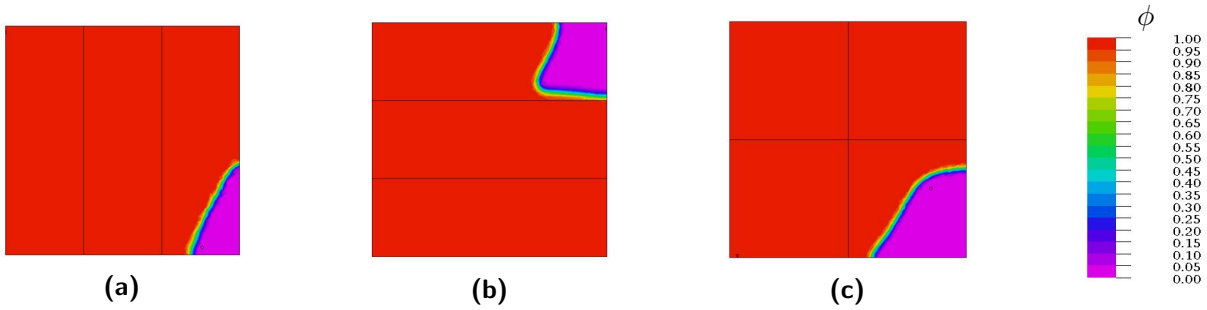

Figure 2. Interface position at $time = 1200s$ for the series (a), parralel (b) and matrix (c) configurations

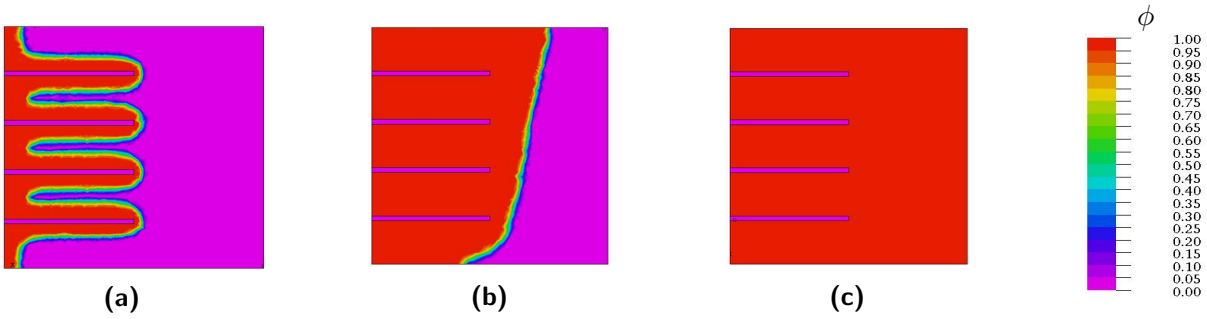

Figure 3. Solid-liquid interface progress in the single PCM slab with fins at time $25s$ (a), 200s (b) and 1200s (c)

Slab Type	Melting temp. (K)	Liquid fraction	Q_{latent} (J)	Q_{total} (J)	Enhancement %
Single	333	0.84	1.64×10^5	2.53×10^5	———
Series (3-PCM)	L=318, M=333, R=348	0.925	2.15×10^5	2.92×10^5	15.4
Parallel (3-PCM)	T=348, M=333, B=318	0.914	1.79×10^5	2.72×10^5	7.5
Matrix (2-PCM)	LD=338, RD=328	0.89	1.74×10^5	2.69×10^5	6.32
Single with fins	333	1	2.28×10^5	3.48×10^5	37.55

L:left, R:right, L:low, T:top, M:medium, D:diagonal

Table 1. Comparison of the energy charged for the different configurations

Conclusions

The phase-field model is an effective method for simulating the solidification/melting process of PCMs. Composite PCM slabs with different melting temperatures or adding highly conductive fins can significantly enhance the total energy charged in the PCMs, depending on the type of arrangements and the thermo-physical properties. Also, the effect of buoyancy driven natural convection plays an important role in the amount of energy charged and energy enhancement during the PCM melting process.

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