

Numerical Simulation of the Solidification Process of Nanofluids

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ABSTRACT

The effects of mass transfer of the nanoparticles on the morphology of the solid-liquid interface and evolving concentration field during solidification of colloids have been reported. The numerical method that has been used was based on the one-fluid-mixture model. The model takes into account the thermal as well as the solutal convection effects. A differentially-heated square cavity was used in the simulation. The colloid was composed of a suspension of copper nanoparticles in water. The temperature difference between the hot and cold sides was 5 degrees centigrade and the loadings of the nanoparticles that have been used in the simulation were 1%, 5%, and 10% by mass. The solid-liquid interface for the case of nanofluid with 10 wt% of nanoparticles evolved from a planar shape at the beginning of the solidification process to a dendritic shape as the solidification process proceeds in time.

Keywords: Nanofluids, colloidal, solidification, mushy zone, dendrites.

1 INTRODUCTION

Investigations of nanofluids which can be considered as a class of colloidal suspensions have been reported by the scientific community for the past few years. The improved thermophysical properties of nanofluids has promoted these colloids to be considered as serious candidates to replace conventional heat transfer fluids. More recently, due to the great demand for improvement of thermal energy storage systems, Khodadadi and Hosseinizadeh [1] proposed the idea of suspending nano-size particles in phase change materials (PCM), in order to improve their properties. This concept is also known as nanoparticle enhanced phase change materials (NEPCM).

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Ideally, NEPCM can go through cycles of melting and solidification through their life span. Modeling of those processes will enable one to better predict their performance. Generally, there are two class of methods that are found in the literature. The first one considers the interaction of a single particle with the solid-liquid interface such as [2] and other one considers the particles as a concentration field and uses the same methods that are used to simulate multi-component mixtures such as binary alloys, and aqueous solutions such as [3]. Peppin et al. [3] developed a similarity solution for the volume fraction and the temperature ahead of the planar interface in the case of unidirectional solidification for hard sphere colloidal suspensions by considering the particles as a concentration field. The same method has been used to solve the solidification of binary mixtures. They developed relations for the mass diffusivity of the particles as a function of the volume fraction using the classical theory of colloidal suspensions. They assumed also that the growth velocity was very small and all the particles have been rejected. They found that for very small particles, from the solid Brownian diffusion is important and the concentration and temperature profiles resemble those observed during alloy solidification. Also, in certain cases they found that the interface can become unstable due to the constitutional supercooling. However, for large particles Brownian diffusion is weak or absent, and a porous medium is formed against the freezing front. Due to the fact that the porous medium is supercooled, it allows for the morphological instability of the interface.

To the best knowledge of the authors there is no study in the literature that considers the solidification of colloidal suspensions, which takes into account the effects of the thermal and solutal convections. So, the objective of the present paper is to employ the one-fluid mixture model, which will account for the complicated convection and phase change process during the dendritic solidification of a NEPCM colloidal suspension. For this purpose, the physical system of a square cavity with vertical sides kept at uniform temperatures has been selected. Initially, the cavity is occupied with water/copper nanoparticles. The suspension is solidified by lowering the right wall temperature below the liquidus temperature that corresponds to the initial concentration.

2 MATHEMATICAL MODEL

The model equations are obtained by integrating the microscopic conservation equations over a small volume element. The volume element is occupied simultaneously by the liquid and solid phases of the colloidal suspension. The model is based on the one-fluid mixture model as described in [4] and implemented by the commercial code FLUENT which uses the enthalpy method, and calculates liquid fraction explicitly. The averaged equations in non-dimensional form that are valid in the liquid and solid regions as well as the mushy zone, can be summarized as the following:

Continuity:

$$\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} = 0, \quad (1)$$

x-direction Momentum:

$$\frac{\partial \bar{u}}{\partial \tau} + (\bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y}) = -\frac{\partial \bar{P}}{\partial x} + \text{Pr} \nabla^2 \bar{u} - \frac{C(1-\lambda)^2 \alpha}{\lambda^3 \rho L} \bar{u} \quad (2)$$

y-direction Momentum:

$$\frac{\partial \bar{v}}{\partial \tau} + (\bar{u} \frac{\partial \bar{v}}{\partial x} + \bar{v} \frac{\partial \bar{v}}{\partial y}) = -\frac{\partial \bar{P}}{\partial y} + \text{Pr} \nabla^2 \bar{v} + \text{Ra} \theta \text{Pr} - \frac{C(1-\lambda)^2}{\lambda^3 \rho L} \bar{v} \quad (3)$$

Thermal Energy:

$$\frac{\partial \theta}{\partial \tau} + (\bar{u} \frac{\partial \theta}{\partial x} + \bar{v} \frac{\partial \theta}{\partial y}) = \nabla^2 \theta - \left(\frac{\partial (1/Ste)}{\partial \tau} \right) + \frac{\partial}{\partial x} (\bar{u}/Ste) + \frac{\partial}{\partial y} (\bar{v}/Ste) \quad (4)$$

Species:

$$\frac{\partial \phi_w}{\partial \tau} + (\bar{u} \frac{\partial \phi_w}{\partial x} + \bar{v} \frac{\partial \phi_w}{\partial y}) = \nabla \cdot \left[\frac{1}{Le} \nabla \phi_w + \frac{1}{Le_T} \frac{\nabla \theta}{\theta} \right] \quad (5)$$

By denoting fluid and particles with subscripts f and p , respectively, the thermal conductivity of the NEPCM can be computed from the following relation:

$$k_1 = \frac{k_p + 2k_f - 2\phi(k_f - k_p)}{k_p + 2k_f + \phi(k_f - k_p)} \quad (6a)$$

$$k_2 = K(\rho C_p) \sqrt{u^2 + v^2} \phi d_p \quad (6b)$$

$$k = k_1 + k_2 \quad (6c)$$

The Brownian diffusivity is calculated from:

$$D_B = \frac{T k_B}{3\pi \mu} (1-\phi)^6 \frac{d(\phi)}{d\phi}, \quad (7a)$$

And for spherical nanoparticles we have:

$$z(\phi) = \frac{1 + (4 - \frac{1}{0.64})\phi + (10 - \frac{4}{0.64})\phi^2 + (18 - \frac{10}{0.64})\phi^3}{1 - \frac{\phi}{0.64}} \quad (7b)$$

Equations (7a-b) are obtained from [3]. The thermophoretic diffusivity is computed from following relation :

$$D_T = \beta_k \frac{\mu}{\rho} \phi, \quad (8)$$

The rest of the thermal physical properties of the NEPCM are determined by using a mixture law.

At the liquid-solid interface, the following relation holds with subscripts l and s referring to the liquid and solid phases, respectively:

$$(\phi_{ws})_{interface} = k_0 (\phi_{wl})_{interface} \quad (9)$$

The geometry that has been selected is shown in Fig 1. The computational domain consisted of 10,000 equally-spaced cells and the time step varied from 0.01 to 0.1 sec. The total number of time steps was 20,000 steps which were sufficient to cover the time span in which all the solidification phenomenon's occurs. The convergence criteria for each time step was that the residuals of the continuity and momentum reached a value below 10^{-5} and those for solute and thermal energy were below 10^{-7} .

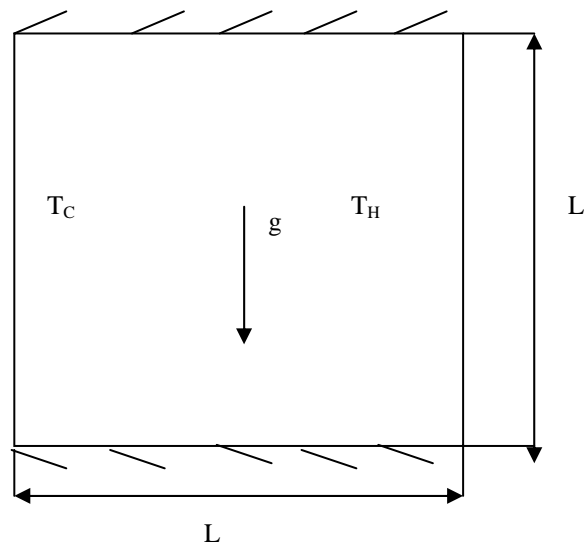


Figure 1 The geometry of the physical model

Benchmarking of the model was conducted by comparing to the detailed one-component melting study by Hannoun et al. [5] of a differentially-heated square cavity. The interface locations after 100 and 200 seconds of initiation of melting are shown in Fig 2. Very good agreement between the results of the model used here and the computational results of [5] is observed.

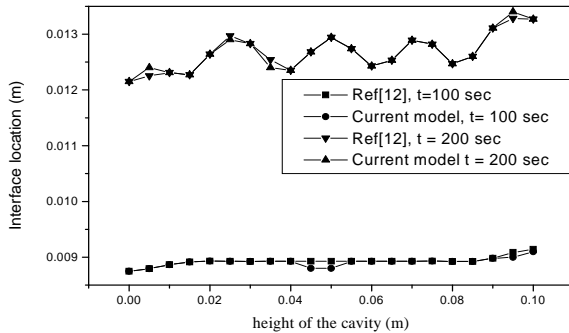


Figure 2 Comparison between the predicted values of the solid-liquid interface and those of Ref [5] after $t = 100$ and 200 sec.

3 RESULTS

The numerical investigations were carried out for the case of unidirectional solidification of water with copper nanoparticles NEPCM contained within a square cavity with the following operational parameters ($\theta_H = 1$, $\theta_C = 0$, and, with $\theta_{initial} = 0.2$) and with the following nanoparticles mass fractions 1%, 5% and 10%. Copper was chosen since a similar colloid was studied earlier [1]. The diameter of the spherical nanoparticles was 10 nm and the segregation coefficient was set to $k_o = 0.1$. As for thermal conductivity of copper, a value for bulk copper was used and quantum effects were not considered.

As shown from Fig. 3, the interface tends to be planar at the early stages of the solidification process, however at later times the solid-liquid interface assumes a dendritic shape due to the phenomena of constitutional supercooling which has been observed experimentally during colloidal solidification [3]. Fig. 4 shows the development of concentration field. It is clearly shown that at $t = 100$ s, concentration is nearly uniform throughout the domain except near the interface. However, at $t = 1000$ sec, the nanoparticles move away from the interface due to the solutal convection and segregate in the space between the dendrites.

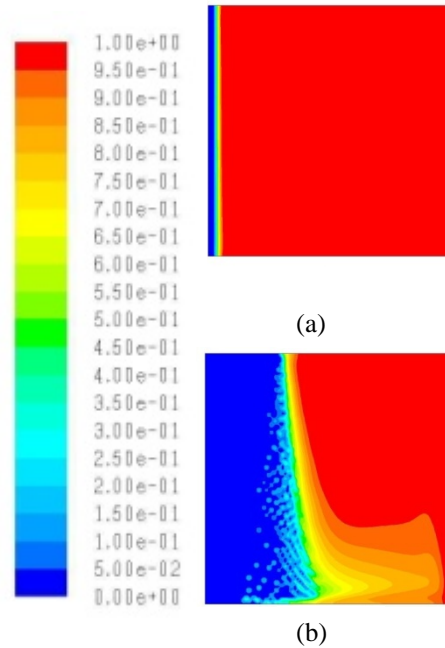


Figure 3 Development of the liquid fraction field at different time instants: (a) 100 s and (b) 1,000 s for an initial concentration field of 10 percent.

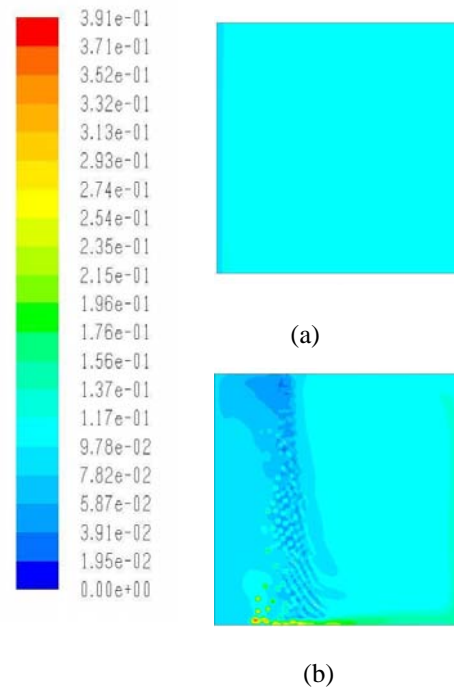


Figure 4 Development of the nanoparticle concentration field at different time instants (a) 100 s, and (b) 1,000s, for an initial concentration field of 10 percent.

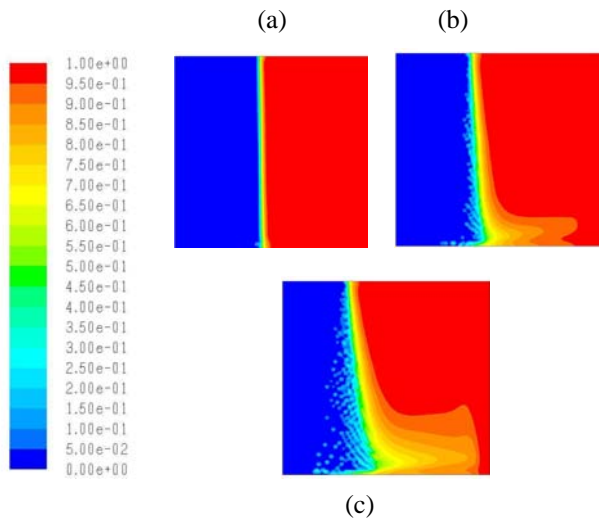


Figure 5 Comparison between the contours of the liquid fraction for the case of (a) $\phi_w = 1\%$ and (b) $\phi_w = 5\%$ and (c) $\phi_w = 1\%$ after $t=1000$ s.

As shown in Fig 5, as the initial nanoparticles concentration increases the shape of the solid-liquid interface changes from a planar shape to a dendritic shape.

4 CONCLUSIONS

The solidification process of copper–water nanofluid has been investigated. It has been observed that the movement of the nanoparticles significantly affect of the shape of the interface. Also it has been shown that solutal convection plays a role in the distribution of the nanoparticles.

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NOMENCLATURE

L	Length of enclosure (m)	Ra	Rayleigh number $\frac{g\beta(T_H - T_C)L^3}{\nu\alpha}$
D_B	Brownian Difusivity (m^2s^{-1})	L_h	Latent heat
		Ste	Stefan number , $\frac{c_p(T_H - T_C)}{L_h}$

Le	Lewis number (α/D_B)	Pr	Prandtl number, $\frac{\mu c_p}{k}$
Le_T	(α/D_T)	\bar{u}	uL/α
T	temperature	\bar{v}	vL/α
u	Velocity in x direction	θ	$(T-T_C)/(T_H-T_C)$
v	Velocity in y direction	τ	$\frac{t\alpha}{L^2}$
α	Thermal diffusivity	β	Thermal expansion coefficient

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