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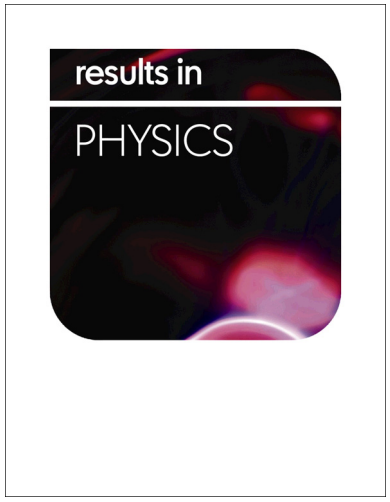

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Effects of Nanoparticles on Melting Process with Phase-Change Using the Lattice Boltzmann Method

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ABSTRACT

In this work, the problem of nanoparticles dispersion effects on coupled heat transfer and solid-liquid phase change has been studied. The lattice Boltzmann method (LBM) enthalpy-based is employed. The collision model of lattice Bhatangar-Gross-Krook (LBGK) is used to solve the problem of 1D melting by conduction. On the other hand, we use the model of multi-distribution functions (MDF) to calculate the density, the velocity and the temperature for the problem of 2D melting by free convection, associated with different boundary conditions. In these simulations, the volume fractions of copper nanoparticles (0-2%) added to water-base fluid and Rayleigh numbers of 10^3 to 10^5. We use the Chapman-Enskog expansion to derive the governing macroscopic quantities from the mesoscopic lattice Boltzmann equation. The results obtained by these models have been compared to an analytical solution or other numerical methods. The effects of nanoparticles on conduction and natural convection during the melting process have been investigated. Moreover, the influences of nanoparticles on moving of the phase change front, the thermal conductivity and the latent heat of fusion are also studied.

Keywords: Lattice Boltzmann Method, Nanofluids, conduction melting, convection melting, BGK Collision Model.

Introduction

The nanofluid is defined as a diluted fluid with nanoparticles [1]. If nanoparticles with high thermal conductivity are suspended in a base fluid with low thermal conductivity, the effective thermal conductivity and the convective heat transfer coefficient of the base fluid will be enhanced. For example, the thermal conductivities of nanoparticles such as Al_2O_3, CuO, Cu, SiO, TiO, are much higher than thermal conductivities of their base fluids [2-9]. Khanafer et al. [10] studied enhancement of the heat transfer using nanofluids in a 2D enclosure. Also, nanoparticles are employed a rectangular container to investigate their effects on the solidification phase front inside [11]. The problem of nanoparticles dispersion in a concentric annulus was considered by Sebti et al. [12]. In Ref. [13], the lattice Boltzmann method (LBM) was used to study the nanoparticles distributions and flow pattern of nanofluids. Moreover, Nemati et al. [14] used LBM to investigate nanofluids influences on mixed convection flows. Yang and Lai [15] presented LBM numerical study for the problem of flow and heat transfer of the alumina-water nanofluid in a microchannel, while the Al_2O_3-water nanofluid in a plain square cavity was simulated also using LBM by He et al. [16]. Also, Kefayati et al. [17] are employed the LBM simulation for free convection in a tall enclosure. The effect of nanoparticles on solid-liquid phase change materials are studied by Darzi et al. [18]. More studies on melting phase-change are done such as Ref. [20-21]. In Ref. [19], authors developed an LBM for heat transfer coupled with melting process.

The objective of this work is to extend our previous work [19] by considering nanoparticles influence on the melting process using LBM. We consider nanoparticles effects on two problems, namely, melting by conduction, and melting by free convection in a square cavity. The D1Q2 lattice model is used to represent temperature field in melting by conduction, while D2Q9 lattice model is employed to express velocity and temperature. We introduced numerical investigation to get some physical insight. For this purpose, various values of the Rayleigh number with different volume fraction of nanoparticles (0 to 0.02) are used to study the effect of the melting rate. The remaining of this paper is organized as follow. in the first section physical properties of the copper/water nanofluid, while the governing differential equations are presented after that. Then, the LBM technique is introduced.

After that, we presented results and discussions, and finally conclusions are withdrawn.

Physical Properties of Cu/Water nanofluid

It is well known that the when nanoparticles are added into the water, thermal conductivity, viscosity and other physical properties will be changed. The subscript nf stand for nanofluid. The density of the nanofluid is expressed as,

$$\rho_{nf} = (1-\phi)\rho_f + \phi\rho_s \tag{1}$$

where ρ_f, ρ_s are the density of water and the density of copper (Cu) nanoparticles, respectively, while, ϕ is the volume fraction of nanoparticles. The heat capacity of the nanofluid becomes [22],

$$(\rho c_p)_{nf} = (1-\phi)(\rho c_p)_f + \phi(\rho c_p)_s \tag{2}$$

and the Boussinesq term can be written as [22],

$$(\rho\beta)_{nf} = (1-\phi)(\rho\beta)_f + \phi(\rho\beta)_s \tag{3}$$

Also, the nanofluid viscosity may be written as,

$$\mu_{nf} = \frac{\mu_f}{(1-\phi)^{2.5}} \tag{4}$$

The Maxwell-Garnetts approximation is used to formulate the thermal conductivity of the nanofluid as [23],

$$\frac{k_{nf}}{k_f} = \frac{k_s + 2k_f + 2(k_f - k_s)}{k_s + 2k_f - \phi(k_f - k_s)} \tag{5}$$

The latent heat of the nanofluid is represented by the formula,

$$(\rho L)_{nf} = (1-\phi)(\rho L)_f \tag{6}$$

In Table 1, the thermo-physical properties of copper nanoparticles, water and copper/water nanofluid are provided [22].

Table 2: Physical properties of Cu nanoparticles, water, Cu/water nanofluids [22].

	Copper nanoparticles	**Base fluid (water)** $\phi = 0$	**Nanofluid 1** $\phi = 0.1$	**Nanofluid 2** $\phi = 0.2$
$\rho\,[kg \cdot m^{-3}]$	8954	997.1	1792.79	2588.48
$k\ [w\ / m \cdot {}^{\circ}c]$	400	0.6	0.8	1.04748
$c_p\ [J\ / kg \cdot {}^{\circ}c]$	383	4179	2283.107	1552.796
$L_f\,[J\ / kg]$	_	3.35×10^{5}	1.68×10^{5}	1.03×10^{5}
$\mu[Pa \cdot s]$	_	8.9×10^{-4}	1.158×10^{-3}	1.555×10^{-3}
$\alpha[m^2\ / s]$	1.17×10^{-4}	1.44×10^{-7}	1.95×10^{-7}	2.6×10^{-7}
$\beta[1/{}^{\circ}c]$	1.67×10^{-5}	2.1×10^{-4}	1.13×10^{-4}	7.63×10^{-5}

Governing Equations

(I) *Conduction Melting for Nanofluids*

The governing equation of the heat conduction with melting process can be written as,

$$\frac{\partial(\rho H)_{nf}}{\partial t} = \nabla \cdot (k_{nf} \nabla T) \tag{7}$$

where T, κ and ρ are the temperature, thermal conductivity and density, respectively. H is the total enthalpy given as,

$$H_{nf} = (c_p)_{nf} T + L_{nf} f_l \tag{8}$$

where c_p, L_{nf} and f_l are the specific heat at constant pressure, latent heat of melt and the liquid fraction. Note that the total enthalpy is composed of the sensible enthalpy and the latent enthalpy. Accordingly, Eq. (7) can be written as,

$$\frac{\partial((\rho c_p)_{nf} T)}{\partial t} = \nabla \cdot (\kappa_{nf} \nabla T) - \frac{\partial((\rho L_f)_{nf} f_l)}{\partial t} \tag{9}$$

For constant physical properties, we can get

$$\frac{\partial T}{\partial t} = \alpha_{nf} \nabla^2 T - \frac{L_{nf}}{(c_p)_{nf}} \frac{\partial f_l}{\partial t} \tag{10}$$

Where $\alpha_{nf} = \frac{k_{nf}}{(\rho c_p)_{nf}}$ is the thermal diffusivity.

(II) ***Convection Melting for Nanofluids***

The governing equations for convection melting, with assuming that fluids are Newtonian and incompressible can be described as follows [19, 24, 33]:

$$\nabla \cdot \mathbf{u} = 0 \tag{11}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot (\nabla \mathbf{u}) = -\nabla p + \nu_{nf} \nabla^2 \mathbf{u} + F_b \tag{12}$$

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot (\nabla T) = \alpha_{nf} \nabla^2 T + q \tag{13}$$

where $\mathbf{u}, p, \nu_{nf}, \alpha_{nf}$ and T are the velocity, the pressure, the kinematic viscosity, the thermal diffusivity and the temperature, respectively. F_b is the body force that donates the buoyancy force, and q is the heat source. Considering the Boussinesq approximation, F_b in momentum equation may be described as,

$$F_b = -g \beta_{nf} (T - T_{ref}) \tag{14}$$

where g is the gravity acceleration, β_{nf} is the thermal expansion coefficient, T_{ref} is the reference temperature. The source term q can be described as,

$$q = -\frac{1}{(\rho c_p)_{nf}} \left[\frac{\partial (\rho_{nf} \Delta H)}{\partial t} + \nabla \cdot (\rho_{nf} \mathbf{u} \Delta H) \right] \tag{15}$$

where ΔH is the latent enthalpy for pure the material. The second term can be neglected because the latent enthalpy for the liquid is uniform. Thus,

$$q = -\frac{1}{(\rho c_p)_{nf}} \frac{\partial (\rho_{nf} \Delta H)}{\partial t} = -\frac{1}{(\rho c_p)_{nf}} \frac{\partial (\rho_{nf} L_{nf} f_l)}{\partial t} = -\frac{L_{nf}}{(c_p)_{nf}} \frac{\partial f_l}{\partial t} \tag{16}$$

Here f_l is the volume-phase fraction of the liquid phase $(0 \le f_l \le 1)$, while L_{nf} is the melt latent heat. Therefore, the governing equations of the free convection with solid-liquid phase change may be rewritten in the dimensionless form as,

$$\nabla \cdot \mathbf{u}^* = 0 \tag{17}$$

$$\frac{\partial \mathbf{u}^*}{\partial t^*} + \mathbf{u}^* \cdot (\nabla \mathbf{u}^*) = -\nabla p^* + \Pr \nabla^2 \mathbf{u}^* - \Pr RaT^* \tag{18}$$

$$\frac{\partial T^*}{\partial t^*} + \mathbf{u}^* \cdot (\nabla T^*) = \nabla^2 T^* - \frac{1}{Ste} \frac{\partial f_l}{\partial t^*} \tag{19}$$

such that,

$$T^* = \frac{T - T_c}{T_h - T_c} \quad t^* = \frac{\alpha t}{l^2} \quad x^* = \frac{x}{l} \quad y^* = \frac{y}{l} \tag{20}$$

where l is a length scale (will be taken as the height of the cavity), $\Pr = \frac{\nu_{nf}}{\alpha_{nf}}$ is the prandtl number, $Ra = \frac{g \beta_{nf} \Delta T l^3}{\nu_{nf} \alpha_{nf}}$ is the Rayleigh number, and $Ste = \frac{(c_p)_{nf} \Delta T}{(L_f)_{nf}}$ is the Stefan number.

Phase change treatment using LBM

Nowadays, the LBM is considered a powerful tool for the computational modeling of fluids flow and transport phenomena that appear in different physical systems. Double distribution function (DDF) model is used for solving flow and thermal fields [25-29] and discussed in details in our previous work [19]. The consistency between LB equation and macroscopic equations with phase change is analyzed by the Chapman-Enskog expansion. Employing the enthalpy technique is important to avoid the requirement for conditions at the front of the phase change. Hence, we apply the modified version of the LBM to express conduction and convection melting of the pure substance. This modified method, is an enthalpy-based iterative method, employed to solve the temperature and the liquid fraction. In this approach, the melting term is represented as a source for solidification and as a sink for melting, in the collision term of the LB equation. The temperature at the time step *n* and the iteration *k*, is computed by,

$$T^{n,k} = \sum_i g_i^{n,k} \tag{64}$$

Here, $T^{n,k} \equiv T^k (t = n)$.

The local enthalpy is given by,

$$En^{n,k} = cT^{n,k} + L_f f_l^{n,k-1} \tag{65}$$

such that f_l is calculated at the previous iteration step. Then, at the current iteration level, one may have,

$$f_l^{n,k} = \begin{cases} 0 & if\ En^{n,k} < En_s = cT_m \\ \dfrac{En^{n,k} - En_s}{En_l - En_s} & if\ En_s \le En^{n,k} \le En_l = En_s + L_f \\ 1 & if\ En^{n,k} > En_l \end{cases} \tag{66}$$

Finally, the temperature distribution can be given as,

$$g_i^{n,k}(x + e_i \Delta t, t + \Delta t) = g_i(x,t) - \frac{1}{\tau_g}(g_i(x,t) - g_i^{eq}(x,t)) - \omega_i \frac{L_f}{c}(f_l^{n,k} - f_l^{n-1}) \tag{67}$$

In addition to three different types of thermal boundary conditions including Dirichlet, adiabatic and bounce-back boundary conditions are employed [19].

Results and Discussions

Firstly, in order to verify our model, we carried out 1D LB simulation for melting with heat transfer enhancement using nanoparticles. Secondly, in order to get physical insight, we performed some numerical experiments to simulate melting in a square cavity.

The 1D conduction-induced melting of ice and Cu/water nanofluids in a semi-infinite domain (Fig. 1) is solved using the LBM. Table 1 illustrates thermo-physical properties of the materials. At the beginning (t=0), the substance was at a constant temperature T_0, such that $(T_0 = -5.0\,^{\circ}C < T_m = 0.0)$. Also, the initial temperature on the left wall is raised to $(T_b = 90.0\,^{\circ}C)$. So, the substance is expected to melt under the influence of the heat conduction. The analytical solution which is given in Refs. [19,31], is employed to verify the proposed LB model. Comparisons between the LBM and analytical results for the temperature distribution and the location of solid-liquid phase interface in the

conduction-induced melting are presented in our previous work [19], which show good agreements.

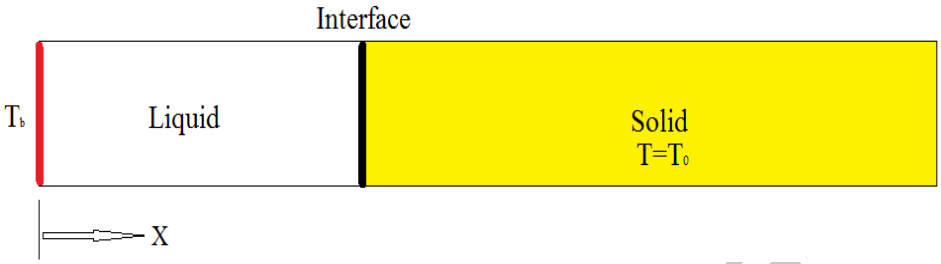


Fig. 1: Schematic of one-dimensional conduction-induced melting with the coordinate and boundary condition shown.

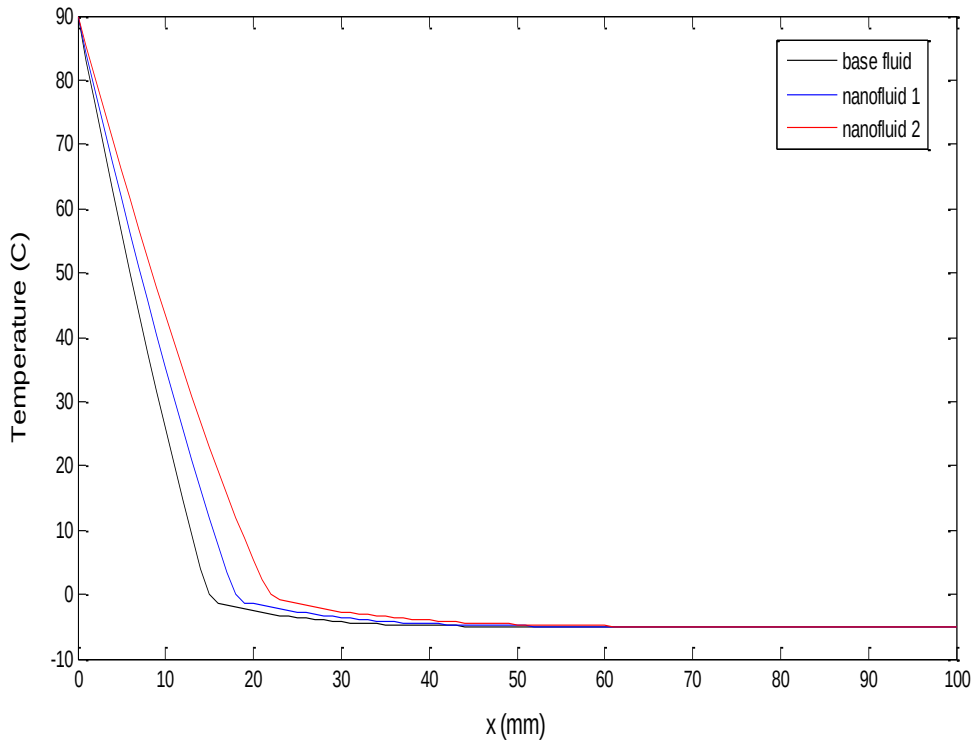


Fig. 2: Comparisons between temperature distributions in the conduction-induced melting for base fluid ($\phi = 0.0$) and nanofluids ($\phi = 0.1 and\ \phi = 0.2$) at t=100 s.

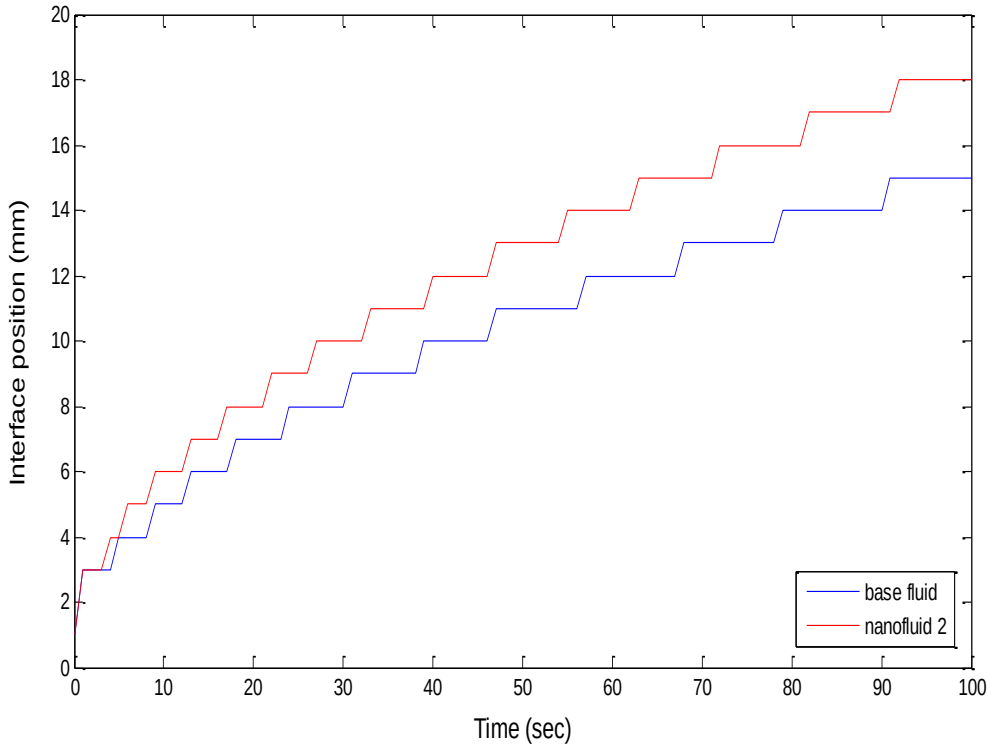
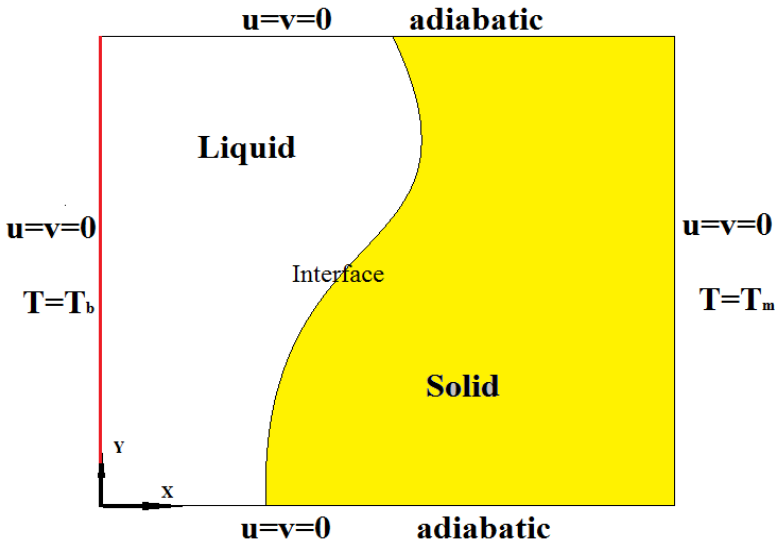


Fig. 3: Comparisons between locations of solid-liquid interface in the conduction-induced melting for base fluid ($\phi = 0.0$) and nanofluid ($\phi = 0.2$).

In order to show the effect of nanoparticles (Cu) suspended in water, the temperature distribution of pure water ($\phi = 0.0$) and Cu/water nanofluid ($\phi = 0.01, 0.02$) for different solid fractions are plotted in Fig. 2. It can be seen from this figure that by increasing the volume fraction the conduction heat transfer increases. Fig. 3 shows the comparisons between locations of the solid-liquid interface in the conduction-induced melting for base fluid ($\phi = 0.0$) and nanofluid ($\phi = 0.2$). The melting process is faster due to nanoparticles enhancement of the heat transfer during phase change.

In the following, we use the LBM for further simulation of the melting problem coupled with the natural convection. This case considers a 2D melting problem

in a square cavity with hot left wall (Fig. 4). In the beginning of the simulation the domain contents only a solid phase with initial melting temperature T_m, while, the temperature on the left wall is raised to T_b ($T_b > T_m$). The right wall temperature is T_m and the horizontal walls are assumed to be adiabatic. The thermo-physical properties of copper particles, water-base and nanofluids were taken in Table 1.



$$u = v = \frac{\partial T}{\partial y} = 0 \qquad at \;\; y = 0, l \;\; and \;\; 0 \le x \le l$$

$$u = v = 0, T = T_b \qquad at \;\; x = 0 \;\; and \;\; 0 \le y \le l$$

$$u = v = 0, T = T_m \qquad at \;\; x = l \;\; and \;\; 0 \le y \le l$$

Fig. 4: Schematic diagram of 2D melting in a square cavity.

The influence of volume fractions of nanoparticles on the melting rate is studied for various values of Ra=10^3,10^4 and 10^5 with Pr=6.2 and Ste=1. This model is validated against for the case of natural convection in a square cavity in Ref. [32]. The evaluation is fulfilled at three different Rayleigh numbers, 10^3,10^4 and 10^5; and its results are shown in Table 2. This Table shows the

accuracy of the present work through the comparison with the benchmark solutions [32].

Table 2: The validation of the current results in a square cavity.

	$\frac{u_{\max}H}{\alpha}$	$\frac{v_{\max}H}{\alpha}$	Nu_m
$Ra=10^3$			
Ref. [32]	3.649	3.697	1.118
Present study	3.352	3.952	1.085
$Ra=10^4$			
Ref. [32]	16.187	19.617	2.243
Present study	15.71	20.15	2.2394
$Ra=10^5$			
Ref. [32]	34.730	68.590	4.519
Present study	35.54	70.341	4.56

Fig. 5 shows the comparison of temperature contours for various solid concentrations (0 *to* 0.02) at fixed Rayleigh number 10^4. As the time steps increases, the top parts melt faster. By increasing the volume fraction from 0 to 2%, it can enhance the melting rate.

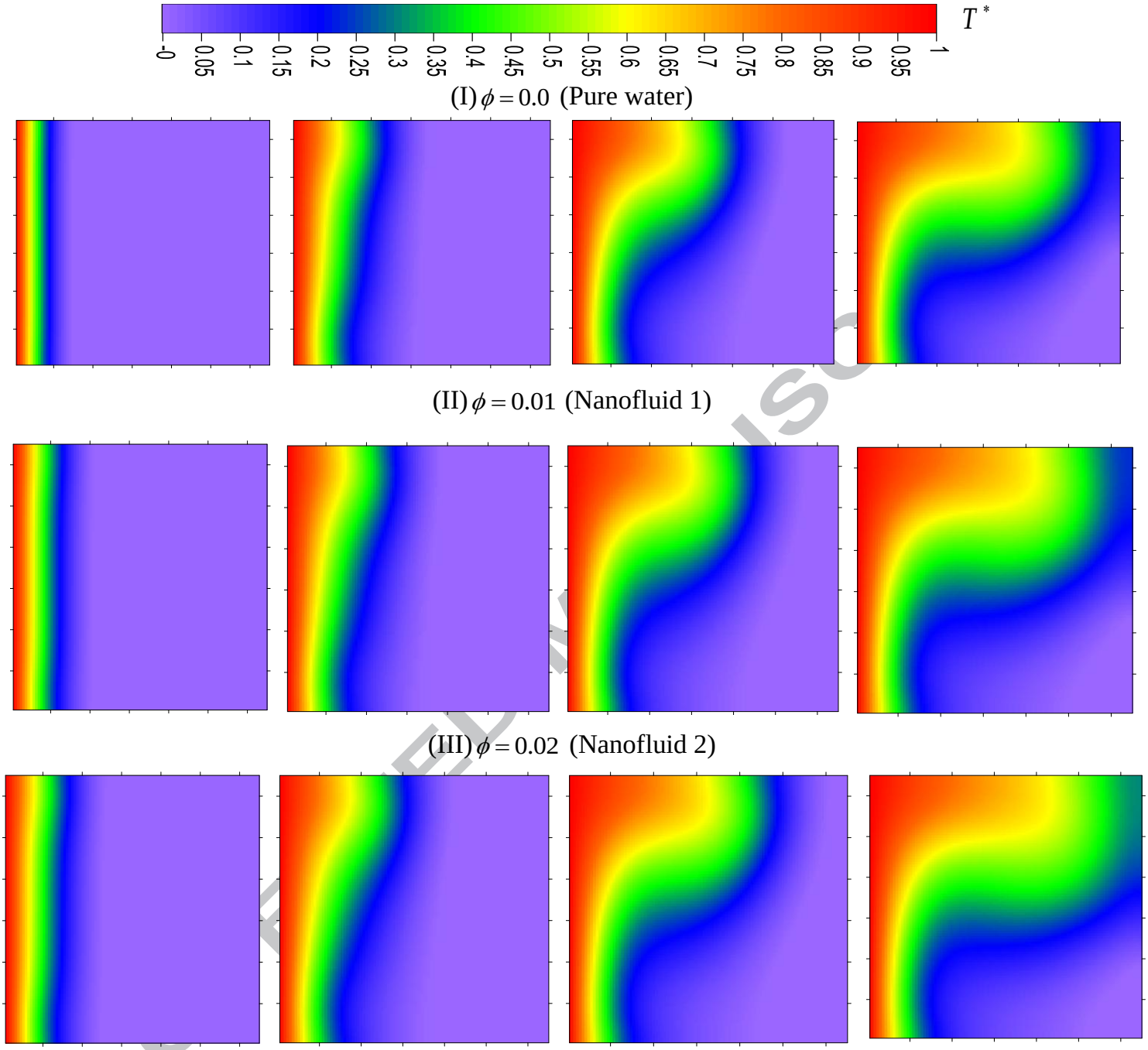
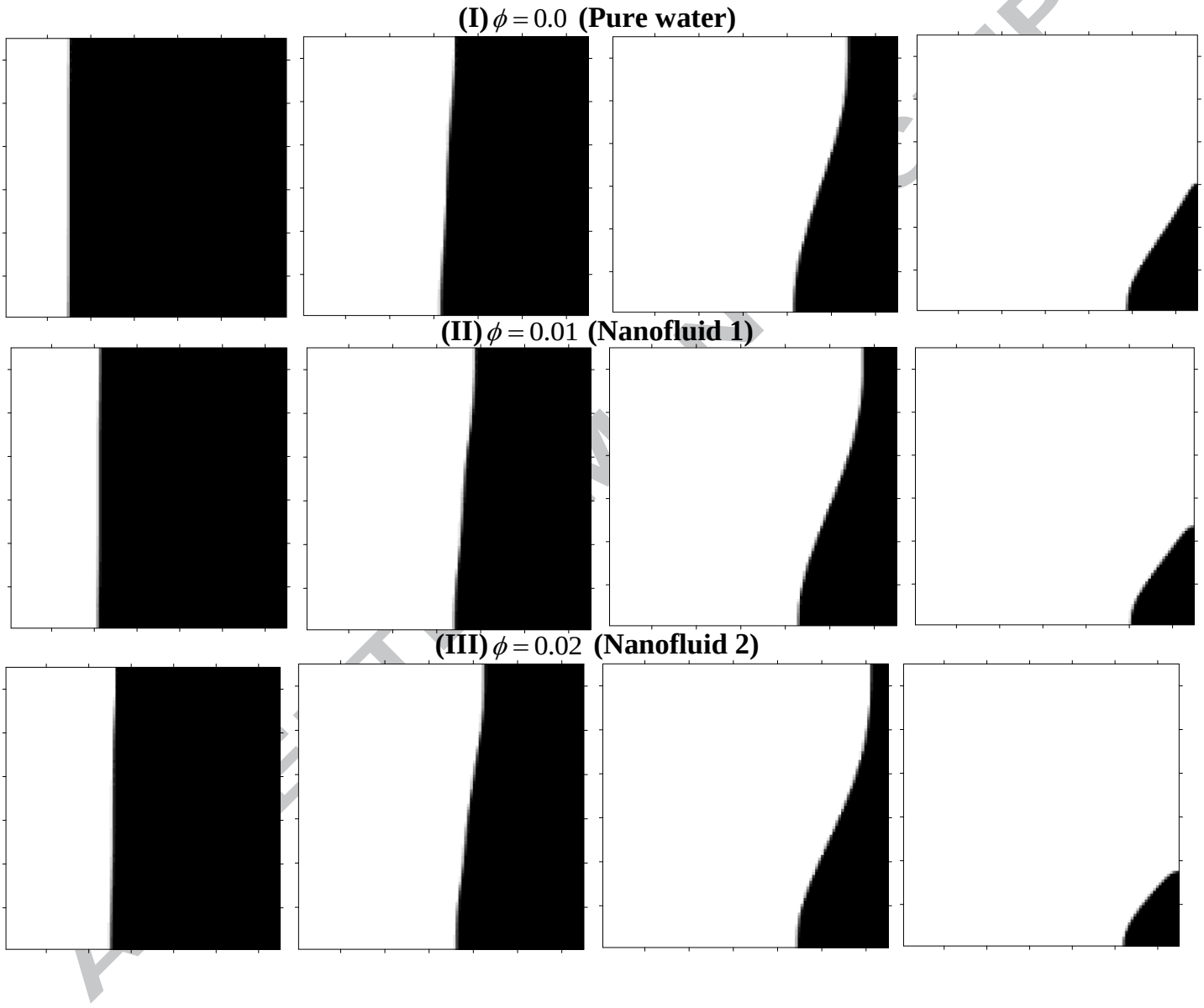


Fig. 7: Contours of temperature in a cavity for (I) $\phi = 0$, (II) $\phi = 0.01$ and (III) $\phi = 0.02$ with different times and $Ra = 10^4$.

Comparison of solid-liquid interface location with different values of solid concentrations at fixed *Ra* is presented in Fig. 8. It may be noted from this figure that the effective thermal conductivity of the nanofluid increases as the

temperature of the left wall increases. Also, the nanoparticles enhance the solid-liquid interface moving as time elapses, in particular at the top part of the cavity. This is because of the convective heat transfer augmentation at this region.



Time steps = 1000, 5000, 10000, 15000 (from left to right).

Fig. 8: Interface position for a cavity with (I) $\phi = 0$, (II) $\phi = 0.01$ and (III) $\phi = 0.02$ at different dimensionless times and $Ra = 10^4$.

Conclusions

In this paper, we employed the LBM enthalpy-based to study the nanoparticles effects of the coupled melting and heat transfer. The Bhatnagr-Gross-Krook (BGK) model was applied to simulate the one-dimensional conduction melting however, we used the multi-distribution function to simulate the two-dimensional convection melting process. A comparison between the present results and analytical solution or previous numerical results was carried out. We found that heat transfer by conduction dominants at the beginning of the melting process, then, the natural convection takes place. Also, it can be concluded that the existence of nanoparticles in the PCM, enhances the phase change front moving. Moreover, it is reported that adding copper nanoparticles enhances the thermal conductivity and reduces of the latent heat and the melting rate.

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Highlights:

- LBM is used to simulate nanoparticles dispersion heat transfer with phase-change.
- MDF D2Q9 model is used to determine physical parameters.
- Effects of nanoparticles on conduction/convection/melting process are investigated.
- Effects on the phase change front moving and the latent heat of fusion are studied.