

## NUMERICAL ANALYSIS OF MELTING OF NANOENHANCED PHASE CHANGE MATERIAL IN LATENT HEAT THERMAL ENERGY STORAGE SYSTEM

by

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*The heat transfer enhancement in the latent heat thermal energy storage system through dispersion of nanoparticle is reported. The resulting nanoparticle-enhanced phase change materials exhibit enhanced thermal conductivity in comparison to the base material. Calculation is performed for nanoparticle volume fraction from 0 to 0.08. In this study rectangular and cylindrical containers are modeled numerically and the effect of containers dimensions and nanoparticle volume fraction are studied. It has been found that the rectangular container requires half of the melting time as for the cylindrical container of the same volume and the same heat transfer area and also, higher nanoparticle volume fraction result in a larger solid fraction. The increase of the heat release rate of the nanoparticle-enhanced phase change materials shows its great potential for diverse thermal energy storage application.*

Keywords: nanoparticle, phase change material, melting, thermal energystorage

### Introduction

One of the most efficient ways to conserve thermal energy is latent heat storage. Since phase change materials (PCM) can absorb-release high latent heat during the melting-solidifying process, they have received a great interest in many applications. In order to develop and design an efficient and cost effective latent heat thermal energy storage system, many researchers in the past have investigated numerous problems considered to latent heat thermal energy storage and utilization. Also, a lot of research was done on numerical modeling of convection in the liquid phase of a PCM, both during cooling and heating [1, 2].

Duanet *al.* [3] conducted a numerical investigation of the solidification of a pure n-hexadecane inside a rectangular enclosure based on an enthalpy formulation of the energy equation. The effects of the cold wall temperature, initial liquid superheat and aspect ratio of the enclosure were studied in terms of the solid fraction and the shape of the solid-liquid phase front. Semma *et al.* [4] adopted the lattice Boltzmann method (LBM) to solve melting and solidification problems. Recently, a comprehensive and efficient numerical model for melting with natural convection is developed by Wang *et al.* [5]. The model is based on the finite volume approach and temperature transforming model. A new method for solid velocity

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correction with an explicit update for melting front and buoyancy force is proposed and shown to be very effective in eliminating inconsistencies. Moreover, there are several review papers about phase change materials. Khanafer *et al.* [6] studied heat transfer enhancement in a two-dimensional enclosure utilizing nanofluids for various considered parameters Kenisarin and Mahkamov [7] presented a review on the assessment of the thermal properties of various PCM, methods of heat transfer enhancement and design configurations of heat storage facilities to be used as a part of different solar systems. Zalba *et al.* [8] performed a detailed review on thermal energy storage that dealt with phase change materials, heat transfer studies and applications. Jegadheeswaran and Pohekar [9] presented a review on the influence of enhancement techniques on the thermal response of the PCM in terms of phase change rate and amount of latent heat stored/retrieved has been addressed as a main aspect. Dutil *et al.* [10] presented a review of the present models of phase change material based on the first law and on the second law of thermodynamics and showed selected results for several configurations, from numerous authors.

The major drawback of PCM is low thermal conductivities which lead to decreasing the rates of heat storage and retrieval during melting and solidification processes that in turn limit their utility areas. To overcome this problem, a wide range of investigations were carried out to enhance the thermal conductivity of the organic PCM or increase heat transfer performance. Conductivity enhancement can be done in a number of ways including the use of nanoparticles. The enhanced PCM is found to exhibit lengthened melt times and shortened cool-down times. The presence of the nanoparticles in the fluids increases appreciably the effective thermal conductivity of the fluid and consequently enhances the heat transfer characteristics. A review of the unique features of nanofluids, such as enhancement of heat transfer, improvement in thermal conductivity, increase in surface volume ratio, Brownian motion, thermophoresis and in addition, the outline of the recent research in experimental and theoretical studies on forced and free convective heat transfer in nanofluids, their thermo-physical properties and their applications is performed by Godson *et al.* [11].

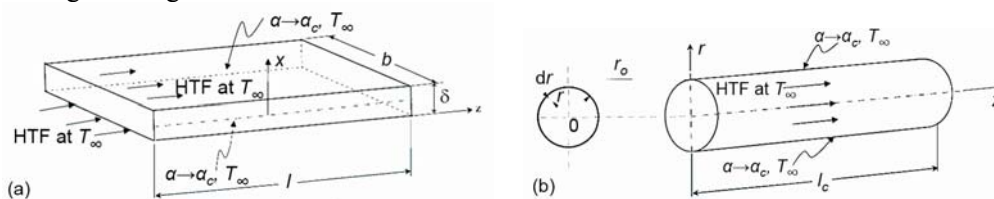
Khodadadi and Hosseinizadeh [12] were the first to report on improved functionality of PCM through dispersion of nanoparticles. They found that the resulting nanoparticle-enhanced (NEPCM) exhibit enhanced thermal conductivity in comparison to the base material. Ranjbar *et al.* [13] investigated the influence of utilizing nanoparticle on enhancement of heat transfer in a three dimensional cavity. Khodadadi and Fan [14] utilized an analytic/integral approach to solve the Stefan problem with a 1-D model for a nanofluid that undergoes freezing. Their model accounts for the thermal property jumps between the liquid and solid phases and showed that the freezing time to decrease as the volume fraction of the nanoparticle is raised. Wu *et al.* [15] studied the potential of  $\text{Al}_2\text{O}_3\text{-H}_2\text{O}$  nanofluids as a new PCM for the thermal energy storage of cooling systems. The thermal response test shows the addition of  $\text{Al}_2\text{O}_3$  nanoparticles remarkably decreases the supercooling degree of water, advances the beginning freezing time and reduces the total freezing time. They showed that only adding 0.2 wt.%  $\text{Al}_2\text{O}_3$  nanoparticles, the total freezing time of  $\text{Al}_2\text{O}_3\text{-H}_2\text{O}$  nanofluids can be reduced by 20.5%. Recently, Zhu *et al.* [16] numerically simulated the phase change behavior and heat transfer enhancement in a 2-D enclosure considering different volume fractions of the  $\text{SiC-H}_2\text{O}$  nanofluids. Besides using nanoparticles, the geometrical pattern can be useful in improving the heat transfer performance. Flow and heat transfer from irregular surfaces are often encountered in many engineering applications to enhance heat transfer. In this study the melting behavior of the NEPCM and the various parameters affecting melting in a cylindrical container and rectangular container are studied.

**Problem formulation and governing equations**

As shown in fig. 1, the physical models under investigation are rectangular and cylindrical enclosures filled with Cu-CaCl<sub>2</sub>·6H<sub>2</sub>O nanofluid as phase change material. The diameter of solid copper nanoparticles is considered to be 10 nm. The thermophysical properties are given in tab. 1. Lateral sides of the rectangular container are well insulated and heat transfer occurs only on side  $x = 0$  and  $x = \delta$ . The rectangular container, made of stainless steel with dimensions of  $l = b = 100$  mm and  $\delta = 20$  mm is filled with the calcium chloride hexahydrate and well isolated on the lateral sides. The containers with the solid PCM are assumed in the constant temperature bath, which is lower than melting temperature. At  $t = 0$ , are exposed to  $T_\infty = 60^\circ\text{C}$  as well as the air velocity is assumed to be  $w = 5$  m/s. Since  $T_\infty$  is higher than the temperature of exposed surface of containers, natural convection heat transfer occurs between the air (HTF) and exposed surface and consequently heat is transferred to PCM through conduction mechanism. Finally, phase change take places and large amount of energy can be stored. The convection heat transfer coefficient between the air and the container wall is determined using the correlation given in Incropera and DeWitt [17], and is calculated to be  $\alpha_{\text{conv}} = 16 \text{ W/m}^2\text{K}$ .

Also, a cylindrical container is studied in this paper and its results will be compared with those of the rectangular container, fig. 1(b). The dimensions of the containers are chosen in such a manner that the volume as well as the convective heat transfer area for both the cylindrical and rectangular containers to be equal. The fixed dimensions are chosen to be the length of the cylindrical container  $l_c = 20$  mm.

The nanofluid is treated as an incompressible and Newtonian fluid, [6, 12], as well as homogenous and isotropic. The phase change process in the PCM is assumed to be isothermal and conduction is considered as dominant mechanism of heat transfer. Thermophysical properties of the nanofluid are assumed to be constant and the PCM behaves ideally, *i. e.* such phenomena as property degradation and supercooling are not accounted for. Also, the thermal resistance across the wall of the container and heat loss from the container to its surroundings are neglected.



**Figure 1. Schematic of the studied configuration**

In order to simulate phase change of NEPCM in an enclosure with vertical walls, enthalpy-porosity method [18,19] is used. It is worth to note here that Bertrand *et al.* [20] presented the results of a comparison exercise in which various numerical approaches were applied to a phase-change problem that included coupled natural convection and melting. Their results indicate that enthalpy methods are to be used in most phase-change problems where a solid-liquid interfacial region is present between the phases. Considering the nanofluid as a continuous media with thermal equilibrium between the base fluid and the solid nanoparticles, the governing equations are:

$$\frac{\partial H}{\partial t} = \frac{\partial}{\partial z} \left( \frac{k}{\rho} \frac{\partial T}{\partial z} \right) \tag{1}$$

$$mc_p \frac{\partial T_{\text{air}}}{\partial z} = \alpha_{\text{conv}} A_{\text{ht}} (T - T_{\text{air}}) \quad (2)$$

**Table 1. Thermophysical properties of the Cu nanoparticles and base fluid (CaCl<sub>2</sub>·6H<sub>2</sub>O)**

	Copper nanoparticles	Base fluid
$\rho$ [kgm <sup>-3</sup> ]	8954	Solid = 1710
		Liquid = 1530
$c_p$ [Jkg <sup>-1</sup> K <sup>-1</sup> ]	383	Solid = 2200
		Liquid = 1400
$k$ [Wm <sup>-1</sup> k <sup>-1</sup> ]	400	Solid = 1.09
		Liquid = 0.53
$L$ [Jkg <sup>-1</sup> ]	–	187000
Melting point [°C]	–	29.9

An alternative form of above equation can be obtained by splitting the total enthalpy  $H$  into sensible and latent heat components:

$$H = h + Lf_1 \quad (3)$$

where

$$h = \int_{T_m}^T c_p dT \quad (4)$$

and  $T_m$  is the melting temperature of the PCM. For the problem of isothermal phase change, the local liquid fraction  $f_1$  is defined as:

$$f_1(T) = \begin{cases} 1 & \text{if } T > T_m \\ 0 & \text{if } T < T_m \end{cases} \quad (5)$$

Substituting eq. 3 into eq. 1 gives:

$$\frac{\partial h}{\partial t} = \text{div} \left( \frac{k}{\rho} \text{grad } T \right) - L \frac{\partial f_1}{\partial t} \quad (6)$$

Equation 6 should be solved with the appropriate initial and boundary conditions and also appropriate nanofluid properties which are described below.

The density of the nanofluid is given by:

$$\rho_{\text{nf}} = (1 - \phi)\rho_f + \phi\rho_s \quad (7)$$

Whereas the heat capacitance of the nanofluid and part of the Boussinesq term are:

$$(\rho c_p)_{\text{nf}} = (1 - \phi)(\rho c_p)_f + \phi(\rho c_p)_s \quad (8)$$

$$(\rho\beta)_{\text{nf}} = (1 - \phi)(\rho\beta)_f + \phi(\rho\beta)_s \quad (9)$$

With  $\phi$  being the volume fraction of the solid particles and subscripts f, nf, and s stand for base fluid, nanofluid, and solid, respectively. The effective dynamic viscosity of the Nanofluid containing a dilute suspension of small rigid spherical particles given by the recent models of Corcione[21] which seems to be more accurate is:

$$\frac{\mu_{\text{nf}}}{\mu_f} = \frac{1}{1 - 34.87 \left( \frac{d_p}{d_f} \right)^{-0.3} \phi^{1.03}} \quad 0 \leq \phi \leq 0.08 \quad (10)$$

$$d_f = 0.1 \left[ \frac{6M}{N\pi\rho_{f,0}} \right]^{1/3} \quad (11)$$

$K_{\text{eff}}$  is the mixture conductivity of solid and liquid NEPCM given as:

$$k_{\text{eff}} = (k_{\text{nf,liquid}} + k_d)f + k_{\text{nf,solid}}(1 - f) \quad (12)$$

Whereas the thermal conductivity of the stagnant (subscript 0) nanofluid and the effective thermal conductivity of the nanofluid according to Maxwell [22], are:

$$\frac{k_{\text{nf0}}}{k_f} = \frac{k_s + 2k_f - 2\phi(k_f - k_s)}{k_s + 2k_f + \phi(k_f - k_s)} \quad (13)$$

Experiments showed that heat transfer enhancement of nanofluids exceed the thermal conductivity enhancement of nanofluids. This extra enhancement might be explained by thermal dispersion, which occurs due to the random motion of nanoparticles in the flow. In our modeling, the nanofluid is treated as a single phase fluid but the additional heat transfer enhancement obtained with nanofluids is considered by modeling the dispersion phenomenon. It was noted that thermal dispersion occurs in nanofluid flow due to the random motion of nanoparticles and considering the fact that this random motion creates small perturbations in velocity and temperature. The thermal conductivity enhancement term due to thermal dispersion is given by [12]:

$$k_d = C(\rho c_p)_{\text{nf}} \sqrt{u^2 + v^2} \phi d_p \quad (14)$$

The empirically-determined constant  $C$  is evaluated following the work of Wakao and Kagueli [23].

Also the latent heat that is evaluated using:

$$(\rho L)_{\text{nf}} = (1 - \phi)(\rho L)_f \quad (15)$$

The governing equation for the case of the cylindrical container has the following form:

$$\frac{\partial H}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{k}{\rho} \frac{\partial T}{\partial r} \right) \quad (16)$$

In eq. (16),  $H$  represents the total enthalpy, which can be split into its sensible and latent component. The solution methodology and numerical procedure for eq. 15 is the same as for eq. 1.

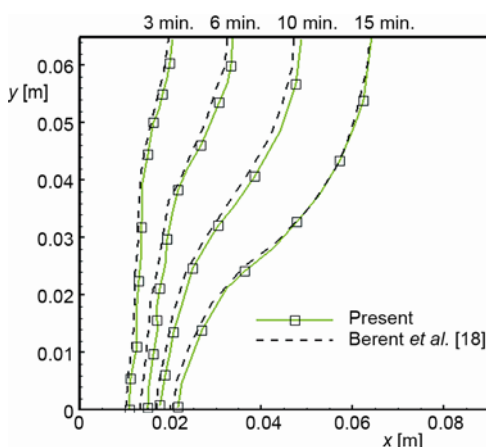
### Computational methodology

The numerical solution of the problem uses the enthalpy-porosity approach, Brent *et al.* [18]. By this approach, the porosity in each cell is set equal to the liquid fraction in that cell. Based on an enthalpy balance, the liquid fraction (which is based on volume)  $f_l$  is computed at each iteration.  $f_l$  takes the value  $f_l = 1$  in the liquid phase,  $f_l = 0$  in the solid phase and  $0 < f_l < 1$  in the mushy zone (partially solidified region).

A home-generated FORTRAN code based on the finite volume method on collocated body-fitted grids using the SIMPLE algorithm has been developed to solve the governing equations. The governing equations are discretized using a control volume approach. For a typical run, the time step is 0.1s and the number of sweeps for each time step is 400. The QUICK differencing scheme is used for solving the momentum and energy equations, whereas the PRESTO scheme is adopted for the pressure correction equation. The under-relaxation factors for the velocity components, pressure correction, thermal energy and liquid fraction are 0.5, 0.3, 1 and 0.9, respectively. In enthalpy method, the solution is based on a fixed grid and governing equations are modified such that they are valid for both phases. Also the mushy zone constant is set to  $10^5$  [ $\text{kgm}^{-3}\text{s}$ ].

### Validation of the model

To verify the validity and accuracy of the results of present study, the obtained results are compared with other available numerical and experimental results. In order to evaluate the ability of the enthalpy-porosity method in modeling of phase change process the numerical results of melting gallium in a rectangular cavity obtained by Brent *et al.*[18]



**Figure 2. Progress of melting front with time: comparison among predictions of Brent *et al.* [18] and present work**  
(for color image see journal web-site)

A reasonably good agreement is obtained where the relative error value between the two results is less than 5%.

The present numerical result is validated against the results of Khanafer *et al.* [6] for natural convection of Cu-water nanofluid in a rectangular enclosure with as shown in fig. 3. The horizontal walls are assumed to be insulated, while the left and right vertical walls are kept at high and low temperatures, respectively. This figure shows the effect of Grashof number ( $Gr$ ) and nanoparticle dispersion into pure fluid on the temperature and velocity profiles at the mid-sections of the cavity. The results obtained for  $Gr = 10^4$ ,  $10^5$  and  $\phi = 0.2$ . The velocities at the center of the cavity for higher values of  $Gr$  are small as compared to those at the boundaries, where the fluid has higher velocities. This comparison revealed good agreements between results.

From the results shown in fig. 4, it can be concluded that the agreement between present study and experimental data of Zivkovic and Fujii study [24] is good. In their study, a simple computational model for isothermal phase change material encapsulated in a single container was presented. In this analysis all initial and boundary conditions and also the physical model

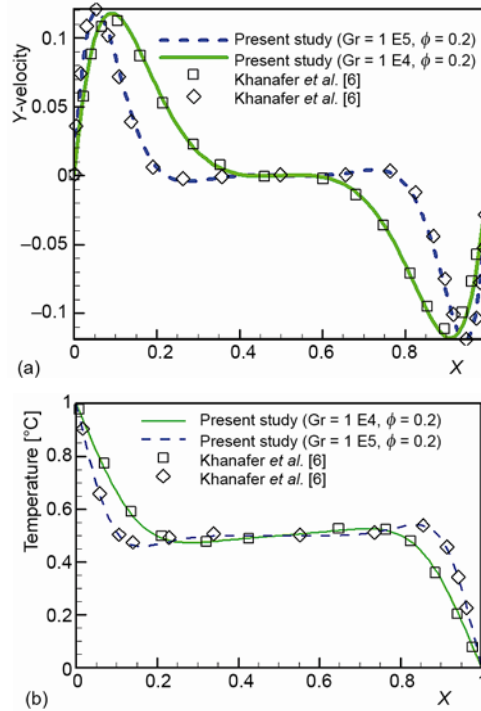
are compared with their results in fig. 2. As it is clear from this figure, the melting starts from the left wall, since the temperature of hot wall is kept over the melting temperature of gallium. The melting phase front travels to the right as well as liquid phase occupies a major part of the cavity expediting melting process and advection in liquid phase as time goes by.

and PCM are the same as what are used in present study. As shown in fig. 4, the temperature of center of the container increases until reaches to the melting point. Then the PCM absorb energy to change phase from solid to liquid in a constant temperature, then, the temperature will increase.

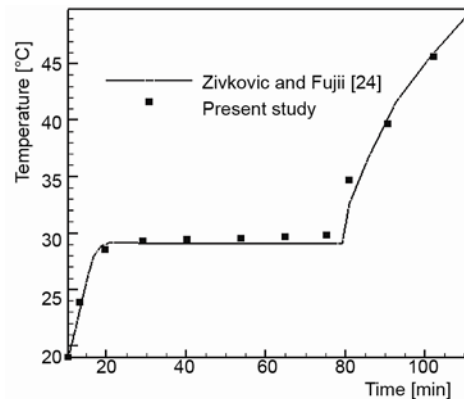
**Results and discussions**

Figure 5 shows the variation with time of the PCM temperature in the center of both the rectangular and cylindrical containers for the different dimensions of the containers and also for different nanoparticle volume fraction. For small values of  $\delta$  and  $r_o$ , the difference in melting time between the rectangular and cylindrical containers is not so pronounced. However, on increasing the mass of the PCM filling the container, *i. e.* with increasing  $\delta$  for the rectangular container and  $r_o$  for the cylindrical container, the difference in the melting time increases considerably, with the rectangular container showing a much shorter melting time than the cylindrical container of the same volume and heat transfer area. Also, the effect of nanoparticle volume fraction on the time variation of the temperature of the PCM at the center point is illustrated in fig. 5. As it is shown, increasing the nanoparticle volume fraction leads to smaller melting time. The influence of the amount of PCM filling the container on the melting time of PCM is shown in fig. 6. Results show that for larger quantities of the material filling the container, the difference in the melting time between the rectangular and cylindrical containers is more pronounced, with the melting time of the cylindrical container being nearly twice that of the rectangular one.

Also, increasing the nanoparticle volume fraction has great effect on the melting time of the PCM. It can be observed that the nanofluid heat transfer rate increases with an increase in the nanoparticles volume fraction. The instantaneous dimensionless volumes of the nanofluid within the containers are presented in fig. 7 for all the cases under investigation. The solid volume that continuously decreases from the start of the melting exhibits strong sensitivity



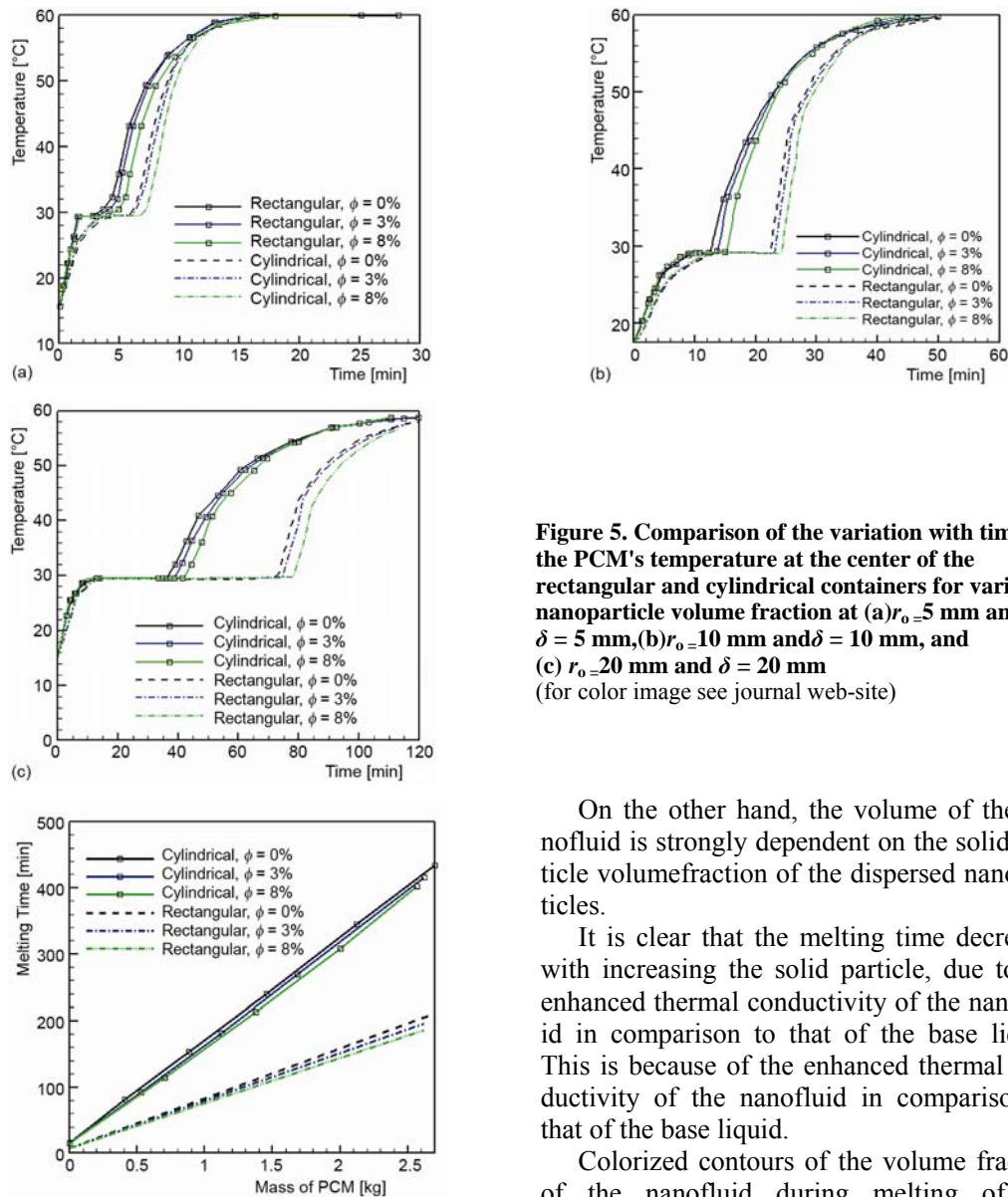
**Figure 3. Comparison of the Y-velocity (a) and the temperature (b) profiles of nanofluid for  $Gr = 10^4-10^5$  and  $\phi=0.2$  obtained by present study and the work of Khanafar *et al.*[6] (for color image see journal web-site)**



**Figure4. Variation with time of PCM's temperature at the center of the rectangular container**

of the solid volume that continuously decreases from the start of the melting exhibits strong sensitivity

to the shape of container. The observed higher heat release rate of the rectangular container is a clear indicator of its great potential for thermal energy storage applications in comparison with cylindrical containers.



**Figure 5.** Comparison of the variation with time of the PCM's temperature at the center of the rectangular and cylindrical containers for various nanoparticle volume fraction at (a)  $r_o = 5$  mm and  $\delta = 5$  mm, (b)  $r_o = 10$  mm and  $\delta = 10$  mm, and (c)  $r_o = 20$  mm and  $\delta = 20$  mm (for color image see journal web-site)

On the other hand, the volume of the nanofluid is strongly dependent on the solid particle volume fraction of the dispersed nanoparticles.

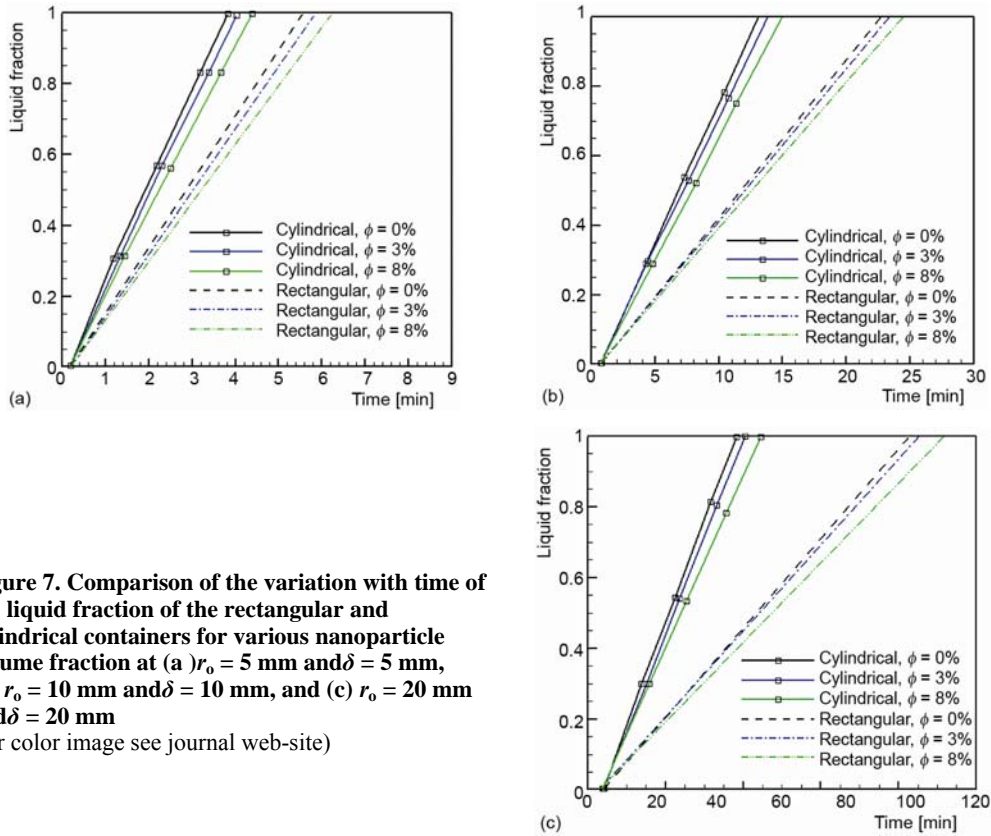
It is clear that the melting time decreases with increasing the solid particle, due to the enhanced thermal conductivity of the nanofluid in comparison to that of the base liquid. This is because of the enhanced thermal conductivity of the nanofluid in comparison to that of the base liquid.

Colorized contours of the volume fraction of the nanofluid during melting of the NEPCM at various time instants are shown in fig. 8 at 20 and 34 min in the rectangular container. It should be mentioned that the color red is used to identify the liquid phase, whereas color blue is indicative of the frozen solid phase. It is seen clearly that the solid front move to the center of the container faster by increasing the nanoparticle volume fraction.

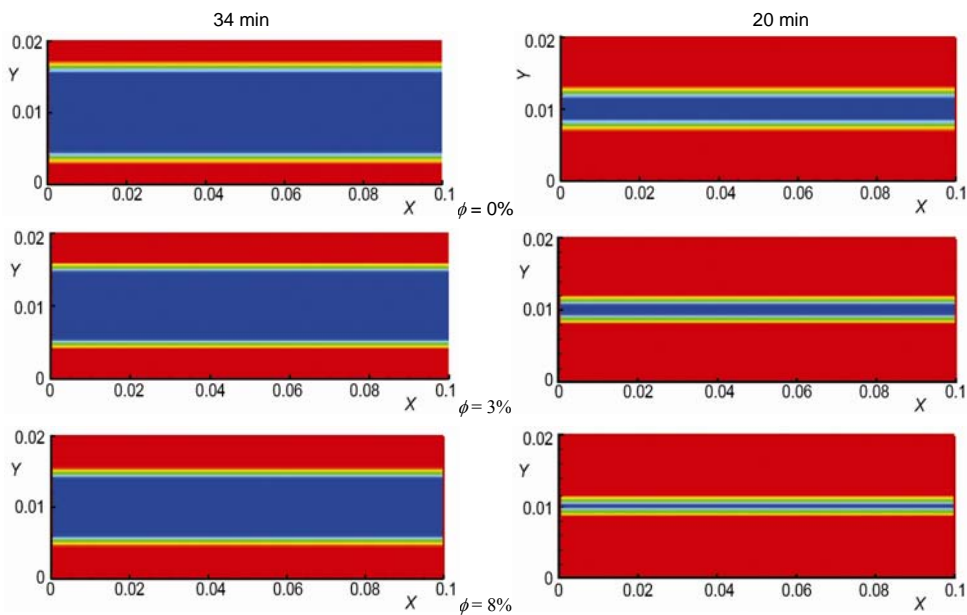
**Figure 6.** Comparison of the melting time for rectangular and cylindrical containers of equal volume and heat transfer area (for color image see journal web-site)

It is seen clearly that the solid front move to the center of the container faster by increasing the nanoparticle volume fraction.





**Figure 7. Comparison of the variation with time of the liquid fraction of the rectangular and cylindrical containers for various nanoparticle volume fraction at (a)  $r_o = 5$  mm and  $\delta = 5$  mm, (b)  $r_o = 10$  mm and  $\delta = 10$  mm, and (c)  $r_o = 20$  mm and  $\delta = 20$  mm (for color image see journal web-site)**



**Figure 8. Colorized contours of the volume fraction of the nanofluid at various time (for color image see journal web-site)**

## Conclusions

Melting inside rectangular and cylindrical containers filled with nanoenhanced phase change material has been studied numerically using a pressure based finite volume method with an enthalpy porosity technique. The effects of nanoparticle dispersion during melting with various volume fractions of Cu as well as the shape of container and its dimension on the melting phase front are investigated. It is found that the nanoparticle dispersion in a phase change material results in an approximately 30% increase in thermal conductivity and enhanced heat transfer rate and consequently, decreases the melting time about 15%. Furthermore, the rate of heat transfer increased by increasing nanoparticle volume fraction. It can be concluded from the obtained results that for the same volume and heat transfer area of two containers, rectangular container shows much shorter melting time as compared to cylindrical container which is more pronounced for higher values of PCM mass. So it is preferable to use rectangular containers for energy storage system than cylindrical ones. Finally it is shown that the potential of energy storage system can be improved by using proper suspension of nanoparticles within conventional phase change materials and by choosing proper geometry for containers.

## Nomenclature

$A_{ht}$  – heat transfer surface, [m]  
 $b$  – width of rectangular enclosures, [m]  
 $c_p$  – specific heat at constant pressure, [Jkg<sup>-1</sup>K<sup>-1</sup>]  
 $d_p$  – nanoparticle diameter, [m]  
 $f$  – liquid fraction  
 $Gr$  – Grashof number ( $= g\beta\Delta T l^3 \nu^{-2}$ )  
 $H$  – total enthalpy, [Jkg<sup>-1</sup>]  
 $h$  – sensible enthalpy, [Jkg<sup>-1</sup>]  
 $k$  – fluid thermal conductivity, [Wm<sup>-1</sup>K<sup>-1</sup>]  
 $L$  – latent heat of fusion, [Jkg<sup>-1</sup>]  
 $l$  – length of rectangular enclosures, [m]  
 $l_c$  – length of cylindrical container, [m]  
 $M$  – molecular weight of the base fluid, [kg]  
 $m$  – mass, [kg]  
 $N$  – Avogadro number =  $6.022 \cdot 10^{23} \text{ mol}^{-1}$   
 $r$  – radial co-ordinate, [m]  
 $T$  – temperature, [K]  
 $T_m$  – melting temperature, [K]  
 $T_\infty$  – air temperature [°C]  
 $t$  – time, [s]  
 $u, v$  – velocity components, [ms<sup>-1</sup>]

$w$  – velocity, [ms<sup>-1</sup>]  
 $x, y, z$  – Cartesian coordinates, [m]

### Greek symbols

$\alpha$  – convection heat transfer coefficient, [Wm<sup>-2</sup>K<sup>-1</sup>]  
 $\beta$  – thermal expansion coefficient, [K<sup>-1</sup>]  
 $\delta$  – height of rectangular enclosures, [m]  
 $\mu$  – dynamic viscosity, [m<sup>2</sup>s<sup>-1</sup>]  
 $\nu$  – kinematic viscosity (m<sup>2</sup>s<sup>-1</sup>)  
 $\rho$  – density, [kgm<sup>-3</sup>]  
 $\phi$  – particle volume fraction

### Subscripts

0 – stagnant  
conv – convection  
d – thermal dispersion  
eff – effective  
f – fluid  
nf – nanofluid  
p – particle  
s – solid

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