NUMERICAL HEAT TRANSFER STUDIES OF A LATENT HEAT STORAGE SYSTEM CONTAINING NANO-ENHANCED PHASE CHANGE MATERIAL

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. The effects of nanoparticle volume fraction and some other parameters such as natural convection are studied in terms of solid fraction and the shape of the solid-liquid phase front. It has been found that higher nanoparticle volume fraction result in a larger solid fraction. The present results illustrate that the suspended nanoparticles substantially increase the heat transfer rate and also the nanofluid heat transfer rate increases with an increase in the nanoparticles volume 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.

Key words: nanoparticle, phase change material, solidification, thermal storage

Introduction

Because of the problems of fast depletion of conventional energy sources and ever increasing demand of energy, many researches all around the world started paying attention to renewable energy sources and energy storage systems. Energy storage is essential, whenever, the supply or consumption of energy varies independently with time. Basically there are three methods of storing thermal energy: sensible, latent, and thermo-chemical heat or cold storage. Thermal storage systems, based on the latent heat storage, have been relevant, especially in solar thermal applications. Solid-liquid phase change during heat storage and recovery processes provides considerable advantages such as high storage capacity and nearly isothermal behavior during charging and discharging processes. There are several promising developments going on in the field of application of phase change material (PCM) for heating and cooling of building. Zalba et al. [1] performed a detailed review on thermal energy storage that dealt with PCM, heat transfer studies, and applications. Farid et al. [2] also presented a review on the analysis of PCM, hermetic encapsulation, and application of PCM.

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Mehling et al. [3] summarized the investigations and developments on using PCM in buildings. Kenisarin et al. [4] presented a review of investigations and developments carried out during the last 10-15 years in the field of PCM, enhancing heat conductivity, available fields of using PCM, and clarifying typical questions. Rajeev et al. [5] presented a numerical solution of inward solidification of phase change material contained in cylinder/sphere. Shen et al. [6] worked on thermal management of mobile devices. Their paper presented the experimental study of using phase change material in the cooling of the mobile devices. It investigated the thermal performance of transient charging and discharging of mobile devices in three different situations; making phone calls frequently, making long duration calls, and making occasional calls. The results showed that mobile devices are heated up fastest during the long duration usage. Ganaoui et al. [7] developed and qualified a numerical scheme coupling lattice Boltzmann and finite volumes approaches for test cases of phase change problems. Anandan et al. [8] presented a review of thermal management of electronics devices dealing with various aspects of cooling methods. During these years, researchers have tried to find new way to develop energy storage system. Using nano technology to increase the heat transfer shows great opportunity in storage system. Because of low thermal conductivity of conventional heat transfer fluids such as water, oil, and ethylene glycol mixture, nanotechnology is considered to enhance thermal characteristics with substantially higher conductivities. The presence of the nanoparticles in the fluids increases appreciably the effective thermal conductivity of the fluid and consequently enhances the heat transfer characteristics. Masuda et al. [9] reported on enhanced thermal conductivity of dispersed ultra-fine (nanosize) particles in liquids. Soon thereafter, Choi [10] was the first to coin the term “nanofluids” for this new class of fluids with superior thermal properties. Khanafer et al. [11] studied heat transfer enhancement in a two-dimensional enclosure utilizing nanofluids for various pertinent parameters. Khodadadi et al. [12] were the first to report on improved functionality of PCM through dispersion of nanoparticles. They found that the resulting nanoparticle-enhanced phase change materials (NEPCM) exhibit enhanced thermal conductivity in comparison to the base material. In this study the solidification behavior of the NEPCM and the various parameters affecting solidification in an enclosure were studied.

Problem statement

The analysis was carried out in two separate but related stages. Firstly, steady-state buoyancy driven convection in a differentially heated cavity containing a nanofluid was studied. Consider a 3-D cavity with adiabatic walls except left \((T_h)\) and right \((T_c)\) walls which are maintained at constant temperatures where \(T_h > T_c\). (fig. 1).

Gravity acts parallel to the active walls pointing toward the bottom wall. The fluid is treated as an incompressible and Newtonian fluid. Thermophysical properties of the nanofluid are assumed to be constant, where as the density variation in the buoyancy...
force term is handled by Boussinesq approximation. Thermophysical properties of the nanofluid is shown at tab. 1.

Table 1. Thermophysical properties of the nanofluid

<table>
<thead>
<tr>
<th>Nanofluid</th>
<th>Copper nanoparticles</th>
<th>Base fluid</th>
<th>Nanofluid $\phi = 0.025$</th>
<th>Nanofluid $\phi = 0.05$</th>
<th>Nanofluid $\phi = 0.1$</th>
<th>Nanofluid $\phi = 0.15$</th>
<th>Nanofluid $\phi = 0.2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$ [kgm$^{-3}$]</td>
<td>8954</td>
<td>997.1</td>
<td>1196.02</td>
<td>1394.95</td>
<td>1792.79</td>
<td>2190.64</td>
<td>2588.48</td>
</tr>
<tr>
<td>$\mu$ [kgms$^{-1}$]</td>
<td>–</td>
<td>8.9·10$^{-4}$</td>
<td>9.48·10$^{-4}$</td>
<td>1.10$^{-3}$</td>
<td>1.158·10$^{-3}$</td>
<td>1.33·10$^{-3}$</td>
<td>1.555·10$^{-3}$</td>
</tr>
<tr>
<td>$c_p$ [Jkg$^{-1}$K$^{-1}$]</td>
<td>383</td>
<td>4179</td>
<td>3468.54</td>
<td>2960.67</td>
<td>2283.107</td>
<td>1851.64</td>
<td>1552.796</td>
</tr>
<tr>
<td>$k$ [Wm$^{-1}$K$^{-1}$]</td>
<td>400</td>
<td>0.6</td>
<td>0.648</td>
<td>0.698</td>
<td>0.8</td>
<td>0.915</td>
<td>1.04748</td>
</tr>
<tr>
<td>$\alpha$ [m$^2$s$^{-1}$]</td>
<td>–</td>
<td>1.17·10$^{-4}$</td>
<td>1.44·10$^{-2}$</td>
<td>1.682·10$^{-2}$</td>
<td>1.7·10$^{-2}$</td>
<td>1.95·10$^{-2}$</td>
<td>2.25·10$^{-2}$</td>
</tr>
<tr>
<td>$L$ [Jkg$^{-1}$]</td>
<td>–</td>
<td>3.35·10$^4$</td>
<td>2.72·10$^3$</td>
<td>2.27·10$^3$</td>
<td>1.68·10$^3$</td>
<td>1.29·10$^3$</td>
<td>1.03·10$^3$</td>
</tr>
<tr>
<td>Ste</td>
<td>–</td>
<td>0.125</td>
<td>0.1275</td>
<td>0.1304</td>
<td>0.136</td>
<td>0.1435</td>
<td>0.150</td>
</tr>
</tbody>
</table>

**Governing equation**

Considering the nanofluid as a continuous media with thermal equilibrium between the base fluid and the solid nanoparticles, the governing equations are:

- Continuity

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

(1)

- X-momentum equation

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = \frac{1}{\rho_{nf}} \left[ -\frac{\partial p}{\partial x} + \mu_{nf} \nabla^2 u + (\rho \beta_{nf}) g_x (T - T_{ref}) \right]$$

(2)

- Y-momentum equation

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = \frac{1}{\rho_{nf}} \left[ -\frac{\partial p}{\partial y} + \mu_{nf} \nabla^2 v + (\rho \beta_{nf}) g_y (T - T_{ref}) \right]$$

(3)

- Z-momentum equation

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = \frac{1}{\rho_{nf}} \left[ -\frac{\partial p}{\partial z} + \mu_{nf} \nabla^2 w + (\rho \beta_{nf}) g_z (T - T_{ref}) \right]$$

(4)

- Energy equation

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} = \frac{\partial}{\partial x} \left[ \frac{(k_{nf0} + k_d)}{\rho_{nf} c_p} \frac{\partial T}{\partial x} \right] +$$

$$\frac{\partial}{\partial y} \left[ \frac{(k_{nf0} + k_d)}{\rho_{nf} c_p} \frac{\partial T}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{(k_{nf0} + k_d)}{\rho_{nf} c_p} \frac{\partial T}{\partial z} \right]$$

(5)
The density of the nanofluid is given by:
\[ \rho_{nf} = (1 - \phi)\rho_f + \phi\rho_s \]  
whereas the heat capacitance of the nanofluid and part of the Boussinesq term are:
\[ (\rho c_p)_{nf} = (1 - \phi)(\rho c_p)_f + \phi(\rho c_p)_s \]  
\[ (\rho\beta)_{nf} = (1 - \phi)(\rho\beta)_f + \phi(\rho\beta)_s \]
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 viscosity of the nanofluid containing a dilute suspension of small rigid spherical particles is given by:
\[ \mu_{nf} = \frac{\mu_f}{(1 - \phi)^{2.5}} \]
whereas the thermal conductivity of the stagnant (subscript 0) nanofluid is:
\[ k_{nf0} = \frac{k_s + 2k_f - 2\phi(k_f - k_s)}{k_s + 2k_f + \phi(k_f - k_s)} \]

The effective thermal conductivity of the nanofluid is:
\[ k_{eff} = k_{nf0} + k_d \]
and the thermal conductivity enhancement term due to thermal dispersion is given by:
\[ k_d = C(\rho c_p)_{nf}\sqrt{u^2 + v^2}\phi d_p \]

The empirically-determined constant \( C \) is evaluated following the work of Wakao et al. [13].

Also the latent heat that is evaluated using:
\[ (\rho L)_{nf} = (1 - \phi)(\rho L)_f \]

**Computational methodology**

The numerical solution of the problem uses the enthalpy-porosity approach. 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 \( \beta \) is computed at each iteration. \( \beta \) takes the value \( \beta = 1 \) in the liquid phase, \( \beta = 0 \) in the solid phase and \( 0 < \beta < 1 \) in the mushy zone (partially solidified region).

The governing equations are discretized using a control volume approach. For a typical run, the time step is 0.1 s and the number of sweeps for each time step is 400. The QUICK differencing scheme was used for solving the momentum and energy equations, whereas the PRESTO scheme was adopted for the pressure correction equation. The under-relaxation factors for the velocity components, pressure correction, thermal energy, and liquid fraction were 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 was set to \( 10^5 \) kg/m’s.
Validation of the model

Melting of gallium was simulated numerically by Brent et al. [14] with one vertical wall cooled while the opposite wall was heated. The top and bottom walls were adiabatic. The phase front propagation obtained in the present work is compared with their results in fig. 2. A reasonably good agreement is obtained.

The results of the recent work of Khanaf er et al. [11] were used to benchmark the present computations for the case of natural convection of nanofluids within a differentially-heated square cavity. The predicted horizontal velocity component on the vertical mid-plane of the square cavity for the present study with a 81x81 grid system and that of Khanaf er et al. [11] are compared in fig. 3 for Gr = 10^4 and 10^5.

Regardless of the volume fraction of the nanoparticles, the well-established trends of the horizontal fluid velocity exhibiting accelerated flow near the horizontal walls and weak flow in the center of the cavity point to the observation that nanofluids behave more like a fluid [11] as opposed to flow of mm- or micron-size suspensions. The comparison for the cases of buoyancy-driven convection of a pure fluid (zero volume fraction) for the two Grashof numbers is excellent. According to Khanaf er et al. [12], the dimensionless velocity was related to the inverse of the temperature difference between the two active walls. Consequently, the dimensionless velocity for Gr = 10^5 is lower compared to the corresponding Gr = 10^4 case. For a fixed Grashof number, as the loading of the nanoparticles is increased, “irregular and random” [11] motion of the nanoparticles promote greater momentum and energy transport throughout the cavity. Consequently, the extra thermal conductivity due to dispersion is enhanced. It should be noted that in the study of Khanaf er et al. [11], both the Prandtl and Grashof numbers were evaluated using the properties of the base fluid. In our work, these dimensionless groupings were evaluated using the properties of the specific nanofluids. In effect, it appears that there are discrepancies between our predictions and those of Khanaf er et al. [11] for non-zero solid volume fractions. The reader should not be alarmed on this matter in view of the different scaling parameters used to form the dimensionless groupings.

Figure 2. Progress of melting front with time: comparison among predictions of Brent et al. [14] and present work

Figure 3. Comparison of the predicted horizontal velocity component on the vertical mid-plane of the square cavity for the present study and those of Khanaf er et al. [11] with Gr = 10^4 and Gr = 10^5
The phase front for wall temperature of 15 °C at a time of 6 minutes was simulated numerically by Duan et al. [15] is shown in fig. 4, in order to investigate the effect of natural convection on the solidification of n-hexadecane. Also, fig. 5 shows the solid fraction vs. time for wall temperature of 15 °C. The numerical results agree very well with present work.

![Figure 4. Phase front propagation at 6 minutes for wall temperature of 15 °C](image)

![Figure 5. Solid fraction vs. time for wall temperature at 15 °C](image)

From the results shown in fig. 6, it can be concluded that the agreement between present study and experimental data of Fuji and Zivkovic study [16] is well. In their study, a simple computational model for isothermal phase change material encapsulated in a single container was presented. As shown in fig. 6, the temperature of centre of the container increases until reach to the melting point. Then the PCM absorb energy to change phase from solid to liquid in a constant temperature, and finally, the temperature will increase rapidly again.

Following preliminary tests, a grid of $51^3$ nodes in the fluid, selectively refined towards the walls, proved to yield an almost complete grid-independence of the results. Corresponding CPU times were of the order of 24 hours per test case on a 1500 MHz PC with 1024 megabytes RAM.

**Results and discussion**

Starting at time $t = 0$, the temperature of active left and right walls were held below the freezing temperature of the base fluid where the temperature of left wall is 273.15 °C and
the temperature of right wall is 283.15 °C. Consequently, the nanofluid will start freezing on the right wall and the solid front travels to the left. The remaining boundary conditions were unchanged in comparison to the conditions prior to $t = 0$. Colorized contours of the volume fraction of the nanofluid during freezing of the NEPCM at various time instants are shown in fig. 7 for wall temperature of 10 and 25 minutes for $Gr = 10^6$. 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.

Figure 7. Colorized contours of the volume fraction of the nanofluid at $Gr = 10^6$
(color image see on our to web site)
The instantaneous dimensionless volume of the nanofluid within the square cavity is presented in fig. 8 for all cases that were investigated. The liquid volume that continuously decreases from the start of the freezing exhibits little sensitivity to the value of the initial Grashof number except near the conclusion of the freezing process. 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 because of the enhanced thermal conductivity of the nanofluid in comparison to that of the base liquid, by increasing the solid particle volume fraction the freezing time become lower.

In fig. 9 the temperature of the center line of the cavity is shown at different time at Grashof number of $10^5$. It can be seen that the temperature of the center line decreases by time and a significant drop occur near the cold wall. Also, in fig. 10 the temperature profiles of the center line of the cavity for two nanoparticle volume fractions are shown. It could be found from these figures that the effect of natural convection will descend by the time. This is because of the decrease in the liquid domain.

Figure 11 shows solid front at a certain time for three different Grashof numbers ($Gr = 10^5$, $10^6$, and $10^7$). It is clear that natural convection effect descends by decreasing the Grashof number.
The instantaneous streamlines within the nanofluid for the initial 10 s during the freezing of NEPCM for an initial Gr =10^5, Ste = 0.150, and a solid particle volume fraction of 0.2 are shown in Fig. 11. Also, to study the effect of natural convection, the streamlines within the nanofluid for various Grashof number are shown in Fig.13. The streamlines at t = 0 correspond to a similar case studied by Khanafet et al. [11] and a clockwise rotating vortex is clearly observed. As a result of the sudden lowering of the temperatures of the two active walls at t = 0, the clockwise rotating vortex diminishes in strength and spatial coverage due to formation of a counter clockwise rotating vortex next to the left wall. The creation of the dual-vortex flow pattern was examined in greater detail by lowering the time step to 0.1 s for this case. Note that the formation, growth and equilibration of the counter clockwise vortex during the initial 10 s involves a dynamic interaction with the initially strong clockwise vortex. At the t = 10 s instant, two vortices rotating in opposite direction s and nearly equal in size are observed squeezed between the left wall and a thin frozen layer next to the right wall. For the remainder of the freezing process, the dual-vortex structure will persist however due to the leftward movement of the freezing front, the vortices will shrink in coverage space and their strength will decay. It should be noted that the actual Grashof number for this unsteady freezing problem decreases with time due to the continuous shrinking of the distance between the left wall and the liquid-solid interface.
Figure 12. Streamline patterns at various time instants for the initial 10 s during the freezing of water with copper nanoparticles (solid particle volume fraction of 0.2) for an initial $Gr = 10^5$ and $St_e = 0.150$
Figure 13. Streamline patterns at various Grashof number at $t = 0$ and $10$ s during the freezing of water with copper nanoparticles (solid particle volume fraction of 0.2)
In order to study the temperature distribution in the domain, the temperature profiles along the middle of the enclosure for the six different nanoparticle volume fraction at 5 and 12 minutes are shown in fig. 14. There is a significant temperature drop in the solid region, with hardly any noticeable temperature difference in the liquid region. The liquid temperature is near the melting temperature of 273 K. This shows that the temperature gradient in the liquid is too small to cause a significant natural convection in the liquid. Thus, heat conduction is the dominant mode of heat transfer in both solid and liquid.

![Image of temperature profiles](image)

**Figure 14. The temperature profiles along the middle of the enclosure**

**Conclusions**

Solidification inside rectangular container has been studied numericaly to investigate the effect of utilizing nanoparticle on the solidification phase front. The present results illustrate that the suspended nanoparticles substantially increase the heat transfer rate and also the nanofluid heat transfer rate increases with an increase in the nanoparticles volume fraction. Also, it was found that the temperature gradient in the liquid is too small to cause a significant natural convection in the liquid. Thus, heat conduction is the dominant mode of heat transfer in both solid and liquid.

**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>C</td>
<td>constant</td>
</tr>
<tr>
<td>$c_p$</td>
<td>specific heat, [Jkg$^{-1}$K$^{-1}$]</td>
</tr>
<tr>
<td>$d_p$</td>
<td>nanoparticle diameter, [m]</td>
</tr>
<tr>
<td>$f$</td>
<td>liquid fraction</td>
</tr>
<tr>
<td>$Gr$</td>
<td>Grashof number (= $\rho^2\beta\Delta T H^3/l^3$)</td>
</tr>
<tr>
<td>$H$</td>
<td>height of the enclosure, [m]</td>
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<tr>
<td>$k$</td>
<td>thermal conductivity, [Wm$^{-1}$K$^{-1}$]</td>
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<tr>
<td>$L$</td>
<td>latent heat of fusion, [Jkg$^{-1}$]</td>
</tr>
<tr>
<td>$p$</td>
<td>pressure, [Pa]</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number (= $\mu C_p/k$)</td>
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<tr>
<td>$T$</td>
<td>temperature, [K]</td>
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<table>
<thead>
<tr>
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<tbody>
<tr>
<td>$t$</td>
<td>time, [s]</td>
</tr>
<tr>
<td>$u, v, w$</td>
<td>velocity components, [m$s^{-1}$]</td>
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<tr>
<td>$x, y, z$</td>
<td>Cartesian co-ordinates</td>
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<table>
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<td>$\beta$</td>
<td>volumetric expansion coefficient, [K$^{-1}$]</td>
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<tr>
<td>$\varepsilon$</td>
<td>constant</td>
</tr>
<tr>
<td>$\mu$</td>
<td>dynamic viscosity, [kgm$^{-1}s^{-1}$]</td>
</tr>
<tr>
<td>$\rho$</td>
<td>density, [kgm$^{-3}$]</td>
</tr>
<tr>
<td>$\phi$</td>
<td>volume fraction of solid particles</td>
</tr>
</tbody>
</table>
Subscripts
ave – average
c – cold
d – thermal dispersion
f – based fluid
h – enthalphy

References