Solidification of Nano-Enhanced Phase Change Materials (NEPCM) in a Trapezoidal Cavity: A CFD Study

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Abstract  The solidification process of nanofluid (water + copper nanoparticles) has been studied numerically in this paper. The horizontal walls of the cavity are insulated while inclined walls are kept at constant but different temperatures. The effects of nanoparticle dispersions ($\phi = 0\%, 10\%$ and $20\%$) and the temperature difference between hot and cold wall on the solidification of Cu-water nanofluid inside the cavity is investigated numerically. Enthalpy-porosity technique is used to trace the solid-liquid interface. It is illustrated that the suspended nanoparticles substantially increase the heat transfer rate which is further increased by the temperature difference.

Keywords  Solidification, Phase Change Materials, Nanofluid, Trapezoidal Cavity

1. Introduction

A continuous increase of the gap between the energy demand and supply and the depletion of fossil fuels has received the attention of researchers in the last few decades. Consequently, there have been many efforts to find alternate energy resources or to store energy as sensible heat or latent heat. Although sensible heat storage systems are widely used in many industrial applications, latent thermal energy storages (LTES) are more attractive and promising due to its high energy storage density. Therefore, melting and freezing processes are used in a wide range of applications such as, solar energy collector, manufacturing processes (drilling, welding, and metal casting etc.) and in particular, as a thermal energy storage. Design and development of an efficient and cost effective latent heat thermal energy storage system has been greatly assisted by many experimental and numerically investigations. The purpose of the present work is to analyze the solidification of water-Cu nanofluid filled in an isosceles trapezoidal cavity using the Ansys-Fluent CFD commercial package. The effects of nanoparticle volume fractions and temperature differences between hot and cold walls on the solidification will be presented. The solidification time of the nanofluid in the trapezoidal cavity and a square cavity will be compared keeping the internal area of the both cavities equal.

2. Literature Review

Low thermal conductivity of all PCMs is the primary limitation in many engineering devices but the dispersion of solid particles in the PCM enhances the conductivity. The term nanofluid was used by Choi et al [2] for the mixture of dispersed nanoparticles into the base fluid. Khodadadi and Hosseinizadeh[7] were the first to report the improved functionality of PCM through dispersion of nanoparticles. They reported that NEPCM requires less time to solidify in comparison to the base fluid because of their enhanced thermal conductivity. Similar study was conducted by Zhu et al. [14] using SiC-H$_2$O nanofluid and found that adding 5% SiC nanoparticles into water can save the total solidification time by 17.4%. Song and Viskanta[9] investigated experimentally the solidification of a porous medium saturated with an aqueous salt solution filled in a square cavity and the effect of porous matrix permeability was examined over a wide range of parameters. F.L. Tan[10] experimentally investigated the solidification of aqueous ammonium chloride solution in a rectangular enclosure with solidification from the bottom (upward solidification) or the top (downward solidification), respectively. Yang and Zhao[13] analyzed the solidification of PCM within a single encapsulated particle and developed a technique which combines the Explicit Euler method and Implicit Euler method in finite element method scheme to solve the Stefan problem.

Besides using nanoparticles, the geometrical structures can also be used to improve the heat transfer performance of the nanofluid. Mahmud et al.[8] conducted a numerical study to predict the natural convection heat transfer in an enclosure with two wavy vertical walls. They mentioned in their study that heat transfer decreases with the increase of surface...
waviness. Das and Mahmud[3] investigated the natural convection heat transfer in an enclosure with horizontal wavy walls. They found that at low Grashof number, heat transfer increases when amplitude wavelength ratio changes from zero to other values, after that it has negligible effect on average heat transfer rate. Ismail et al.[5] conducted numerical and experimental study for the solidification of PCM around a curved cold tube to determine the effect of Dean number. Natural convection in a differentially heated cavity is considered to be a prototype of many industrial applications and in particular, trapezoidal cavity has received significant attention of researchers due to its applicability in various fields. Trapezoidal section is of vital importance in the moderate concentrating solar collector.

Presence of sloping walls makes the convective flow analysis more difficult in a trapezoidal cavity than square and rectangular geometry. Recently Nasrin and Parvin (2012) investigated numerically the natural convection flow and heat transfer in a trapezoidal cavity filled with Cu-Water nanofluid. They found that the Cu nanoparticles with the highest Pr and the lowest AR are more effective in enhancing performance of heat transfer rate. Varol et al.[11] performed a numerical study of buoyancy driven flow and heat transfer for a porous medium filled in a trapezoidal cavity having different aspect ratios and Rayleigh number. They found that existence of buoyancy driven force reversal resulting from maximum density effect, reduces the strength of convective flow and the average Nusselt number.

Although many researchers have considered the trapezoidal cavity in their studies, still there is a serious lack of information regarding the problems related to heat transfer enhancement in trapezoidal section filled with nanofluid. To the best of our knowledge, a very little investigation of the solidification/melting process by natural convection heat transfer of NEPCM in a trapezoidal cavity has been undertaken yet. Therefore, the purpose of the present work is to analyze the problem of solidification by natural convection in water-Cu nanofluid filled in trapezoidal cavity. The effects of nanoparticle volume fraction and temperature difference between hot and cold wall on the solidification phenomenon have been presented graphically. Considering the internal area of both cavities is equal, the solidification time for nanofluid in trapezoidal cavity and square cavity has also been compared.

### 3. Research Methodology

#### 3.1. Mathematical Formulation

A trapezoidal cavity of 10 mm² internal area, as shown in Fig 1, has been considered in this numerical study. Length (L) of the cavity is 10 mm. The horizontal walls are assumed to be insulated, non-conducting, and impermeable to heat transfer. The left and right inclined walls are kept at constant temperatures, $T_h = 283.15 \text{ K}$ and $T_c = 273.15 \text{ K}$ respectively. The nanofluid within the cavity is Newtonian, laminar, and incompressible. Thermo-physical properties (Table 1) of the nanofluid are assumed to be constant, whereas the density variation in the buoyancy force is based on the Boussinesq approximation. The nanoparticles are assumed to have a uniform shape and size (10 nm diameter). The left lower corner of the cavity was the origin of the coordinate system. Gravity acts in the negative y-coordinate direction, $g_x = 0$, and $g_y = -y$.

The initial and boundary conditions for the present investigation are follows: at the left inclined wall $T = T_c$ at the right inclined wall $T = T_c$ at horizontal surfaces $\frac{\partial T}{\partial y} = 0$ at all solid boundaries $u = v = 0$

![Figure 1. Sketch of the two dimensional trapezoidal cavity](image)

Table 1. Thermo-physical properties of the base fluid (water) and the Cu nanoparticles

|                     | Copper nanoparticles | Base fluid (water) |
|---------------------|----------------------|--------------------|
| $\rho \ [kg \ m^3]$ | 8954                 | 997.1              |
| $\mu \ [Pa \ s]$   | 8.9 x 10^{-4}       |                    |
| $c_p \ [J/kg \ K]$ | 383                  | 4179               |
| $k \ [W/m \ K]$    | 400                  | 0.6                |
| $\beta \ [1/K]$    | 1.67 x 10^{-5}      | 2.1 x 10^{-4}     |
| $l \ [J/kg]$       | -                    | 3.35 x 10^5       |
| $Pr$                | -                    | 6.2                |
| $St_e$              | -                    | 0.125              |
| $d_p \ [nm]$       | 10^{-9}              | -                  |

The continuity, momentum considering the Boussinesq approximation and energy equation for the above mentioned assumptions can be written in the following form:
Continuity
\[ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \] (1)

X-momentum
\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \frac{1}{\rho_i} \left( -\frac{\partial P}{\partial x} + \mu_i \nabla^2 u + (\rho \beta_i) \frac{\partial T}{\partial x} \right), \] (2)

Y-momentum
\[ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = \frac{1}{\rho_i} \left( -\frac{\partial P}{\partial y} + \mu_i \nabla^2 v + (\rho \beta_i) \frac{\partial T}{\partial y} \right), \] (3)

Energy equation
\[ \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{\partial}{\partial x} \left( \frac{k_{f} + k_{p}}{(\rho c_{p})_{f}} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{k_{f} + k_{p}}{(\rho c_{p})_{f}} \frac{\partial T}{\partial y} \right), \] (4)

The density of the nanofluid is given by:
\[ \rho_{nf} = (1 - \phi) \rho_f + \phi \rho, \] (5)

The viscosity of nanofluid is given by Brinkman (Brinkman, 1952):
\[ \mu_{nf} = \frac{\mu_f}{(1 - \phi)^{2/3}}. \] (6)

The heat capacitance of the nanofluid and part of the Boussinesq are:
\[ (\rho c_{p})_{nf} = (1 - \phi)(\rho c_{p})_{f} + \phi(\rho c_{p})_{f}, \] (7)
\[ (\rho \beta)_{nf} = (1 - \phi)(\rho \beta)_{f} + \phi(\rho \beta)_{f}. \] (8)

The latent heat of the nanofluid is evaluated using
\[ (\rho L)_{nf} = (1 - \phi)(\rho L)_{f}. \] (9)

Where L is the latent heat and φ is the nanoparticle volume fraction.

Thermal conductivity of the quiescent (subscript 0) nanofluid is:
\[ \frac{k_{nf0}}{k_f} = \frac{k_z + 2k_f - 2\phi(k_f - k_z)}{k_z + 2k_f + 2\phi(k_f - k_z)}. \] (10)

Whereas the effective thermal conductivity of the nanofluid is:
\[ k_{nf} = k_{nf0} + k_d. \] (11)

And the thermal conductivity enhancement term due to thermal dispersion is given by:
\[ k_d = C(\rho c_{p})_{nf} \sqrt{\frac{u^2}{v^2} + \frac{\phi d_p}{v^2}}. \] (12)

The empirically-determined constant C is evaluated following the work of Wakao and Kagyei [12].

### 3.2. Numerical Method

The numerical solution of the problem uses the enthalpy-porosity approach. In this technique, the porosity in each cell is set equal to the liquid fraction in that cell and this fraction is computed at each iteration. The SIMPLE method of the commercial code ANSYS FLUENT is used for solving the governing Eqs. 1-4. Orthogonal and uniform grid size of 6500 elements is used. The time step size for all the simulations in this study is 0.5 s and number of iterations for each time step are 800. The under-relaxation factor all the components, such as velocity components, pressure correction, thermal energy etc. is kept at 0.3. Convergence criteria are set at 10^{-7} for continuity and momentum and 10^{-9} for thermal energy. The QUICK differencing scheme was used for solving the momentum and energy equations, whereas the Pressure Staggering Option (PRESTO) scheme was used for pressure correction equations. 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^{7} [kg/m^3 s].
4. Results

4.1. Validation of the Model

Experimental results of Gau and Viskanta [4], numerical predictions by Brent et al. (1988) and Khodadadi and Hosseinizadeh [7] for melting of solid gallium in a rectangular cavity are compared with the current numerical data in Fig 2. A two dimensional rectangular cavity of 8.89 cm × 6.35 cm size completely filled with solid gallium was considered and qualitatively, the trends are agreeable among all four approaches, whereas the present computational results are more close to the experimental data and previous numerical predictions.

4.2. Effect of Nanoparticle Volume Fraction on Solidification Time

Numerical simulations of solidification begin with the steady state natural convection within the trapezoidal cavity filled with nanofluid (Cu-H$_2$O). The nanofluid was maintained at uniform temperature 273.15 K throughout the cavity at t = 0s. Then, the temperatures of both inclined walls are lowered by equal amount (10°C). Consequently, solidification of nanofluid begins at the right wall and the solid-liquid interface travels towards left until the complete solidification of the nanofluid within cavity. Fig 3 shows the coloured contours of the volume fraction of the nanofluid during freezing of NEPCM at various time instants (100s, 600s and 1200s). Colour red is used to identify the liquid phase, whereas blue colour is indicative of solid phase. Fig 4 shows the comparison of total solidification time of trapezoidal cavity of internal area 10 mm$^2$ and inclination angle 2.72°. Comparison of this time with the time taken by square cavity of the same internal area has also been made and presented in the figure 5. Trapezoidal cavity takes lesser time to completely solidify as compared to square cavity. This is because the surface area normal to the direction of heat flow is more in trapezoidal section.

Figure 2. Comparison of the progress of the melting phase front with time.

Figure 3. Colourized contours of the volume fraction of nanofluid for the nanoparticle volume fraction of 0% (pure water) and 20%
4.3. Effect of Temperature Difference between Hot and Cold Wall on the Total Solidification Time

Variation of liquid fraction against solidification time for five different temperature differences, ΔT = 10°, 20°, 30°, 55° and 110° and inclination angle, θ = 2.72° are shown in fig 6. It is necessary to consider the intensity of various factors such as conduction or convection effect, heat transfer surface area etc. on the solidification process of nanofluid in a cavity. Fig. 6 shows that for all values of temperature difference (Gr), the solidification time consistently decreases. For low temperature differences (ΔT=10°, 20°, and 30°), the influence of convection is negligible compared to conduction, therefore the phase front propagates parallel to the cold wall (Fig. 5). For large temperature differences (ΔT=55°and 110°), more powerful buoyancy-driven heat transfer exists which expedites the solidification process.

![Figure 4](image4.png)

**Figure 4.** Effect of nanoparticle volume fraction on solidification time of nanofluid within the square and trapezoidal cavity of θ = 2.72°.

![Figure 5](image5.png)

**Figure 5.** Effect of temperature difference on the solidification of nanofluid of 20% nanoparticle volume fraction inside cavity of θ = 2.72°.

5. Conclusions

The solidification of nanofluid by natural convection heat transfer in the isosceles trapezoidal cavity has been studied numerically and the results obtained are as follows:

- The solidification time for a trapezoidal cavity of θ = 2.72° is almost 10% lesser than that of a square cavity (θ = 0°). Further inclination will increase the heat transfer rate within the nanofluid and decrease the solidification time. The vertical wall inclination (θ) can be used as a critical parameter for controlling the solidification time.
- Increasing nanoparticle volume fraction decreases the solidification time e.g. total solidification time for pure fluid (water) is 3000s and that of nanofluid of 10% solid Cu nanoparticles is 1890s. Further increasing nanoparticle concentration to 20%, it requires only 1300s to completely solidify.
- The heat transfer rate greatly depends upon the temperature difference and increasing temperature difference increases the heat transfer rate for all values of nanoparticle volume fraction.

This numerical study can be helpful for designing thermal energy storage systems for solar energy collector or casting and mold design. Further numerical and experimental study by changing the inclination angles, considering the wall thickness, and the effect of various nondimensional numbers on solidification process can be studied for deeper insight of this subject.

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