Numerical simulation of melting behavior of nano-enhanced phase change material in differentially heated cavity

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Abstract: The melting and solidification process in enclosures filled with phase change materials has wide applications in metal casting, thermal energy storage, building insulation and battery thermal management. In the current study, the melting and heat transfer characteristics of Nano Enhanced Phase Change Material (NEPCM) are numerically investigated in a differentially heated square cavity. The NEPCM consists of ice as the phase change material (PCM) into which Single Walled Carbon Nano-tubes (SWCNT) particles of uniform size is dispersed. The left and right walls of the enclosed cavity are maintained at a constant wall temperature and considered as hot and cold walls and the remaining walls are treated as adiabatic and the simulation is performed using Ansys Fluent 19.2. The temperature difference between the hot and cold walls are varied and further investigations are performed by considering the effects of nanoparticle volume fraction on the melting behavior of NEPCM. The results are analyzed by plotting the stream function, melting interface temperature and velocity contours. The results indicate that the addition of SWCNT nanoparticles significantly influences the heat transfer characteristics and melting rate of phase change material. It is also found that the increase in nanoparticle volume fraction enhances the average melting and heat transfer rate of phase change material. The present results are validated and are in excellent agreement with the benchmark results available in literature.

1.Introduction
We come across many fluids in our day-to-day life. Simple fluids such as ethanol, pure water, and ethylene glycol have a poor heat conduction ability and thermal properties[1]. This problem can be corrected by adding nanoparticles that are thermally conductive to the base fluid and such nano-particles are known as nano-fluids.[2&3]. Xing et al[4] conducted experiments using SWCNT nanofluids and experimentally obtained results by varying volume fraction and temperature. He concluded that SWCNT show more heat conduction in laminar region. A PCM is a substance which absorbs/ emits energy in form of latent heat when its state changes. The temperature of PCM remains constant at the time of latent heat of absorption / heat release and the energy consumption by power grids are reduced. There has been excessive studies going on PCM based energy storage [5]. Some authors made out studies especially highlighting the advantages of PCM[6&7] such as low cost, chemical stability, high latent heat storage and density storage. These properties allow PCM to be used in refrigeration, air conditioning, space industry, photovoltaic electric systems, solar energy and preservation of food. Some
innovations are made in PCM to increase its efficiency where the PCM was capsulated inside a nano-shell to prevent energy leakage[8]. This material was named as NEPCM(Nano-Encapsulated Phase Change Material) and the advantage was energy can be absorbed/ released by both the core layer and PCM at the time of solidification/ melting. There is also another class of materials with the same abbreviation NEPCM(Nano- Enhanced Phase Change Materials). In later, simply solid nanoparticles are added to improve the thermal behavior of PCM [9-13]. Melting of PCM has its applications in latent heat thermal engineering systems, electronic cooling [14]. From the above studies, the heat transfer characteristics of phase change materials in the presence of Single wall carbon nanotubes (SWCNT) needs further understanding and this has been the motivation for the present study. A two dimensional numerical study is performed in a differentially heated cavity filled with phase change material and nanoparticles. Ice is taken as the phase change material because of its high latent heat of fusion(333J/g) into which SWCNT nanoparticles are dispersed. The parametric study is performed by varying the temperature differences and nanoparticle volume fractions inside the cavity.

**Nomenclature**

\[ \rho \] density [kg/m\(^3\)]  
\[ C_p \] specific heat [J/kg K]  
\[ k \] thermal conductivity [W/m-K]  
\[ \mu \] viscosity [kg/m-s]  
\[ \phi \] volume fraction  
\[ n \] empirical shape factor

**Subscripts**

\[ T_L \] temperature in left wall  
\[ T_R \] temperature in right wall  
\[ vf \] volume fraction  
\[ bf \] base fluid  
\[ np \] nano particle
2. Methodology

2.1. Geometry description
The numerical simulation is carried out in a differentially heated 2-D square cavity. The top and bottom walls are maintained as adiabatic and the left wall and right wall are maintained at constant temperatures ($T_L$ and $T_R$) respectively where $T_L > T_R$ as seen in figure 1. Thermo-physical properties of base fluid and nano-particle are kept constant. The temperature difference between the left and right walls and volume fraction of SWCNT and base fluid is varied and results are compared.

2.2 Governing equations and thermo-physical properties
The numerical analysis is done in two separate but related stages. Firstly ice was chosen as phase change material (base fluid) and a steady-state driven numerical analysis is carried out in a differentially heated two dimensional square enclosure. Secondly, SWCNT nano particle of uniform size is dispersed with

### Table 1. Thermo physical properties of Nanoparticles dispersed in PCM

|                  | $\rho$ [kg/m$^3$] | $C_p$ [J/kg K] | $k$ [W/m-K] | $\mu$ [kg/m-s] |
|------------------|-------------------|----------------|-------------|---------------|
| ice only         | 916               | 2050.0         | 2.22        | 0.79          |
| ice+1%vf SWCNT   | 927.8             | 1876.6         | 1.03        | 0.81          |
| ice+2.5%vf SWCNT | 945.6             | 1875.1         | 1.07        | 0.84          |
| ice+5%vf SWCNT   | 975.2             | 1872.2         | 1.15        | 0.89          |
| SWCNT            | 1400              | 4.33           | 3000        | 0             |
ice and the same analysis is carried. The following equations of density, specific heat, thermal conductivity and viscosity are used to determine the boundary conditions [table 1].

\[ \rho C_p^{\text{mix}} = (1-\phi)(\rho C_p)_{bf} + \phi(\rho C_p)_{np} \]  

(1)

\[ \rho^{\text{mix}} = (1-\phi)(\rho)_{bf} + \phi(\rho)_{np} \]  

(2)

\[ \mu^{\text{mix}} = \frac{(\mu)_{bf}}{(1-\phi)^{\frac{3}{5}}} \]  

(3)

\[ k^{\text{mix}} = \frac{k_{np} + (n-1)k_{np} + (n-1)\phi(k_{np} - k_{bp})}{k_{np} + (n-1)k_{np} - \phi(k_{np} - k_{bp})} \]  

(4)

The above equations from [15] were used to compute the density, co-efficient of specific heat, thermal conductivity and viscosity of ice+SWCNT. Subscripts mix, np, bf represent mixture (SWCNT+ice), nano-particle(SWCNT) and base fluid (ice) respectively.

2.3 Initial and boundary conditions

The FLUENT 19.2 version is used to solve these governing equations. A pressure based steady-state analysis is carried out with the effect of gravity being vertically upwards. The parameters of pressure, body forces, momentum, liquid fraction, density and energy are set to 0.3, 1, 0.7, 0.9, 1 and 1 respectively. The flow and energy equation modes are turned on at the time of iterations. An absolute convergence criterion is followed with equations residual of continuity, x-velocity, y-velocity and energy of the range 10^{-6}. The solution initialization is standard and the reference frame used is ‘relative to cell zone’. The initialization is computed from the heated wall and results are presented below.

2.4 Grashof Number

It is a dimension-less parameter that is used to co-relate the heat and mass transfer by thermally driven natural convection in a solid surface that is immersed in a fluid. It is calculated using the following equation:

\[ G_r = \frac{gl^3 \varepsilon \Delta t}{\nu^2} \]  

(5)

Where,

- \( g \)= acceleration due to gravity (m/s²)
- \( l \)= dimension of the cavity
- \( \varepsilon \)= co-efficient of expansion of fluid (K⁻¹)
- \( \Delta t \)= temperature difference between the walls (k)
- \( \nu \)= kinematic viscosity (m²/s)

The Grashof number is calculated using the values from Table1 for ice and ice+SWCNT at different volume fractions.

3. Results and discussions
The temperature and pressure contours of melting of ice is shown in figure 2 and 3. The red region denotes that the wall is at higher temperature(left wall) and blue region denotes that the wall is at a lower temperature(right wall). The heat transfer occurs from left to right wall as shown in figure 2.

**Figure 2.** Temperature contour of melting of ice

**Figure 3.** Pressure contour of melting of ice
Figure 4. Comparison of pressure contours of ice+SWNCT at 1%vf at temperature difference of 40°C, 50°C and 60°C.

Figure 5. Comparison of temperature contours of ice+SWNCT at 1%vf at temperature difference of 40°C, 50°C and 60°C.

Figure 6. Comparison of longitudinal velocity contours of ice+SWNCT at 1%vf at temperature difference of 40°C, 50°C and 60°C.
In figure 4, a comparison of pressure contours of Ice+SWCNT at 1% vf at different temperature differences is displayed. It can be noticed that the pressure in the wall boundaries is more than the middle region of the cavity. Similarly, a comparison of temperatures, longitudinal velocities, and normal velocities contours of Ice+SWCNT at 1% vf at different temperature differences are shown in figures 5, 6, and 7 respectively. From the comparison of above contours, it is observed that the intensity of heat transfer characteristics and velocity distributions is higher in case of ice dispersed with SWCNT (NEPCM) than pure ice.

Following figures 2-7, some points are taken from the contours and plotted as graphs in figures 8-10. Figure 8 represents a comparison plot of temperatures of Ice+SWCNT at 2.5% vf at different temperature differences. There is a drop in temperature from left to right wall because of the given boundary conditions ($T_L > T_R$).
Figure 9. Comparison of longitudinal and normal velocity plots of ice+SWCNT at 2.5%vf at 40°C, 50°C, and 60°C.

Figures 9 indicates the comparison plots of longitudinal and normal velocity plots of ice+SWCNT at 2.5%vf indicates that the mid-height temperature and velocity distribution increases linearly with increase from 40°C to 60°C. Moreover, it is found that the increase in temperature difference from 40°C to 60°C enhances the longitudinal and normal velocities by 47.05% and 30% respectively. This is attributed to the increase in thermal convection which enhances the flow and melting rates of PCM.

Figure 10. Comparison of temperature and velocity plots of ice+SWCNT at different vf at 50°C.

Figure 11 and 12 represents the comparison plots of longitudinal and normal velocities of Ice+SWCNT at 50°C at different volume fractions. It is noticed that the velocity distributions are suppressed at the mid-section of the cavity with increase in SWCNT volume fraction. This is due to the fact that the addition of nanoparticles decreases the thermal convection at the mid-section of the cavity; however, the effects of volume fraction on velocity distribution is not visualized near the left and right walls of the cavity. This is due to influence of no-slip and constant wall temperature boundary conditions. For 2.5% and 5% volume fraction of SWCNT dispersed in ice, the longitudinal velocities were decreased by 2.5% and 9.7% in comparison with pure ice.
Table 2: Computation of Grashof number

| Materials             | Grashof number |
|-----------------------|----------------|
| Ice                   | 1742.9         |
| Ice+SWCNT(vf 1%)      | 769.2          |
| Ice+SWCNT(vf 2.5%)    | 743.1          |
| Ice+SWCNT(vf 5%)      | 711.4          |

Table 2 indicates the variations of Grashof number (Gr) for different material properties and it is observed that the Gr values of pure ice are higher than the cases dispersed with SWCNT nanoparticles. It is also interesting to note that the Grashof number decreases with increase in volume fraction of nanoparticles. Hence the decrease in Grashof number suppresses the thermal convection and destabilizes the motion of phase change melt zone and the reduction in temperature and velocity distributions visualized in Figure 10 are due to the influence of lower Grashof number at higher nanoparticle volume fractions.

4. Conclusions

Numerical simulation is carried out to investigate heat and flow transfer characteristics in a differentially heated enclosure filled with ice and single wall carbon nanotube nanoparticles. The flow and thermo-physical properties of base fluid (ice) with SWCNT nano-particles are reported at different temperature differences and volume fractions. The results indicate that the intensity of heat transfer and velocity distributions increases with increase in temperature difference for pure ice and ice dispersed with SWCNT (NEPCM). This is due to the increase in thermal convection which enhances the flow and melting rates of PCM. It is also found that for fixed temperature difference, the velocity distributions are suppressed at the mid-section of the cavity with increase in SWCNT volume fraction. This is due to the fact that the addition of nanoparticles decreases the thermal convection at the mid-section of the cavity; however the effects of volume fraction on velocity distribution were not visualized near the left and right walls of the cavity. Moreover, it is found that the increase in temperature difference from 40°C to 60°C enhances the longitudinal and normal velocities by 47.05% and 30% respectively. The results from the present study will be useful in designing an effective nano-enhanced phase change material for energy and thermal storage applications.

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