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Numerical investigation of the effect of nanoparticles on thermal efficiency of phase change materials

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Abstract. In this study, in order to examine the thermal properties of different materials, the effect of different nanoparticles (Np) in phase change materials on the heat transfer rate in the melting and freezing processes of these materials has been numerically investigated. In the present study, carbon nanotubes and aluminum oxide as an enhancement nanoparticle as well as paraffin and a combination of hydrated salts as a phase-change material have been used. The finite difference method is used based on the enthalpy method for the phase change problem for numerical solution. The simulation results indicate an increase in the heat transfer rate due to the addition of nanoparticles to the phase change material. For both of the phase change materials considered in the present study, the results show the higher efficiency of carbon nanotubes compared to aluminum oxide to increase the heat transfer rate. The highest increase compared to the base state at the speed of the processes involved the addition of carbon nanotubes to paraffin, which according to the simulation is about 30 %. The lowest increase is related to the state of aluminum oxide in the composition of hydrated salts (about 4.5 %). The results of this study can be used to determine the heat transfer speed required for storing and releasing energy.

Key words. Energy storage, phase change material, nanoparticles, carbon nanotubes, enthalpy method, melting, freezing.

1. Introduction

Today, with increased demand for energy and reduction of fossil fuels, as well as the polluting and expensiveness of these fuels, the need for renewable energies has been felt more and more and this concerned researchers to this type of energy such as sun, geothermal energy, wind energy, and so on. In general, renewable energies need to be restrained, stored, and released in accordance with the need. In fact, materials can be used to store this low-energy depending on the need and at high speeds to

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prevent the loss of energy. One of the ways to increase the storage and release speed is to increase the thermal conductivity of materials that are stored and released in the process of energy storage and release, and due to the high thermal conductivity found in nanoparticles, and in particular carbon nanotubes, these materials is one of the best options.

In 2005, Pirkandi et al. [1] examined the process of phase change in a phase-change material in an energy storage device with two co-axial pipes. They used enthalpy method for the melting and freezing process in their work.

In 2018, Aldalbahi et al. [2], explored a variety of energy storage technologies based on phased-change materials and the use of nanotechnology. In 2011, Sebti et al. [3] investigated the numerical work of the heat transfer process during freezing inside two annular central cylinders by adding nanoparticles. With addition of nanoparticles, an increase in the rate of heat transfer was observed. In their work, they used finite volume method through enthalpy technique to find the boundaries of solid and liquid phases. Copper oxide was also used as a nanoparticle. In 2015, Mondragón et al. [4] investigated the numerical process of heat transfer in a cryogenic energy storage system In 2014, Sharmat et al. [5] studied the process of freezing of nano-fluid containing water and copper oxide numerically. The effect of different volume fractions and temperature difference between two cold and hot walls in the freezing process was investigated and it was observed that the increase of nanoparticle volume fraction had the most effect on increasing the heat transfer.

Most studies have used copper oxide or other spherical nanoparticles. For this reason, we decided to examine the effect of carbon nanotubes and compare them with the results of other nanoparticles. In this study, the numerical study of the effect of nanoparticles to phase-change material on the speed of the melting and freezing process has been investigated, and a comparison has been made between different nanoparticles. The purpose of this study was to investigate the effect of nanoparticles on the efficiency of phase-change materials using enthalpy method for phase change process.

2. Problem geometry

The geometric model of the problem, as shown in Fig. 1 consists of a layer containing a phase change material with dimensions of 73×5.2,cm and two adjacent channels in which the air flows. On the right side of the air flows from the bottom to up, but on the left side the air is constant. In both channels, heat transfer is provided free of charge. Open channel dimensions are 73×5 centimeters. The air in the left side has a constant temperature, which, at the time of the freezing and melting process, has a value of 0 and 30 °C, respectively. The available air on the right side of the layer containing the phase change material at a temperature of 20 °C entered the canal and is affected by the heat transfer process of the free movement in the channel and its temperature rises. Also, in the process of melting the constant thermal flux , $200\,\mathrm{W/m^2}$, from the left to the layer containing the phase change material is applied, and in the freezing process, the constant thermal flux -$200\,\mathrm{W/m^2}$ is applied to the layer from the left.

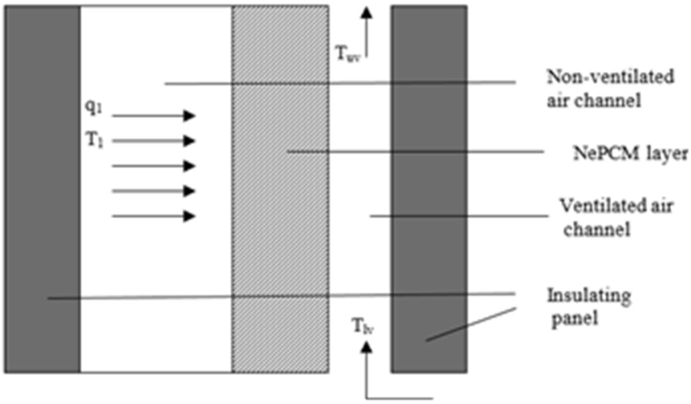

Fig. 1. Geometric model of the problem

In this study, the desired fluid was air, and among the phase change material, a combination of hydrated salts (water + calcium chloride (2CaCl) + potassium chloride (KCl) + other added substances) and paraffin as a phase change material were selected. among the various types of paraffin, Nano-Ocodacane was used for application and the properties are listed in the following Table 1. There were many options to choose for a nanoparticle in phase change material, among carbon nanotubes with regard to their unique properties we used. Aluminum oxide nanoparticles were also used to compare the results.

Table 1. Thermophysical properties of paraffin and carbon nanotubes

Material	Parameters				
	Density (kg/m^3) (Solid/ Liquid)	Specific heat capacity (J/(kg K)) (Solid/ Liquid)	Thermal conductivity (W/(m K)) (Solid/ Liquid)	Phase change temperature (°C)	Latent heat (kJ/kg)
Paraffin (*n*-octadecane)	(770/685)	(2196/1934)	(0.148/0.358)	27	243
Carbon nanotube	1350	600	K	-	-
Aluminum oxide	3600	765	36	-	-
Mixture of hydrates	1070	(2207/1832)	(0.58/0.82)	27	184.276

The prediction of thermophysical properties enhanced phase material in both solid and liquid phases depend on the phase change material and the volume fraction of the nanoparticles, is made to vary the density, specific heat capacity, and the latent heat of the theory combination has been used. The density ρ_{eff} of enhanced phase material is given below:

$$\rho_{\mathrm{eff}} = (1 - \Phi_{\mathrm{vol}})\rho_{\mathrm{PCM}} + \Phi_{\mathrm{vol}}\rho_{\mathrm{NP}}\,. \tag{1}$$

In this equation, Φ_{vol} represents the volume fraction of nanoparticles, ρ_{NP} is their specific mass and ρ_{PCM} denotes the specific mass of phase-change material. The specific heat capacity of enhanced phase material is as follows:

$$(\rho C_{\mathrm{p}})_{\mathrm{eff}} = (1 - \Phi_{\mathrm{vol}})\,(\rho C_{\mathrm{p}})_{\mathrm{PCM}} + \Phi_{\mathrm{vol}}(\rho C_{\mathrm{p}})_{\mathrm{NP}}\,, \tag{2}$$

where ρC_{p} denotes the specific heat.

According to the assumptions, nanoparticles are not in latent heat, the effective latent heat L of enhanced phase material is obtained as follows:

$$(\rho L_{\mathrm{eff}}) = (1 - \Phi_{\mathrm{vol}})\,(\rho L)_{\mathrm{PCM}}\,. \tag{3}$$

In order to predict the thermal conductivity enhanced phase material, the NANO model has been used for solid phase in the form

$$\frac{K_{\mathrm{eff}}}{K_{\mathrm{b}}} = \frac{3 + \Phi(B_x + B_z)}{3\Phi B_x}\,. \tag{4}$$

This model was modified by considering the effective length parameter by Sang et al. In the present work, the effective length is considered an average of one. It is defined as follows

$$\frac{K_{\mathrm{eff}}}{K_{\mathrm{b}}} = \frac{\frac{K_{\mathrm{p,m}}}{K_{\mathrm{b}}} + \alpha - \alpha\Phi_{\mathrm{N}}\left[1 - \frac{K_{\mathrm{p,m}}}{K_{\mathrm{b}}}\right]}{\frac{K_{\mathrm{p,m}}}{K_{\mathrm{b}}} + \alpha + \alpha\Phi_{\mathrm{N}}\left[1 - \frac{K_{\mathrm{p,m}}}{K_{\mathrm{b}}}\right]}\,. \tag{5}$$

In the above equations, K denotes the thermal conductivity, C_{p} denotes the specific heat, H denotes the enthalpy, Q_1 represents the input energy to the energy storage layer, T is the temperature,

For the present study, the value $2.1\times5^{-9}\,\mathrm{m^2K/W}$, which has a great degree of magnitude compared to experimental work, is considered to be thermal resistance. Another nano-particle is aluminum oxide, which is a spherical nanoparticle. Apart from effective thermal conductivity, other thermo-physical properties of enhanced phase change material by this nanoparticle is the same as the staus used by carbon nanotubes. In order to calculate the thermal conductivity of enhanced phase change material, the following equation is used:

$$k_{\mathrm{n-pcm}} = \frac{k_{\mathrm{np}} + 2k_{\mathrm{pcm}} - 2(k_{\mathrm{pcm}} - k_{\mathrm{np}})\Phi_{\mathrm{np}}}{k_{\mathrm{np}} + 2k_{\mathrm{pcm}} + (k_{\mathrm{pcm}} - k_{\mathrm{np}})\Phi_{\mathrm{np}}}k_{\mathrm{pcm}} + {}$$
$$+ \beta k_1 \rho_{\mathrm{pcm}} C_{\mathrm{p,pcm}}\sqrt{\frac{KT}{\rho_{\mathrm{np}} d_{\mathrm{np}}}}f(T, \Phi_{\mathrm{np}})\,. \tag{6}$$

The first part of this equation indicates the Maxwell model, and the second part indicates Brownian motion, which indicates thermal dependence for effective thermal conductivity. Also, for calculating the conductivity of carbon nanotubes, the equation below has been used:

$$k = [3.7 \times 10^{-7} T + 9.7 \times 10^{-10} T^2 + 9.3 \left(1 + \frac{0.5}{L_{\mathrm{CNT}}}\right) T^{-2}]^{-1} . \tag{7}$$

The parameters used in equation of thermal conductivity are listed in Table 2.

Table 2. Parameters used in the equations of thermal conductivity

Parameter	Value	Unit
$d_{\mathrm{np,Al_2O_3}}$, $d_{\mathrm{np,CNT}}$, $L_{\mathrm{np,CNT}}$	59×10^{-9}, 1.7×10^{-9}, 5×10^{-6}	m
$C_{\mathrm{1np,Al_2O_3}}$, $C_{\mathrm{2np,Al_2O_3}}$, c_1	0.9830, 12.959, -3.91123×10^{-3}	-
c_2, c_3, c_4	28.217×10^{-3}, 3.917×10^{-3}, -30.699×10^{-3}	-
$S_{\mathrm{1np,Al_2O_3}}$, $S_{\mathrm{2np,Al_2O_3}}$	8.4407, -1.07304	-
T_{ref}	298.15	k
K	1.381×10^{-23}	J/K
k_1	5×10^4	-

3. Results and discussion

A numerical simulation was performed for the conditions mentioned in the previous sections for storing and releasing energy. In the next step, the effect of adding different nanoparticles to phase change materials will be studied and compared at the speed of melting and freezing processes. The speed of melting and freezing processes for aluminum oxide nanoparticles and carbon nanotubes—enhanced phase change material (paraffin) with a volume fraction of 5 % has been investigated. The calculation of the melting and freezing process for paraffin and various nanoparticles is shown in Figs. 2 and 3.

Increasing the heat transfer rate due to the addition of nanoparticles due to the high thermal conductivity and thus the acceleration of the melting and freezing processes is predictable, which can be seen in Figs. 3 and 4. It should be noted, that the process of melting of aluminum oxide nanoparticles and carbon nanotubes—enhanced phase change material (paraffin) experienced an increase of 30 % and 16 % at execution. The values for the freezing process of this material are 14.5 % and 5.5 %. By doing the same for the other phase change material (a combination of hydrated salts), the results were similar to those given for paraffin. These results are shown in Figs 5 and 6, which are related to the melting and freezing processes.

In this study, for drawing the diagram of the duration of the melting and freezing processes, the time for these processes to be considered for the longest time, and the rest of the time is proportional to it. In Fig. 6, in order to sum up the contents, the rate of melting and freezing processes for all the materials is presented for comparison.

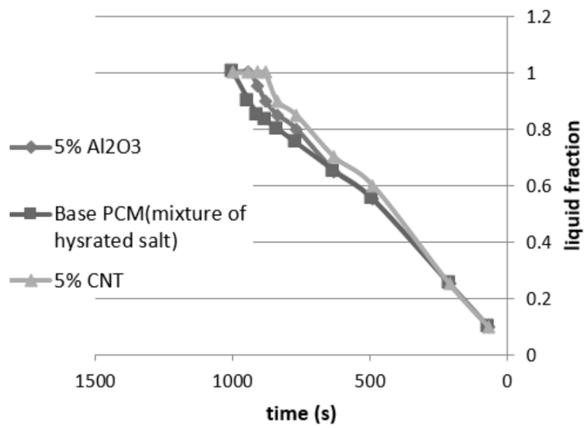

Fig. 2. Melting process of aluminum oxide nanoparticles and carbon nanotubes—enhanced phase change material (paraffin)

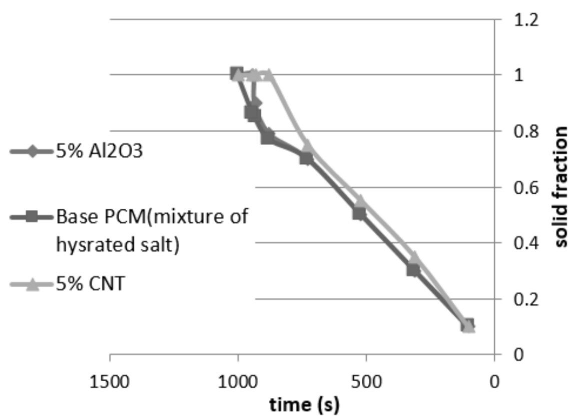

Fig. 3. Freezing process of aluminum oxide nanoparticles and carbon nanotubes—enhanced phase change material (paraffin)

As shown in Fig.. 6, the greatest increase in the speed of the processes is related to the state of the carbon nanotubes added to paraffin. There are two main reasons for this. The first reason is that the thermal conductivity of paraffin as a base phase material is very low about 0.15 W/mK. The second reason is the high thermal conductivity of nanotube carbon fiber, about 3000 W/mK. Also, according to the results, the least increase in the speed of the processes in relation to the base state is the one used to combine aluminum oxide with hydrated salts.

4. Conclusion

In the present study, a numerical study was carried out to estimate the effect of increasing the thermal conductivity through the addition of carbon nanotubes and

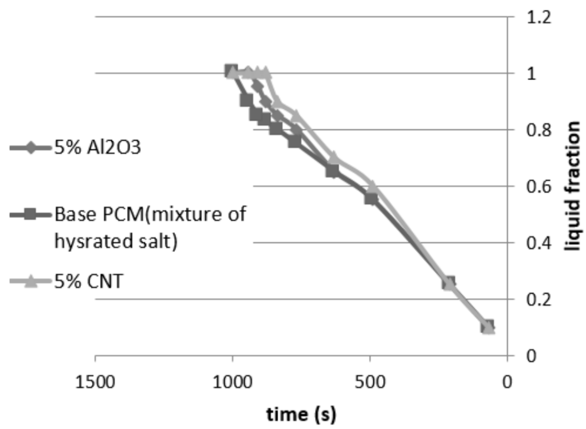

Fig. 4. Melting process of aluminum oxide nanoparticles and carbon nanotubes—enhanced phase change material (hydrate salts composition)

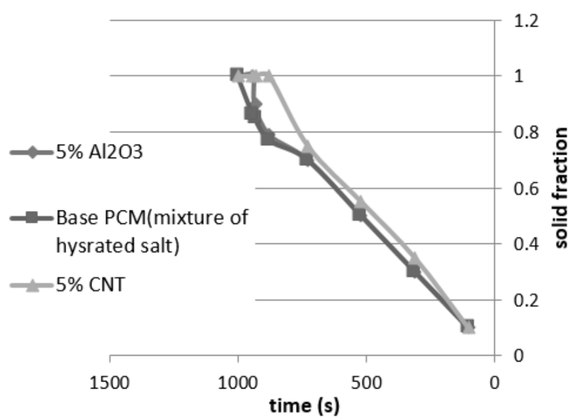

Fig. 5. Freezing process of aluminum oxide nanoparticles and carbon nanotubes—enhanced phase change material (hydrate salts composition)

aluminum oxide to various phase change materials on the thermal efficiency of the resulting material. Based on the present study, it can be noted that the thermal performance of the phase change material is enhanced by the addition of aluminum oxide nanoparticles and carbon nanotubes to these materials and, in fact, the heat transfer rate is controllable. For both nano particles, the thermal efficiency of the phase change material is better than the base state, but the use of carbon nanotubes results in better results than aluminum oxide. Generally, the use of nanoparticles increases the speed of melting and freezing processes. Of course, it is unlikely that the use of nanoparticles is now economically justifiable for energy storage processes that have so far been low.

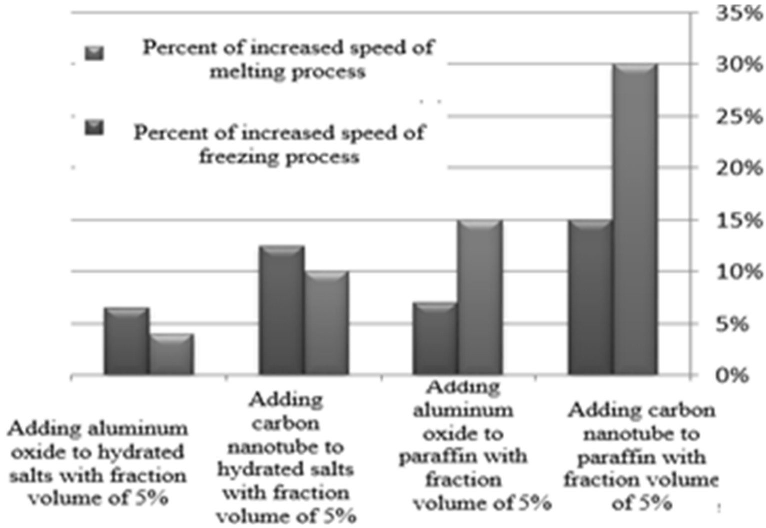

Fig. 6. Effect of adding nanoparticles too phase change materials on increasing the speed of melting and freezing processes thab base- phase change materials

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